



## Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 08:43 am GMT

PDB ID : 7AJT  
EMDB ID : EMD-11807  
Title : Cryo-EM structure of the 90S-exosome super-complex (state Pre-A1-exosome)  
Authors : Cheng, J.; Lau, B.; Flemming, D.; Venuta, G.L.; Berninghausen, O.; Beckmann, R.; Hurt, E.  
Deposited on : 2020-09-29  
Resolution : 4.60 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

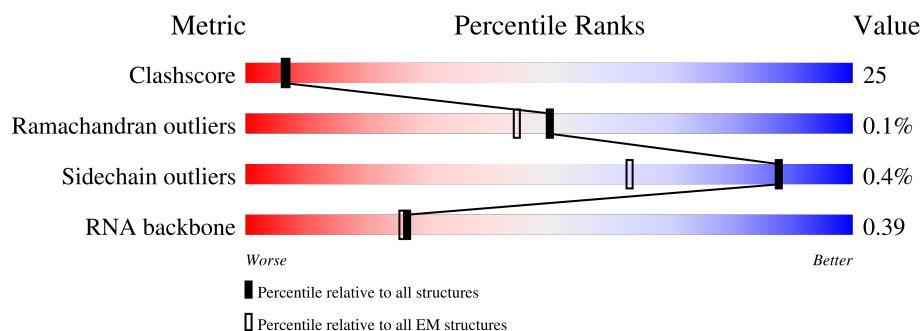
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




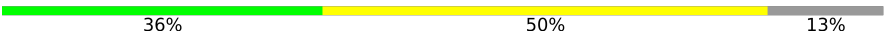
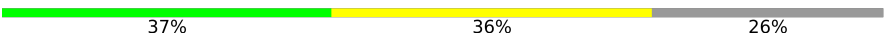
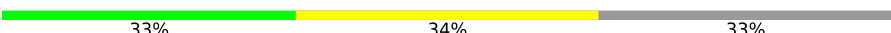

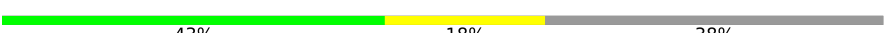



















Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	CA	327	
1	CB	327	
2	DA	255	
3	JA	1056	
3	JB	1056	
4	UA	923	
5	UB	810	


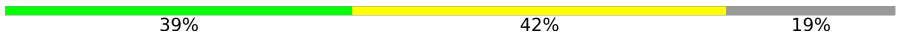



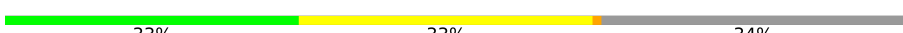










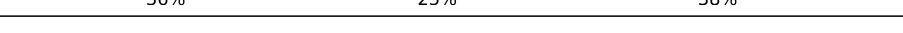








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Mol	Chain	Length	Quality of chain
6	UC	610	
7	UD	776	
8	UE	643	
9	UF	440	
10	UG	554	
11	UH	713	
12	UI	575	
13	UJ	1769	
14	UK	250	
15	UL	943	
16	UM	817	
17	UN	899	
18	UO	513	
19	UP	214	
20	UQ	896	
21	UR	594	
22	US	552	
23	UT	2493	
24	UU	939	
25	UV	1237	
26	UX	189	
27	UZ	274	
28	CD	504	
29	CE	511	
30	CF	126	





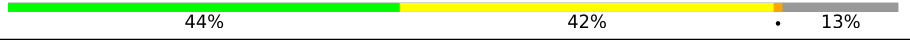


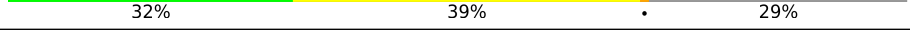
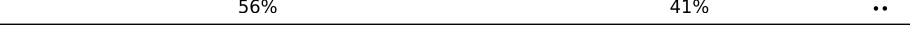
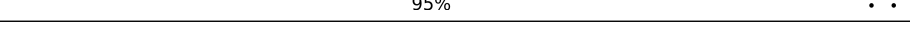
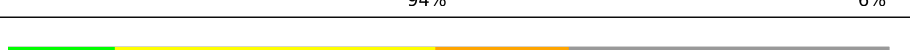
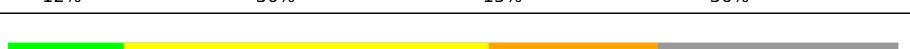
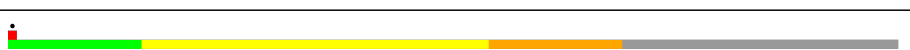
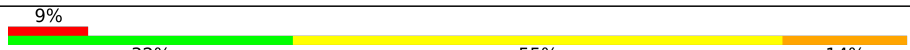
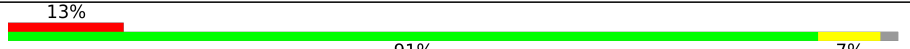
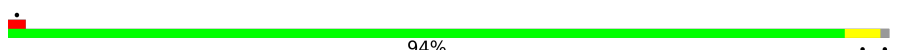

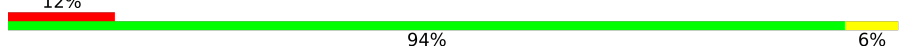
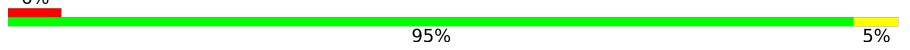

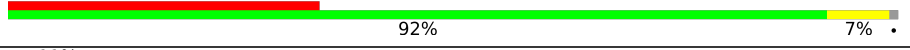
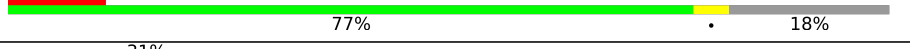

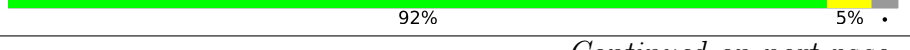

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Mol	Chain	Length	Quality of chain
30	CG	126	
31	CH	573	
32	CI	183	
33	CJ	290	
34	CK	593	
35	CL	1183	
36	CM	367	
37	CN	297	
38	JC	707	
39	JF	252	
39	JG	252	
40	JH	483	
41	JI	1729	
42	JJ	274	
43	JK	534	
44	JM	217	
45	JN	346	
46	JO	316	
47	JP	489	
48	JQ	206	
49	DE	261	
50	DF	225	
51	DG	236	
52	DH	190	
53	DI	200	

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Mol	Chain	Length	Quality of chain
54	DJ	197	
55	DL	156	
56	DN	151	
57	DO	137	
58	DQ	143	
59	DS	146	
60	DW	130	
61	DX	145	
62	DY	135	
63	Db	82	
64	Dc	67	
65	D2	700	
66	D3	1808	
67	D4	333	
68	EA	22	
69	EB	305	
70	EC	246	
71	ED	394	
72	EE	223	
73	EF	267	
74	EG	250	
75	EH	240	
76	EI	359	
77	EJ	292	
78	EK	1001	

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Mol	Chain	Length	Quality of chain
79	EN	1073	<div><div></div><div>35%</div><div></div><div>79%</div><div></div><div>10%</div><div></div><div>10%</div></div>

## 2 Entry composition [i](#)

There are 82 unique types of molecules in this entry. The entry contains 256149 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called rRNA 2'-O-methyltransferase fibrillarin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	CA	242	Total	C	N	O	S	0	0
			1881	1193	338	340	10		
1	CB	228	Total	C	N	O	S	0	0
			1782	1131	320	321	10		

- Molecule 2 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	DA	240	Total	C	N	O	S	0	0
			1912	1209	354	345	4		

- Molecule 3 is a protein called RNA cytidine acetyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	JA	812	Total	C	N	O	S	0	0
			5916	3745	1044	1102	25		
3	JB	835	Total	C	N	O		0	0
			4132	2462	835	835			

- Molecule 4 is a protein called Periodic tryptophan protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	UA	834	Total	C	N	O	S	0	0
			6635	4223	1140	1253	19		

- Molecule 5 is a protein called Nucleolar complex protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	UB	507	Total	C	N	O	S	0	0
			3734	2367	663	695	9		

- Molecule 6 is a protein called Something about silencing protein 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	UC	128	Total	C	N	O		
			1026	633	204	189	0	0

- Molecule 7 is a protein called U3 small nucleolar RNA-associated protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	UD	675	Total	C	N	O	S		
			5361	3395	929	1015	22	0	0

- Molecule 8 is a protein called U3 small nucleolar RNA-associated protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	UE	475	Total	C	N	O	S		
			3772	2400	649	710	13	0	0

- Molecule 9 is a protein called U3 small nucleolar RNA-associated protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	UF	293	Total	C	N	O	S		
			2487	1605	435	434	13	0	0

- Molecule 10 is a protein called U3 small nucleolar RNA-associated protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	UG	533	Total	C	N	O	S		
			4218	2646	758	802	12	0	0

- Molecule 11 is a protein called U3 small nucleolar RNA-associated protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	UH	442	Total	C	N	O	S		
			2701	1680	494	524	3	0	0

- Molecule 12 is a protein called U3 small nucleolar RNA-associated protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	UI	104	Total	C	N	O	S		
			860	556	152	150	2	0	0

- Molecule 13 is a protein called U3 small nucleolar RNA-associated protein 10.



Mol	Chain	Residues	Atoms					AltConf	Trace
13	UJ	1116	Total	C	N	O	S	0	0
			8961	5802	1468	1666	25		

- Molecule 14 is a protein called U3 small nucleolar RNA-associated protein 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	UK	242	Total	C	N	O	S	0	0
			2021	1254	389	371	7		

- Molecule 15 is a protein called U3 small nucleolar RNA-associated protein 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	UL	842	Total	C	N	O	S	0	0
			6726	4303	1129	1267	27		

- Molecule 16 is a protein called U3 small nucleolar RNA-associated protein 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	UM	762	Total	C	N	O	S	0	0
			5969	3785	1007	1149	28		

- Molecule 17 is a protein called U3 small nucleolar RNA-associated protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	UN	147	Total	C	N	O	S	0	0
			1227	765	233	227	2		

- Molecule 18 is a protein called U3 small nucleolar RNA-associated protein 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	UO	493	Total	C	N	O	S	0	0
			3911	2462	702	735	12		

- Molecule 19 is a protein called Bud site selection protein 21.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	UP	60	Total	C	N	O	0	0
			495	310	101	84		

- Molecule 20 is a protein called NET1-associated nuclear protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	UQ	832	Total	C	N	O	S	0	0
			6662	4236	1124	1283	19		

- Molecule 21 is a protein called U3 small nucleolar RNA-associated protein 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	UR	482	Total	C	N	O	S	0	0
			3799	2405	669	715	10		

- Molecule 22 is a protein called Nucleolar complex protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	US	494	Total	C	N	O	S	0	0
			3622	2326	617	667	12		

- Molecule 23 is a protein called U3 small nucleolar RNA-associated protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	UT	2255	Total	C	N	O	S	0	0
			17290	11076	2927	3235	52		

- Molecule 24 is a protein called U3 small nucleolar RNA-associated protein 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	UU	848	Total	C	N	O	S	0	0
			6678	4241	1149	1267	21		

- Molecule 25 is a protein called U3 small nucleolar RNA-associated protein 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	UV	1081	Total	C	N	O	S	0	0
			8736	5681	1440	1591	24		

- Molecule 26 is a protein called rRNA-processing protein FCF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	UX	174	Total	C	N	O	S	0	0
			1395	890	255	240	10		

- Molecule 27 is a protein called Ribosome biogenesis protein UTP30.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	UZ	247	Total	C	N	O	S	0	0
			2006	1284	356	358	8		

- Molecule 28 is a protein called Nucleolar protein 56.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	CD	380	Total	C	N	O	S	0	0
			2994	1898	513	574	9		

- Molecule 29 is a protein called Nucleolar protein 58.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	CE	435	Total	C	N	O	S	0	0
			3325	2093	571	653	8		

- Molecule 30 is a protein called 13 kDa ribonucleoprotein-associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	CF	123	Total	C	N	O	S	0	0
			931	594	160	173	4		
30	CG	123	Total	C	N	O	S	0	0
			928	591	160	173	4		

- Molecule 31 is a protein called Ribosomal RNA-processing protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	CH	465	Total	C	N	O	S	0	0
			3725	2365	653	697	10		

- Molecule 32 is a protein called U3 small nucleolar ribonucleoprotein protein IMP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	CI	182	Total	C	N	O	S	0	0
			1530	967	287	269	7		

- Molecule 33 is a protein called U3 small nucleolar ribonucleoprotein protein IMP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	CJ	282	Total	C	N	O	S	0	0
			2296	1441	430	418	7		

- Molecule 34 is a protein called U3 small nucleolar RNA-associated protein MPP10.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	CK	207	Total	C	N	O	S	0	0
			1667	1034	297	332	4		

- Molecule 35 is a protein called Ribosome biogenesis protein BMS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	CL	781	Total	C	N	O	S	0	0
			6332	4063	1122	1117	30		

- Molecule 36 is a protein called RNA 3'-terminal phosphate cyclase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	CM	360	Total	C	N	O	S	0	0
			2781	1781	473	516	11		

- Molecule 37 is a protein called Ribosomal RNA-processing protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	CN	232	Total	C	N	O	S	0	0
			1893	1213	322	351	7		

- Molecule 38 is a protein called Ribosome biogenesis protein ENP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	JC	354	Total	C	N	O	S	0	0
			2845	1795	489	552	9		

- Molecule 39 is a protein called Ribosomal RNA small subunit methyltransferase NEP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	JF	216	Total	C	N	O	S	0	0
			1701	1079	296	315	11		
39	JG	230	Total	C	N	O	S	0	0
			1799	1142	313	333	11		

- Molecule 40 is a protein called Essential nuclear protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	JH	261	Total	C	N	O		0	0
			1295	773	261	261			

- Molecule 41 is a protein called rRNA biogenesis protein RRP5.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	Jl	265	Total	C	N	O	0	0
			1314	784	265	265		

- Molecule 42 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	JJ	182	Total	C	N	O	S	0	0
			1442	923	259	256	4		

- Molecule 43 is a protein called Protein BFR2.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	JK	42	Total	C	N	O	0	0
			334	213	54	67		

- Molecule 44 is a protein called rRNA-processing protein FCF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	JM	135	Total	C	N	O	S	0	0
			1137	721	211	201	4		

- Molecule 45 is a protein called Protein FAF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	JN	186	Total	C	N	O	S	0	0
			1428	879	287	259	3		

- Molecule 46 is a protein called KRR1 small subunit processome component.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	JO	230	Total	C	N	O	S	0	0
			1876	1203	330	332	11		

- Molecule 47 is a protein called Protein SOF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	JP	461	Total	C	N	O	S	0	0
			3765	2354	686	709	16		

- Molecule 48 is a protein called Regulator of rDNA transcription protein 14.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	JQ	63	Total	C	N	O	0	0
			381	234	69	78		

- Molecule 49 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	DE	245	Total	C	N	O	S	0	0
			1944	1245	360	336	3		

- Molecule 50 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	DF	213	Total	C	N	O	S	0	0
			1669	1045	307	314	3		

- Molecule 51 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	DG	218	Total	C	N	O	S	0	0
			1755	1102	337	313	3		

- Molecule 52 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	DH	184	Total	C	N	O	0	0
			1481	951	265	265		

- Molecule 53 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	DI	177	Total	C	N	O	S	0	0
			1399	869	279	249	2		

- Molecule 54 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	DJ	185	Total	C	N	O	S	0	0
			1494	943	289	261	1		

- Molecule 55 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	DL	140	Total	C	N	O	S	0	0
			1129	724	215	187	3		

- Molecule 56 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	DN	150	Total	C	N	O	S	0	0
			1192	759	224	207	2		

- Molecule 57 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	DO	120	Total	C	N	O	S	0	0
			881	544	167	167	3		

- Molecule 58 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
58	DQ	125	Total	C	N	O		
			973	625	174	174	0	0

- Molecule 59 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
59	DS	104	Total	C	N	O		
			516	308	104	104	0	0

- Molecule 60 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	DW	129	Total	C	N	O	S	0	0
			1021	650	188	180	3		

- Molecule 61 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	DX	103	Total	C	N	O	S	0	0
			786	503	144	137	2		

- Molecule 62 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
62	DY	134	Total	C	N	O	0	0
			1073	676	208	189		

- Molecule 63 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Db	81	Total	C	N	O	S	0	0
			610	382	110	113	5		

- Molecule 64 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	Dc	63	Total	C	N	O	S	0	0
			497	306	99	91	1		

- Molecule 65 is a RNA chain called 5'ETS RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	D2	446	Total	C	N	O	P	0	0
			9508	4250	1682	3130	446		

- Molecule 66 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	D3	1327	Total	C	N	O	P	0	0
			28287	12644	5022	9294	1327		

- Molecule 67 is a RNA chain called U3 snoRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	D4	230	Total	C	N	O	P	0	0
			4869	2180	841	1618	230		

- Molecule 68 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	EA	22	Total	C	N	O	P	0	0
			366	161	43	140	22		

- Molecule 69 is a protein called Exosome complex component RRP45.



Mol	Chain	Residues	Atoms				AltConf	Trace
69	EB	299	Total	C	N	O	0	0
			1475	877	299	299		

- Molecule 70 is a protein called Exosome complex component SKI6.

Mol	Chain	Residues	Atoms				AltConf	Trace
70	EC	244	Total	C	N	O	0	0
			1204	716	244	244		

- Molecule 71 is a protein called Exosome complex component RRP43.

Mol	Chain	Residues	Atoms				AltConf	Trace
71	ED	317	Total	C	N	O	1	0
			1571	937	317	317		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
ED	363	MET	VAL	conflict	UNP P25359

- Molecule 72 is a protein called Exosome complex component RRP46.

Mol	Chain	Residues	Atoms				AltConf	Trace
72	EE	223	Total	C	N	O	1	0
			1107	661	223	223		

- Molecule 73 is a protein called Exosome complex component RRP42.

Mol	Chain	Residues	Atoms				AltConf	Trace
73	EF	267	Total	C	N	O	1	0
			1326	792	267	267		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EF	-1	GLY	-	expression tag	UNP Q12277
EF	0	HIS	-	expression tag	UNP Q12277
EF	138	ILE	VAL	conflict	UNP Q12277

- Molecule 74 is a protein called Exosome complex component MTR3.

Mol	Chain	Residues	Atoms				AltConf	Trace
74	EG	215	Total	C	N	O	0	0
			1058	628	215	215		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EG	75	SER	THR	conflict	UNP P48240

- Molecule 75 is a protein called Exosome complex component RRP40.

Mol	Chain	Residues	Atoms				AltConf	Trace
75	EH	237	Total	C	N	O	0	0
			1170	696	237	237		

- Molecule 76 is a protein called Exosome complex component RRP4.

Mol	Chain	Residues	Atoms				AltConf	Trace
76	EI	293	Total	C	N	O	0	0
			1440	854	293	293		

- Molecule 77 is a protein called Exosome complex component CSL4.

Mol	Chain	Residues	Atoms				AltConf	Trace
77	EJ	222	Total	C	N	O	0	0
			1091	647	222	222		

- Molecule 78 is a protein called Exosome complex exonuclease DIS3.

Mol	Chain	Residues	Atoms				AltConf	Trace
78	EK	970	Total	C	N	O	1	0
			4818	2878	970	970		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EK	171	ASN	ASP	conflict	UNP Q08162
EK	551	ASN	ASP	conflict	UNP Q08162

- Molecule 79 is a protein called ATP-dependent RNA helicase DOB1.

Mol	Chain	Residues	Atoms				AltConf	Trace
79	EN	964	Total	C	N	O	0	0
			4767	2842	964	961		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EN	80	MET	VAL	conflict	UNP P47047

- Molecule 80 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
80	UX	1	Total	Zn	0
			1	1	
80	Db	1	Total	Zn	0
			1	1	
80	EK	1	Total	Zn	0
			1	1	

- Molecule 81 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
81	UX	1	Total	Mg	0
			1	1	
81	CL	1	Total	Mg	0
			1	1	
81	EK	1	Total	Mg	0
			1	1	

- Molecule 82 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).

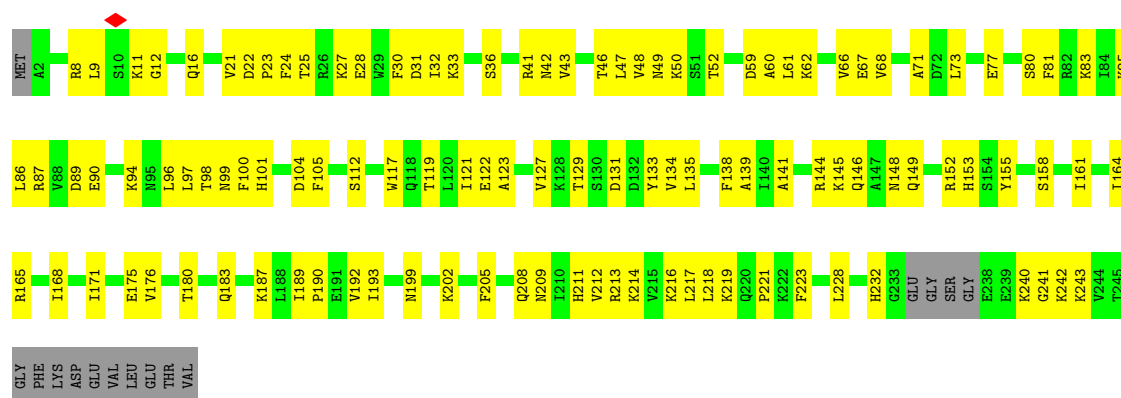


Mol	Chain	Residues	Atoms					AltConf
82	CL	1	Total	C	N	O	P	0
			32	10	5	14	3	



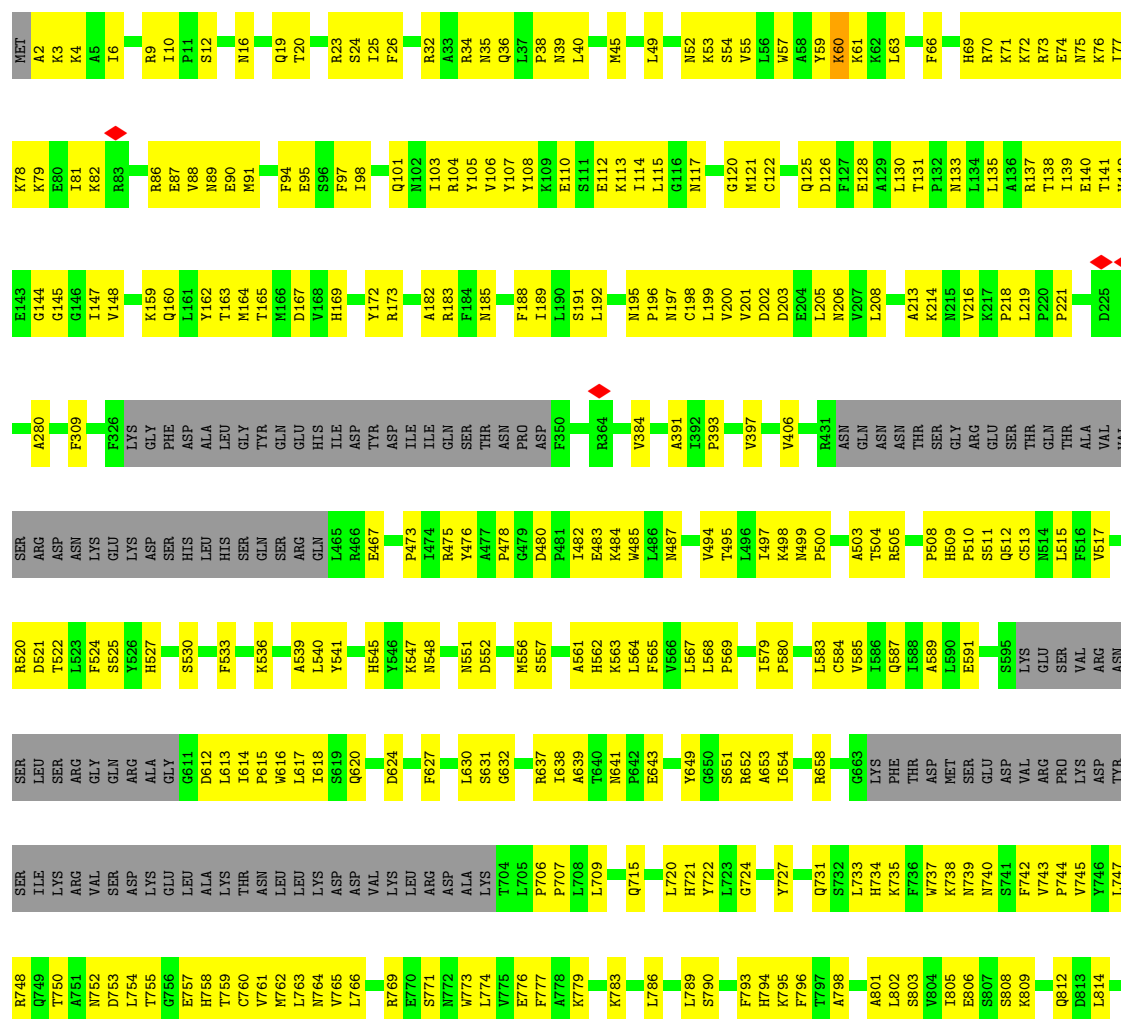
• Molecule 2: 40S ribosomal protein S1-A

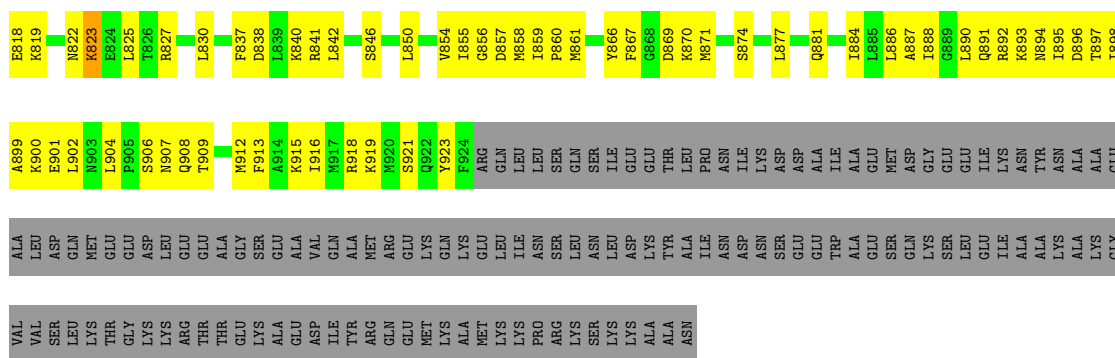
Chain DA:  50% 44% 6%



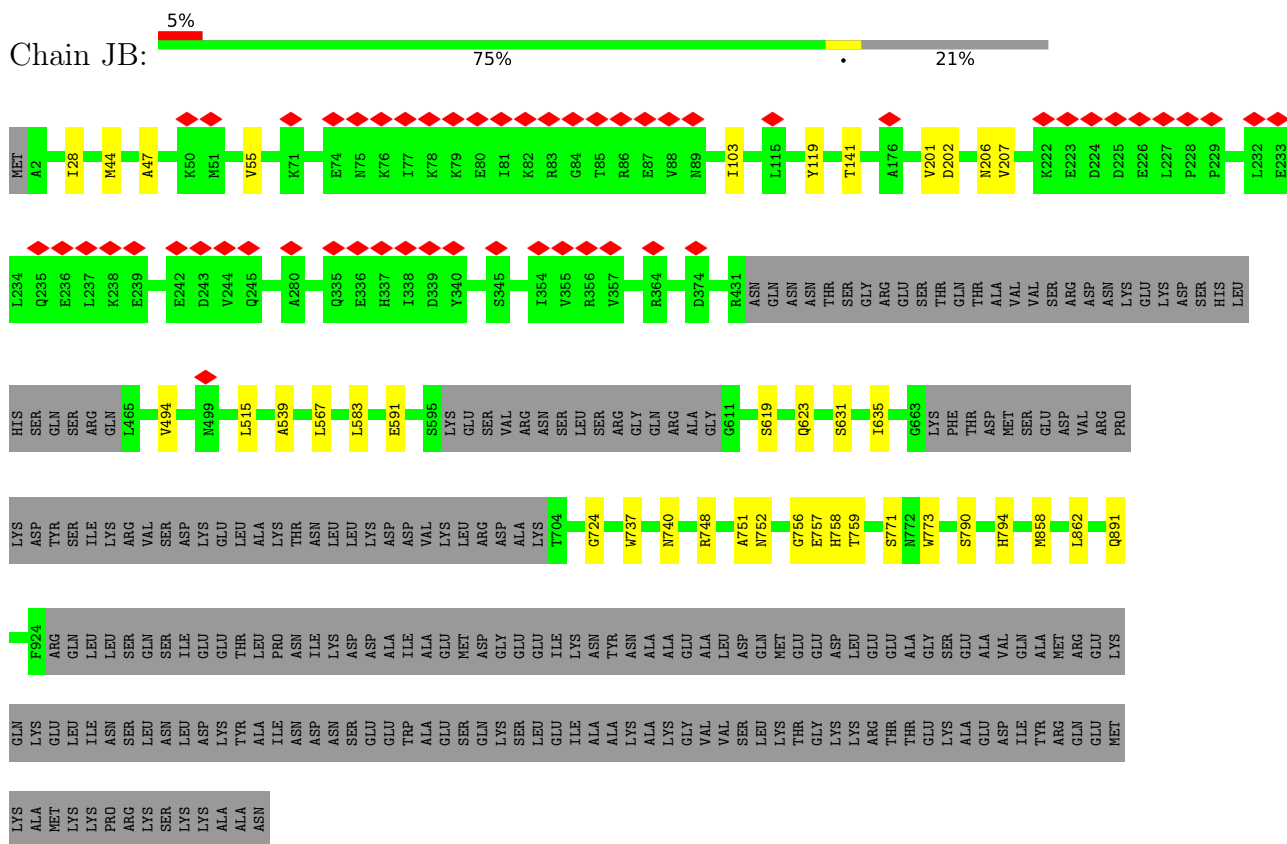
• Molecule 3: RNA cytidine acetyltransferase

Chain JA:  45% 32% 23%





- Molecule 3: RNA cytidine acetyltransferase



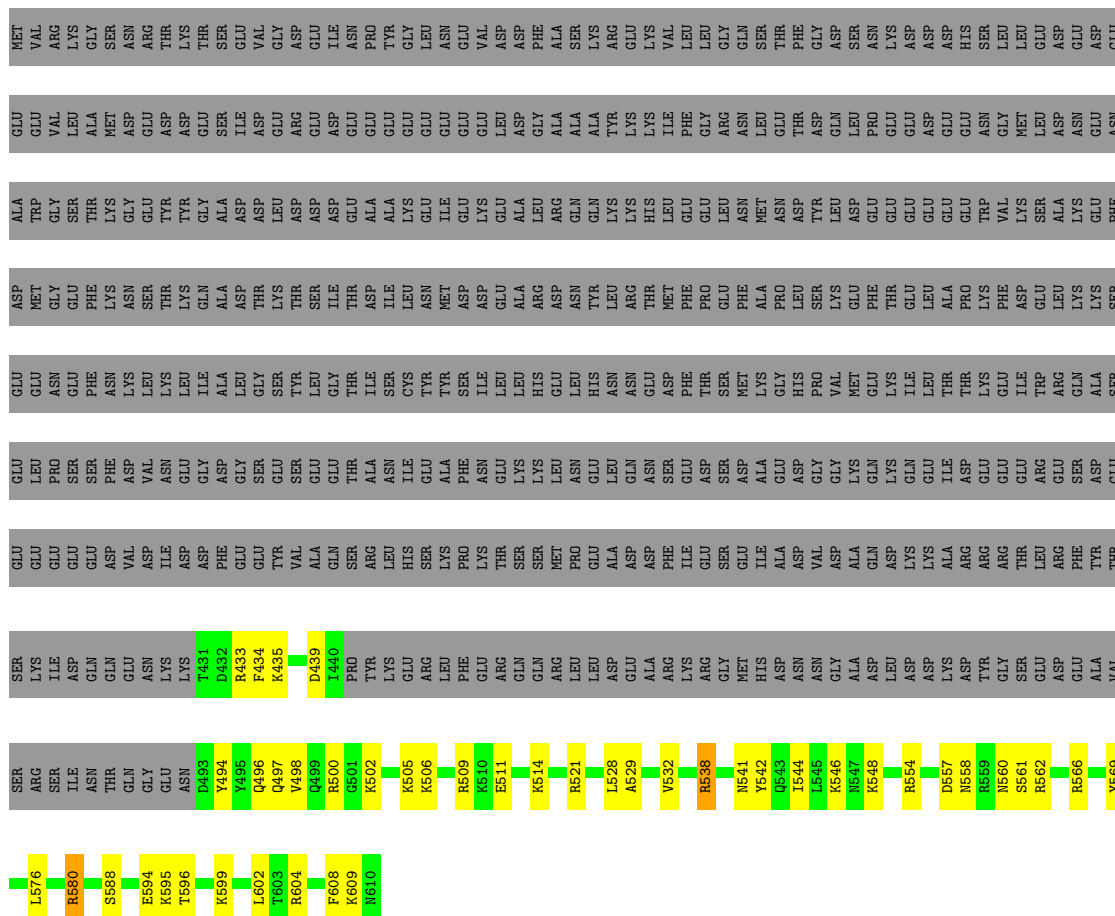
- Molecule 4: Periodic tryptophan protein 2







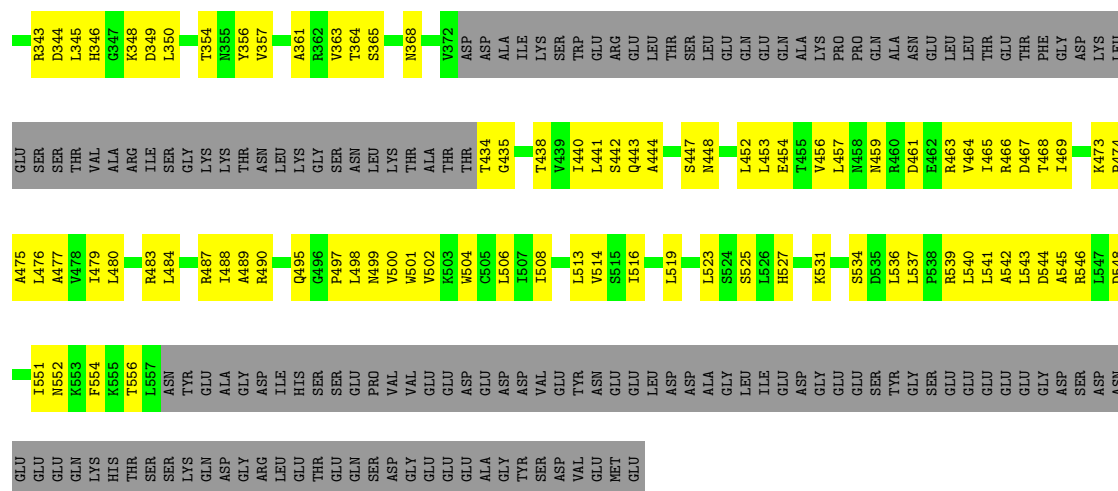
- Molecule 6: Something about silencing protein 10



- Molecule 7: U3 small nucleolar RNA-associated protein 4

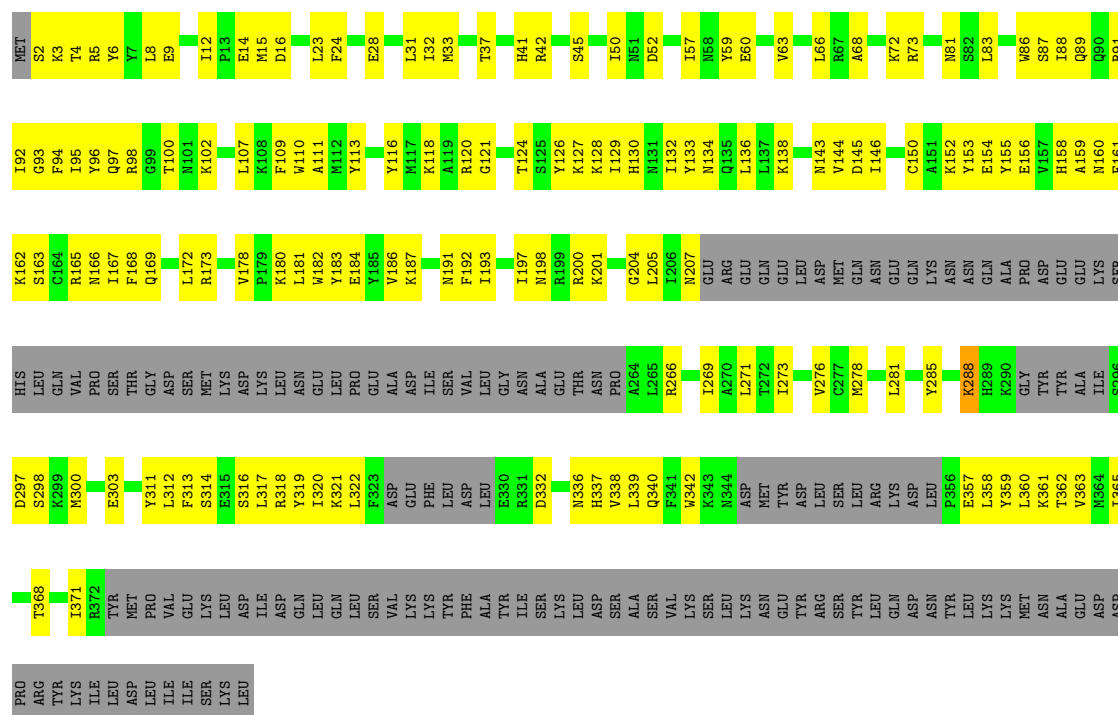






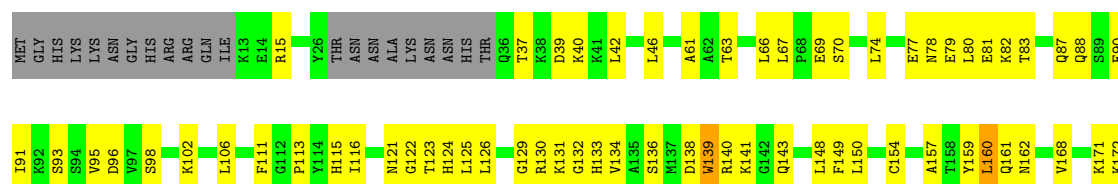
• Molecule 9: U3 small nucleolar RNA-associated protein 6

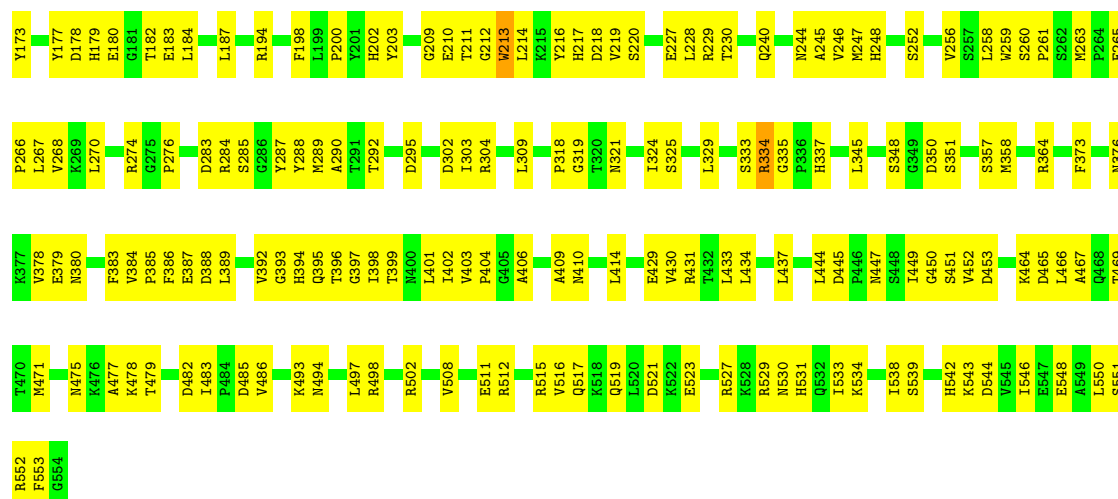
Chain UF: 33% 34% 33%



• Molecule 10: U3 small nucleolar RNA-associated protein 7

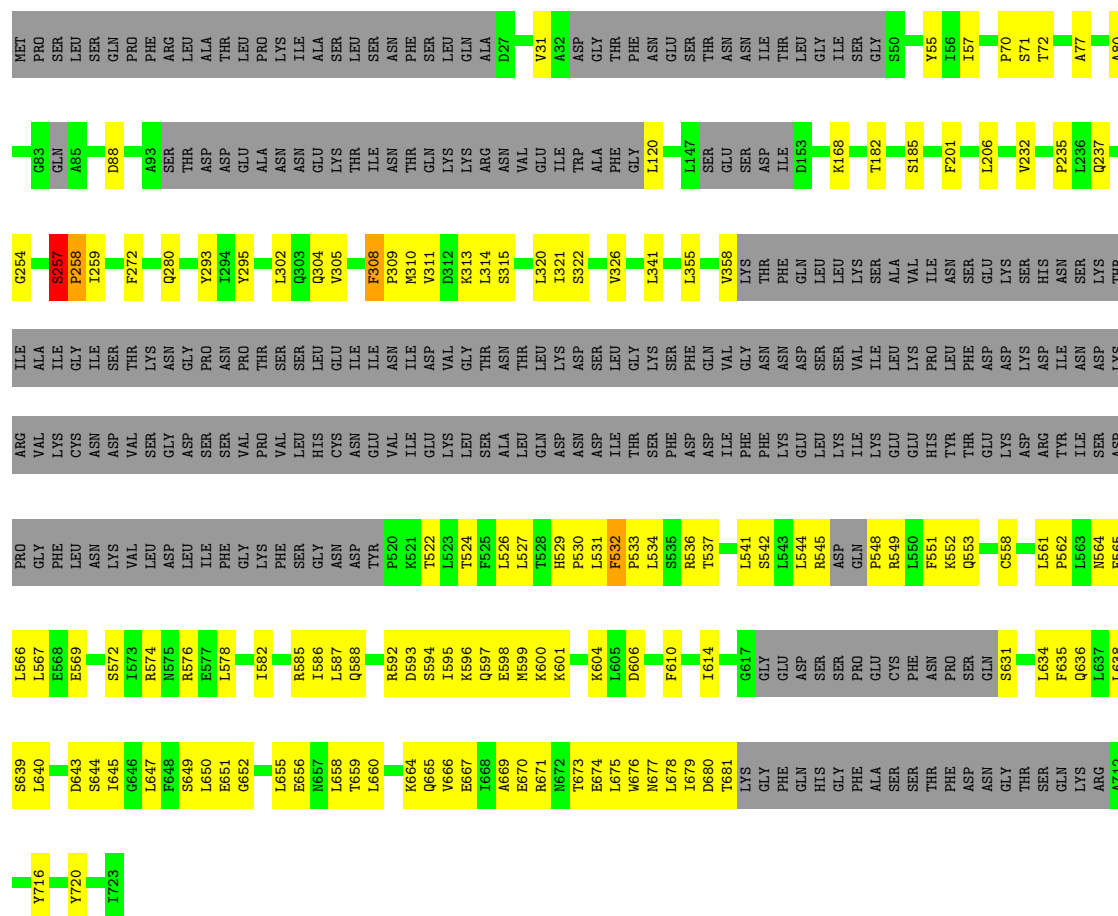
Chain UG: 55% 41% . .





- Molecule 11: U3 small nucleolar RNA-associated protein 8

Chain UH: 43% 18% 38%

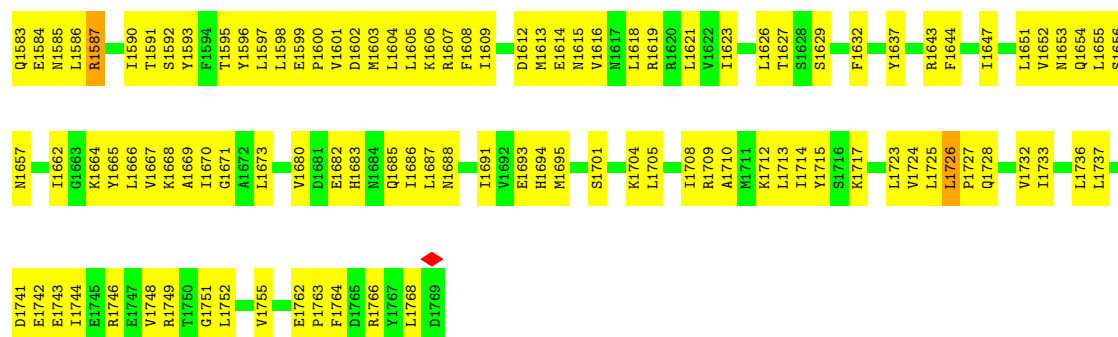


- Molecule 12: U3 small nucleolar RNA-associated protein 9

Chain UI: 5% 13% 82%







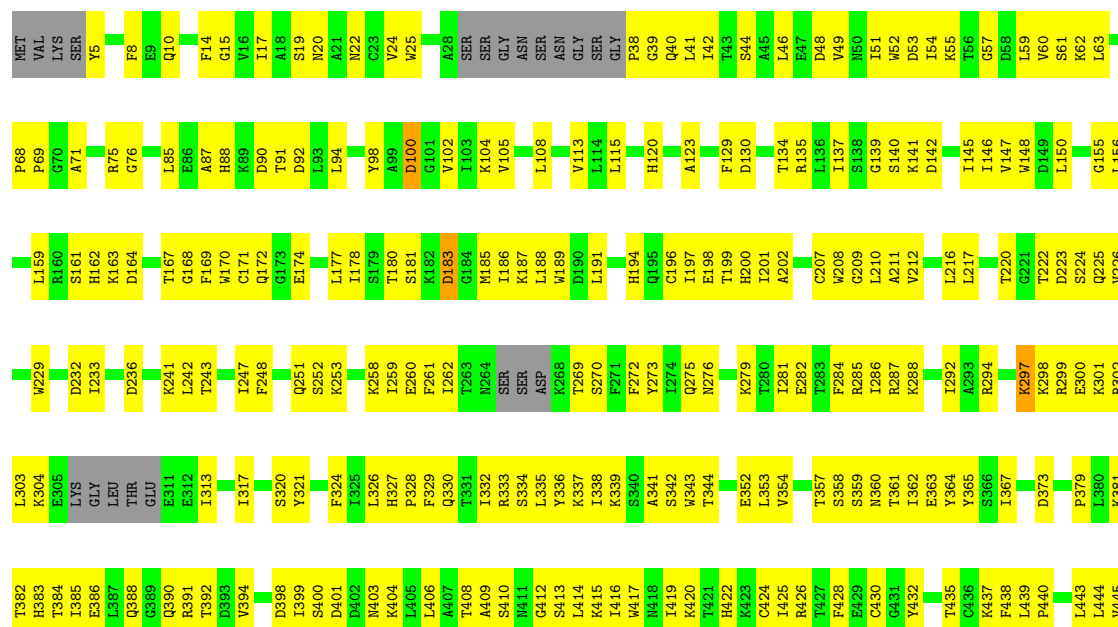
• Molecule 14: U3 small nucleolar RNA-associated protein 11

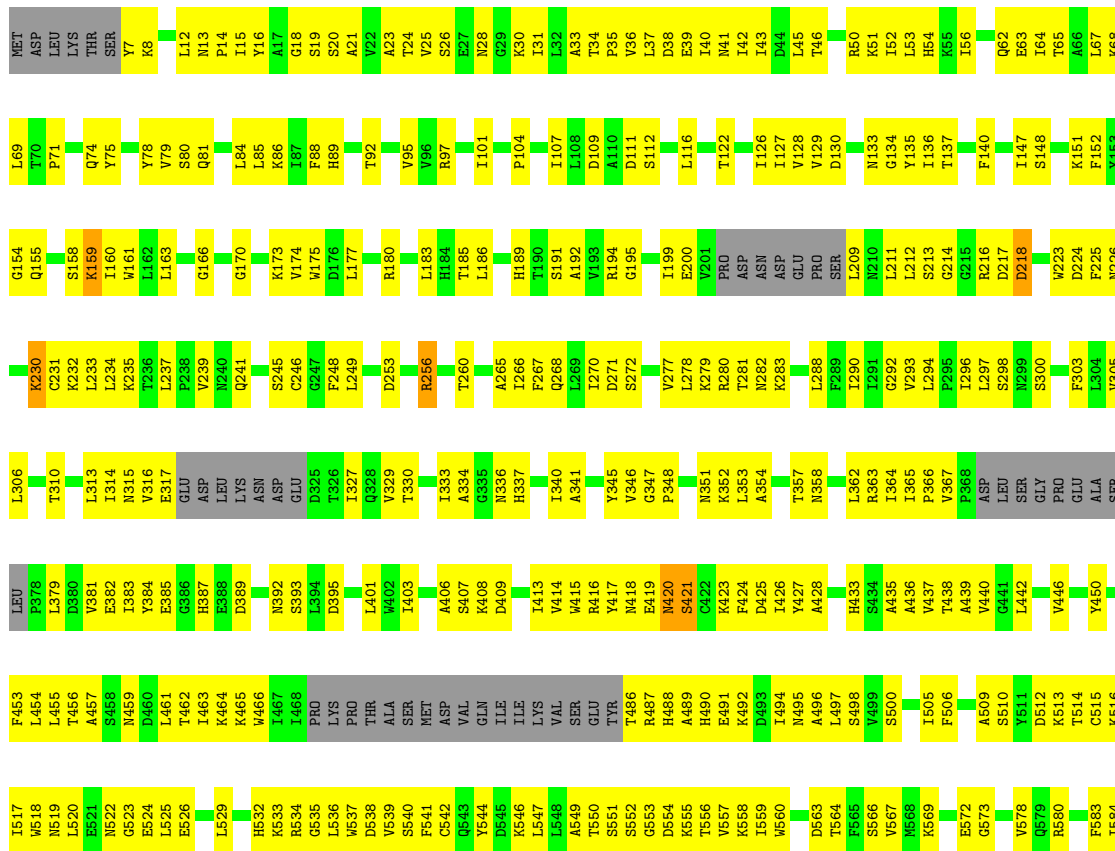
Chain UK: 41% 55%



• Molecule 15: U3 small nucleolar RNA-associated protein 12

Chain UL: 44% 45% 11%





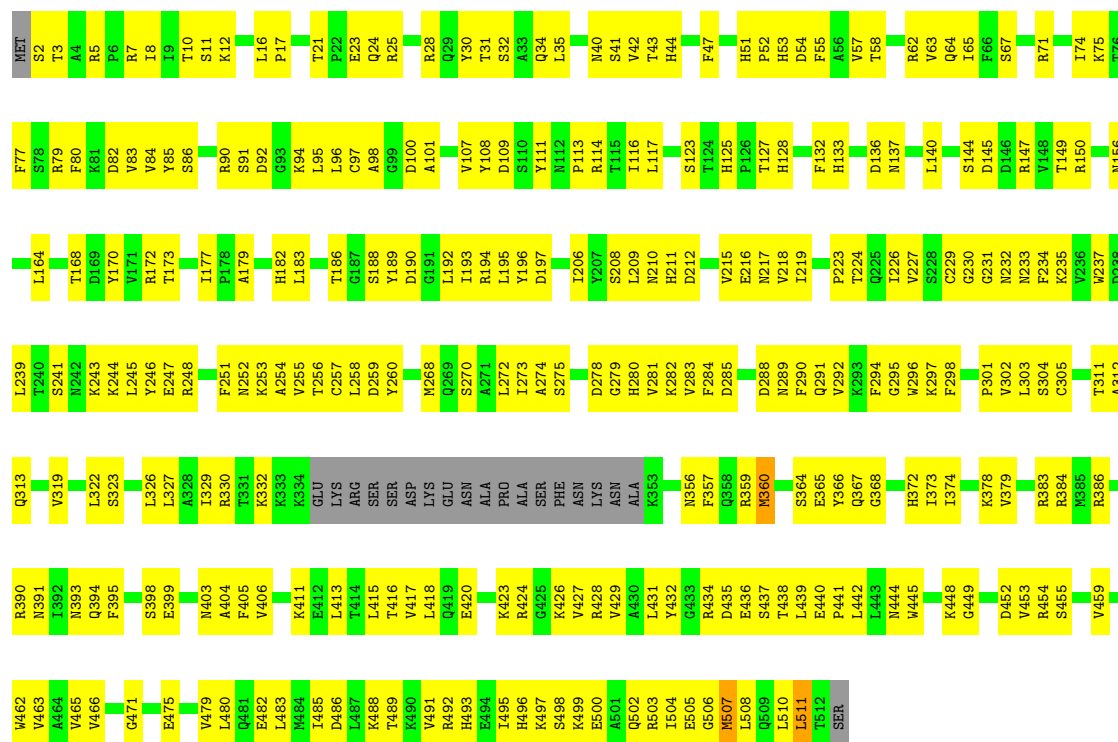






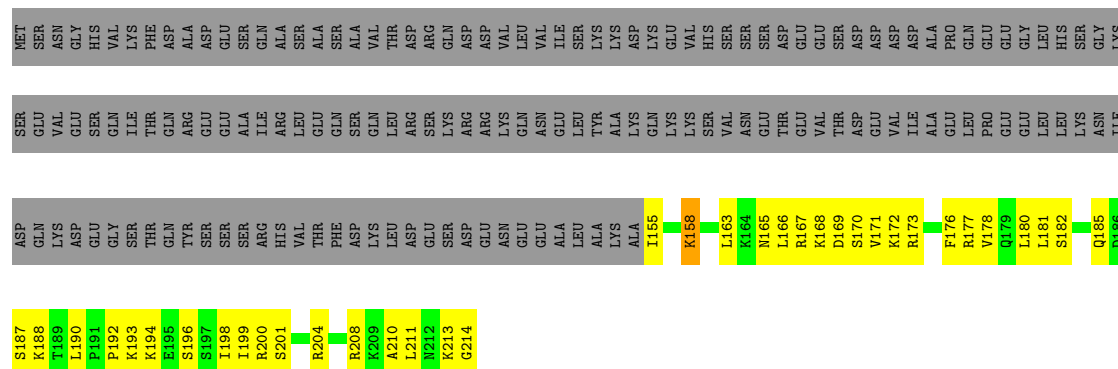
- Molecule 18: U3 small nucleolar RNA-associated protein 15

Chain UO: 42% 53% ..



- Molecule 19: Bud site selection protein 21

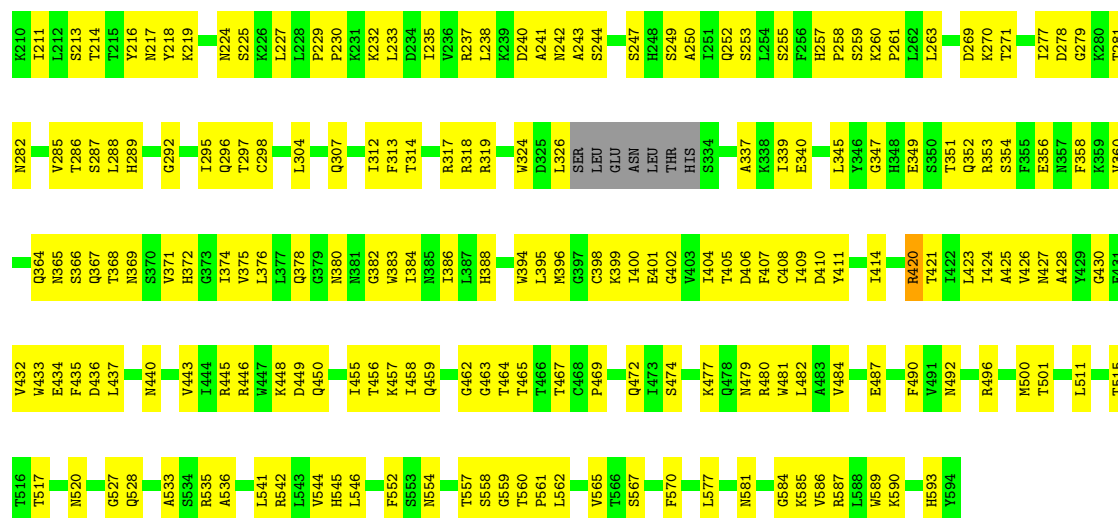
Chain UP: 11% 16% 72%



- Molecule 20: NET1-associated nuclear protein 1

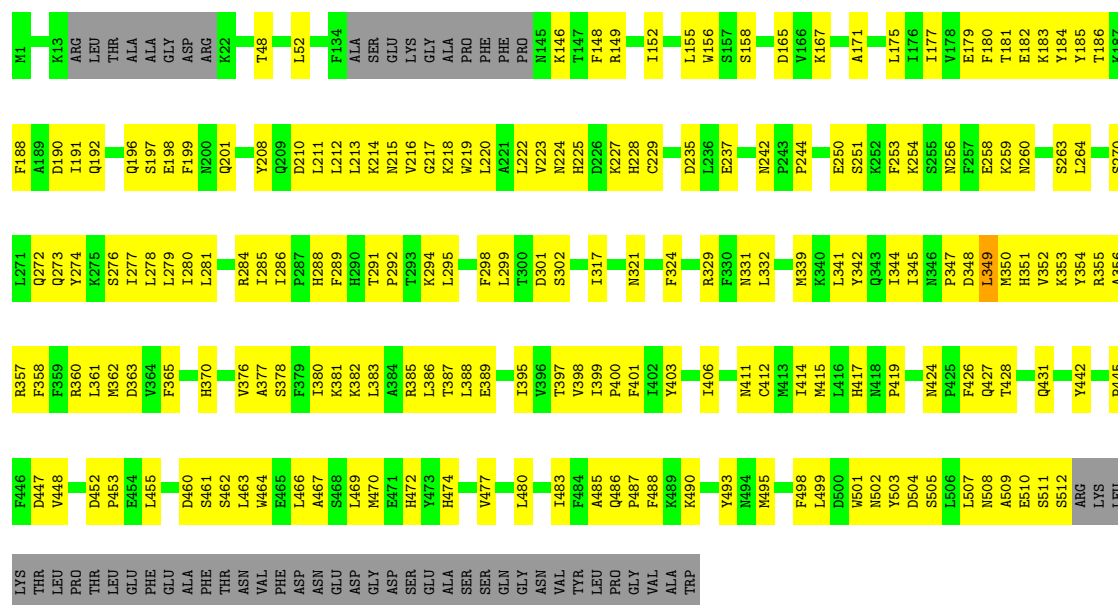
Chain UQ: 43% 49% 7%

MET	THR	GLN	SER	LEU	GLY	ILE	GLU	Q9	Y10	V15	S16	G17	G18	K19	P20	N24	L25	T29	G30	N31	N32	N33	I34	A35	R36	L37	S38	Q39	D40	Q41	R42	N43	P47	F48	N49	N50	Q51	I52	K53	V54	Y55	S56	V57	R60	K64	T65	L66	K67	L73	I77	F78																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
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F157	K158	D159	PRO	GLN	LYS	ALA	HIS	N166	S167	L168	Q169	S170	Y171	R172	L173	Y174	D179	D180	A181	K182	K183	Q184	H189	E192	N195	V196	I197	S199	N200	I201	L207	L208	A209	H210	M211	C212	K213	D214	V215	S216	T217	K218	D219	S224	I225	S226	V227	V228	S229	F231																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
D232	V235	N236	L237	S238	F239	P240	S243	L244	S245	S246	S247	Q248	T249	Q250	L252	S253	Y254	N255	T256	R257	Y258	V259	M262	I264	D265	N266	Q270	L271	A272	G274	F275	A276	S277	I282	V283	I290	R291	L292	L293	K294	W295	H296	I297	D298	S299	S302	F305	S306																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
G309	S310	Y311	N386	L312	L313	S314	W317	E318	K319	V320	M321	S322	L323	W324	N329	S330	Q331	L334	P335	R336	L337	N338	G339	I340	D343	C344	Q345	V346	L347	S354	S355	L356	I357	E362	N363	N364	S365	F366	T367	T368	D368	F371	L372	L373	N375	A376	S377	D378	L379	T380	S381																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
K382	L383	S384	I385	N386	G387	P388	P389	V391	F392	I396	K397	H398	Q401	F402	I403	M406	N407	T408	K409	M410	S411	N412	S413	I414	S420	K421	K422	Q424	S425	R426	K427	L428	I429	K430	R433	Q434	D435	F436	T437	T438	N439	V440	N443	K447	N448	I449	Y450	H453	I454																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
S455	A456	V457	Q458	I459	F460	D461	F462	Y463	Q467	V468	N469	Y470	Q471	L472	T473	S475	G476	N478	K483	S554	V555	P556	F557	L557	T558	L561	P562	S570	C573	D497	L498	K499	F500	D503	O504	Q505	W506	M507	F508	T509	Y510	F511	T512	E513	Y514	P515	D518	S522	R523	D524																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
H527	I528	L529	K530	N531	W532	T533	N535	E538	T539	N540	W541	N542	K544	T545	K546	V547	I548	I553	S554	V555	P556	F557	L557	T558	L561	P562	S570	C573	D497	L498	K499	F500	D503	O504	Q505	W506	M507	F508	T509	Y510	F511	T512	E513	Y514	P515	D518	S522	R523	D524																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
S608	S612	S616	S617	S618	S619	S620	F623	H624	G625	F626	D627	D628	Q631	L632	L633	D634	F635	D636	F637	K638	K639	E642	S657	E658	L660	T661	F662	L663	L664	L665	N669	L670	T674	R675	T676	L677	L678	N682	L683	L689	M690	D693	L694	Y695	F696	F697	V698	Y701																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
Y702	K703	N704	H705	H706	H707	D708	R709	S781	T782	T783	G784	T785	VAL	ASN	THR	GLN	LEU	SER	ASP	GLU	VAL	ASN	ASN	GLY	LEU	ASP	GLY	VAL	SER	ASN	GLN	THR	ILE	THR	SER	ALA	SER	S818	S819	D820	I821	F822	O825	L826	L829	SER	ARG	GLY	LYS	SER																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
D773	F774	T775	F776	L777	D778	L779	S780	T781	T782	T783	G784	T785	VAL	ASN	THR	GLN	LEU	SER	ASP	GLU	VAL	ASN	ASN	GLY	LEU	ASP	GLY	VAL	SER	ASN	GLN	THR	ILE	THR	SER	ALA	SER	S818	S819	D820	I821	F822	O825	L826	L829	SER	ARG	GLY	LYS	SER																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
ASP	THR	ARG	ASP	LYS	ASN	THR	ASN	ASP	N846	D849	E850	I853	K862	K863	N864	K865	N868	S871	F872	N875	F876	D877	N878	I879	Q880	N884	D885	T886	F887	R890	V894	L895	T896	S897	S898	D899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935	L936	L937	L938	L939	L940	L941	L942	L943	L944	L945	L946	L947	L948	L949	L950	L951	L952	L953	L954	L955	L956	L957	L958	L959	L960	L961	L962	L963	L964	L965	L966	L967	L968	L969	L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980	L981	L982	L983	L984	L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999	L1000	L1001	L1002	L1003	L1004	L1005	L1006	L1007	L1008	L1009	L1010	L1011	L1012	L1013	L1014	L1015	L1016	L1017	L1018	L1019	L1020	L1021	L1022	L1023	L1024	L1025	L1026	L1027	L1028	L1029	L1030	L1031	L1032	L1033	L1034	L1035	L1036	L1037	L1038	L1039	L1040	L1041	L1042	L1043	L1044	L1045	L1046	L1047	L1048	L1049	L1050	L1051	L1052	L1053	L1054	L1055	L1056	L1057	L1058	L1059	L1060	L1061	L1062	L1063	L1064	L1065	L1066	L1067	L1068	L1069	L1070	L1071	L1072	L1073	L1074	L1075	L1076	L1077	L1078	L1079	L1080	L1081	L1082	L1083	L1084	L1085	L1086	L1087	L1088	L1089	L1090	L1091	L1092	L1093	L1094	L1095	L1096	L1097	L1098	L1099	L1100	L1101	L1102	L1103	L1104	L1105	L1106	L1107	L1108	L1109	L1110	L1111	L1112	L1113	L1114	L1115	L1116	L1117	L1118	L1119	L1120	L1121	L1122	L1123	L1124	L1125	L1126	L1127	L1128	L1129	L1130	L1131	L1132	L1133	L1134	L1135	L1136	L1137	L1138	L1139	L1140	L1141	L1142	L1143	L1144	L1145	L1146	L1147	L1148	L1149	L1150	L1151	L1152	L1153	L1154	L1155	L1156	L1157	L1158	L1159	L1160	L1161	L1162	L1163	L1164	L1165	L1166	L1167	L1168	L1169	L1170	L1171	L1172	L1173	L1174	L1175	L1176	L1177	L1178	L1179	L1180	L1181	L1182	L1183	L1184	L1185	L1186	L1187	L1188	L1189	L1190	L1191	L1192	L1193	L1194	L1195	L1196	L1197	L1198	L1199	L1200	L1201	L1202	L1203	L1204	L1205	L1206	L1207	L1208	L1209	L1210	L1211	L1212	L1213	L1214	L1215	L1216	L1217	L1218	L1219	L1220	L1221	L1222	L1223	L1224	L1225	L1226	L1227	L1228	L1229	L1230	L1231	L1232	L1233	L1234	L1235	L1236	L1237	L1238	L1239	L1240	L1241	L1242	L1243	L1244	L1245	L1246	L1247	L1248	L1249	L1250	L1251	L1252	L1253	L1254	L1255	L1256	L1257	L1258	L1259	L1260	L1261	L1262	L1263	L1264	L1265	L1266	L1267	L1268	L1269	L1270	L1271	L1272	L1273	L1274	L1275	L1276	L1277	L1278	L1279	L1280	L1281	L1282	L1283	L1284	L1285	L1286	L1287	L1288	L1289	L1290	L1291	L1292	L1293	L1294	L1295	L1296	L1297	L1298	L1299	L1300	L1301	L1302	L1303	L1304	L1305	L1306	L1307	L1308	L1309	L1310	L1311	L1312	L1313	L1314	L1315	L1316	L1317	L1318	L1319	L1320	L1321	L1322	L1323	L1324	L1325	L1326	L1327	L1328	L1329	L1330	L1331	L1332	L1333	L1334	L1335	L1336	L1337	L1338	L1339	L1340	L1341	L1342	L1343	L1344	L1345	L1346	L1347	L1348	L1349	L1350	L1351	L1352	L1353	L1354	L1355	L1356	L1357	L1358	L1359	L1360	L1361	L1362	L1363	L1364	L1365	L1366	L1367	L1368	L1369	L1370	L1371	L1372	L1373	L1374	L1375	L1376	L1377	L1378	L1379	L1380	L1381	L1382	L1383	L1384	L1385	L1386	L1387	L1388	L1389	L1390	L1391	L1392	L1393	L1394	L1395	L1396	L1397	L1398	L1399	L1400	L1401	L1402	L1403	L1404	L1405	L1406	L1407	L1408	L1409	L1410	L1411	L1412	L1413	L1414	L1415	L1416	L1417	L1418	L1419	L1420	L1421	L1422	L1423	L1424	L1425	L1426	L1427	L1428	L1429	L1430	L1431	L1432	L1433	L1434	L1435	L1436	L1437	L1438	L1439	L1440	L1441	L1442	L1443	L1444	L1445	L1446	L1447	L1448	L1449	L1450	L1451	L1452	L1453	L1454	L1455	L1456	L1457	L1458	L1459	L1460	L1461	L1462	L1463	L1464	L1465	L1466	L1467	L1468	L1469	L1470	L1471	L1472	L1473	L1474	L1475	L1476	L1477	L1478	L1479	L1480	L1481	L1482	L1483	L1484	L1485	L1486	L1487	L1488	L1489	L1490	L1491	L1492	L1493	L1494	L1495	L1496	L1497	L1498	L1499	L1500	L1501	L1502	L1503	L1504	L1505	L1506	L1507	L1508	L1509	L1510	L1511	L1512	L1513	L1514	L1515	L1516	L1517	L1518	L1519	L1520	L1521	L1522	L1523	L1524	L1525	L1526	L1527	L1528	L1529	L1530	L1531	L1532	L1533	L1534	L1535	L1536	L1537	L1538	L1539	L1540	L1541	L1542	L1543	L1544	L1545	L1546	L1547	L1548	L1549	L1550	L1551	L1552	L1553	L1554	L1555	L1556	L1557	L1558	L1559	L1560	L1561	L1562	L1563	L1564	L1565	L1566	L1567	L1568	L1569	L1570	L1571	L1572	L1573	L1574	L1575	L1576	L1577	L1578	L1579	L1580	L1581	L1582	L1583	L1584	L1585	L1586	L1587	L1588	L1589	L1590	L1591	L1592	L1593	L1594	L1595	L1596	L1597	L1598	L1599	L1600	L1601	L1602	L1603	L1604	L1605	L1606	L1607	L1608	L1609	L1610	L1611	L1612	L1613	L1614	L1615	L1616	L1617	L1618	L1619	L1620	L1621	L1622	L1623	L1624	L1625	L1626	L1627	L1628	L1629	L1630	L1631	L1632	L1633	L1634	L1635	L1636	L1637	L1638	L1639	L1640	L1641	L1642	L1643	L1644	L1645	L1646	L1647	L1648	L1649	L1650	L1651	L1652	L1653	L1654	L1655	L1656	L1657	L1658	L1659	L1660	L1661	L1662	L1663	L1664	L1665	L1666	L1667	L1668	L1669	L1670	L1671	L1672	L1673	L1674	L1675	L1676	L1677	L1678	L1679	L1680	L1681	L1682	L1683	L1684	L1685	L1686	L1687	L1688	L1689	L1690	L1691	L1692	L1693	L1694	L1695	L1696	L1697	L1698	L1699	L1700	L1701	L1702	L1703	L1704	L1705	L1706	L1707	L1708	L1709	L1710	L1711	L1712	L1713	L1714	L1715	L1716	L1717	L1718	L1719	L1720	L1721	L1722	L1723	L1724	L1725	L1726	L1727	L1728	L1729	L1730	L1731	L1732	L1733	L1734	L1735	L1736	L1737	L1738	L1739	L1740	L1741	L1742	L1743	L1744	L1745	L1746	L1747	L1748	L1749	L1750



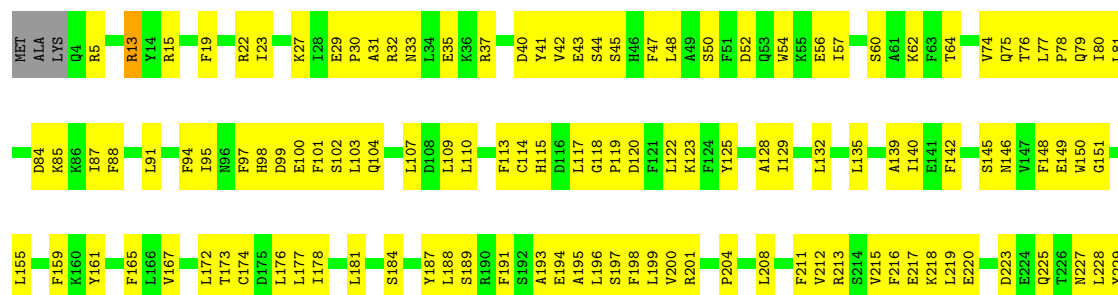
### • Molecule 22: Nucleolar complex protein 4

Chain US: 55% 34% 11%



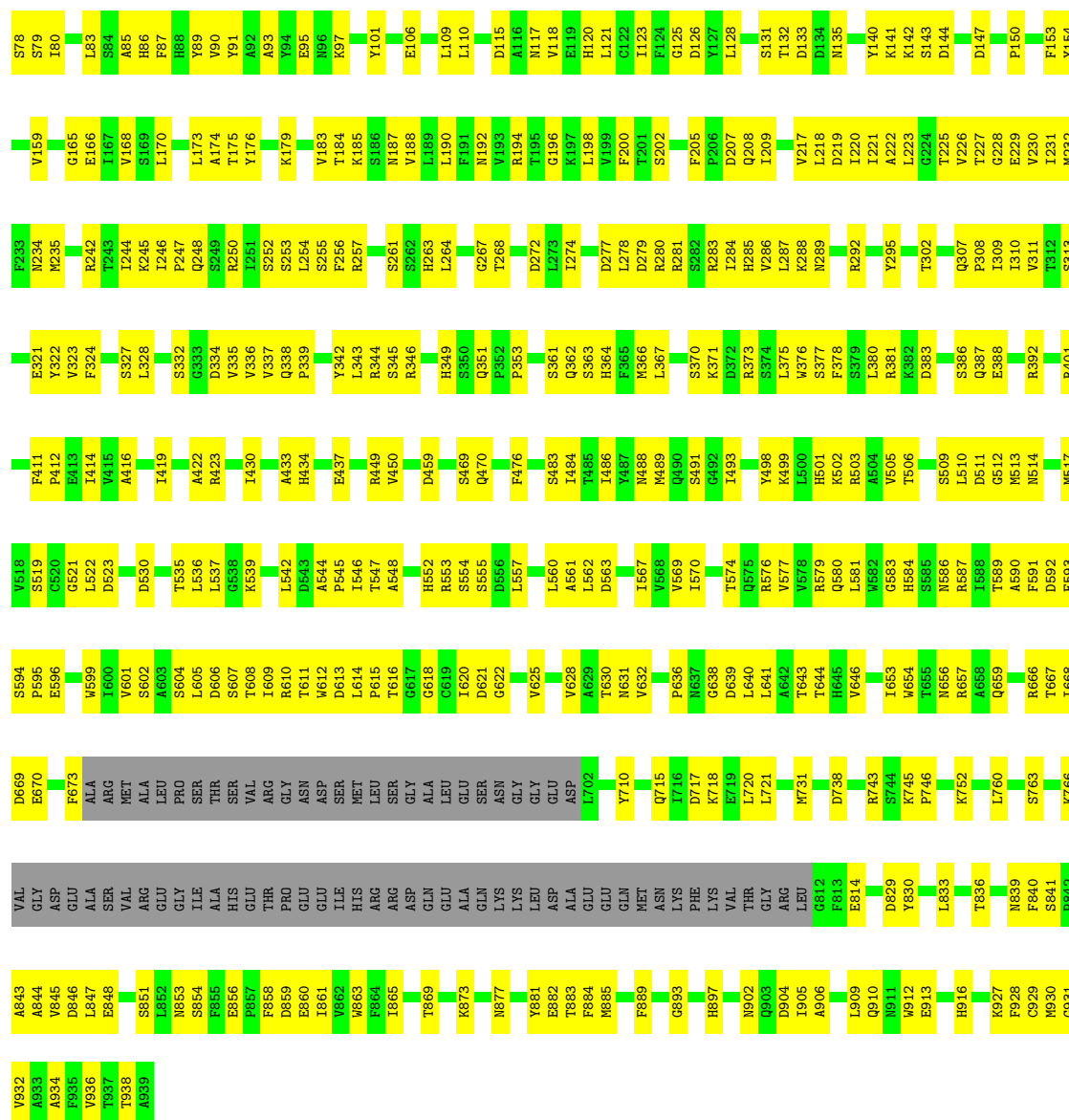
### • Molecule 23: U3 small nucleolar RNA-associated protein 20

Chain UT: 48% 42% 10%



F1288	D1125	L1054	L972	I901	V830	W754	W678	K605	I525	E456	S369	M298	L232
I1289	E1126	R1055	D973	T902	F831	N755	V681	T606	Y526	F457	L374	Y299	L233
G1292	F1127	Q1056	Y974	T903	L832	S756	F682	L607	R527	I458	L303	Q300	I234
V1295	A1130	Q1057	F977	L905	F838	I758	D683	L610	GLU	S460	L386	N303	L235
P1296	M1134	G1058	F978	T906	K839	S759	N687	P616	ASP	I461	D391	L306	P236
E1297	Q1140	L1059	G979	S910	N840	S760	V688	D617	ASP	R462	C392	T237	E238
L1298	S981	K1060	N980	S910	I841	T761	V689	S620	ALA	D463	T309	E239	T241
I1301	H1141	S1063	H982	K914	V844	E763	T690	S621	GLY	F393	L309	R133	S242
V1305	K1143	V1065	S986	D917	E845	E764	D692	S622	N535	E395	L309	I314	T243
L1308	E1144	F1066	S987	E918	E849	P771	L895	G623	N536	F396	L309	I315	T246
N1309	A1145	E1067	K988	K919	L850	I772	V696	V624	L537	F397	L309	K316	L247
M1310	V1146	F1068	K989	V920	H851	S773	W697	V625	R539	Q398	L309	V317	L248
T1311	T1147	V1069	T990	V921	L852	L773	L625	I625	T540	F399	L309	L318	H248
S1312	G1148	D1239	L991	N922	H853	I774	K698	E626	T540	R402	L309	T319	S249
S1313	T1149	T1240	K992	P923	L854	R775	L699	I641	N535	R403	L309	T320	K250
S1314	I1150	F1073	T993	Y924	H855	W776	V700	T631	N536	L403	L309	T321	A251
R1315	I1151	D1074	I994	V925	V856	Q777	L701	L632	Y480	S404	L309	V322	K252
M1316	A1154	S1078	R995	L926	L857	W781	S702	Q633	W481	Y406	L309	V323	A253
D1320	D1155	M1079	R996	R927	L858	W782	F703	N634	R482	E406	L309	V324	I254
S1326	S1156	T1079	M997	T928	C859	W783	L704	A635	A483	R407	L309	E325	M255
K1329	I1157	M1082	T998	F929	S860	S784	K705	R636	I484	V408	L309	E326	S256
K1332	N1163	V1083	G999	F930	H861	L706	L706	D637	I485	F486	L309	G327	V257
E1333	H1166	W1087	V1001	Q934	N862	P707	P707	L638	N412	K487	L309	R328	L258
D1334	D1169	K1088	N1002	V935	T863	D708	D708	R641	G413	Y488	L309	R329	L259
G1335	C1178	P1089	I1003	R943	D864	Q711	Q711	I642	L414	L414	L309	I330	H260
Y1336	I1181	K1090	N1005	S939	V865	E790	D714	K644	K491	K415	L309	P331	A261
S1340	L1185	D1096	S1006	S939	L868	D795	Y715	V645	Q492	K493	L309	D332	E262
E1341	Y1186	D1097	L1008	G940	A869	I796	Y715	V645	N494	T494	L309	W333	L263
L1342	Y1187	W1098	S1009	Q941	L870	P718	P718	E648	E495	K422	L309	I336	L264
E1343	K1188	Q1100	V1010	R943	L873	P719	L719	G650	E495	Q428	L309	T337	K265
W1344	L1189	Q1101	L1011	S944	L874	F799	F799	K651	I497	I340	L309	I340	S266
V1345	SER	P1102	R1012	R945	A875	Y801	G723	T652	I498	K431	L309	I343	E269
L1346	D1191	S1103	R1013	K946	I876	N802	A724	K653	P499	L434	L309	Q346	R270
L1347	S1194	L1105	N1014	T947	R877	D803	K726	T654	L500	F435	L309	S347	S271
L1348	F1198	R1107	L1015	A948	N878	F804	W727	D655	E502	F436	L309	E348	V272
F1349	L1199	L1108	F1016	V949	N878	LYS	L728	K656	R503	L437	L309	ASN	S273
F1350	W1200	Q1023	P1016	V949	L881	THR	W729	L657	F508	F438	L309	CYS	L275
F1351	L1201	L1024	R958	S951	L881	THR	D790	V658	A509	V439	L309	ALA	S276
L1352	L1202	I1027	K958	V952	Y884	LYS	S731	S658	S510	D440	L309	ALA	D277
T1355	Y1028	Y1028	P959	L953	R885	ASP	S732	S659	S510	D441	L309	SER	L278
N1356	A1033	A1033	P960	P954	D886	GLU	W733	F662	P511	K442	L309	LEU	W279
K1358	L1118	L1118	S961	N955	N887	GLU	V734	N588	N588	P443	L309	SER	M280
A1362	Y1119	Y1119	K957	F956	L888	ASP	R735	L666	N513	E444	L309	Q355	N281
L1363	Q1120	Q1120	R958	S957	K899	MET	L736	L591	F514	L445	L309	D356	I282
E1285	E1207	E1207	K958	K957	N890	GLU	L736	F667	T515	Q446	L309	K357	I282
E1286	F1121	F1121	P959	S957	L891	ASN	T740	G668	T515	Q446	L309	K357	I282
L1287	Y1123	Y1123	S969	S969	L892	GLU	T740	D593	K516	K447	L309	V358	I288
T1365	I1211	Y1124	R971	R971	D894	ARG	H745	D593	D517	V448	L309	V358	I288
						VAL	H746	T596	M518	R449	L309	F362	L291
						THR	W747	R597	V519	E450	L309	A363	L292
						THR	S748	T600	G520	V451	L309	L364	P293
						GLY	K749	L603	T521	M452	L309	F365	V294
						S822	W749	L603	L522	F453	L309	I366	Y295
							S822	L603	L522	R367	L309	R367	E296
									K524	E455	L309	N368	V297



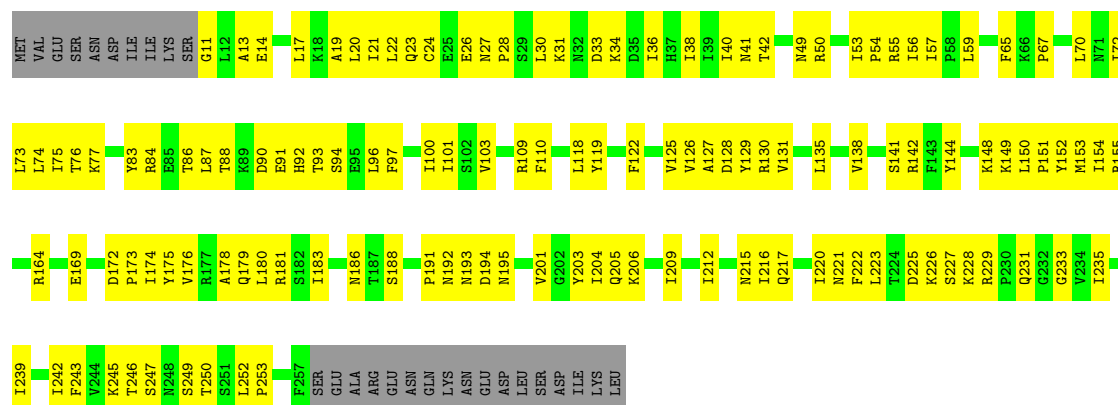






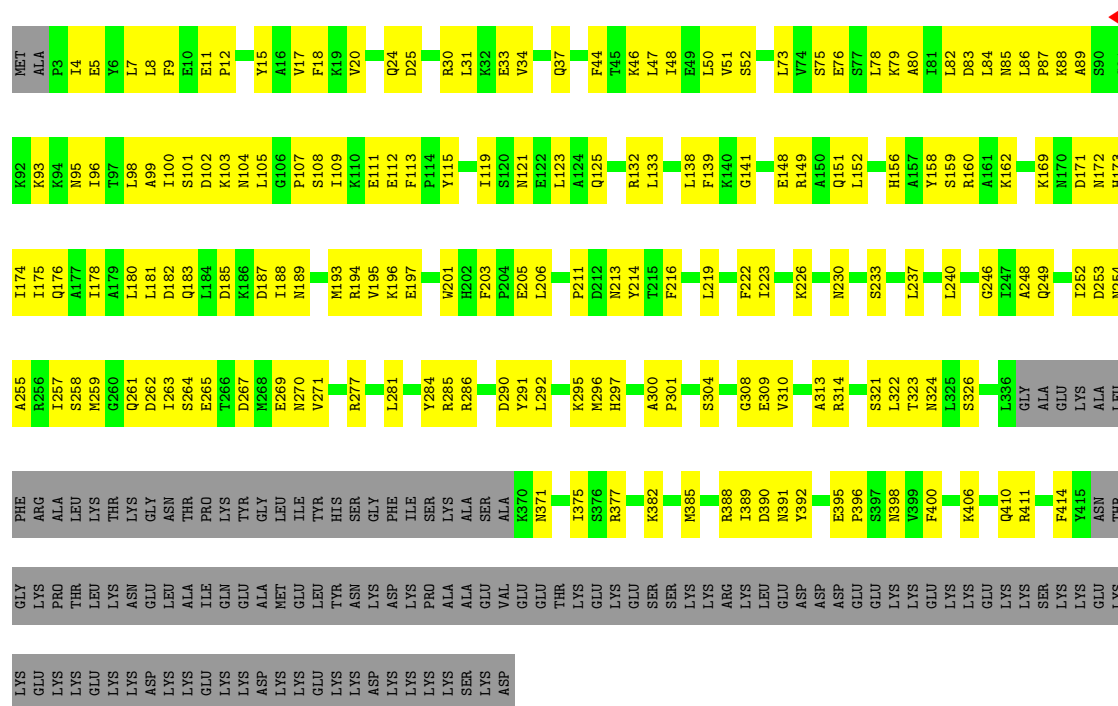
• Molecule 27: Ribosome biogenesis protein UTP30

Chain UZ:  43% 47% 10%



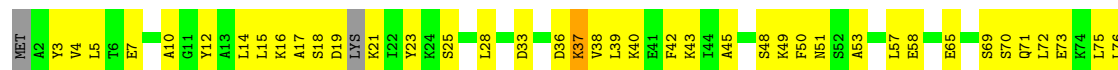
• Molecule 28: Nucleolar protein 56

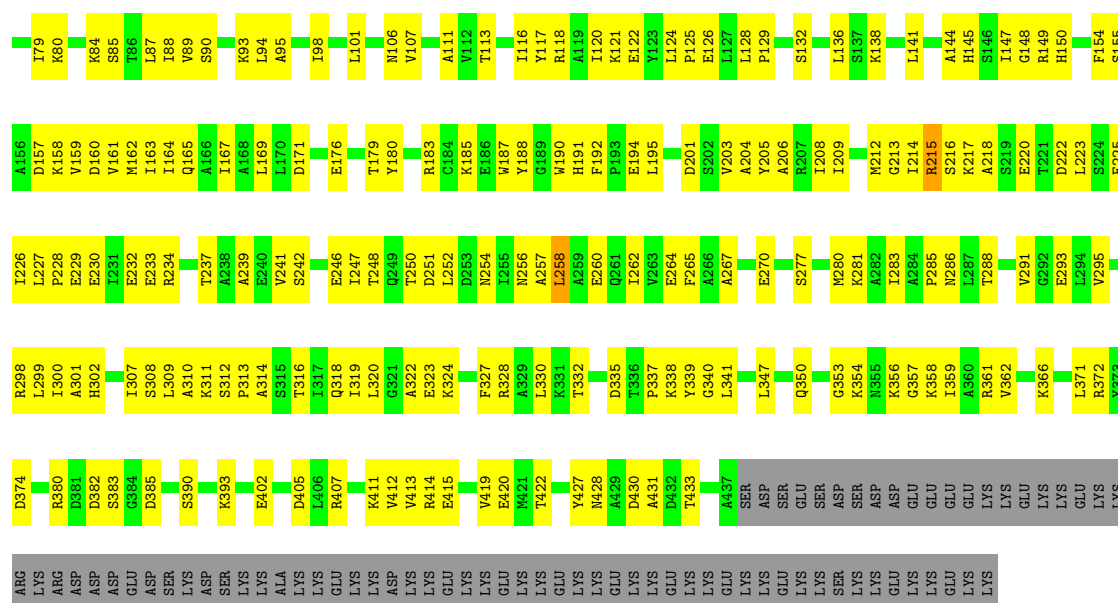
Chain CD:  41% 34% 25%



• Molecule 29: Nucleolar protein 58

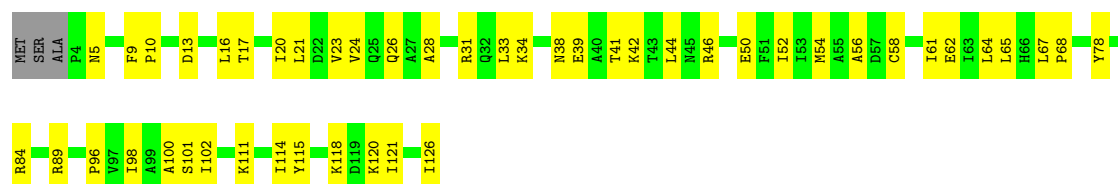
Chain CE:  41% 44% 15%





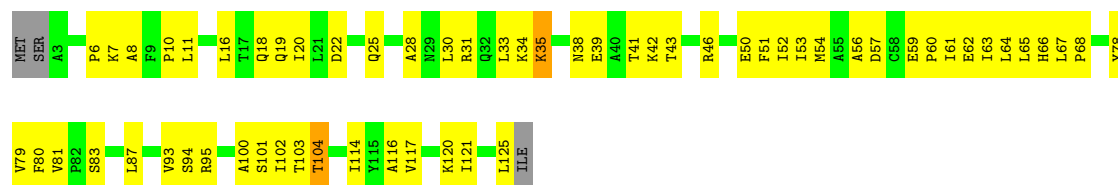
- Molecule 30: 13 kDa ribonucleoprotein-associated protein

Chain CF: 60% 37% .



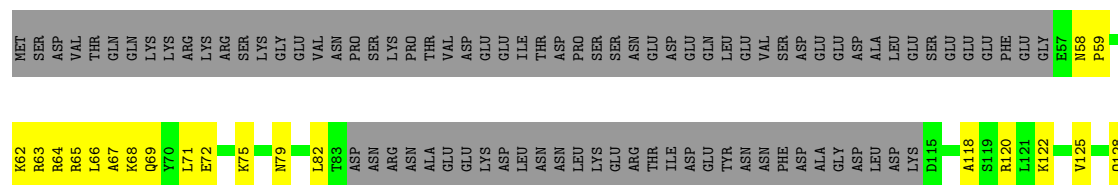
- Molecule 30: 13 kDa ribonucleoprotein-associated protein

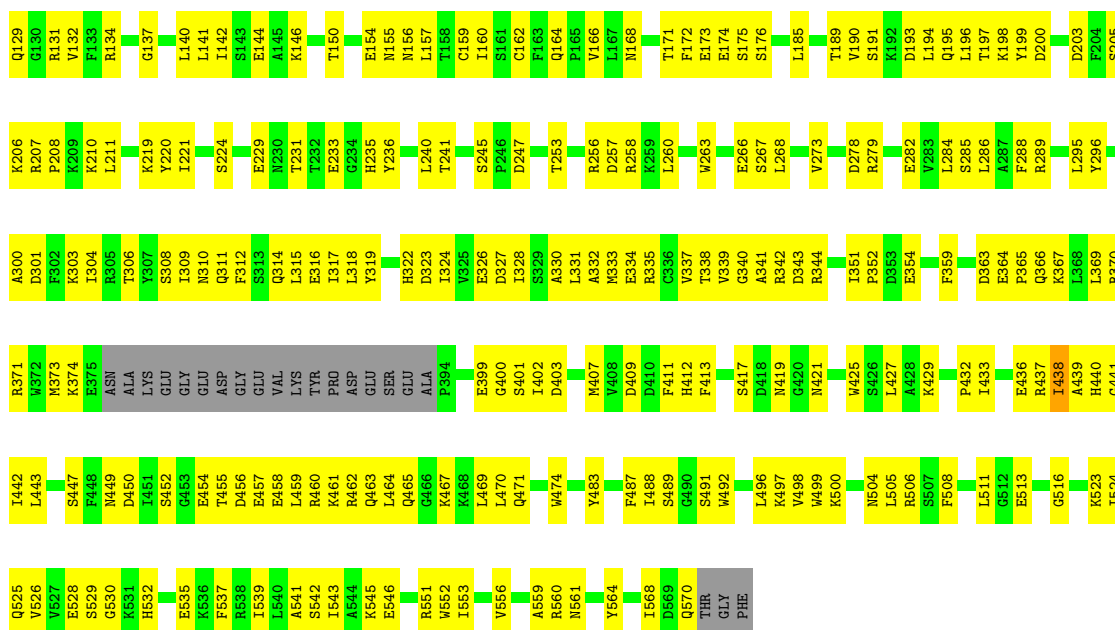
Chain CG: 50% 46% . .



- Molecule 31: Ribosomal RNA-processing protein 9

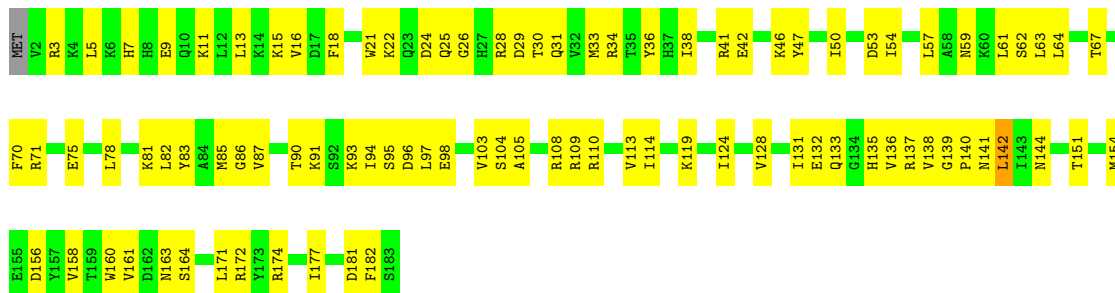
Chain CH: 39% 42% 19%





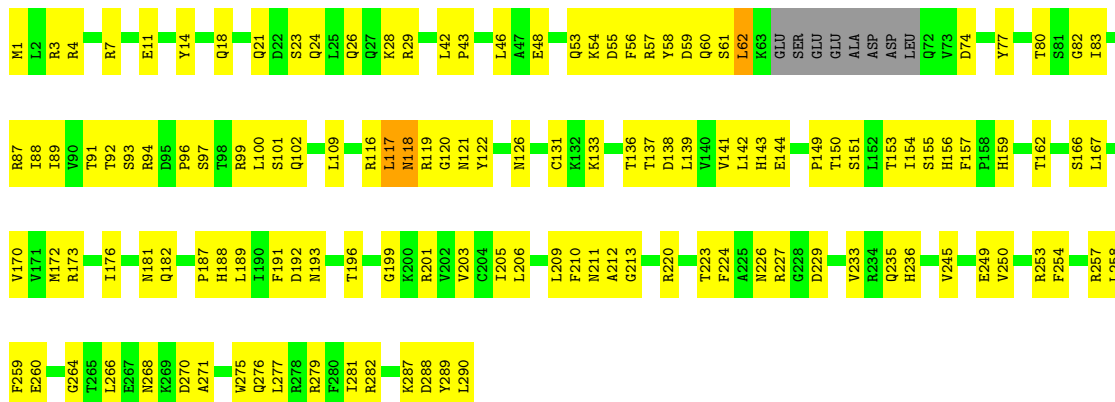
- Molecule 32: U3 small nucleolar ribonucleoprotein protein IMP3

Chain CI: 50% 49% ..



- Molecule 33: U3 small nucleolar ribonucleoprotein protein IMP4

Chain CJ: 52% 44% ..



- Molecule 34: U3 small nucleolar RNA-associated protein MPP10

Chain CK:  19% 15% 65%

MET	GLN	GLN	TYR	THR	Q304	THR	S464	RS34
SER	VAL	VAL	GLY	LYS	I306	ARG	L465	RS38
LEU	TRP	TRP	ILE	GLU	E306	LYS	E466	AS39
PHE	GLN	GLN	ASN	PRO	I307	SER	E467	ASN
GLY	VAL	VAL	ASP	VAL	R308	GLN	R468	LEU
VAL	GLY	GLY	LYS	LYS	K309	ARG	Y469	PRO
LEU	LEU	LEU	PHE	LYS	G310	PRO	E470	ASN
LYS	VAL	VAL	PHE	HIS	I311	GLN	T473	ASN
ASN	ASP	ASP	LEU	SER	E312	PHE	T474	LYS
SER	ILE	ILE	GLU	VAL	E315	GLU	E477	ARG
ALA	SER	SER	LYS	LYS	N316	SER	D478	LYS
GLY	ILE	ILE	PHE	PRO	E317	VAL	A479	ASN
ARG	ASP	ASP	ASN	LYS	A318	LYS	A480	ASP
ILE	GLY	GLY	ASP	GLU	V319	SER	P481	VAL
LEU	LEU	LEU	THR	GLU	W324	LYS	L482	VAL
LYS	ILE	ILE	LEU	GLU	S325	LYS	Y483	ASP
ASP	GLN	GLN	ALA	GLU	L326	SER	Y484	THR
PRO	GLY	GLY	ALA	LEU	K327	LEU	S485	LEU
ASN	ILE	ILE	ALA	ASP	G328	ALA	S488	LYS
GLU	GLU	GLU	ASP	GLU	E329	GLU	L490	ALA
THR	LEU	LEU	ASN	TYR	V330	ILE	A491	LYS
LYS	LYS	LYS	GLU	GLU	K331	GLY	P492	ILE
ASP	ASP	ASP	ALA	HIS	A332	ASP	E494	THR
VAL	VAL	VAL	SER	ASP	R335	TYR	I495	VAL
LYS	VAL	VAL	GLY	LYS	L340	ASP	Y496	ILE
ALA	THR	THR	GLY	VAL	L341	THR	Y497	ASN
TYR	PRO	PRO	ASP	GLY	T342	ARG	V498	GLY
GLY	LYS	LYS	GLU	VAL	E343	ALA	A501	GLU
ASP	HIS	HIS	ASP	LYS	E344	GLU	G505	LYS
SER	ASN	ASN	GLU	LYS	F347	SER	E506	LYS
SER	ASN	ASN	ILE	LEU	D348	L426	S427	ASP
VAL	LEU	LEU	ASP	LEU	R349	A427	E428	VAL
ALA	ASP	ASP	ALA	PHE	T358	E429	R508	SER
THR	GLY	GLY	ALA	TYR	E360	K432	N511	GLY
CYS	SER	SER	ARG	PHE	V361	A433	G512	LYS
LYS	THR	THR	GLU	ALA	E366	H434	V513	THR
LYS	GLY	GLY	ASP	ASN	D367	A442	A514	LYS
LYS	GLU	GLU	ASP	ALA	R370	N443	M515	LYS
ALA	GLU	GLU	GLU	ALA	I373	L444	S516	SER
LEU	LEU	LEU	GLU	VAL	F378	V445	K517	ARG
ASP	GLY	GLY	ALA	GLY	E378	L448	E518	SER
GLU	ILE	ILE	ILE	GLU	L381	D449	E519	PRO
THR	ALA	ALA	TYR	ALA	Q382	R522	R523	ASP
VAL	GLU	GLU	GLU	SER	R383	D524	E454	SER
SER	ARG	ARG	GLU	ASP	K296	S452	V454	ASN
ASP	VAL	VAL	ASP	ASP	L297	O455	H455	ILE
GLY	PHE	PHE	PHE	LEU	E301	F456	R530	LYS
LEU	LYS	LYS	ASP	ASP	I386	V457	A531	LEU
ASP	ALA	ALA	LYS	PRO	LEU	P458		
ALA	LYS	LYS	PRO	PRO	ILE			

• Molecule 35: Ribosome biogenesis protein BMS1

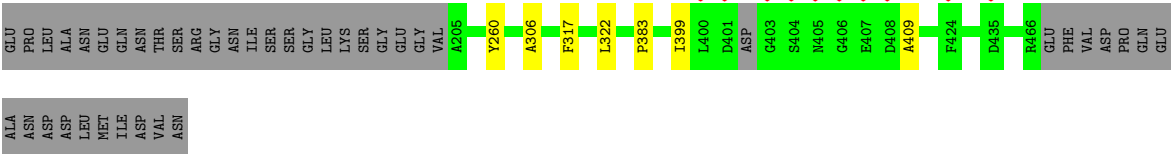
Chain CL:  33% 33% 34%

MET	R61	D124	L207	P279	L353
GLU	T62	L125	S208	L280	I354
GLN	P63	N126	G209	M281	M358
SER	E64	A127	V210	S282	S359
ASN	D65	I128	I211	T286	V364
LYS	D66	M129	N212	G213	L365
GLN	P67	K133	R214	R214	M366
HIS	P68	I134	P216	A291	D367
ARG	P69	A135	F70	G292	D369
LYS	I71	D136	E219	D295	Y372
ALA	V72	L137	I220	V298	G376
LYS	A73	V138	L221	A299	LYS
LYS	V74	L139	N222	Q300	ASN
ASN	V75	L140	I227	K303	GLU
THR		L141	M230	L304	GLU
LYS	P78	I142	K231	P305	PRO
LYS	G79	D143	F232	D306	PHE
LYS	T80	G144	K236	T310	VAL
LYS	G81	N145	W237	P311	PRO
LEU	K82	F146	R238	F312	GLY
HIS	G147	F148	H241	K316	ARG
GLN	L85	E149	P242	R322	GLY
GLY	R87	M150	M243	GLY	GLU
HIS	S88	E151	L245	MET	GLU
ASN	L89	T152	A246	GLY	GLU
ALA	V90	M153	R248	LYS	GLU
LYS	R91	E154	F249	ALA	LEU
ALA	R92	F155	D251	LYS	MET
PHE	M93	H161	L252	THR	THR
ALA	T94	R166	G169	ALA	GLY
VAL	K95	V167	T172	ASN	LEU
ALA	S96	L168	H173	GLY	GLN
ALA	N99	G174	P104	ILE	VAL
GLY	D100	L175	T106	THR	GLU
LYS	I101	D176	T106	THR	GLN
LYS	Q102	L177	L107	ALA	SER
ASP	A40	F177	V108	ILE	THR
VAL	R41	L183	S109	THR	GLN
SER	T42	R184	G110	ALA	SER
GLY	T42	K111	D48	THR	ALA
LYS	T42	H112	S46	LYS	LYS
THR	N43	R113	D48	ARG	PHE
LYS	Q44	R115	N50	ARG	ASP
LYS	R45	L116	E51	ARG	GLY
LYS	S46	F117	R52	ARG	VAL
SER	S47	R193	K53	ARG	VAL
ARG	D48	L118	F117	ASP	LEU
SER	K111	E119	E118	ASP	GLN
GLY	V49	C120	V56	LEU	LEU
PRO	N50	P121	P57	ASP	GLN
ASP	E51	F206	M58	LEU	PHE
LYS	R113	Y206	V59	SER	SER
LYS	R115		D60		

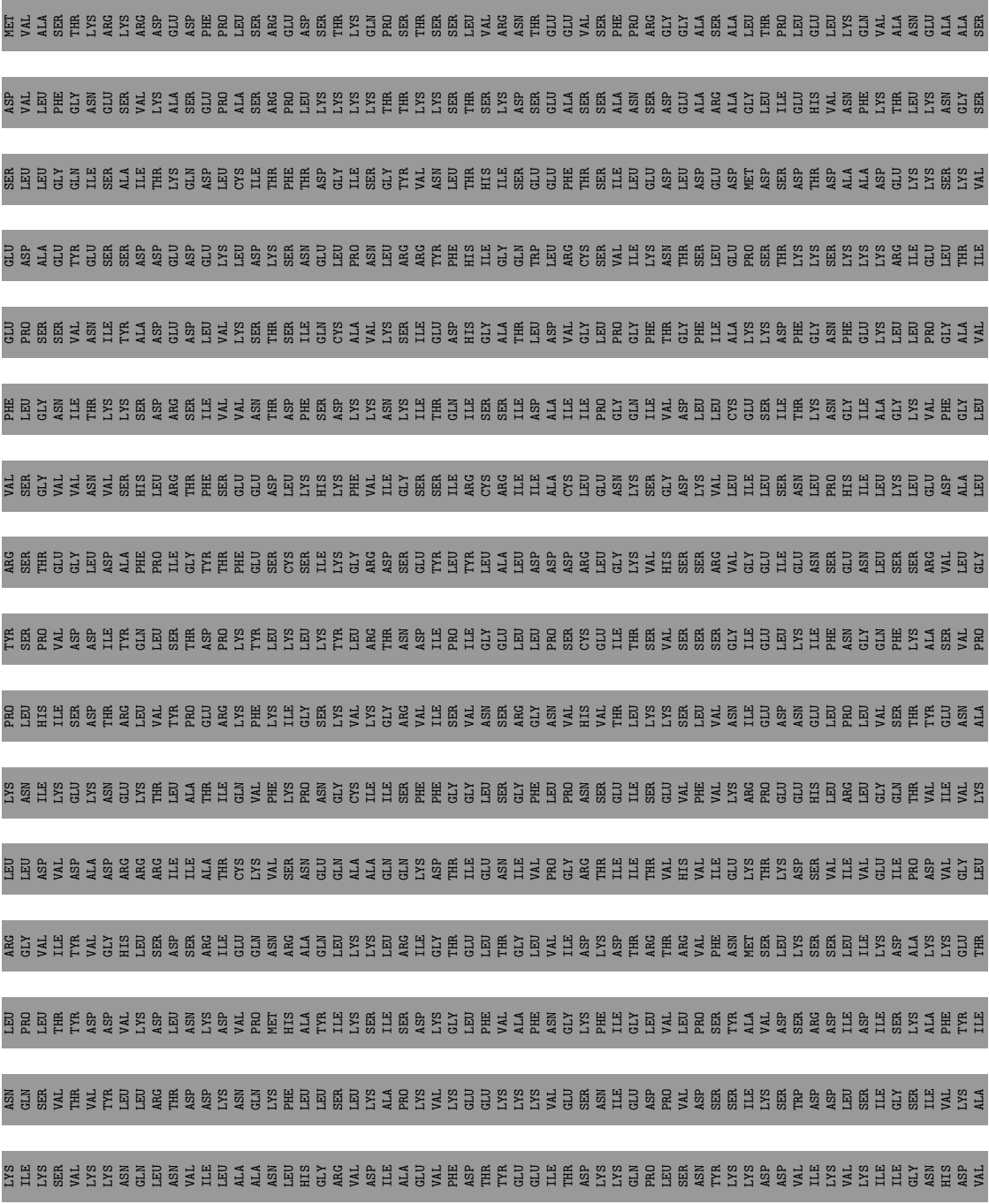








● Molecule 41: rRNA biogenesis protein RRP5





- Molecule 42: Pre-rRNA-processing protein PNO1

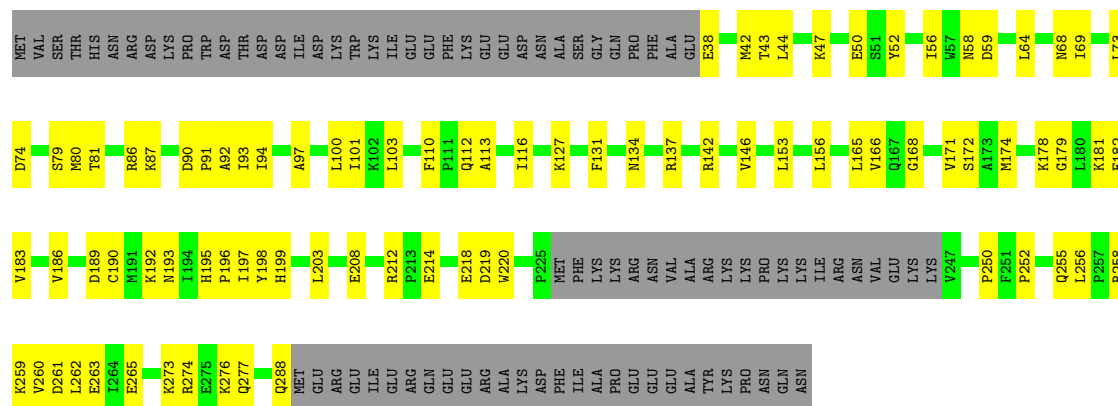
- Molecule 43: Protein BFR2

MET	GLU	LYS	SER	LEU	ALA	ASP	GLN	ILE	SER	ASP	ILE	ALA	LYS	PRO	VAL	ASN	LYS	ASP	PHE	ASP	ILE	GLU	GLU	GLU	ASN	ALA	SER	LEU	PHE	GLN	GLN	ASN	GLU	LYS	ASN	GLY	GLY	GLU	SER	ASP	LEU	SER	SER	ASP	ASP	THR	THR	GLU	GLU	THR	LYS	LYS	ALA	HIS	HIS	TYR	LEU
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



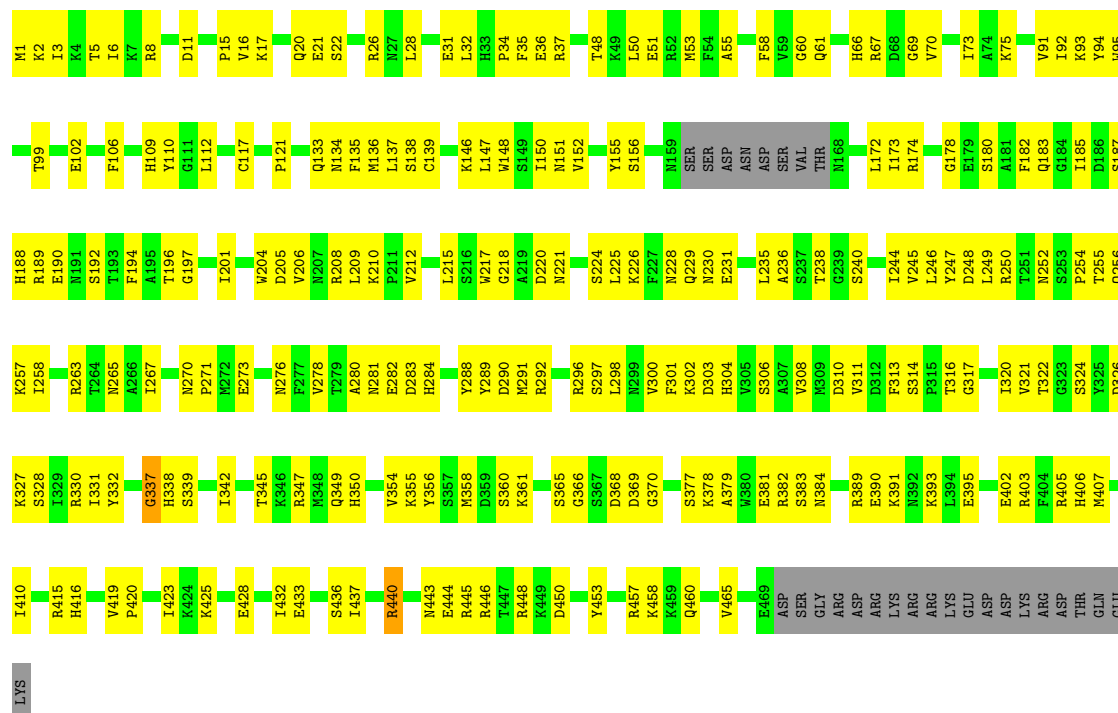
- Molecule 46: KRR1 small subunit processome component

Chain JO: 



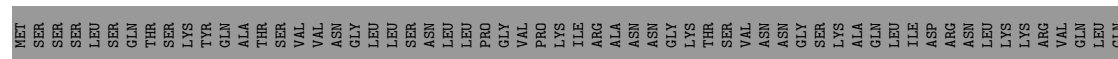
- Molecule 47: Protein SOF1

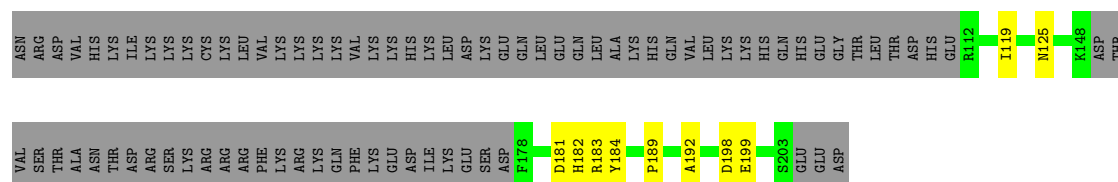
Chain JP:  49% 45% 6%



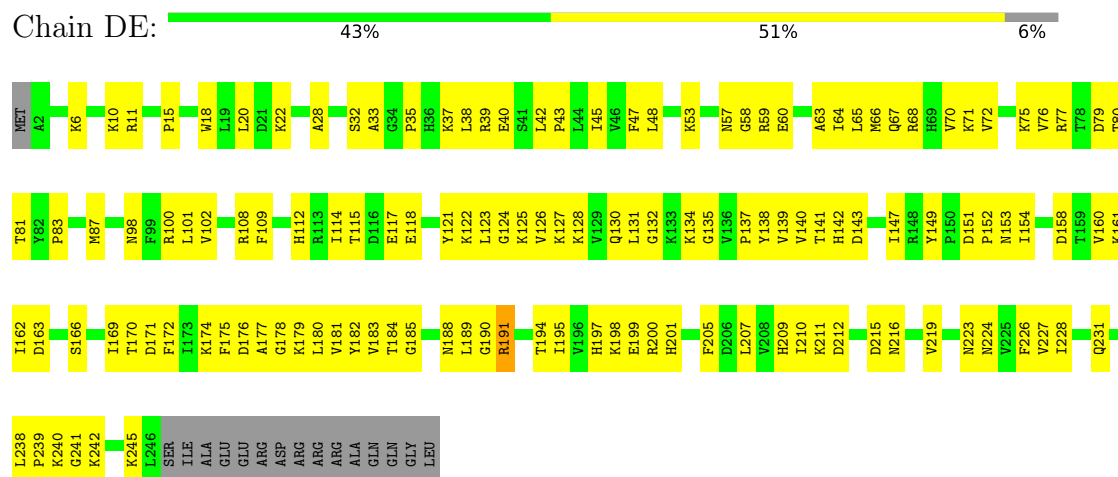
- Molecule 48: Regulator of rDNA transcription protein 14

Chain JQ:  26% 5% 69%





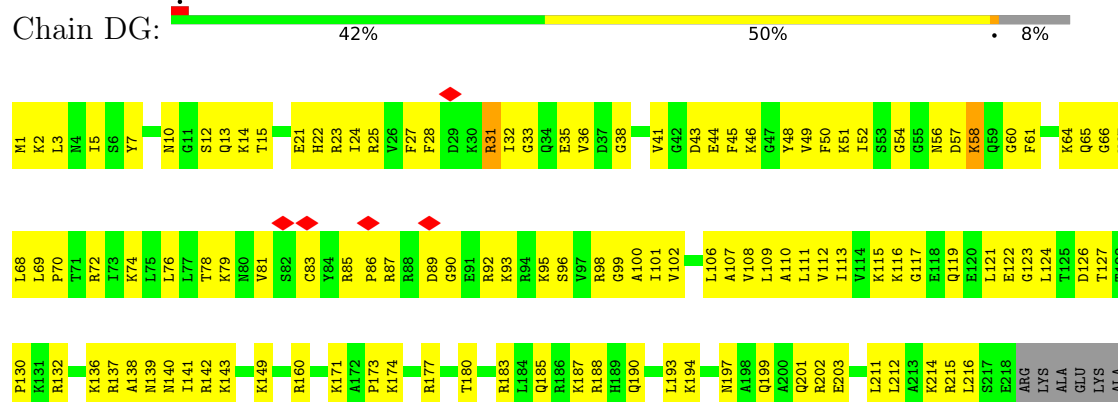
• Molecule 49: 40S ribosomal protein S4-A



• Molecule 50: 40S ribosomal protein S5



• Molecule 51: 40S ribosomal protein S6-A

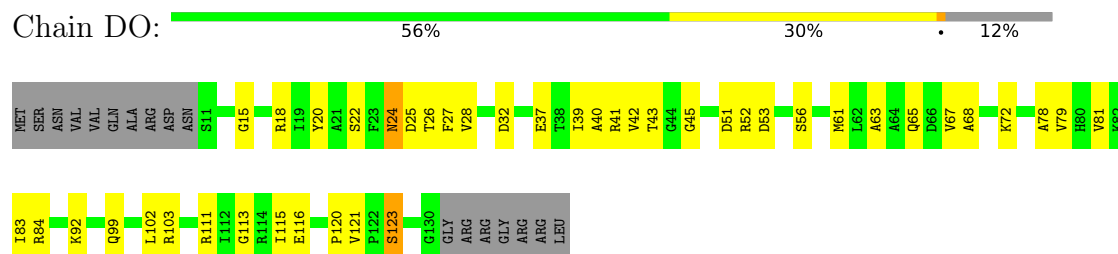




- Molecule 56: 40S ribosomal protein S13



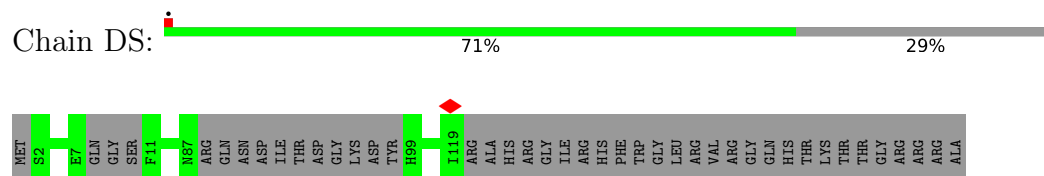
- Molecule 57: 40S ribosomal protein S14-A



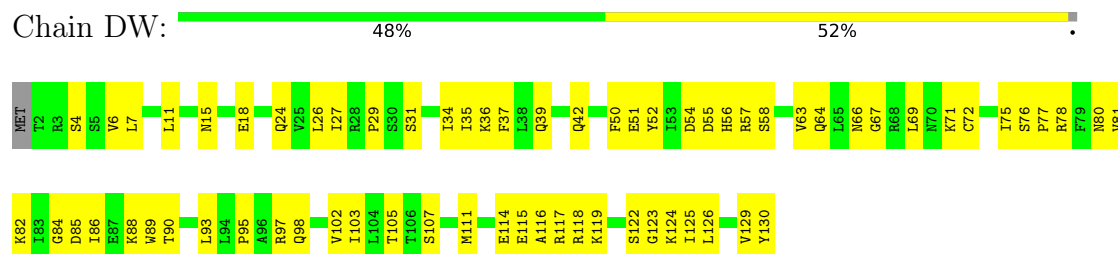
- Molecule 58: 40S ribosomal protein S16-A



- Molecule 59: 40S ribosomal protein S18-A



- Molecule 60: 40S ribosomal protein S22-A



- Molecule 61: 40S ribosomal protein S23-A

SER	A67	I68	R69	K70	V74	Q75	L76	I77	G80	A85	F86	V87	P88	N89	D90	G91	C92	L93	N94	F95	E98	N99	D100	E101	L104	R109	K112	A113	K114	I117	P118	G119	V120	R121	F122	K123	V124	V130	S131	L132	L133	A134	L135	W136	K137	E138	K139	E141	R144						
	GLY	LYS	GLY	LYS	PRO	ARG	GLY	LEU	ASN	SER	ALA	ARG	LYS	LEU	ARG	VAL	HIS	ARG	ASN	ASN	ARG	TRP	ALA	GLU	ASN	ASN	TYR	LYS	LYS	ARG	LEU	LEU	GLY	THR	ALA	PHE	LYS	SER	SER	P42	F43	G44	G45	S46	S47	H48	A49	K50	G51	I52	I59	E60	G63	P64	N65

- |     |     |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| A97 | E98 | K99 | V100 | E101 | K102 | A103 | S104 | Q105 | R106 | Q107 | R108 | K109 | Q110 | K111 | K112 | N113 | R114 | R124 | L125 | A126 | K127 | K128 | R131 | D135 | MET | S2 | R8 | K11 | V12 | I13 | S14 | N15 | P16 | L17 | L18 | A19 | R20 | K21 | Q22 | F23 | V24 | V25 | H29 | K37 | D38 | E39 | L40 | K49 | A50 | E51 | K52 | D53 | A54 | V55 | S56 | G59 | F60 | G71 | L74 | V75 | Y76 | N77 | E81 | K84 | F85 | E86 | Y89 | A90 | L91 | V92 | R93 | L95 |
|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

- 
- ```

graph TD
    MET[MET] --- V2[V2]
    V2 --- L21[L21]
    L21 --- F79[F79]
    F79 --- R80[R80]
    R80 --- R81[R81]
    R81 --- K82[K82]
  
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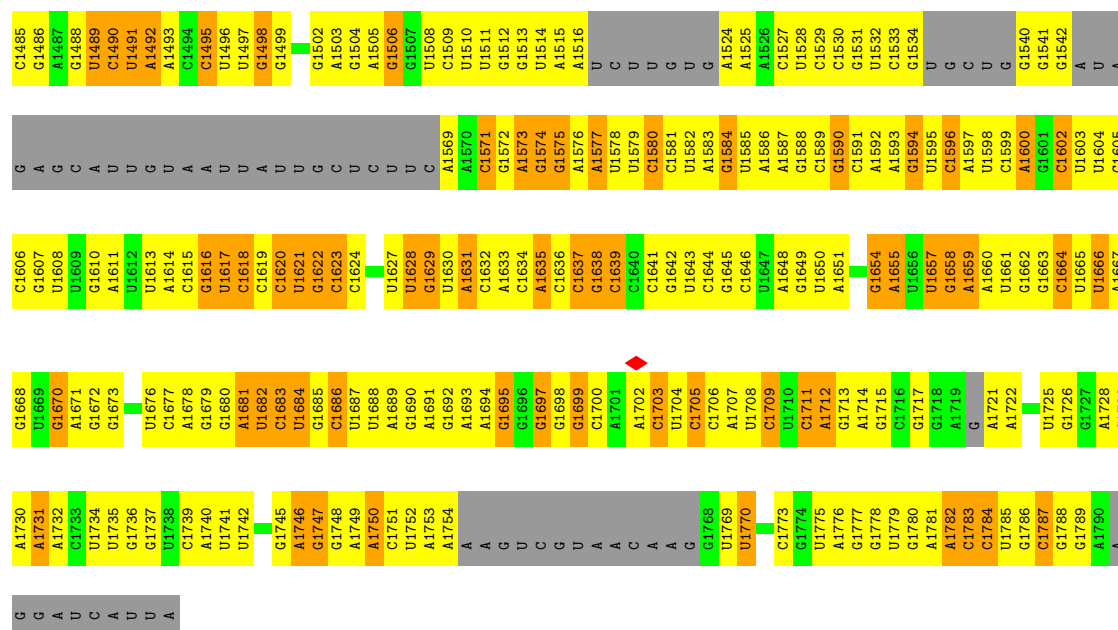
- MET  
ASP  
ASN  
LYS  
T5  
R67

- |      |      |      |     |
|------|------|------|-----|
| C186 | A124 | U64  | A1  |
| A187 | G125 | U65  | U2  |
| A188 | A126 | C166 | G3  |
|      |      | G67  | C4  |
| U191 | U129 | U68  | G5  |
| G192 | G130 | U69  | A6  |
| G193 | C131 | A70  | A7  |
| G194 | C132 | U    | A8  |
| A195 | U133 | G    | G9  |
| A196 | A134 | U    | C10 |
| G197 | G135 | U    | A11 |
| A198 | U136 | U    | G12 |
| A199 | C137 | U    | U13 |
| A200 | U138 | U    | U14 |
| U201 | C139 | G    | G15 |
| U202 | U140 | U    | A16 |
| C203 | A141 | A80  | A17 |
| G204 | U142 | A81  | G18 |
| C205 | A143 | A82  | A19 |
| A206 | C144 | U83  | C20 |
| G207 | U145 | G84  | A21 |
| A208 | G146 | G85  | A22 |
| G209 | C147 | C86  | G23 |
| U210 | G148 | C87  | U24 |
| G211 | A149 | U88  | U   |
| U212 | G150 | C89  | C   |
| G213 | U151 | G90  | G   |
| U214 | U152 | U91  | A   |
| U215 | U153 | C92  | A   |
| U216 | A154 | A93  | A   |
| C217 | A155 | A94  | A   |
| U218 | U156 | A95  | G   |
| U219 | U157 | C96  | A   |
| U220 | G158 | G97  | G   |
| U221 | A159 | G98  | U   |
| G222 | C160 | U99  | U   |
| C223 | A161 | G100 | U   |
| G224 | U162 | G101 | G   |
| U225 | C163 | A102 | G   |
| U226 | G164 | G103 | A   |
| U227 | G165 | A104 | A   |
| A228 | U166 | G105 | A   |
| A229 | U167 | A106 | A   |
|      | G168 | G107 | C   |
| U232 | A169 | U108 | C   |
| G233 | U170 | C109 | A   |
| A234 | G171 | G110 | A   |
| A235 | C172 | C111 | U   |
| C236 | G173 | U112 | C   |
| U237 | U174 | A113 | G   |
| G238 |      | G114 | A   |
| U239 | U177 | G115 | G   |
| C240 | A179 | U116 | U   |
| U241 | G180 | G117 | A   |
| C242 | A181 | A118 | G   |
| A243 | G182 | U119 | G56 |
| U244 | A183 | C120 | C57 |
| G245 | U184 | G121 | U58 |
| G246 | A185 | U122 |     |
| G247 | A186 | C122 | C59 |

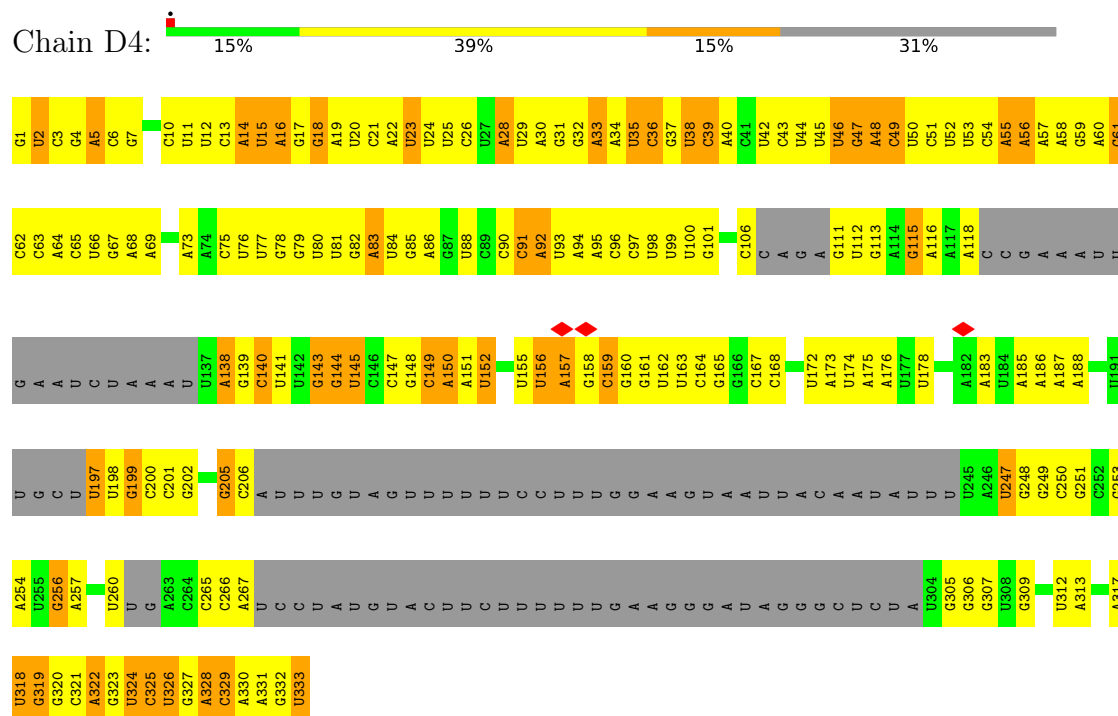




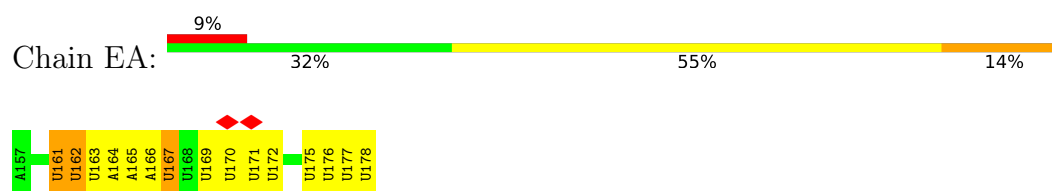




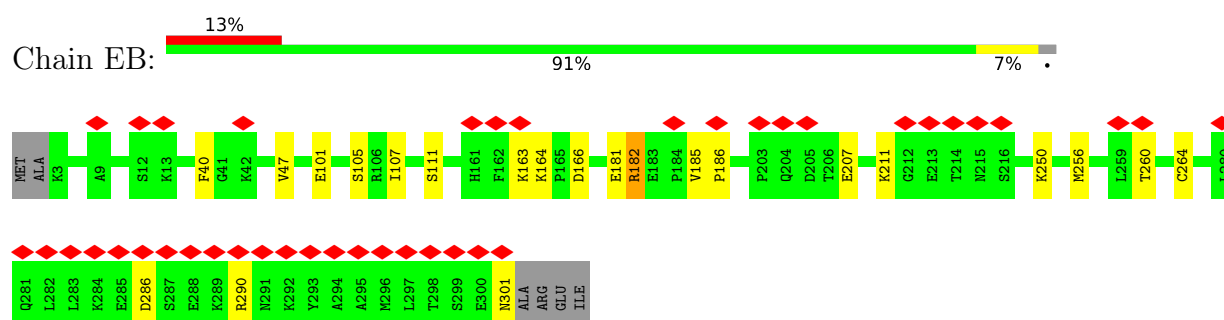
● Molecule 67: U3 snoRNA



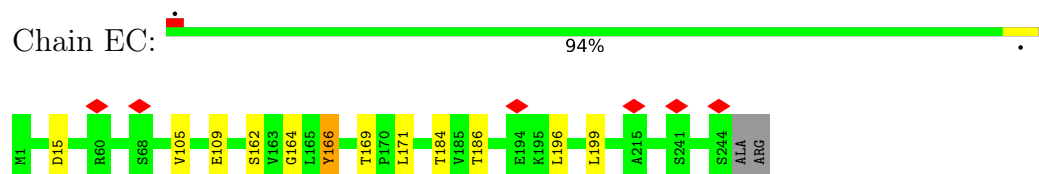
● Molecule 68: RNA



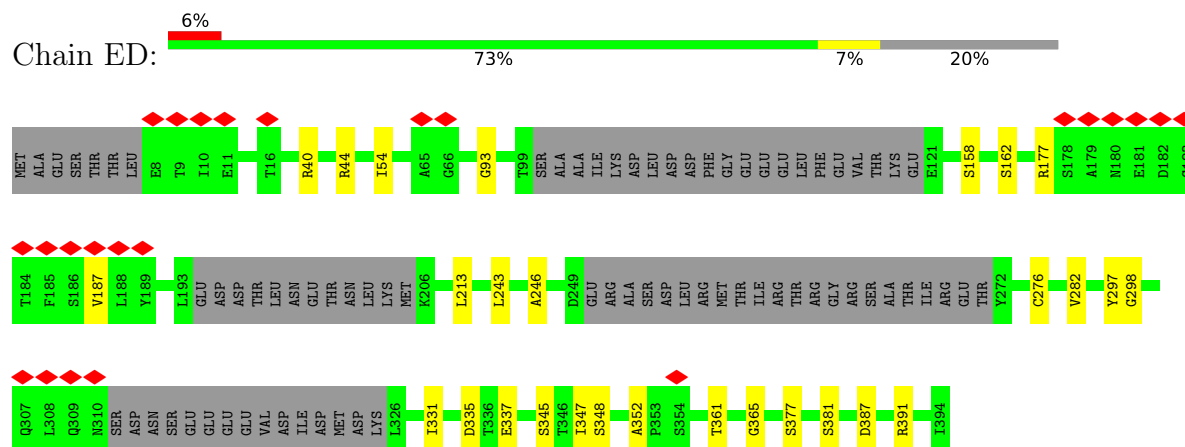
● Molecule 69: Exosome complex component RRP45



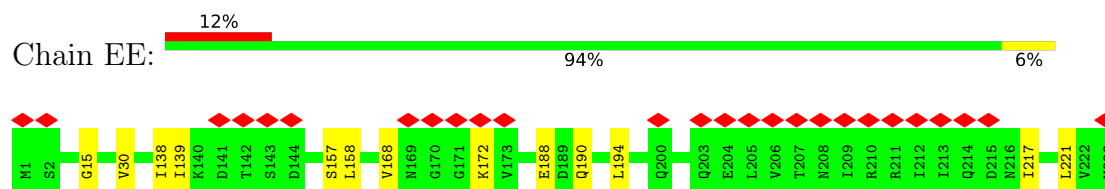
- Molecule 70: Exosome complex component SKI6



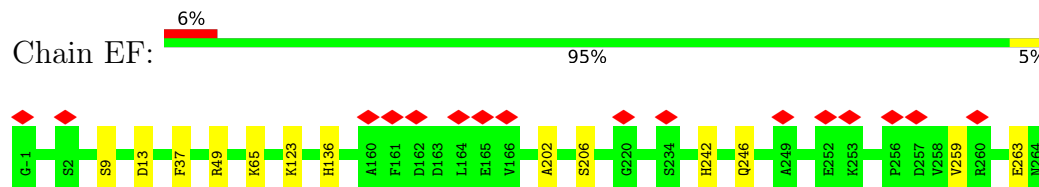
- Molecule 71: Exosome complex component RRP43



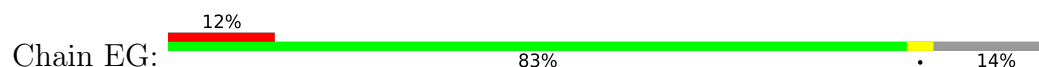
- Molecule 72: Exosome complex component RRP46

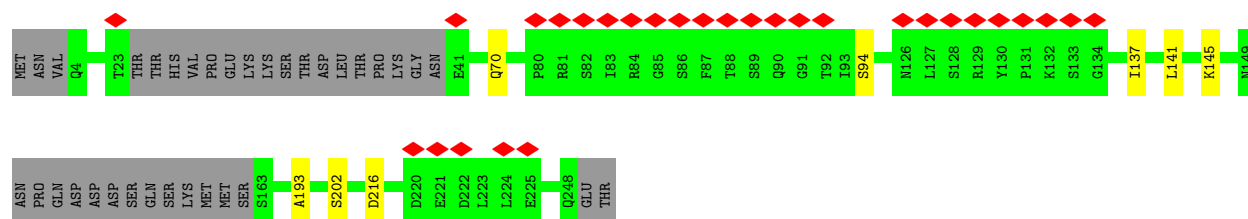


- Molecule 73: Exosome complex component RRP42

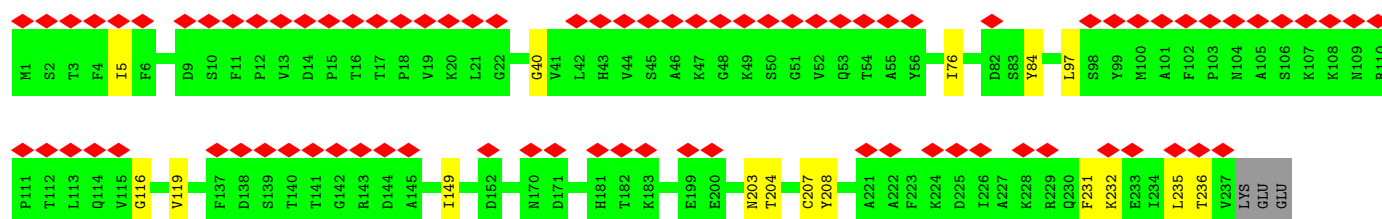
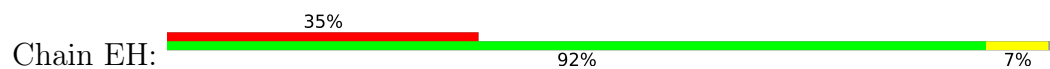


- Molecule 74: Exosome complex component MTR3

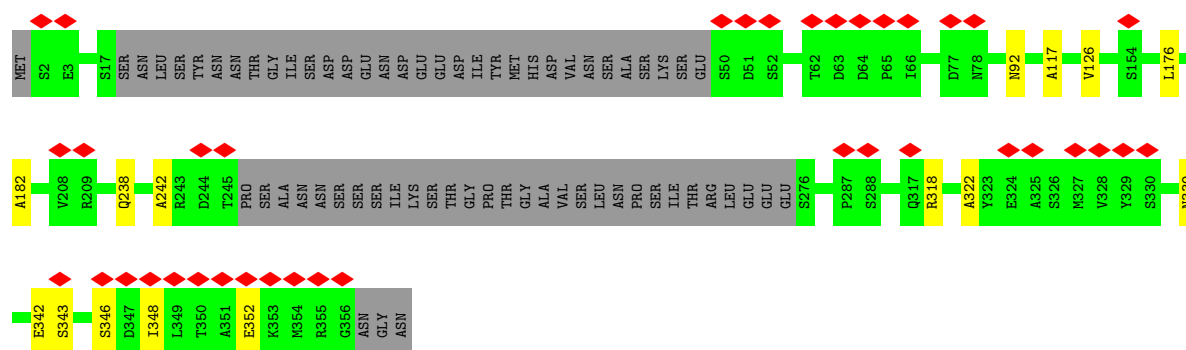
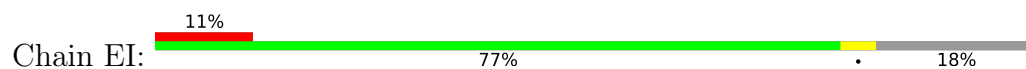




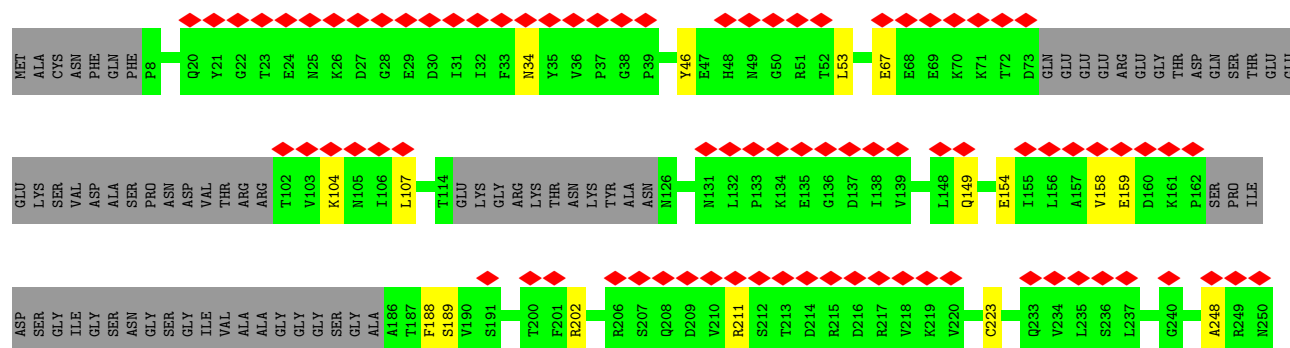
• Molecule 75: Exosome complex component RRP40



• Molecule 76: Exosome complex component RRP4

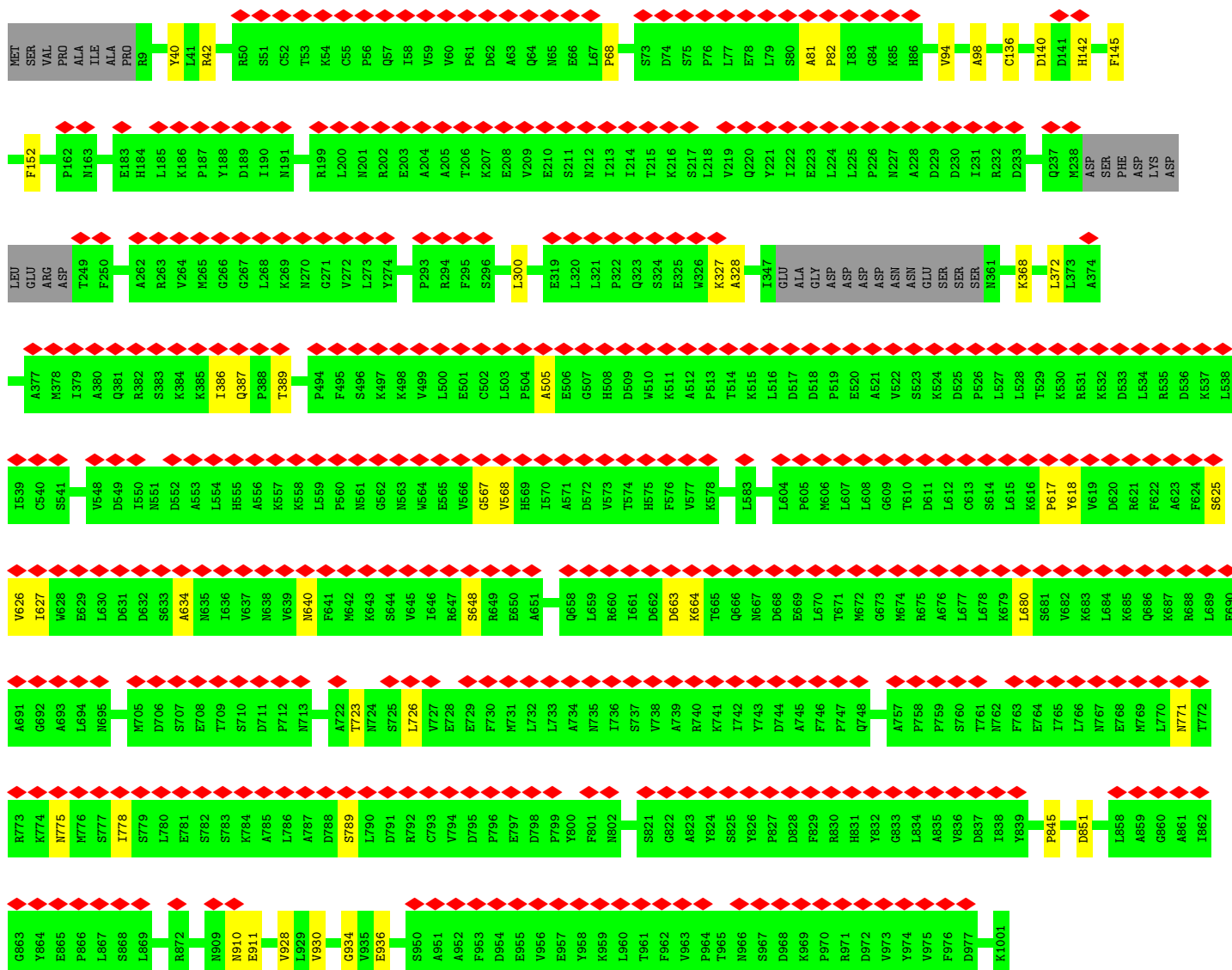
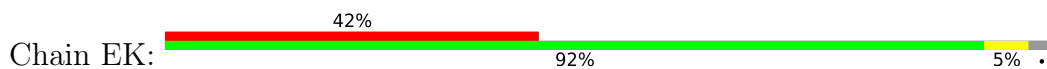


• Molecule 77: Exosome complex component CSL4

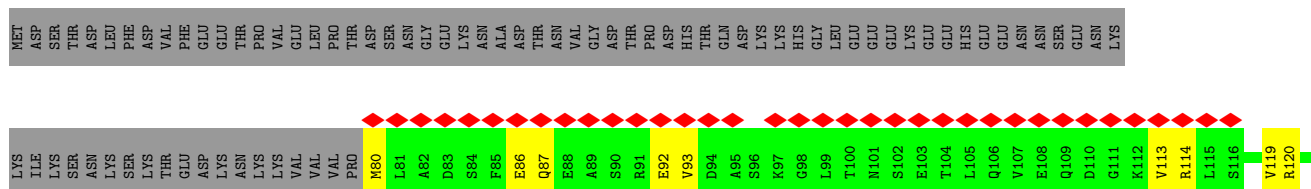
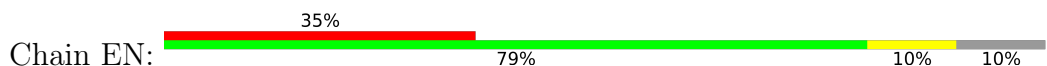


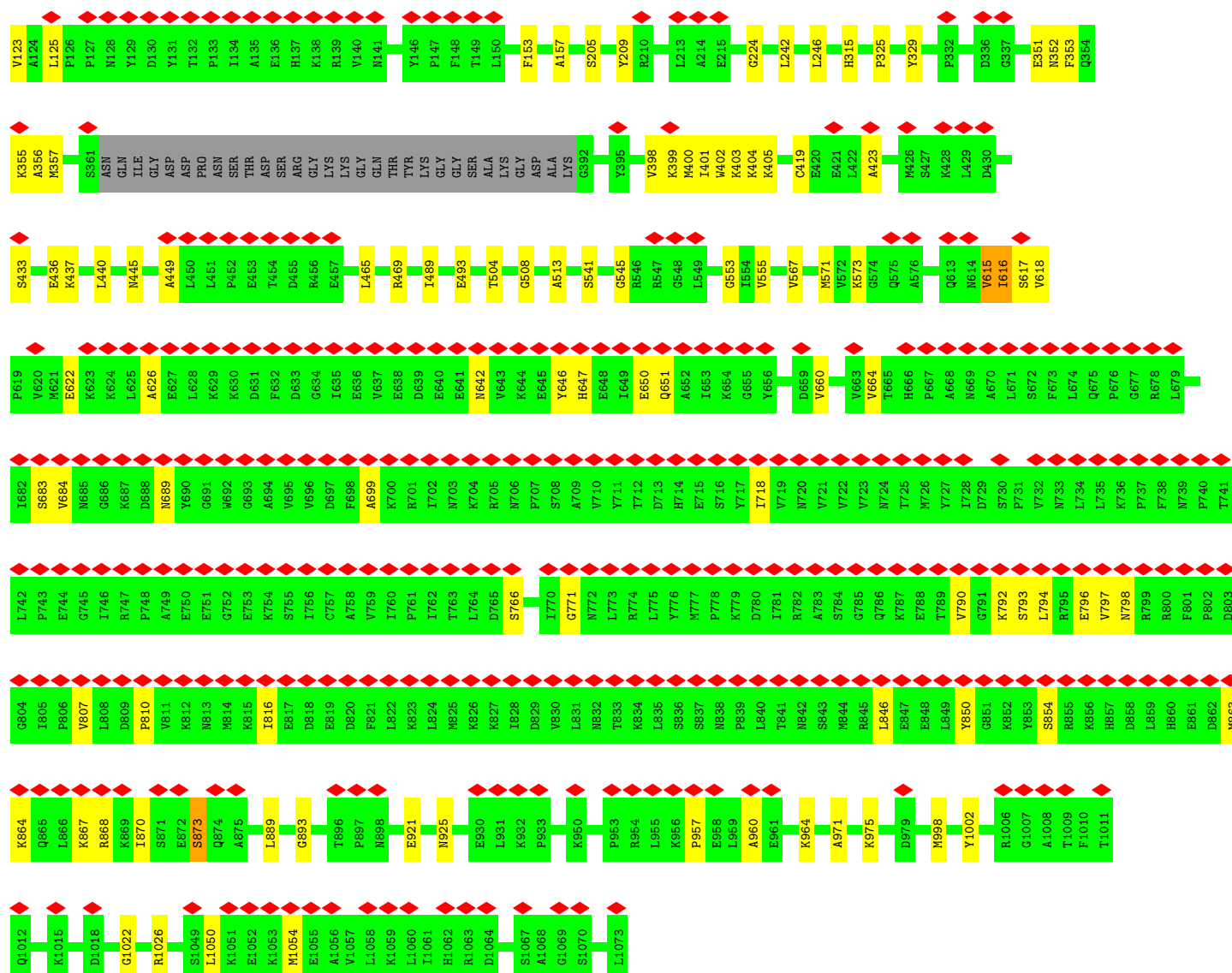


• Molecule 78: Exosome complex exonuclease DIS3



• Molecule 79: ATP-dependent RNA helicase DOB1





## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 6024                                    | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 44                                      | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 0.259                                   | Depositor |
| Minimum map value                    | -0.204                                  | Depositor |
| Average map value                    | 0.001                                   | Depositor |
| Map value standard deviation         | 0.007                                   | Depositor |
| Recommended contour level            | 0.01                                    | Depositor |
| Map size (Å)                         | 571.86, 571.86, 571.86                  | wwPDB     |
| Map dimensions                       | 540, 540, 540                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.059, 1.059, 1.059                     | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GTP, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |               | Bond angles |                |
|-----|-------|--------------|---------------|-------------|----------------|
|     |       | RMSZ         | $\# Z  > 5$   | RMSZ        | $\# Z  > 5$    |
| 1   | CA    | 0.66         | 0/1917        | 0.66        | 1/2588 (0.0%)  |
| 1   | CB    | 0.40         | 0/1815        | 0.61        | 1/2448 (0.0%)  |
| 2   | DA    | 0.43         | 0/1937        | 0.59        | 0/2593         |
| 3   | JA    | 0.28         | 0/6021        | 0.50        | 0/8176         |
| 3   | JB    | 0.24         | 0/4128        | 0.41        | 0/5747         |
| 4   | UA    | 0.52         | 0/6780        | 0.62        | 2/9175 (0.0%)  |
| 5   | UB    | 0.31         | 0/3787        | 0.50        | 1/5126 (0.0%)  |
| 6   | UC    | 0.52         | 0/1034        | 0.63        | 1/1365 (0.1%)  |
| 7   | UD    | 0.39         | 0/5461        | 0.57        | 0/7395         |
| 8   | UE    | 0.37         | 0/3840        | 0.57        | 0/5208         |
| 9   | UF    | 0.45         | 0/2538        | 0.56        | 0/3405         |
| 10  | UG    | 0.62         | 2/4302 (0.0%) | 0.68        | 2/5805 (0.0%)  |
| 11  | UH    | 0.28         | 0/2716        | 0.51        | 0/3721         |
| 12  | UI    | 0.28         | 0/875         | 0.59        | 1/1176 (0.1%)  |
| 13  | UJ    | 0.35         | 0/9111        | 0.52        | 1/12323 (0.0%) |
| 14  | UK    | 0.51         | 0/2047        | 0.65        | 1/2711 (0.0%)  |
| 15  | UL    | 0.34         | 0/6857        | 0.56        | 1/9253 (0.0%)  |
| 16  | UM    | 0.33         | 0/6070        | 0.56        | 0/8216         |
| 17  | UN    | 0.53         | 0/1252        | 0.66        | 0/1688         |
| 18  | UO    | 0.40         | 0/3993        | 0.58        | 3/5413 (0.1%)  |
| 19  | UP    | 0.32         | 0/499         | 0.56        | 0/659          |
| 20  | UQ    | 0.37         | 0/6794        | 0.55        | 1/9203 (0.0%)  |
| 21  | UR    | 0.50         | 0/3883        | 0.61        | 0/5265         |
| 22  | US    | 0.33         | 0/3703        | 0.53        | 1/5053 (0.0%)  |
| 23  | UT    | 0.29         | 0/17584       | 0.49        | 1/23824 (0.0%) |
| 24  | UU    | 0.46         | 0/6815        | 0.58        | 1/9213 (0.0%)  |
| 25  | UV    | 0.31         | 0/8945        | 0.48        | 0/12097        |
| 26  | UX    | 0.64         | 0/1418        | 0.70        | 0/1906         |
| 27  | UZ    | 0.36         | 0/2041        | 0.54        | 0/2745         |
| 28  | CD    | 0.44         | 0/3041        | 0.57        | 0/4098         |
| 29  | CE    | 0.40         | 0/3362        | 0.59        | 1/4533 (0.0%)  |
| 30  | CF    | 0.46         | 0/944         | 0.63        | 0/1284         |



| Mol | Chain | Bond lengths |               | Bond angles |                 |
|-----|-------|--------------|---------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5       | RMSZ        | # Z  >5         |
| 30  | CG    | 0.52         | 0/941         | 0.66        | 0/1281          |
| 31  | CH    | 0.39         | 0/3798        | 0.55        | 0/5113          |
| 32  | CI    | 0.76         | 0/1559        | 0.77        | 1/2097 (0.0%)   |
| 33  | CJ    | 0.57         | 0/2337        | 0.68        | 1/3148 (0.0%)   |
| 34  | CK    | 0.44         | 0/1685        | 0.63        | 0/2261          |
| 35  | CL    | 0.47         | 0/6471        | 0.61        | 0/8708          |
| 36  | CM    | 0.34         | 0/2832        | 0.53        | 0/3825          |
| 37  | CN    | 0.30         | 0/1934        | 0.48        | 0/2604          |
| 38  | JC    | 0.29         | 0/2908        | 0.52        | 0/3938          |
| 39  | JF    | 0.31         | 0/1727        | 0.53        | 0/2329          |
| 39  | JG    | 0.37         | 0/1828        | 0.58        | 0/2470          |
| 40  | JH    | 0.23         | 0/1293        | 0.35        | 0/1801          |
| 41  | JI    | 0.23         | 0/1313        | 0.36        | 0/1830          |
| 42  | JJ    | 0.31         | 0/1469        | 0.55        | 0/1980          |
| 43  | JK    | 0.29         | 0/342         | 0.45        | 0/462           |
| 44  | JM    | 0.46         | 0/1156        | 0.59        | 0/1536          |
| 45  | JN    | 0.52         | 0/1435        | 0.63        | 1/1907 (0.1%)   |
| 46  | JO    | 0.45         | 0/1910        | 0.58        | 0/2569          |
| 47  | JP    | 0.67         | 0/3844        | 0.72        | 0/5174          |
| 48  | JQ    | 0.32         | 0/385         | 0.52        | 0/529           |
| 49  | DE    | 0.33         | 0/1985        | 0.53        | 0/2675          |
| 50  | DF    | 0.47         | 0/1690        | 0.59        | 0/2285          |
| 51  | DG    | 0.29         | 0/1779        | 0.49        | 0/2379          |
| 52  | DH    | 0.35         | 0/1506        | 0.54        | 0/2028          |
| 53  | DI    | 0.28         | 0/1422        | 0.49        | 0/1899          |
| 54  | DJ    | 0.54         | 0/1519        | 0.67        | 1/2035 (0.0%)   |
| 55  | DL    | 0.26         | 0/1155        | 0.50        | 1/1557 (0.1%)   |
| 56  | DN    | 0.41         | 0/1215        | 0.58        | 0/1638          |
| 57  | DO    | 0.41         | 0/892         | 0.56        | 0/1202          |
| 58  | DQ    | 0.67         | 0/990         | 0.70        | 1/1335 (0.1%)   |
| 59  | DS    | 0.24         | 0/513         | 0.40        | 0/711           |
| 60  | DW    | 0.56         | 0/1038        | 0.66        | 0/1395          |
| 61  | DX    | 0.51         | 0/798         | 0.65        | 0/1065          |
| 62  | DY    | 0.40         | 0/1087        | 0.60        | 1/1449 (0.1%)   |
| 63  | Db    | 0.45         | 0/620         | 0.66        | 1/838 (0.1%)    |
| 64  | Dc    | 0.45         | 0/499         | 0.68        | 0/670           |
| 65  | D2    | 0.76         | 0/10633       | 0.94        | 11/16564 (0.1%) |
| 66  | D3    | 0.67         | 0/31617       | 0.89        | 16/49213 (0.0%) |
| 67  | D4    | 0.76         | 1/5432 (0.0%) | 0.90        | 2/8439 (0.0%)   |
| 68  | EA    | 0.77         | 0/405         | 1.53        | 6/625 (1.0%)    |
| 69  | EB    | 0.47         | 0/1474        | 0.57        | 0/2050          |
| 70  | EC    | 0.47         | 0/1203        | 0.58        | 0/1673          |
| 71  | ED    | 0.43         | 0/1569        | 0.61        | 0/2179          |

| Mol | Chain | Bond lengths |                 | Bond angles |                  |
|-----|-------|--------------|-----------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5          |
| 72  | EE    | 0.46         | 0/1109          | 0.61        | 0/1545           |
| 73  | EF    | 0.42         | 0/1328          | 0.60        | 0/1851           |
| 74  | EG    | 0.45         | 0/1055          | 0.59        | 0/1462           |
| 75  | EH    | 0.44         | 0/1169          | 0.64        | 0/1626           |
| 76  | EI    | 0.44         | 0/1437          | 0.62        | 0/1992           |
| 77  | EJ    | 0.40         | 0/1087          | 0.62        | 0/1504           |
| 78  | EK    | 0.39         | 0/4818          | 0.57        | 0/6720           |
| 79  | EN    | 0.40         | 0/4765          | 0.58        | 0/6636           |
| All | All   | 0.48         | 3/264486 (0.0%) | 0.65        | 63/368214 (0.0%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2   | DA    | 0                   | 1                   |
| 3   | JA    | 0                   | 1                   |
| 4   | UA    | 0                   | 1                   |
| 6   | UC    | 0                   | 1                   |
| 9   | UF    | 0                   | 1                   |
| 11  | UH    | 0                   | 3                   |
| 15  | UL    | 0                   | 2                   |
| 16  | UM    | 0                   | 3                   |
| 20  | UQ    | 0                   | 1                   |
| 21  | UR    | 0                   | 1                   |
| 23  | UT    | 0                   | 2                   |
| 30  | CG    | 0                   | 1                   |
| 31  | CH    | 0                   | 1                   |
| 33  | CJ    | 0                   | 1                   |
| 34  | CK    | 0                   | 1                   |
| 38  | JC    | 0                   | 1                   |
| 44  | JM    | 0                   | 1                   |
| 47  | JP    | 0                   | 3                   |
| 56  | DN    | 0                   | 1                   |
| 57  | DO    | 0                   | 1                   |
| 58  | DQ    | 0                   | 1                   |
| 63  | Db    | 0                   | 1                   |
| 70  | EC    | 0                   | 1                   |
| 71  | ED    | 0                   | 3                   |
| 72  | EE    | 0                   | 1                   |
| 73  | EF    | 0                   | 1                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 74  | EG    | 0                   | 2                   |
| 76  | EI    | 0                   | 1                   |
| 77  | EJ    | 0                   | 1                   |
| 79  | EN    | 0                   | 3                   |
| All | All   | 0                   | 43                  |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 10  | UG    | 139 | TRP  | CB-CG  | -5.96 | 1.39        | 1.50     |
| 67  | D4    | 197 | U    | C1'-N1 | 5.53  | 1.57        | 1.48     |
| 10  | UG    | 213 | TRP  | CB-CG  | -5.39 | 1.40        | 1.50     |

All (63) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 68  | EA    | 167  | U    | N1-C2-O2  | 13.96  | 132.57      | 122.80   |
| 68  | EA    | 167  | U    | N3-C2-O2  | -11.26 | 114.32      | 122.20   |
| 68  | EA    | 167  | U    | C2-N1-C1' | 11.18  | 131.12      | 117.70   |
| 24  | UU    | 143  | SER  | C-N-CA    | 10.16  | 147.09      | 121.70   |
| 68  | EA    | 167  | U    | C6-N1-C1' | -8.20  | 109.72      | 121.20   |
| 65  | D2    | 332  | U    | C2-N1-C1' | 7.99   | 127.29      | 117.70   |
| 66  | D3    | 1060 | U    | N1-C2-O2  | 7.74   | 128.22      | 122.80   |
| 32  | CI    | 142  | LEU  | CB-CG-CD2 | -7.52  | 98.22       | 111.00   |
| 65  | D2    | 332  | U    | N3-C2-O2  | -7.42  | 117.01      | 122.20   |
| 66  | D3    | 1060 | U    | C2-N1-C1' | 7.13   | 126.25      | 117.70   |
| 65  | D2    | 332  | U    | N1-C2-O2  | 7.00   | 127.70      | 122.80   |
| 20  | UQ    | 513  | GLU  | C-N-CA    | 6.95   | 139.07      | 121.70   |
| 62  | DY    | 114  | ARG  | CB-CG-CD  | 6.76   | 129.17      | 111.60   |
| 33  | CJ    | 62   | LEU  | CA-CB-CG  | 6.66   | 130.61      | 115.30   |
| 66  | D3    | 1060 | U    | N3-C2-O2  | -6.64  | 117.55      | 122.20   |
| 65  | D2    | 329  | A    | N1-C6-N6  | -6.48  | 114.71      | 118.60   |
| 12  | UI    | 497  | LEU  | CA-CB-CG  | 6.33   | 129.85      | 115.30   |
| 66  | D3    | 1083 | G    | C4-N9-C1' | 6.31   | 134.71      | 126.50   |
| 6   | UC    | 538  | ARG  | NE-CZ-NH1 | -6.19  | 117.21      | 120.30   |
| 10  | UG    | 160  | LEU  | CA-CB-CG  | 6.18   | 129.53      | 115.30   |
| 66  | D3    | 1083 | G    | N3-C4-N9  | 6.09   | 129.65      | 126.00   |
| 22  | US    | 349  | LEU  | CA-CB-CG  | 6.05   | 129.22      | 115.30   |
| 58  | DQ    | 52   | LEU  | CA-CB-CG  | 5.94   | 128.96      | 115.30   |
| 66  | D3    | 1083 | G    | C8-N9-C1' | -5.93  | 119.28      | 127.00   |
| 66  | D3    | 959  | U    | N3-C2-O2  | -5.91  | 118.06      | 122.20   |
| 65  | D2    | 390  | C    | N1-C2-O2  | -5.89  | 115.37      | 118.90   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 66  | D3    | 490  | C    | C2-N1-C1' | 5.83  | 125.22      | 118.80   |
| 29  | CE    | 258  | LEU  | CA-CB-CG  | 5.79  | 128.60      | 115.30   |
| 18  | UO    | 360  | MET  | CG-SD-CE  | -5.70 | 91.08       | 100.20   |
| 65  | D2    | 239  | U    | C2-N1-C1' | 5.66  | 124.50      | 117.70   |
| 4   | UA    | 521  | LEU  | CB-CG-CD1 | -5.66 | 101.38      | 111.00   |
| 55  | DL    | 71   | LEU  | CA-CB-CG  | 5.64  | 128.27      | 115.30   |
| 68  | EA    | 161  | U    | C5-C6-N1  | 5.62  | 125.51      | 122.70   |
| 1   | CA    | 306  | LEU  | CA-CB-CG  | 5.60  | 128.18      | 115.30   |
| 23  | UT    | 1399 | LEU  | CA-CB-CG  | 5.58  | 128.13      | 115.30   |
| 68  | EA    | 167  | U    | C5-C6-N1  | 5.50  | 125.45      | 122.70   |
| 14  | UK    | 217  | ARG  | NE-CZ-NH2 | -5.49 | 117.56      | 120.30   |
| 67  | D4    | 18   | G    | C4-N9-C1' | 5.46  | 133.60      | 126.50   |
| 15  | UL    | 100  | ASP  | CB-CG-OD2 | 5.44  | 123.20      | 118.30   |
| 4   | UA    | 535  | LEU  | CA-CB-CG  | 5.43  | 127.79      | 115.30   |
| 63  | Db    | 21   | LEU  | CA-CB-CG  | 5.42  | 127.77      | 115.30   |
| 45  | JN    | 215  | LEU  | CB-CG-CD2 | -5.41 | 101.80      | 111.00   |
| 18  | UO    | 507  | MET  | CB-CG-SD  | 5.40  | 128.60      | 112.40   |
| 65  | D2    | 387  | C    | C6-N1-C2  | -5.38 | 118.15      | 120.30   |
| 13  | UJ    | 1726 | LEU  | CA-CB-CG  | 5.37  | 127.66      | 115.30   |
| 66  | D3    | 562  | G    | C4-N9-C1' | -5.37 | 119.52      | 126.50   |
| 18  | UO    | 511  | LEU  | CA-CB-CG  | 5.31  | 127.52      | 115.30   |
| 66  | D3    | 1580 | C    | C2-N1-C1' | 5.30  | 124.62      | 118.80   |
| 67  | D4    | 55   | A    | N1-C2-N3  | 5.29  | 131.94      | 129.30   |
| 66  | D3    | 4    | C    | N3-C2-O2  | -5.26 | 118.22      | 121.90   |
| 65  | D2    | 387  | C    | C2-N1-C1' | 5.24  | 124.57      | 118.80   |
| 66  | D3    | 1083 | G    | N3-C4-C5  | -5.24 | 125.98      | 128.60   |
| 1   | CB    | 236  | MET  | CB-CG-SD  | -5.22 | 96.72       | 112.40   |
| 65  | D2    | 448  | G    | N3-C4-C5  | -5.19 | 126.00      | 128.60   |
| 5   | UB    | 598  | LEU  | CA-CB-CG  | 5.09  | 127.01      | 115.30   |
| 66  | D3    | 576  | G    | C4-C5-N7  | 5.08  | 112.83      | 110.80   |
| 65  | D2    | 394  | U    | C2-N1-C1' | 5.06  | 123.77      | 117.70   |
| 10  | UG    | 434  | LEU  | CA-CB-CG  | 5.03  | 126.87      | 115.30   |
| 54  | DJ    | 49   | LEU  | CA-CB-CG  | -5.03 | 103.74      | 115.30   |
| 66  | D3    | 1145 | U    | C2-N1-C1' | 5.01  | 123.72      | 117.70   |
| 65  | D2    | 233  | G    | C2-N3-C4  | -5.01 | 109.40      | 111.90   |
| 66  | D3    | 959  | U    | N1-C2-O2  | 5.01  | 126.30      | 122.80   |
| 66  | D3    | 959  | U    | C2-N1-C1' | 5.00  | 123.70      | 117.70   |

There are no chirality outliers.

All (43) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group   |
|-----|-------|------|------|---------|
| 30  | CG    | 104  | THR  | Peptide |
| 31  | CH    | 340  | GLY  | Peptide |
| 33  | CJ    | 117  | LEU  | Peptide |
| 34  | CK    | 453  | SER  | Peptide |
| 2   | DA    | 104  | ASP  | Peptide |
| 56  | DN    | 3    | ARG  | Peptide |
| 57  | DO    | 123  | SER  | Peptide |
| 58  | DQ    | 13   | LYS  | Peptide |
| 63  | Db    | 79   | PHE  | Peptide |
| 70  | EC    | 166  | TYR  | Peptide |
| 71  | ED    | 335  | ASP  | Peptide |
| 71  | ED    | 352  | ALA  | Peptide |
| 71  | ED    | 54   | ILE  | Peptide |
| 72  | EE    | 188  | GLU  | Peptide |
| 73  | EF    | 136  | HIS  | Peptide |
| 74  | EG    | 141  | LEU  | Peptide |
| 74  | EG    | 216  | ASP  | Peptide |
| 76  | EI    | 92   | ASN  | Peptide |
| 77  | EJ    | 149  | GLN  | Peptide |
| 79  | EN    | 541  | SER  | Peptide |
| 79  | EN    | 573  | LYS  | Peptide |
| 79  | EN    | 615  | VAL  | Peptide |
| 3   | JA    | 739  | ASN  | Peptide |
| 38  | JC    | 53   | PHE  | Peptide |
| 44  | JM    | 135  | HIS  | Peptide |
| 47  | JP    | 102  | GLU  | Peptide |
| 47  | JP    | 337  | GLY  | Peptide |
| 47  | JP    | 95   | TRP  | Peptide |
| 4   | UA    | 289  | LEU  | Peptide |
| 6   | UC    | 580  | ARG  | Peptide |
| 9   | UF    | 45   | SER  | Peptide |
| 11  | UH    | 257  | SER  | Peptide |
| 11  | UH    | 308  | PHE  | Peptide |
| 11  | UH    | 532  | PHE  | Peptide |
| 15  | UL    | 183  | ASP  | Peptide |
| 15  | UL    | 552  | ASP  | Peptide |
| 16  | UM    | 218  | ASP  | Peptide |
| 16  | UM    | 421  | SER  | Peptide |
| 16  | UM    | 705  | SER  | Peptide |
| 20  | UQ    | 179  | ASP  | Peptide |
| 21  | UR    | 367  | GLN  | Peptide |
| 23  | UT    | 1926 | PHE  | Peptide |
| 23  | UT    | 706  | LEU  | Peptide |

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | CA    | 1881  | 0        | 1928     | 99      | 0            |
| 1   | CB    | 1782  | 0        | 1826     | 149     | 0            |
| 2   | DA    | 1912  | 0        | 2023     | 113     | 0            |
| 3   | JA    | 5916  | 0        | 5463     | 317     | 0            |
| 3   | JB    | 4132  | 0        | 1819     | 21      | 0            |
| 4   | UA    | 6635  | 0        | 6525     | 334     | 0            |
| 5   | UB    | 3734  | 0        | 3432     | 169     | 0            |
| 6   | UC    | 1026  | 0        | 1080     | 58      | 0            |
| 7   | UD    | 5361  | 0        | 5364     | 358     | 0            |
| 8   | UE    | 3772  | 0        | 3806     | 203     | 0            |
| 9   | UF    | 2487  | 0        | 2533     | 147     | 0            |
| 10  | UG    | 4218  | 0        | 4223     | 231     | 0            |
| 11  | UH    | 2701  | 0        | 1951     | 127     | 0            |
| 12  | UI    | 860   | 0        | 922      | 79      | 0            |
| 13  | UJ    | 8961  | 0        | 9273     | 525     | 0            |
| 14  | UK    | 2021  | 0        | 2098     | 165     | 0            |
| 15  | UL    | 6726  | 0        | 6764     | 390     | 0            |
| 16  | UM    | 5969  | 0        | 6006     | 388     | 0            |
| 17  | UN    | 1227  | 0        | 1223     | 68      | 0            |
| 18  | UO    | 3911  | 0        | 3906     | 273     | 0            |
| 19  | UP    | 495   | 0        | 561      | 51      | 0            |
| 20  | UQ    | 6662  | 0        | 6588     | 394     | 0            |
| 21  | UR    | 3799  | 0        | 3783     | 237     | 0            |
| 22  | US    | 3622  | 0        | 3214     | 181     | 0            |
| 23  | UT    | 17290 | 0        | 16616    | 924     | 0            |
| 24  | UU    | 6678  | 0        | 6651     | 339     | 0            |
| 25  | UV    | 8736  | 0        | 8850     | 468     | 0            |
| 26  | UX    | 1395  | 0        | 1473     | 70      | 0            |
| 27  | UZ    | 2006  | 0        | 2118     | 117     | 0            |
| 28  | CD    | 2994  | 0        | 3018     | 166     | 0            |
| 29  | CE    | 3325  | 0        | 3414     | 215     | 0            |
| 30  | CF    | 931   | 0        | 983      | 47      | 0            |
| 30  | CG    | 928   | 0        | 976      | 71      | 0            |
| 31  | CH    | 3725  | 0        | 3746     | 220     | 0            |
| 32  | CI    | 1530  | 0        | 1572     | 99      | 0            |
| 33  | CJ    | 2296  | 0        | 2325     | 133     | 0            |
| 34  | CK    | 1667  | 0        | 1701     | 98      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 35  | CL    | 6332  | 0        | 6515     | 416     | 0            |
| 36  | CM    | 2781  | 0        | 2878     | 140     | 0            |
| 37  | CN    | 1893  | 0        | 1875     | 100     | 0            |
| 38  | JC    | 2845  | 0        | 2761     | 234     | 0            |
| 39  | JF    | 1701  | 0        | 1767     | 102     | 0            |
| 39  | JG    | 1799  | 0        | 1872     | 106     | 0            |
| 40  | JH    | 1295  | 0        | 570      | 4       | 0            |
| 41  | JI    | 1314  | 0        | 610      | 0       | 0            |
| 42  | JJ    | 1442  | 0        | 1513     | 72      | 0            |
| 43  | JK    | 334   | 0        | 313      | 24      | 0            |
| 44  | JM    | 1137  | 0        | 1188     | 52      | 0            |
| 45  | JN    | 1428  | 0        | 1425     | 67      | 0            |
| 46  | JO    | 1876  | 0        | 1968     | 76      | 0            |
| 47  | JP    | 3765  | 0        | 3714     | 232     | 0            |
| 48  | JQ    | 381   | 0        | 255      | 12      | 0            |
| 49  | DE    | 1944  | 0        | 2030     | 126     | 0            |
| 50  | DF    | 1669  | 0        | 1724     | 110     | 0            |
| 51  | DG    | 1755  | 0        | 1846     | 119     | 0            |
| 52  | DH    | 1481  | 0        | 1572     | 102     | 0            |
| 53  | DI    | 1399  | 0        | 1431     | 94      | 0            |
| 54  | DJ    | 1494  | 0        | 1573     | 69      | 0            |
| 55  | DL    | 1129  | 0        | 1196     | 65      | 0            |
| 56  | DN    | 1192  | 0        | 1255     | 79      | 0            |
| 57  | DO    | 881   | 0        | 910      | 40      | 0            |
| 58  | DQ    | 973   | 0        | 1029     | 69      | 0            |
| 59  | DS    | 516   | 0        | 222      | 0       | 0            |
| 60  | DW    | 1021  | 0        | 1060     | 73      | 0            |
| 61  | DX    | 786   | 0        | 843      | 69      | 0            |
| 62  | DY    | 1073  | 0        | 1132     | 63      | 0            |
| 63  | Db    | 610   | 0        | 630      | 0       | 0            |
| 64  | Dc    | 497   | 0        | 535      | 0       | 0            |
| 65  | D2    | 9508  | 0        | 4781     | 404     | 0            |
| 66  | D3    | 28287 | 0        | 14261    | 1182    | 0            |
| 67  | D4    | 4869  | 0        | 2468     | 191     | 0            |
| 68  | EA    | 366   | 0        | 184      | 1       | 0            |
| 69  | EB    | 1475  | 0        | 658      | 13      | 0            |
| 70  | EC    | 1204  | 0        | 530      | 9       | 0            |
| 71  | ED    | 1571  | 0        | 699      | 12      | 0            |
| 72  | EE    | 1107  | 0        | 499      | 6       | 0            |
| 73  | EF    | 1326  | 0        | 580      | 6       | 0            |
| 74  | EG    | 1058  | 0        | 478      | 3       | 0            |
| 75  | EH    | 1170  | 0        | 528      | 8       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 76  | EI    | 1440   | 0        | 648      | 7       | 0            |
| 77  | EJ    | 1091   | 0        | 500      | 12      | 0            |
| 78  | EK    | 4818   | 0        | 2108     | 32      | 0            |
| 79  | EN    | 4767   | 0        | 2109     | 59      | 0            |
| 80  | Db    | 1      | 0        | 0        | 0       | 0            |
| 80  | EK    | 1      | 0        | 0        | 0       | 0            |
| 80  | UX    | 1      | 0        | 0        | 0       | 0            |
| 81  | CL    | 1      | 0        | 0        | 0       | 0            |
| 81  | EK    | 1      | 0        | 0        | 0       | 0            |
| 81  | UX    | 1      | 0        | 0        | 0       | 0            |
| 82  | CL    | 32     | 0        | 12       | 2       | 0            |
| All | All   | 256149 | 0        | 219009   | 11280   | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (11280) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:UU:228:GLY:CA  | 24:UU:246:ILE:O    | 1.81                     | 1.28              |
| 11:UH:341:LEU:HA  | 11:UH:358:VAL:O    | 1.15                     | 1.27              |
| 4:UA:77:GLY:HA3   | 4:UA:95:PHE:O      | 1.33                     | 1.24              |
| 24:UU:228:GLY:HA3 | 24:UU:246:ILE:O    | 1.04                     | 1.18              |
| 16:UM:30:LYS:HA   | 16:UM:45:LEU:O     | 1.42                     | 1.18              |
| 78:EK:94:VAL:O    | 78:EK:98:ALA:HB3   | 1.44                     | 1.16              |
| 7:UD:397:SER:O    | 7:UD:421:THR:HA    | 1.47                     | 1.13              |
| 4:UA:482:SER:O    | 4:UA:486:SER:HA    | 1.60                     | 1.01              |
| 79:EN:616:ILE:O   | 79:EN:618:VAL:N    | 1.93                     | 1.01              |
| 11:UH:341:LEU:CA  | 11:UH:358:VAL:O    | 2.10                     | 1.00              |
| 38:JC:189:ASN:O   | 38:JC:193:GLY:HA2  | 1.62                     | 0.99              |
| 20:UQ:302:SER:HG  | 20:UQ:344:CYS:HG   | 1.10                     | 0.98              |
| 21:UR:382:GLY:CA  | 21:UR:400:ILE:O    | 2.12                     | 0.98              |
| 15:UL:767:GLU:HB3 | 15:UL:771:ARG:HH12 | 1.30                     | 0.97              |
| 30:CG:95:ARG:NH2  | 67:D4:253:G:N7     | 2.13                     | 0.97              |
| 21:UR:382:GLY:HA3 | 21:UR:400:ILE:O    | 1.66                     | 0.96              |
| 66:D3:1061:A:H2'  | 66:D3:1062:A:H4'   | 1.46                     | 0.96              |
| 35:CL:252:LEU:O   | 35:CL:268:LYS:HB3  | 1.66                     | 0.95              |
| 4:UA:561:SER:HG   | 4:UA:577:SER:HG    | 1.01                     | 0.95              |
| 1:CB:308:PRO:HG3  | 14:UK:130:SER:H    | 1.32                     | 0.94              |
| 35:CL:109:SER:O   | 35:CL:113:ARG:HB3  | 1.66                     | 0.94              |
| 39:JF:99:LEU:O    | 39:JF:105:ASN:ND2  | 2.00                     | 0.94              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:UK:111:ARG:HE   | 14:UK:212:LYS:HG2  | 1.30                     | 0.94              |
| 31:CH:560:ARG:NH2  | 67:D4:249:G:N7     | 2.15                     | 0.93              |
| 3:JA:122:CYS:HB2   | 3:JA:148:VAL:HG12  | 1.51                     | 0.93              |
| 4:UA:434:ASN:HD21  | 4:UA:450:LEU:HD23  | 1.33                     | 0.93              |
| 42:JJ:206:ALA:HA   | 42:JJ:213:LYS:HE3  | 1.49                     | 0.93              |
| 45:JN:306:LEU:HG   | 45:JN:308:ILE:HD11 | 1.51                     | 0.93              |
| 47:JP:327:LYS:HG2  | 47:JP:350:HIS:H    | 1.34                     | 0.93              |
| 78:EK:42:ARG:CB    | 78:EK:152:PHE:O    | 2.18                     | 0.92              |
| 23:UT:296:GLU:HG2  | 23:UT:300:GLN:HE22 | 1.35                     | 0.91              |
| 10:UG:140:ARG:HH11 | 13:UJ:20:LEU:HD21  | 1.34                     | 0.91              |
| 20:UQ:36:ARG:NH1   | 20:UQ:91:ILE:O     | 2.04                     | 0.91              |
| 78:EK:94:VAL:O     | 78:EK:98:ALA:CB    | 2.19                     | 0.91              |
| 53:DI:105:ASP:HA   | 53:DI:164:ARG:HH22 | 1.33                     | 0.91              |
| 51:DG:2:LYS:HB3    | 51:DG:108:VAL:HG12 | 1.53                     | 0.91              |
| 1:CA:264:GLN:HA    | 1:CA:320:TYR:O     | 1.71                     | 0.90              |
| 23:UT:870:LEU:HD11 | 23:UT:888:LEU:HB3  | 1.54                     | 0.90              |
| 78:EK:617:PRO:HA   | 78:EK:648:SER:CB   | 2.02                     | 0.90              |
| 33:CJ:116:ARG:NH1  | 66:D3:1581:C:OP1   | 2.05                     | 0.90              |
| 65:D2:242:C:H2'    | 65:D2:243:A:H8     | 1.35                     | 0.90              |
| 69:EB:166:ASP:CB   | 69:EB:182:ARG:CB   | 2.51                     | 0.90              |
| 30:CG:42:LYS:NZ    | 67:D4:112:U:OP2    | 2.03                     | 0.89              |
| 1:CB:306:LEU:HD11  | 1:CB:315:ILE:HG13  | 1.52                     | 0.89              |
| 35:CL:72:VAL:HG12  | 35:CL:137:LEU:HB2  | 1.53                     | 0.89              |
| 20:UQ:510:TYR:HH   | 20:UQ:527:HIS:HD1  | 1.17                     | 0.89              |
| 35:CL:830:ARG:NH2  | 61:DX:138:GLU:OE2  | 2.06                     | 0.89              |
| 45:JN:304:ARG:NH1  | 66:D3:1084:A:N7    | 2.20                     | 0.89              |
| 15:UL:217:LEU:HB3  | 15:UL:229:TRP:HB2  | 1.52                     | 0.89              |
| 29:CE:125:PRO:HA   | 29:CE:128:LEU:HD13 | 1.52                     | 0.89              |
| 66:D3:390:G:H1     | 66:D3:407:A:H62    | 1.20                     | 0.89              |
| 65:D2:470:U:H3     | 67:D4:48:A:H61     | 1.21                     | 0.89              |
| 39:JG:112:VAL:HG23 | 39:JG:124:VAL:HB   | 1.53                     | 0.88              |
| 1:CA:281:ASP:OD1   | 1:CA:282:ALA:N     | 2.07                     | 0.88              |
| 6:UC:538:ARG:HH12  | 35:CL:912:ARG:NH1  | 1.72                     | 0.88              |
| 1:CA:123:ILE:HG12  | 44:JM:152:ILE:HG22 | 1.56                     | 0.88              |
| 7:UD:399:VAL:HB    | 7:UD:420:LEU:HB2   | 1.55                     | 0.88              |
| 35:CL:92:ARG:HH21  | 35:CL:221:LEU:HD11 | 1.38                     | 0.88              |
| 21:UR:295:ILE:HD11 | 21:UR:298:CYS:HB3  | 1.55                     | 0.87              |
| 46:JO:58:ASN:HD22  | 65:D2:347:U:H5''   | 1.39                     | 0.87              |
| 10:UG:265:GLU:OE1  | 17:UN:834:LYS:NZ   | 2.06                     | 0.87              |
| 61:DX:63:GLN:NE2   | 66:D3:559:C:O2     | 2.07                     | 0.87              |
| 7:UD:264:PHE:HB2   | 7:UD:274:GLN:HB2   | 1.56                     | 0.87              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 20:UQ:16:SER:HB2   | 20:UQ:783:LEU:HB2   | 1.57                     | 0.87              |
| 5:UB:660:ILE:HG12  | 22:US:388:LEU:HD11  | 1.55                     | 0.87              |
| 10:UG:132:GLY:HA3  | 10:UG:150:LEU:O     | 1.74                     | 0.87              |
| 20:UQ:283:VAL:HG12 | 20:UQ:290:ILE:HG22  | 1.57                     | 0.86              |
| 51:DG:21:GLU:OE1   | 51:DG:25:ARG:NH1    | 2.08                     | 0.86              |
| 39:JF:144:LEU:HD13 | 39:JF:150:ILE:HG12  | 1.56                     | 0.86              |
| 20:UQ:118:VAL:HB   | 20:UQ:130:LYS:HB2   | 1.57                     | 0.86              |
| 66:D3:1697:G:H1    | 66:D3:1704:U:H3     | 1.21                     | 0.86              |
| 11:UH:254:GLY:O    | 11:UH:258:PRO:HA    | 1.75                     | 0.86              |
| 47:JP:393:LYS:NZ   | 67:D4:35:U:O2'      | 2.07                     | 0.86              |
| 13:UJ:166:ASN:OD1  | 29:CE:407:ARG:NH1   | 2.09                     | 0.86              |
| 35:CL:45:ARG:NH1   | 66:D3:27:U:O2'      | 2.08                     | 0.86              |
| 17:UN:294:GLU:OE2  | 47:JP:250:ARG:NH2   | 2.09                     | 0.85              |
| 24:UU:35:ASN:HD22  | 24:UU:55:GLY:H      | 1.19                     | 0.85              |
| 25:UV:182:ASP:HB2  | 25:UV:208:THR:HB    | 1.59                     | 0.85              |
| 1:CA:155:ILE:HD11  | 1:CA:162:LEU:HD22   | 1.56                     | 0.85              |
| 6:UC:599:LYS:NZ    | 66:D3:498:G:OP1     | 2.08                     | 0.85              |
| 3:JA:860:PRO:HB3   | 3:JA:892:ARG:HH21   | 1.40                     | 0.85              |
| 3:JA:612:ASP:O     | 3:JA:616:TRP:HB2    | 1.76                     | 0.85              |
| 21:UR:181:GLU:OE1  | 24:UU:242:ARG:NH1   | 2.09                     | 0.85              |
| 24:UU:289:ASN:O    | 24:UU:292:ARG:NH1   | 2.10                     | 0.85              |
| 46:JO:127:LYS:NZ   | 66:D3:929:A:O2'     | 2.09                     | 0.85              |
| 8:UE:513:LEU:HD11  | 18:UO:511:LEU:HG    | 1.59                     | 0.85              |
| 25:UV:528:ASP:HA   | 25:UV:614:ARG:HH21  | 1.42                     | 0.84              |
| 8:UE:88:TYR:HA     | 8:UE:95:VAL:HA      | 1.59                     | 0.84              |
| 23:UT:1358:LYS:HD2 | 23:UT:1410:LEU:HD13 | 1.57                     | 0.84              |
| 17:UN:306:ARG:NH1  | 66:D3:-5:G:OP1      | 2.09                     | 0.84              |
| 30:CF:84:ARG:HD2   | 30:CF:96:PRO:HB3    | 1.59                     | 0.84              |
| 5:UB:678:PHE:O     | 5:UB:682:ARG:NH2    | 2.10                     | 0.84              |
| 12:UI:502:ARG:HG2  | 18:UO:510:LEU:HD21  | 1.59                     | 0.84              |
| 21:UR:426:VAL:HG22 | 21:UR:432:VAL:HG22  | 1.59                     | 0.84              |
| 7:UD:92:GLU:HB2    | 7:UD:428:ILE:HD13   | 1.58                     | 0.84              |
| 24:UU:343:LEU:HG   | 24:UU:344:ARG:H     | 1.41                     | 0.84              |
| 37:CN:16:VAL:HB    | 37:CN:37:MET:HB2    | 1.58                     | 0.84              |
| 47:JP:174:ARG:NH2  | 47:JP:206:VAL:O     | 2.10                     | 0.84              |
| 13:UJ:278:ALA:HA   | 21:UR:208:LEU:HD21  | 1.60                     | 0.84              |
| 16:UM:30:LYS:HD3   | 16:UM:46:THR:HB     | 1.57                     | 0.84              |
| 33:CJ:149:PRO:HG2  | 33:CJ:170:VAL:HG11  | 1.59                     | 0.84              |
| 15:UL:760:ILE:HG13 | 15:UL:831:LYS:HB3   | 1.59                     | 0.83              |
| 26:UX:161:LYS:HG2  | 26:UX:172:LEU:HD21  | 1.58                     | 0.83              |
| 1:CA:156:MET:SD    | 1:CA:309:TYR:OH     | 2.35                     | 0.83              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 15:UL:357:THR:HG1   | 15:UL:361:THR:HG1   | 1.13                     | 0.83              |
| 18:UO:192:LEU:HA    | 18:UO:209:LEU:O     | 1.77                     | 0.83              |
| 56:DN:100:LYS:HG2   | 56:DN:104:ARG:HH22  | 1.43                     | 0.83              |
| 4:UA:793:GLU:OE2    | 24:UU:721:LEU:N     | 2.12                     | 0.83              |
| 24:UU:574:THR:OG1   | 24:UU:576:ARG:NH2   | 2.11                     | 0.83              |
| 39:JF:55:ILE:O      | 39:JF:63:ASP:HA     | 1.79                     | 0.83              |
| 58:DQ:42:GLU:HG2    | 58:DQ:45:ARG:HH21   | 1.42                     | 0.83              |
| 52:DH:48:GLU:HG2    | 52:DH:88:ARG:HH22   | 1.44                     | 0.83              |
| 25:UV:403:GLY:HA2   | 25:UV:410:LYS:HA    | 1.60                     | 0.83              |
| 3:JA:89:ASN:HA      | 35:CL:95:LYS:HZ3    | 1.44                     | 0.83              |
| 4:UA:482:SER:O      | 4:UA:486:SER:CA     | 2.27                     | 0.83              |
| 35:CL:78:PRO:HD3    | 35:CL:122:ALA:CB    | 2.09                     | 0.83              |
| 3:JA:88:VAL:O       | 35:CL:95:LYS:NZ     | 2.12                     | 0.82              |
| 21:UR:129:ASP:OD2   | 24:UU:192:ASN:ND2   | 2.13                     | 0.82              |
| 21:UR:317:ARG:HH12  | 65:D2:233:G:H22     | 1.24                     | 0.82              |
| 35:CL:831:ARG:NH1   | 35:CL:877:GLU:O     | 2.11                     | 0.82              |
| 1:CA:103:GLU:OE2    | 6:UC:594:GLU:N      | 2.11                     | 0.82              |
| 8:UE:253:LEU:HB3    | 8:UE:279:ILE:HB     | 1.60                     | 0.82              |
| 13:UJ:1637:TYR:O    | 13:UJ:1643:ARG:NH2  | 2.12                     | 0.82              |
| 26:UX:79:LYS:NZ     | 45:JN:308:ILE:O     | 2.12                     | 0.82              |
| 30:CG:25:GLN:NE2    | 31:CH:323:ASP:OD2   | 2.12                     | 0.82              |
| 4:UA:780:LYS:NZ     | 4:UA:819:THR:O      | 2.11                     | 0.82              |
| 1:CB:251:ARG:NH2    | 7:UD:178:GLU:OE1    | 2.11                     | 0.82              |
| 11:UH:558:CYS:H     | 11:UH:585:ARG:HH12  | 1.24                     | 0.82              |
| 14:UK:150:LYS:NZ    | 65:D2:192:G:O2'     | 2.12                     | 0.82              |
| 18:UO:453:VAL:HG23  | 18:UO:454:ARG:H     | 1.45                     | 0.82              |
| 23:UT:1616:LEU:HD22 | 23:UT:1635:ILE:HD13 | 1.59                     | 0.82              |
| 4:UA:73:ILE:HD12    | 4:UA:102:VAL:HG21   | 1.61                     | 0.82              |
| 20:UQ:471:GLN:HE22  | 20:UQ:541:TRP:H     | 1.26                     | 0.82              |
| 65:D2:2:U:HO2'      | 65:D2:69:U:HO2'     | 1.20                     | 0.82              |
| 69:EB:301:ASN:O     | 78:EK:505:ALA:O     | 1.98                     | 0.82              |
| 4:UA:650:ASN:ND2    | 4:UA:655:ASP:O      | 2.13                     | 0.82              |
| 23:UT:13:ARG:NH1    | 62:DY:84:LYS:O      | 2.13                     | 0.82              |
| 49:DE:178:GLY:O     | 49:DE:231:GLN:NE2   | 2.12                     | 0.82              |
| 78:EK:930:VAL:O     | 78:EK:934:GLY:HA2   | 1.80                     | 0.82              |
| 18:UO:279:GLY:HA3   | 18:UO:298:PHE:O     | 1.80                     | 0.82              |
| 21:UR:535:ARG:NH2   | 65:D2:234:A:OP1     | 2.10                     | 0.82              |
| 23:UT:1477:LYS:HE3  | 23:UT:1480:SER:HB3  | 1.60                     | 0.82              |
| 35:CL:78:PRO:HD3    | 35:CL:122:ALA:HB1   | 1.62                     | 0.82              |
| 35:CL:80:THR:HG23   | 35:CL:172:THR:HG21  | 1.59                     | 0.82              |
| 19:UP:169:ASP:HB2   | 19:UP:180:LEU:HD23  | 1.62                     | 0.81              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:CJ:193:ASN:HB3  | 33:CJ:226:ASN:HB3  | 1.61                     | 0.81              |
| 49:DE:87:MET:HE1   | 49:DE:123:LEU:H    | 1.45                     | 0.81              |
| 5:UB:444:ASN:H     | 5:UB:446:GLN:HE21  | 1.25                     | 0.81              |
| 30:CG:95:ARG:HH11  | 31:CH:551:ARG:H    | 1.28                     | 0.81              |
| 7:UD:306:GLN:HE22  | 7:UD:308:SER:HB3   | 1.45                     | 0.81              |
| 35:CL:753:LEU:HG   | 35:CL:757:LYS:HZ3  | 1.45                     | 0.81              |
| 9:UF:152:LYS:HD3   | 44:JM:65:LEU:HD11  | 1.62                     | 0.81              |
| 13:UJ:122:VAL:HA   | 13:UJ:127:ILE:HG12 | 1.61                     | 0.81              |
| 4:UA:581:THR:HG22  | 4:UA:596:GLY:HA2   | 1.61                     | 0.81              |
| 24:UU:715:GLN:NE2  | 24:UU:717:ASP:O    | 2.12                     | 0.81              |
| 38:JC:116:HIS:CE1  | 38:JC:124:GLN:HB2  | 2.15                     | 0.81              |
| 1:CA:225:ARG:HH21  | 1:CA:246:GLN:HG2   | 1.45                     | 0.81              |
| 4:UA:160:PHE:CE2   | 4:UA:183:ALA:HB3   | 2.16                     | 0.81              |
| 35:CL:858:PRO:HA   | 35:CL:885:PHE:HB3  | 1.61                     | 0.81              |
| 49:DE:212:ASP:O    | 49:DE:215:ASP:N    | 2.13                     | 0.81              |
| 4:UA:563:ARG:HB2   | 4:UA:571:ALA:HB2   | 1.63                     | 0.81              |
| 35:CL:295:ASP:OD1  | 35:CL:852:ARG:NH1  | 2.14                     | 0.81              |
| 21:UR:285:VAL:HG12 | 21:UR:286:THR:HG23 | 1.63                     | 0.81              |
| 15:UL:52:TRP:HB3   | 15:UL:59:LEU:HA    | 1.61                     | 0.81              |
| 67:D4:63:C:H2'     | 67:D4:64:A:H8      | 1.46                     | 0.81              |
| 6:UC:433:ARG:HD2   | 39:JF:231:PRO:HG2  | 1.61                     | 0.80              |
| 8:UE:344:ASP:OD1   | 8:UE:345:LEU:N     | 2.14                     | 0.80              |
| 29:CE:430:ASP:OD1  | 29:CE:431:ALA:N    | 2.14                     | 0.80              |
| 33:CJ:7:ARG:NH1    | 33:CJ:11:GLU:OE2   | 2.12                     | 0.80              |
| 39:JG:188:ARG:HE   | 39:JG:190:GLN:HB3  | 1.44                     | 0.80              |
| 7:UD:97:ARG:HH12   | 19:UP:190:LEU:HD13 | 1.45                     | 0.80              |
| 23:UT:54:TRP:HA    | 23:UT:57:ILE:HG22  | 1.64                     | 0.80              |
| 23:UT:957:LYS:HG3  | 23:UT:959:PRO:HD2  | 1.60                     | 0.80              |
| 55:DL:69:LYS:NZ    | 66:D3:304:U:O2     | 2.14                     | 0.80              |
| 16:UM:414:VAL:HB   | 16:UM:428:ALA:HB3  | 1.63                     | 0.80              |
| 13:UJ:246:LEU:O    | 13:UJ:285:ASN:ND2  | 2.14                     | 0.80              |
| 23:UT:707:PRO:O    | 23:UT:775:ARG:NH1  | 2.11                     | 0.80              |
| 13:UJ:231:LEU:HD13 | 13:UJ:268:LEU:HD21 | 1.63                     | 0.80              |
| 14:UK:140:ARG:NH2  | 19:UP:168:LYS:O    | 2.15                     | 0.80              |
| 16:UM:24:THR:HG21  | 16:UM:68:LYS:HD2   | 1.62                     | 0.80              |
| 19:UP:204:ARG:HH21 | 65:D2:170:U:H4'    | 1.47                     | 0.80              |
| 21:UR:382:GLY:HA2  | 21:UR:400:ILE:O    | 1.80                     | 0.80              |
| 23:UT:1710:LEU:O   | 23:UT:1714:SER:HB3 | 1.82                     | 0.80              |
| 23:UT:1738:TYR:HA  | 66:D3:803:A:H1'    | 1.64                     | 0.80              |
| 13:UJ:286:LEU:HD21 | 13:UJ:292:LYS:HG3  | 1.63                     | 0.80              |
| 22:US:179:GLU:OE2  | 22:US:183:LYS:NZ   | 2.14                     | 0.80              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 23:UT:1425:VAL:HA  | 23:UT:1434:PHE:HB3  | 1.63                     | 0.80              |
| 23:UT:1655:ARG:NH2 | 23:UT:1744:GLU:OE1  | 2.14                     | 0.80              |
| 35:CL:74:VAL:HG12  | 35:CL:119:GLU:HA    | 1.63                     | 0.80              |
| 9:UF:66:LEU:HD22   | 21:UR:26:VAL:HG11   | 1.63                     | 0.80              |
| 13:UJ:1749:ARG:NH2 | 23:UT:35:GLU:O      | 2.15                     | 0.80              |
| 16:UM:128:VAL:HG13 | 16:UM:137:THR:HB    | 1.64                     | 0.80              |
| 17:UN:886:LYS:NZ   | 65:D2:485:G:O2'     | 2.15                     | 0.80              |
| 21:UR:137:ILE:O    | 21:UR:143:THR:OG1   | 2.00                     | 0.79              |
| 15:UL:661:TRP:HE1  | 15:UL:677:HIS:HB2   | 1.46                     | 0.79              |
| 20:UQ:368:ASP:HB3  | 20:UQ:389:LEU:HD22  | 1.62                     | 0.79              |
| 23:UT:1099:LEU:HB2 | 23:UT:1142:VAL:HG22 | 1.64                     | 0.79              |
| 30:CG:79:VAL:HG21  | 30:CG:121:ILE:HD12  | 1.62                     | 0.79              |
| 3:JA:55:VAL:HG12   | 3:JA:121:MET:HB2    | 1.64                     | 0.79              |
| 21:UR:181:GLU:HG3  | 24:UU:281:ARG:HH21  | 1.45                     | 0.79              |
| 3:JA:75:ASN:HA     | 3:JA:78:LYS:HZ3     | 1.47                     | 0.79              |
| 5:UB:762:GLU:OE1   | 34:CK:349:ARG:NH1   | 2.16                     | 0.79              |
| 7:UD:271:THR:HG22  | 7:UD:272:LEU:H      | 1.45                     | 0.79              |
| 66:D3:1175:U:O4    | 66:D3:1464:G:N2     | 2.16                     | 0.79              |
| 23:UT:635:ALA:HB1  | 23:UT:676:PRO:HG2   | 1.63                     | 0.79              |
| 17:UN:295:VAL:HG21 | 47:JP:291:MET:HE1   | 1.64                     | 0.79              |
| 24:UU:232:MET:HE1  | 24:UU:256:PHE:HZ    | 1.45                     | 0.79              |
| 24:UU:361:SER:HA   | 24:UU:636:PRO:HG2   | 1.65                     | 0.79              |
| 24:UU:592:ASP:OD1  | 24:UU:593:PHE:N     | 2.15                     | 0.79              |
| 31:CH:447:SER:OG   | 31:CH:449:ASN:OD1   | 2.01                     | 0.79              |
| 14:UK:154:THR:HG22 | 14:UK:167:THR:HA    | 1.63                     | 0.79              |
| 32:CI:151:THR:OG1  | 34:CK:455:HIS:NE2   | 2.14                     | 0.79              |
| 34:CK:480:GLN:HE22 | 34:CK:482:LEU:HB2   | 1.48                     | 0.79              |
| 52:DH:61:PHE:HB3   | 52:DH:95:GLU:HG3    | 1.64                     | 0.79              |
| 4:UA:300:MET:HG3   | 4:UA:328:LEU:HD22   | 1.65                     | 0.79              |
| 13:UJ:349:THR:HG21 | 13:UJ:379:GLU:HG3   | 1.65                     | 0.79              |
| 23:UT:220:GLU:HA   | 23:UT:270:ARG:HH11  | 1.46                     | 0.79              |
| 2:DA:146:GLN:NE2   | 66:D3:1065:A:N3     | 2.31                     | 0.79              |
| 4:UA:296:GLN:OE1   | 4:UA:330:TYR:OH     | 2.01                     | 0.79              |
| 22:US:291:THR:HB   | 22:US:294:LYS:HD3   | 1.64                     | 0.79              |
| 24:UU:743:ARG:NH2  | 34:CK:480:GLN:O     | 2.16                     | 0.79              |
| 35:CL:829:LEU:HD12 | 35:CL:915:ALA:HB1   | 1.65                     | 0.79              |
| 35:CL:833:ARG:NH2  | 61:DX:141:GLU:OE2   | 2.16                     | 0.79              |
| 43:JK:472:ILE:HA   | 43:JK:475:TYR:HB2   | 1.64                     | 0.79              |
| 2:DA:189:ILE:HB    | 2:DA:190:PRO:HD3    | 1.63                     | 0.79              |
| 10:UG:258:LEU:HB2  | 10:UG:268:VAL:HG12  | 1.65                     | 0.79              |
| 20:UQ:408:THR:HG23 | 20:UQ:410:ASN:H     | 1.48                     | 0.79              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 5:UB:475:ARG:HH21   | 22:US:511:SER:HA    | 1.48                     | 0.78              |
| 11:UH:257:SER:O     | 11:UH:259:ILE:N     | 2.12                     | 0.78              |
| 24:UU:309:ILE:HG12  | 24:UU:323:VAL:HG12  | 1.63                     | 0.78              |
| 35:CL:862:THR:HG23  | 35:CL:872:LEU:HD11  | 1.64                     | 0.78              |
| 38:JC:353:CYS:HB2   | 38:JC:356:LEU:HD13  | 1.64                     | 0.78              |
| 30:CG:18:GLN:HE22   | 31:CH:400:GLY:HA2   | 1.46                     | 0.78              |
| 35:CL:562:GLU:HG2   | 35:CL:565:ARG:HE    | 1.48                     | 0.78              |
| 35:CL:754:GLN:HA    | 35:CL:757:LYS:HE2   | 1.64                     | 0.78              |
| 11:UH:308:PHE:O     | 11:UH:310:MET:N     | 2.14                     | 0.78              |
| 14:UK:111:ARG:HH11  | 14:UK:212:LYS:HE3   | 1.47                     | 0.78              |
| 16:UM:294:LEU:HB2   | 16:UM:303:PHE:HB2   | 1.65                     | 0.78              |
| 17:UN:329:ARG:NH2   | 17:UN:339:GLN:OE1   | 2.16                     | 0.78              |
| 18:UO:5:ARG:HA      | 20:UQ:336:ARG:HH22  | 1.45                     | 0.78              |
| 45:JN:209:ARG:NH1   | 45:JN:282:ASP:OD2   | 2.15                     | 0.78              |
| 14:UK:214:VAL:HA    | 14:UK:217:ARG:HD3   | 1.66                     | 0.78              |
| 56:DN:112:LYS:NZ    | 66:D3:975:C:OP1     | 2.16                     | 0.78              |
| 1:CB:99:ALA:O       | 1:CB:104:ASP:HA     | 1.83                     | 0.78              |
| 27:UZ:227:SER:OG    | 27:UZ:228:LYS:NZ    | 2.16                     | 0.78              |
| 7:UD:548:GLY:HA3    | 7:UD:566:LEU:O      | 1.83                     | 0.78              |
| 16:UM:654:GLU:OE1   | 16:UM:658:LYS:NZ    | 2.17                     | 0.78              |
| 21:UR:382:GLY:O     | 21:UR:399:LYS:HA    | 1.83                     | 0.78              |
| 36:CM:200:VAL:HG12  | 36:CM:201:SER:H     | 1.46                     | 0.78              |
| 47:JP:228:ASN:ND2   | 47:JP:230:ASN:O     | 2.17                     | 0.78              |
| 13:UJ:661:ILE:HG22  | 13:UJ:663:SER:H     | 1.49                     | 0.78              |
| 15:UL:123:ALA:HB3   | 15:UL:141:LYS:HD3   | 1.66                     | 0.78              |
| 36:CM:246:VAL:O     | 36:CM:248:GLN:NE2   | 2.17                     | 0.78              |
| 53:DI:86:SER:O      | 66:D3:341:A:O2'     | 2.00                     | 0.78              |
| 57:DO:41:ARG:HH22   | 66:D3:916:U:H3      | 1.31                     | 0.78              |
| 7:UD:401:ILE:HD13   | 7:UD:418:CYS:HB2    | 1.64                     | 0.78              |
| 14:UK:102:GLN:NE2   | 29:CE:335:ASP:OD1   | 2.15                     | 0.78              |
| 20:UQ:510:TYR:OH    | 20:UQ:527:HIS:ND1   | 2.15                     | 0.78              |
| 20:UQ:720:ILE:HD11  | 20:UQ:766:ILE:HG21  | 1.66                     | 0.78              |
| 35:CL:91:ARG:HH22   | 35:CL:214:ARG:HE    | 1.30                     | 0.78              |
| 36:CM:274:LYS:HD2   | 36:CM:278:GLN:HE22  | 1.49                     | 0.78              |
| 39:JG:175:CYS:SG    | 39:JG:176:ARG:N     | 2.56                     | 0.78              |
| 5:UB:649:THR:HG23   | 5:UB:650:VAL:HG23   | 1.66                     | 0.78              |
| 7:UD:354:LYS:O      | 7:UD:374:THR:HA     | 1.84                     | 0.78              |
| 15:UL:760:ILE:HG23  | 15:UL:834:LYS:HZ1   | 1.48                     | 0.78              |
| 23:UT:1658:LEU:HD13 | 23:UT:1661:ILE:HD11 | 1.65                     | 0.78              |
| 23:UT:1671:VAL:HG22 | 23:UT:1713:SER:HB2  | 1.66                     | 0.78              |
| 35:CL:133:LYS:O     | 35:CL:238:ARG:NH1   | 2.16                     | 0.78              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 38:JC:317:ILE:HD12  | 38:JC:333:ASN:HB3   | 1.65                     | 0.78              |
| 55:DL:56:LYS:NZ     | 66:D3:328:A:OP2     | 2.17                     | 0.78              |
| 66:D3:396:G:N2      | 66:D3:399:A:OP2     | 2.17                     | 0.78              |
| 66:D3:502:U:H2'     | 66:D3:503:G:H8      | 1.47                     | 0.78              |
| 4:UA:730:LEU:HD21   | 4:UA:754:VAL:HG23   | 1.64                     | 0.78              |
| 18:UO:384:ARG:NH1   | 65:D2:92:C:OP1      | 2.16                     | 0.78              |
| 23:UT:1640:CYS:HB3  | 23:UT:1680:THR:HG21 | 1.63                     | 0.78              |
| 31:CH:157:LEU:HD23  | 31:CH:191:SER:HB2   | 1.66                     | 0.78              |
| 47:JP:21:GLU:HG2    | 67:D4:39:C:H5''     | 1.64                     | 0.78              |
| 66:D3:956:C:H2'     | 66:D3:957:G:H8      | 1.49                     | 0.78              |
| 4:UA:638:ALA:HB3    | 10:UG:149:PHE:CD1   | 2.18                     | 0.77              |
| 35:CL:864:ASP:OD2   | 35:CL:868:ARG:NH1   | 2.16                     | 0.77              |
| 55:DL:8:GLN:NE2     | 55:DL:12:ALA:O      | 2.16                     | 0.77              |
| 65:D2:484:G:N2      | 65:D2:486:U:O2'     | 2.16                     | 0.77              |
| 30:CF:44:LEU:HD21   | 30:CF:52:ILE:HD11   | 1.67                     | 0.77              |
| 62:DY:113:ASN:ND2   | 66:D3:54:C:OP1      | 2.17                     | 0.77              |
| 78:EK:136:CYS:HA    | 78:EK:145:PHE:CB    | 2.14                     | 0.77              |
| 1:CA:253:ILE:O      | 1:CA:257:SER:OG     | 2.01                     | 0.77              |
| 7:UD:37:ARG:HD2     | 7:UD:756:GLU:HB2    | 1.67                     | 0.77              |
| 16:UM:42:ILE:HG23   | 16:UM:53:LEU:HB3    | 1.65                     | 0.77              |
| 23:UT:367:ARG:HB2   | 23:UT:403:LEU:HD13  | 1.64                     | 0.77              |
| 23:UT:482:ARG:HA    | 23:UT:485:ILE:HD12  | 1.66                     | 0.77              |
| 5:UB:548:ARG:NH1    | 5:UB:638:ASN:OD1    | 2.18                     | 0.77              |
| 8:UE:112:LEU:HD11   | 8:UE:131:LEU:HD11   | 1.65                     | 0.77              |
| 50:DF:76:ARG:CZ     | 58:DQ:122:ARG:HE    | 1.97                     | 0.77              |
| 54:DJ:37:LYS:HE2    | 54:DJ:126:ARG:HH21  | 1.49                     | 0.77              |
| 60:DW:82:LYS:HZ2    | 66:D3:748:U:H5''    | 1.48                     | 0.77              |
| 66:D3:760:A:H3'     | 66:D3:761:G:H4'     | 1.67                     | 0.77              |
| 67:D4:68:A:H2'      | 67:D4:69:A:H8       | 1.50                     | 0.77              |
| 10:UG:183:GLU:OE1   | 32:CI:41:ARG:NH2    | 2.17                     | 0.77              |
| 17:UN:321:HIS:NE2   | 28:CD:93:LYS:O      | 2.17                     | 0.77              |
| 23:UT:1680:THR:HG23 | 23:UT:1681:LEU:HD12 | 1.67                     | 0.77              |
| 25:UV:373:ARG:HH22  | 25:UV:510:ILE:HG23  | 1.49                     | 0.77              |
| 29:CE:176:GLU:HA    | 29:CE:179:THR:HG22  | 1.66                     | 0.77              |
| 35:CL:628:VAL:HG23  | 35:CL:632:LYS:HZ3   | 1.50                     | 0.77              |
| 10:UG:486:VAL:HG23  | 10:UG:523:GLU:HG2   | 1.65                     | 0.77              |
| 20:UQ:658:GLU:OE1   | 20:UQ:675:ARG:NH2   | 2.14                     | 0.77              |
| 66:D3:1472:C:O2     | 66:D3:1534:G:N2     | 2.17                     | 0.77              |
| 12:UI:489:SER:O     | 12:UI:492:ILE:HG22  | 1.85                     | 0.77              |
| 13:UJ:1746:ARG:NH1  | 23:UT:43:GLU:OE2    | 2.16                     | 0.77              |
| 33:CJ:60:GLN:OE1    | 45:JN:207:ARG:NH1   | 2.17                     | 0.77              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 66:D3:1584:G:N2    | 66:D3:1611:A:OP2    | 2.11                     | 0.77              |
| 79:EN:616:ILE:C    | 79:EN:618:VAL:H     | 1.88                     | 0.77              |
| 14:UK:231:LYS:NZ   | 65:D2:236:C:OP2     | 2.18                     | 0.77              |
| 24:UU:126:ASP:H    | 29:CE:433:THR:HG21  | 1.50                     | 0.77              |
| 27:UZ:56:ILE:HA    | 27:UZ:188:SER:HA    | 1.67                     | 0.77              |
| 47:JP:117:CYS:HB3  | 47:JP:137:LEU:HB2   | 1.66                     | 0.77              |
| 62:DY:108:ARG:NH2  | 66:D3:457:G:OP1     | 2.18                     | 0.77              |
| 23:UT:718:PRO:HD3  | 23:UT:758:ILE:HG13  | 1.66                     | 0.77              |
| 25:UV:534:GLY:H    | 25:UV:606:ASN:HB3   | 1.50                     | 0.77              |
| 37:CN:38:PHE:HB2   | 37:CN:56:VAL:HB     | 1.65                     | 0.77              |
| 13:UJ:724:VAL:O    | 13:UJ:755:ARG:NH2   | 2.18                     | 0.76              |
| 10:UG:213:TRP:HE1  | 10:UG:229:ARG:HG3   | 1.50                     | 0.76              |
| 11:UH:645:ILE:HD11 | 11:UH:649:SER:HB3   | 1.66                     | 0.76              |
| 15:UL:22:ASN:ND2   | 15:UL:85:LEU:O      | 2.18                     | 0.76              |
| 20:UQ:678:LEU:HB2  | 20:UQ:694:LEU:HD11  | 1.66                     | 0.76              |
| 23:UT:428:GLN:HB2  | 23:UT:431:LYS:HB2   | 1.65                     | 0.76              |
| 47:JP:183:GLN:N    | 47:JP:197:GLY:O     | 2.13                     | 0.76              |
| 21:UR:242:ASN:ND2  | 21:UR:584:GLY:O     | 2.18                     | 0.76              |
| 50:DF:80:LYS:HB2   | 50:DF:83:ARG:HH21   | 1.48                     | 0.76              |
| 39:JG:89:PRO:HG2   | 39:JG:134:PHE:HZ    | 1.51                     | 0.76              |
| 66:D3:1593:A:N6    | 66:D3:1594:G:O6     | 2.19                     | 0.76              |
| 18:UO:127:THR:HG22 | 18:UO:144:SER:HB2   | 1.68                     | 0.76              |
| 3:JA:866:TYR:HA    | 3:JA:871:MET:HB2    | 1.68                     | 0.76              |
| 36:CM:246:VAL:HG13 | 36:CM:248:GLN:HE21  | 1.50                     | 0.76              |
| 3:JA:748:ARG:NH1   | 3:JA:750:THR:O      | 2.19                     | 0.76              |
| 65:D2:194:G:N2     | 65:D2:203:C:O2      | 2.19                     | 0.76              |
| 13:UJ:1613:MET:HG2 | 13:UJ:1619:ARG:HH12 | 1.49                     | 0.76              |
| 20:UQ:474:THR:O    | 20:UQ:478:ASN:ND2   | 2.17                     | 0.76              |
| 35:CL:794:GLU:HG3  | 35:CL:795:LYS:H     | 1.51                     | 0.76              |
| 45:JN:224:HIS:O    | 45:JN:228:ILE:HG12  | 1.85                     | 0.76              |
| 62:DY:93:ARG:NH2   | 66:D3:526:A:OP2     | 2.15                     | 0.76              |
| 4:UA:538:GLN:NE2   | 4:UA:554:ASP:OD1    | 2.18                     | 0.76              |
| 15:UL:919:GLU:OE2  | 42:JJ:264:ARG:NH1   | 2.18                     | 0.76              |
| 20:UQ:335:PRO:HB3  | 65:D2:86:C:H1'      | 1.65                     | 0.76              |
| 24:UU:242:ARG:HH22 | 24:UU:281:ARG:HG3   | 1.50                     | 0.76              |
| 27:UZ:55:ARG:NH2   | 27:UZ:231:GLN:OE1   | 2.18                     | 0.76              |
| 35:CL:1019:THR:HB  | 35:CL:1022:LEU:HD12 | 1.67                     | 0.76              |
| 66:D3:1671:A:N6    | 66:D3:1730:A:O2'    | 2.18                     | 0.76              |
| 4:UA:461:GLN:NE2   | 66:D3:1631:A:N1     | 2.34                     | 0.76              |
| 5:UB:538:LYS:NZ    | 5:UB:621:THR:O      | 2.19                     | 0.76              |
| 18:UO:386:ARG:NH2  | 65:D2:146:G:OP1     | 2.19                     | 0.76              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:UQ:719:ASN:OD1  | 20:UQ:720:ILE:N    | 2.19                     | 0.76              |
| 23:UT:1646:LYS:O   | 23:UT:1651:ARG:NH2 | 2.17                     | 0.75              |
| 24:UU:499:LYS:NZ   | 50:DF:15:GLU:O     | 2.19                     | 0.75              |
| 35:CL:151:GLU:HG3  | 35:CL:912:ARG:HH22 | 1.51                     | 0.75              |
| 36:CM:52:PHE:HE1   | 36:CM:102:PRO:HG3  | 1.51                     | 0.75              |
| 66:D3:274:G:N2     | 66:D3:282:C:O2     | 2.18                     | 0.75              |
| 70:EC:15:ASP:CB    | 78:EK:40:TYR:CB    | 2.65                     | 0.75              |
| 8:UE:542:ALA:HA    | 11:UH:677:ASN:ND2  | 2.01                     | 0.75              |
| 14:UK:7:ASP:O      | 14:UK:10:LYS:N     | 2.19                     | 0.75              |
| 53:DI:164:ARG:HA   | 53:DI:164:ARG:NH2  | 2.00                     | 0.75              |
| 58:DQ:122:ARG:NH1  | 66:D3:1584:G:O4'   | 2.18                     | 0.75              |
| 5:UB:538:LYS:HE2   | 5:UB:625:GLU:HG3   | 1.67                     | 0.75              |
| 9:UF:129:ILE:HD13  | 9:UF:153:TYR:HE2   | 1.51                     | 0.75              |
| 20:UQ:657:SER:HB2  | 20:UQ:674:THR:HB   | 1.69                     | 0.75              |
| 35:CL:291:ALA:HB1  | 35:CL:853:ARG:HH22 | 1.51                     | 0.75              |
| 47:JP:94:TYR:HD2   | 47:JP:150:ILE:HG21 | 1.49                     | 0.75              |
| 60:DW:15:ASN:HD21  | 60:DW:71:LYS:HG3   | 1.52                     | 0.75              |
| 1:CB:202:ARG:HG3   | 1:CB:205:ARG:HH21  | 1.52                     | 0.75              |
| 7:UD:317:ASN:O     | 7:UD:319:ARG:NH2   | 2.20                     | 0.75              |
| 8:UE:536:LEU:HD11  | 18:UO:453:VAL:HG12 | 1.69                     | 0.75              |
| 24:UU:548:ALA:HB3  | 24:UU:561:ALA:HB3  | 1.69                     | 0.75              |
| 54:DJ:127:VAL:O    | 54:DJ:131:GLN:HB2  | 1.86                     | 0.75              |
| 2:DA:50:LYS:HD3    | 2:DA:52:THR:H      | 1.52                     | 0.75              |
| 7:UD:265:TRP:HD1   | 7:UD:272:LEU:HA    | 1.51                     | 0.75              |
| 13:UJ:745:TYR:HE2  | 13:UJ:747:GLN:HE21 | 1.33                     | 0.75              |
| 16:UM:26:SER:OG    | 16:UM:28:ASN:OD1   | 2.05                     | 0.75              |
| 29:CE:366:LYS:NZ   | 67:D4:82:G:OP1     | 2.14                     | 0.75              |
| 66:D3:542:A:O2'    | 66:D3:543:C:O5'    | 2.05                     | 0.75              |
| 66:D3:956:C:H2'    | 66:D3:957:G:C8     | 2.22                     | 0.75              |
| 13:UJ:33:LEU:O     | 13:UJ:150:ARG:NH2  | 2.20                     | 0.75              |
| 13:UJ:75:SER:HB2   | 21:UR:33:LEU:HD21  | 1.69                     | 0.75              |
| 23:UT:1519:SER:O   | 23:UT:1523:TYR:HB2 | 1.86                     | 0.75              |
| 45:JN:148:ASN:OD1  | 45:JN:149:LEU:N    | 2.18                     | 0.75              |
| 1:CA:91:HIS:HB3    | 1:CA:96:VAL:HG23   | 1.68                     | 0.75              |
| 30:CG:93:VAL:HG22  | 30:CG:94:SER:H     | 1.50                     | 0.75              |
| 38:JC:136:ARG:NH1  | 66:D3:340:U:OP1    | 2.20                     | 0.75              |
| 66:D3:1052:U:H2'   | 66:D3:1053:G:C8    | 2.22                     | 0.75              |
| 21:UR:317:ARG:HH22 | 65:D2:233:G:H21    | 1.33                     | 0.75              |
| 25:UV:855:LEU:HD12 | 25:UV:889:TYR:HD2  | 1.52                     | 0.75              |
| 38:JC:4:LYS:N      | 38:JC:15:GLN:O     | 2.19                     | 0.75              |
| 38:JC:71:CYS:HB3   | 38:JC:84:TYR:HB2   | 1.69                     | 0.75              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 10:UG:213:TRP:CD1  | 10:UG:229:ARG:HA    | 2.20                     | 0.75              |
| 13:UJ:231:LEU:HB3  | 13:UJ:268:LEU:HD11  | 1.69                     | 0.75              |
| 23:UT:1397:ILE:O   | 23:UT:1401:ASN:ND2  | 2.19                     | 0.75              |
| 36:CM:192:THR:HA   | 36:CM:224:ASN:O     | 1.86                     | 0.75              |
| 45:JN:234:VAL:H    | 45:JN:239:ARG:HH11  | 1.31                     | 0.75              |
| 66:D3:1603:U:H2'   | 66:D3:1604:U:H6     | 1.50                     | 0.75              |
| 24:UU:62:ASP:OD1   | 24:UU:63:ALA:N      | 2.20                     | 0.74              |
| 33:CJ:48:GLU:OE1   | 45:JN:224:HIS:N     | 2.18                     | 0.74              |
| 36:CM:151:LEU:HD21 | 36:CM:166:VAL:HB    | 1.67                     | 0.74              |
| 1:CB:117:VAL:HG23  | 1:CB:118:TYR:HD1    | 1.51                     | 0.74              |
| 13:UJ:196:LEU:HD12 | 13:UJ:241:ILE:HD11  | 1.69                     | 0.74              |
| 16:UM:30:LYS:CA    | 16:UM:45:LEU:O      | 2.30                     | 0.74              |
| 18:UO:374:ILE:HG12 | 21:UR:289:HIS:HD2   | 1.52                     | 0.74              |
| 24:UU:470:GLN:OE1  | 24:UU:553:ARG:NH1   | 2.20                     | 0.74              |
| 29:CE:319:ILE:HD11 | 29:CE:337:PRO:HG2   | 1.69                     | 0.74              |
| 35:CL:775:GLU:HA   | 35:CL:779:ARG:HH21  | 1.50                     | 0.74              |
| 4:UA:471:GLY:O     | 4:UA:498:ARG:NH1    | 2.20                     | 0.74              |
| 13:UJ:59:LEU:HD21  | 13:UJ:113:PRO:HB2   | 1.69                     | 0.74              |
| 15:UL:574:LEU:HD12 | 15:UL:594:ASP:HB3   | 1.68                     | 0.74              |
| 16:UM:407:SER:H    | 16:UM:437:VAL:HG23  | 1.52                     | 0.74              |
| 35:CL:1042:MET:HG3 | 35:CL:1044:LEU:HD23 | 1.69                     | 0.74              |
| 66:D3:1170:G:H1    | 66:D3:1469:A:H61    | 1.32                     | 0.74              |
| 13:UJ:760:PHE:O    | 13:UJ:768:LYS:NZ    | 2.19                     | 0.74              |
| 18:UO:390:ARG:O    | 18:UO:394:GLN:NE2   | 2.21                     | 0.74              |
| 2:DA:117:TRP:HZ2   | 66:D3:934:C:H42     | 1.35                     | 0.74              |
| 4:UA:587:PHE:HE2   | 4:UA:688:PRO:HA     | 1.51                     | 0.74              |
| 6:UC:558:ASN:OD1   | 66:D3:592:A:N6      | 2.21                     | 0.74              |
| 8:UE:534:SER:HA    | 8:UE:537:LEU:HD23   | 1.68                     | 0.74              |
| 29:CE:354:LYS:NZ   | 67:D4:86:A:OP2      | 2.20                     | 0.74              |
| 35:CL:977:LYS:NZ   | 66:D3:1598:U:OP2    | 2.18                     | 0.74              |
| 39:JG:44:VAL:HG12  | 39:JG:113:TYR:HB2   | 1.69                     | 0.74              |
| 10:UG:497:LEU:HD21 | 10:UG:519:GLN:HG2   | 1.69                     | 0.74              |
| 10:UG:552:ARG:NH2  | 25:UV:791:LYS:O     | 2.20                     | 0.74              |
| 16:UM:315:ASN:ND2  | 16:UM:317:GLU:OE2   | 2.20                     | 0.74              |
| 16:UM:505:ILE:HD12 | 16:UM:517:ILE:HD11  | 1.68                     | 0.74              |
| 16:UM:591:ILE:HG13 | 16:UM:601:ILE:HD13  | 1.69                     | 0.74              |
| 29:CE:411:LYS:HE2  | 67:D4:68:A:H5''     | 1.68                     | 0.74              |
| 66:D3:1041:G:N2    | 66:D3:1078:C:O2     | 2.19                     | 0.74              |
| 78:EK:930:VAL:O    | 78:EK:934:GLY:N     | 2.19                     | 0.74              |
| 4:UA:453:PHE:HB3   | 4:UA:475:PRO:HA     | 1.70                     | 0.74              |
| 14:UK:180:ASN:ND2  | 48:JQ:125:ASN:O     | 2.21                     | 0.74              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 56:DN:64:ARG:NH2    | 66:D3:861:U:OP2    | 2.20                     | 0.74              |
| 15:UL:426:ARG:NH2   | 15:UL:459:LEU:O    | 2.21                     | 0.74              |
| 22:US:342:TYR:HE2   | 22:US:378:SER:HB3  | 1.53                     | 0.74              |
| 58:DQ:52:LEU:HD13   | 58:DQ:60:PHE:CD2   | 2.22                     | 0.74              |
| 1:CA:186:ASP:OD1    | 1:CA:214:ARG:NH1   | 2.21                     | 0.74              |
| 8:UE:551:ILE:HA     | 8:UE:554:PHE:CE1   | 2.23                     | 0.74              |
| 13:UJ:556:LYS:O     | 13:UJ:592:ARG:NH2  | 2.21                     | 0.74              |
| 14:UK:193:LYS:NZ    | 65:D2:428:A:OP2    | 2.20                     | 0.74              |
| 25:UV:612:PHE:HD2   | 25:UV:614:ARG:HH22 | 1.34                     | 0.74              |
| 25:UV:626:LYS:HZ2   | 25:UV:628:VAL:H    | 1.34                     | 0.74              |
| 33:CJ:14:TYR:OH     | 33:CJ:18:GLN:NE2   | 2.21                     | 0.74              |
| 37:CN:147:LEU:HD11  | 37:CN:154:GLU:HB2  | 1.68                     | 0.74              |
| 38:JC:65:SER:OG     | 38:JC:109:ASP:O    | 2.06                     | 0.74              |
| 55:DL:57:LYS:O      | 55:DL:138:ASN:ND2  | 2.21                     | 0.74              |
| 18:UO:253:LYS:NZ    | 22:US:332:LEU:O    | 2.18                     | 0.74              |
| 35:CL:1138:ARG:NH2  | 66:D3:492:A:N7     | 2.35                     | 0.74              |
| 47:JP:338:HIS:NE2   | 66:D3:1:U:O2'      | 2.20                     | 0.74              |
| 66:D3:5:U:O2        | 66:D3:7:G:N2       | 2.21                     | 0.74              |
| 13:UJ:21:ASP:OD1    | 13:UJ:22:ARG:N     | 2.21                     | 0.73              |
| 21:UR:240:ASP:HB2   | 21:UR:243:ALA:HB2  | 1.68                     | 0.73              |
| 24:UU:60:ILE:HD13   | 24:UU:70:PHE:HB2   | 1.68                     | 0.73              |
| 27:UZ:126:VAL:HG21  | 27:UZ:154:ILE:HG23 | 1.70                     | 0.73              |
| 31:CH:72:GLU:HA     | 31:CH:75:LYS:HG2   | 1.69                     | 0.73              |
| 31:CH:334:GLU:HG2   | 31:CH:351:ILE:HB   | 1.69                     | 0.73              |
| 38:JC:248:SER:HA    | 38:JC:273:ASP:HA   | 1.68                     | 0.73              |
| 78:EK:930:VAL:O     | 78:EK:934:GLY:CA   | 2.35                     | 0.73              |
| 4:UA:262:LYS:H      | 4:UA:280:THR:HG22  | 1.53                     | 0.73              |
| 11:UH:596:LYS:HE2   | 11:UH:644:SER:HA   | 1.70                     | 0.73              |
| 4:UA:275:LEU:HD22   | 4:UA:289:LEU:HD22  | 1.70                     | 0.73              |
| 8:UE:8:SER:OG       | 8:UE:293:ASN:ND2   | 2.22                     | 0.73              |
| 15:UL:258:LYS:HB3   | 15:UL:275:GLN:HB3  | 1.69                     | 0.73              |
| 35:CL:967:LYS:NZ    | 66:D3:557:G:OP1    | 2.20                     | 0.73              |
| 49:DE:178:GLY:N     | 49:DE:195:ILE:O    | 2.19                     | 0.73              |
| 56:DN:20:ARG:NH2    | 66:D3:861:U:O3'    | 2.18                     | 0.73              |
| 10:UG:388:ASP:OD2   | 47:JP:5:THR:OG1    | 2.05                     | 0.73              |
| 21:UR:278:ASP:OD2   | 21:UR:281:THR:OG1  | 2.05                     | 0.73              |
| 22:US:146:LYS:HD2   | 22:US:149:ARG:HH12 | 1.53                     | 0.73              |
| 35:CL:1142:LEU:HD21 | 66:D3:493:U:H5''   | 1.69                     | 0.73              |
| 65:D2:468:A:H61     | 67:D4:49:C:H42     | 1.34                     | 0.73              |
| 66:D3:162:A:H3'     | 66:D3:163:G:H21    | 1.52                     | 0.73              |
| 32:CI:137:ARG:NH2   | 32:CI:139:GLY:O    | 2.22                     | 0.73              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 56:DN:60:VAL:HG13  | 56:DN:66:ILE:HG13  | 1.70                     | 0.73              |
| 16:UM:797:ASP:OD1  | 24:UU:927:LYS:NZ   | 2.21                     | 0.73              |
| 26:UX:63:TYR:HD2   | 26:UX:90:LEU:HD23  | 1.53                     | 0.73              |
| 30:CF:46:ARG:NH1   | 67:D4:326:U:OP1    | 2.21                     | 0.73              |
| 31:CH:62:LYS:HG2   | 31:CH:65:ARG:HH21  | 1.53                     | 0.73              |
| 36:CM:192:THR:H    | 36:CM:248:GLN:HE22 | 1.34                     | 0.73              |
| 38:JC:178:LEU:HD23 | 38:JC:183:VAL:HG22 | 1.70                     | 0.73              |
| 52:DH:101:LYS:H    | 66:D3:639:U:H5     | 1.35                     | 0.73              |
| 66:D3:1679:G:H2'   | 66:D3:1722:A:H61   | 1.52                     | 0.73              |
| 4:UA:324:LEU:HD12  | 4:UA:342:GLN:HE21  | 1.53                     | 0.73              |
| 13:UJ:1605:LEU:HA  | 13:UJ:1608:PHE:HD2 | 1.54                     | 0.73              |
| 35:CL:1024:LYS:O   | 35:CL:1026:LYS:NZ  | 2.20                     | 0.73              |
| 37:CN:219:ASN:ND2  | 66:D3:1057:U:H1'   | 2.03                     | 0.73              |
| 50:DF:100:ASN:HB3  | 50:DF:103:ASN:HB2  | 1.70                     | 0.73              |
| 56:DN:136:PRO:HG2  | 56:DN:139:TRP:HB2  | 1.71                     | 0.73              |
| 15:UL:557:VAL:HB   | 15:UL:567:LEU:HB3  | 1.71                     | 0.73              |
| 18:UO:279:GLY:CA   | 18:UO:298:PHE:O    | 2.37                     | 0.73              |
| 21:UR:382:GLY:HA3  | 21:UR:399:LYS:HG3  | 1.70                     | 0.73              |
| 23:UT:367:ARG:NH1  | 23:UT:403:LEU:O    | 2.21                     | 0.73              |
| 39:JF:52:THR:HG21  | 39:JF:146:HIS:HE1  | 1.53                     | 0.73              |
| 66:D3:1666:U:H3    | 66:D3:1735:U:H3    | 1.37                     | 0.73              |
| 67:D4:147:C:O2     | 67:D4:165:G:N2     | 2.18                     | 0.73              |
| 5:UB:786:ASN:ND2   | 66:D3:1119:G:O4'   | 2.21                     | 0.73              |
| 23:UT:673:ARG:HH22 | 23:UT:773:LEU:HB3  | 1.53                     | 0.73              |
| 24:UU:579:ARG:NH1  | 24:UU:614:LEU:O    | 2.21                     | 0.73              |
| 31:CH:504:ASN:O    | 31:CH:506:ARG:NH1  | 2.22                     | 0.73              |
| 34:CK:341:LEU:HD11 | 35:CL:956:MET:HB3  | 1.71                     | 0.73              |
| 58:DQ:97:VAL:HG12  | 58:DQ:98:ASP:H     | 1.53                     | 0.73              |
| 66:D3:1697:G:H2'   | 66:D3:1698:G:C8    | 2.23                     | 0.73              |
| 1:CB:92:ARG:HG2    | 14:UK:170:GLN:HE22 | 1.54                     | 0.73              |
| 1:CB:264:GLN:HG3   | 1:CB:321:MET:HG3   | 1.70                     | 0.73              |
| 13:UJ:194:SER:HB2  | 24:UU:335:VAL:HG11 | 1.69                     | 0.73              |
| 16:UM:736:LEU:HD22 | 16:UM:763:ILE:HD11 | 1.70                     | 0.73              |
| 32:CI:42:GLU:O     | 32:CI:46:LYS:HG2   | 1.88                     | 0.73              |
| 49:DE:176:ASP:HB2  | 49:DE:179:LYS:HE3  | 1.71                     | 0.73              |
| 66:D3:105:A:H62    | 66:D3:308:C:H42    | 1.37                     | 0.73              |
| 5:UB:647:ILE:HA    | 5:UB:651:TRP:HE3   | 1.53                     | 0.72              |
| 7:UD:246:TYR:OH    | 7:UD:251:ASP:OD1   | 2.05                     | 0.72              |
| 14:UK:95:GLN:OE1   | 14:UK:95:GLN:N     | 2.22                     | 0.72              |
| 24:UU:176:TYR:OH   | 24:UU:219:ASP:OD1  | 2.03                     | 0.72              |
| 30:CG:7:LYS:HG3    | 31:CH:463:GLN:NE2  | 2.04                     | 0.72              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 34:CK:453:SER:O     | 34:CK:455:HIS:N    | 2.22                     | 0.72              |
| 35:CL:931:LYS:NZ    | 66:D3:558:U:OP1    | 2.21                     | 0.72              |
| 49:DE:162:ILE:HD13  | 49:DE:169:ILE:HD13 | 1.71                     | 0.72              |
| 61:DX:109:ARG:HH12  | 61:DX:118:PRO:HA   | 1.54                     | 0.72              |
| 4:UA:644:ILE:HG21   | 10:UG:131:LYS:HB3  | 1.71                     | 0.72              |
| 21:UR:352:GLN:NE2   | 21:UR:378:GLN:O    | 2.21                     | 0.72              |
| 23:UT:440:ASP:HA    | 23:UT:449:ARG:HD2  | 1.71                     | 0.72              |
| 60:DW:7:LEU:HA      | 60:DW:34:ILE:HD11  | 1.71                     | 0.72              |
| 66:D3:377:G:H5''    | 66:D3:378:A:H5'    | 1.70                     | 0.72              |
| 18:UO:356:ASN:OD1   | 18:UO:359:ARG:NH1  | 2.22                     | 0.72              |
| 21:UR:249:SER:OG    | 21:UR:250:ALA:N    | 2.22                     | 0.72              |
| 23:UT:265:LYS:HE3   | 23:UT:309:THR:HG23 | 1.71                     | 0.72              |
| 23:UT:1014:ASN:HD21 | 53:DI:114:GLU:HB3  | 1.55                     | 0.72              |
| 23:UT:1298:LEU:HB3  | 23:UT:1301:ILE:HB  | 1.71                     | 0.72              |
| 25:UV:628:VAL:HG12  | 25:UV:668:VAL:HG13 | 1.71                     | 0.72              |
| 25:UV:949:PHE:O     | 25:UV:960:LYS:NZ   | 2.21                     | 0.72              |
| 44:JM:213:ARG:NH1   | 66:D3:1491:U:OP2   | 2.16                     | 0.72              |
| 45:JN:265:SER:O     | 45:JN:273:ARG:NH1  | 2.22                     | 0.72              |
| 2:DA:141:ALA:HA     | 2:DA:209:ASN:O     | 1.89                     | 0.72              |
| 6:UC:557:ASP:O      | 6:UC:560:ASN:O     | 2.08                     | 0.72              |
| 9:UF:5:ARG:HH12     | 47:JP:26:ARG:HB2   | 1.53                     | 0.72              |
| 16:UM:572:GLU:HG3   | 16:UM:573:GLY:H    | 1.55                     | 0.72              |
| 18:UO:10:THR:HG23   | 18:UO:416:THR:HG21 | 1.71                     | 0.72              |
| 25:UV:1159:ASN:ND2  | 25:UV:1200:LEU:O   | 2.22                     | 0.72              |
| 34:CK:344:GLU:OE2   | 35:CL:960:ARG:NH2  | 2.22                     | 0.72              |
| 39:JG:73:HIS:HB3    | 39:JG:76:LEU:HD21  | 1.70                     | 0.72              |
| 58:DQ:122:ARG:NH2   | 66:D3:1583:A:O2'   | 2.22                     | 0.72              |
| 22:US:155:LEU:HD11  | 22:US:177:ILE:HG12 | 1.72                     | 0.72              |
| 22:US:217:GLY:HA2   | 22:US:220:LEU:HD13 | 1.72                     | 0.72              |
| 23:UT:955:ASN:OD1   | 53:DI:111:GLN:NE2  | 2.22                     | 0.72              |
| 65:D2:182:G:H1      | 65:D2:215:U:H3     | 1.36                     | 0.72              |
| 3:JA:49:LEU:HD11    | 35:CL:304:LEU:HD23 | 1.71                     | 0.72              |
| 3:JA:884:ILE:HD11   | 3:JA:902:LEU:HD11  | 1.70                     | 0.72              |
| 4:UA:310:VAL:HG12   | 4:UA:317:LEU:HG    | 1.72                     | 0.72              |
| 5:UB:484:ARG:NH1    | 5:UB:492:ALA:O     | 2.22                     | 0.72              |
| 7:UD:550:VAL:HG22   | 7:UD:563:LEU:HD12  | 1.70                     | 0.72              |
| 13:UJ:219:ASN:HD22  | 20:UQ:876:PHE:HE2  | 1.36                     | 0.72              |
| 21:UR:165:ARG:HE    | 24:UU:218:LEU:HD23 | 1.53                     | 0.72              |
| 21:UR:434:GLU:OE2   | 21:UR:445:ARG:NH2  | 2.23                     | 0.72              |
| 24:UU:589:THR:HG22  | 24:UU:605:LEU:HD22 | 1.71                     | 0.72              |
| 33:CJ:99:ARG:HE     | 33:CJ:172:MET:HG3  | 1.54                     | 0.72              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 7:UD:57:ILE:HA     | 7:UD:341:SER:HA     | 1.71                     | 0.72              |
| 22:US:356:ALA:HB1  | 22:US:357:ARG:HH21  | 1.53                     | 0.72              |
| 35:CL:933:LYS:NZ   | 66:D3:575:C:OP1     | 2.17                     | 0.72              |
| 35:CL:1093:THR:OG1 | 65:D2:246:G:OP2     | 2.08                     | 0.72              |
| 53:DI:24:LYS:NZ    | 66:D3:400:A:N7      | 2.37                     | 0.72              |
| 66:D3:170:U:H3     | 66:D3:289:U:HO2'    | 1.32                     | 0.72              |
| 25:UV:151:SER:O    | 25:UV:155:ASN:ND2   | 2.23                     | 0.72              |
| 28:CD:301:PRO:HD2  | 28:CD:396:PRO:HG3   | 1.71                     | 0.72              |
| 53:DI:105:ASP:HA   | 53:DI:164:ARG:NH2   | 2.05                     | 0.72              |
| 57:DO:79:VAL:O     | 57:DO:113:GLY:N     | 2.22                     | 0.72              |
| 60:DW:80:ASN:ND2   | 66:D3:747:C:O2'     | 2.23                     | 0.72              |
| 67:D4:152:U:N3     | 67:D4:161:G:O6      | 2.15                     | 0.72              |
| 4:UA:536:LYS:NZ    | 32:CI:181:ASP:O     | 2.23                     | 0.72              |
| 10:UG:218:ASP:OD1  | 10:UG:219:VAL:N     | 2.22                     | 0.72              |
| 13:UJ:408:ILE:HA   | 13:UJ:412:GLU:HB3   | 1.72                     | 0.72              |
| 13:UJ:414:LEU:HA   | 13:UJ:417:LYS:HD2   | 1.70                     | 0.72              |
| 20:UQ:403:ILE:HD11 | 20:UQ:414:ILE:HG13  | 1.72                     | 0.72              |
| 22:US:356:ALA:HA   | 22:US:499:LEU:HD11  | 1.70                     | 0.72              |
| 31:CH:467:LYS:HA   | 31:CH:470:LEU:HD23  | 1.70                     | 0.72              |
| 50:DF:102:ARG:NH2  | 66:D3:1473:U:O2'    | 2.22                     | 0.72              |
| 1:CB:231:ARG:HA    | 1:CB:260:PHE:HZ     | 1.53                     | 0.72              |
| 5:UB:749:LYS:NZ    | 66:D3:1175:U:OP2    | 2.18                     | 0.72              |
| 7:UD:226:LEU:O     | 7:UD:227:HIS:ND1    | 2.23                     | 0.72              |
| 15:UL:412:GLY:HA3  | 15:UL:430:CYS:H     | 1.55                     | 0.72              |
| 20:UQ:690:ASN:ND2  | 20:UQ:749:ASP:O     | 2.23                     | 0.72              |
| 23:UT:233:LEU:HB2  | 23:UT:274:LEU:HD11  | 1.71                     | 0.72              |
| 23:UT:517:ASP:OD2  | 23:UT:715:TYR:OH    | 2.06                     | 0.72              |
| 33:CJ:149:PRO:HD2  | 33:CJ:170:VAL:HG21  | 1.71                     | 0.72              |
| 38:JC:331:THR:OG1  | 38:JC:339:HIS:O     | 2.06                     | 0.72              |
| 39:JG:177:LYS:HB3  | 39:JG:221:VAL:HA    | 1.72                     | 0.72              |
| 3:JA:515:LEU:HD11  | 3:JA:565:PHE:HB3    | 1.72                     | 0.71              |
| 6:UC:521:ARG:NH1   | 66:D3:580:A:OP1     | 2.23                     | 0.71              |
| 13:UJ:1455:LYS:HB3 | 13:UJ:1459:ARG:HH21 | 1.53                     | 0.71              |
| 24:UU:343:LEU:HG   | 24:UU:344:ARG:N     | 2.05                     | 0.71              |
| 24:UU:484:ILE:HD11 | 24:UU:505:VAL:HG11  | 1.71                     | 0.71              |
| 35:CL:304:LEU:O    | 35:CL:788:TYR:HB3   | 1.88                     | 0.71              |
| 39:JF:227:LEU:HD12 | 39:JF:240:LYS:HE2   | 1.71                     | 0.71              |
| 52:DH:67:LEU:HD13  | 52:DH:94:ALA:HB2    | 1.72                     | 0.71              |
| 53:DI:116:HIS:O    | 53:DI:146:ARG:NH1   | 2.23                     | 0.71              |
| 66:D3:111:U:H2'    | 66:D3:112:A:H8      | 1.55                     | 0.71              |
| 9:UF:205:LEU:HD11  | 44:JM:51:LYS:HD3    | 1.71                     | 0.71              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 13:UJ:772:VAL:HG21  | 13:UJ:801:ILE:HG12  | 1.73                     | 0.71              |
| 13:UJ:1397:GLN:HA   | 13:UJ:1400:ILE:HD12 | 1.72                     | 0.71              |
| 15:UL:300:GLU:HA    | 15:UL:303:LEU:HD12  | 1.72                     | 0.71              |
| 15:UL:558:PHE:HB3   | 15:UL:563:MET:HA    | 1.72                     | 0.71              |
| 18:UO:51:HIS:O      | 18:UO:53:HIS:ND1    | 2.22                     | 0.71              |
| 23:UT:552:LEU:HG    | 23:UT:556:ARG:HE    | 1.54                     | 0.71              |
| 23:UT:1523:TYR:OH   | 23:UT:1551:LEU:O    | 2.07                     | 0.71              |
| 35:CL:628:VAL:HG23  | 35:CL:632:LYS:NZ    | 2.05                     | 0.71              |
| 38:JC:50:ILE:HG23   | 38:JC:53:PHE:HB2    | 1.72                     | 0.71              |
| 53:DI:25:ARG:NH2    | 66:D3:386:G:OP1     | 2.23                     | 0.71              |
| 66:D3:92:A:OP1      | 66:D3:398:G:N2      | 2.23                     | 0.71              |
| 66:D3:188:A:OP2     | 66:D3:189:C:N4      | 2.22                     | 0.71              |
| 5:UB:484:ARG:HB3    | 5:UB:492:ALA:HB1    | 1.72                     | 0.71              |
| 7:UD:757:ARG:HG2    | 7:UD:759:PRO:HD3    | 1.72                     | 0.71              |
| 31:CH:551:ARG:NH1   | 67:D4:253:G:OP2     | 2.23                     | 0.71              |
| 35:CL:870:ARG:NH1   | 66:D3:574:G:OP1     | 2.18                     | 0.71              |
| 50:DF:127:GLN:HG3   | 50:DF:128:ASN:H     | 1.55                     | 0.71              |
| 3:JA:744:PRO:HA     | 3:JA:762:MET:HG2    | 1.72                     | 0.71              |
| 10:UG:123:THR:O     | 10:UG:124:HIS:ND1   | 2.23                     | 0.71              |
| 13:UJ:1586:LEU:HD23 | 13:UJ:1590:ILE:HG13 | 1.72                     | 0.71              |
| 18:UO:114:ARG:NH2   | 66:D3:1532:U:OP2    | 2.22                     | 0.71              |
| 29:CE:155:SER:OG    | 29:CE:157:ASP:OD1   | 2.08                     | 0.71              |
| 31:CH:449:ASN:HA    | 31:CH:460:ARG:HD3   | 1.70                     | 0.71              |
| 32:CI:137:ARG:HD3   | 32:CI:161:VAL:HG23  | 1.72                     | 0.71              |
| 52:DH:9:LEU:HD13    | 52:DH:12:ALA:H      | 1.55                     | 0.71              |
| 54:DJ:131:GLN:HE21  | 66:D3:513:U:H4'     | 1.56                     | 0.71              |
| 66:D3:301:A:HO2'    | 66:D3:334:G:H1      | 1.38                     | 0.71              |
| 66:D3:319:U:H4'     | 66:D3:323:A:C4      | 2.25                     | 0.71              |
| 16:UM:211:LEU:HB2   | 16:UM:223:TRP:HB2   | 1.71                     | 0.71              |
| 24:UU:594:SER:HB2   | 24:UU:599:TRP:HB2   | 1.72                     | 0.71              |
| 29:CE:10:ALA:HB2    | 29:CE:136:LEU:HG    | 1.73                     | 0.71              |
| 33:CJ:102:GLN:NE2   | 66:D3:1579:U:O2'    | 2.23                     | 0.71              |
| 35:CL:889:LEU:HD22  | 35:CL:922:ILE:HB    | 1.72                     | 0.71              |
| 51:DG:23:ARG:NH2    | 51:DG:41:VAL:O      | 2.23                     | 0.71              |
| 52:DH:58:LEU:HB3    | 52:DH:88:ARG:HH21   | 1.53                     | 0.71              |
| 7:UD:199:ASP:HA     | 7:UD:215:ALA:O      | 1.90                     | 0.71              |
| 24:UU:327:SER:OG    | 24:UU:336:VAL:O     | 2.05                     | 0.71              |
| 25:UV:396:LEU:HD21  | 25:UV:429:LEU:HD21  | 1.69                     | 0.71              |
| 39:JF:91:ILE:HD13   | 39:JF:94:GLN:HE22   | 1.56                     | 0.71              |
| 46:JO:134:ASN:HB3   | 46:JO:137:ARG:HB3   | 1.73                     | 0.71              |
| 67:D4:16:A:H2'      | 67:D4:17:G:H8       | 1.56                     | 0.71              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:UA:88:ASN:HD21   | 24:UU:659:GLN:HE21 | 1.37                     | 0.71              |
| 16:UM:88:PHE:HA    | 16:UM:95:VAL:HA    | 1.72                     | 0.71              |
| 16:UM:314:ILE:HG22 | 16:UM:329:VAL:HA   | 1.72                     | 0.71              |
| 66:D3:627:C:N3     | 66:D3:972:G:N1     | 2.37                     | 0.71              |
| 67:D4:63:C:H2'     | 67:D4:64:A:C8      | 2.25                     | 0.71              |
| 3:JA:16:ASN:HD21   | 3:JA:218:PRO:HA    | 1.56                     | 0.71              |
| 1:CB:323:SER:O     | 29:CE:118:ARG:NH1  | 2.24                     | 0.71              |
| 8:UE:350:LEU:O     | 20:UQ:60:ARG:NH1   | 2.21                     | 0.71              |
| 9:UF:193:ILE:HG23  | 9:UF:266:ARG:HD3   | 1.73                     | 0.71              |
| 16:UM:346:VAL:HG23 | 16:UM:352:LYS:HB3  | 1.71                     | 0.71              |
| 21:UR:141:ASN:HA   | 21:UR:144:LYS:HG2  | 1.72                     | 0.71              |
| 21:UR:145:LYS:NZ   | 65:D2:309:A:O2'    | 2.24                     | 0.71              |
| 54:DJ:6:ARG:HH21   | 66:D3:38:C:H4'     | 1.55                     | 0.71              |
| 56:DN:46:THR:OG1   | 56:DN:86:GLU:OE1   | 2.07                     | 0.71              |
| 1:CB:159:LEU:HD13  | 1:CB:162:LEU:HD12  | 1.73                     | 0.71              |
| 8:UE:216:ASP:OD2   | 8:UE:219:SER:OG    | 2.08                     | 0.71              |
| 21:UR:235:ILE:HD11 | 21:UR:589:TRP:HB3  | 1.72                     | 0.71              |
| 23:UT:159:PHE:HB3  | 23:UT:199:LEU:HD21 | 1.73                     | 0.71              |
| 30:CF:5:ASN:ND2    | 30:CF:56:ALA:O     | 2.23                     | 0.71              |
| 37:CN:223:LEU:HA   | 37:CN:226:ILE:HD12 | 1.73                     | 0.71              |
| 24:UU:595:PRO:HG2  | 24:UU:638:GLY:HA2  | 1.73                     | 0.71              |
| 31:CH:159:CYS:SG   | 31:CH:523:LYS:NZ   | 2.64                     | 0.71              |
| 33:CJ:249:GLU:OE2  | 33:CJ:253:ARG:NH1  | 2.24                     | 0.71              |
| 53:DI:172:ARG:NH1  | 66:D3:330:G:OP2    | 2.23                     | 0.71              |
| 55:DL:66:ILE:O     | 66:D3:246:G:N2     | 2.17                     | 0.71              |
| 57:DO:51:ASP:OD2   | 57:DO:52:ARG:NH1   | 2.23                     | 0.71              |
| 66:D3:1779:U:O2    | 66:D3:1782:A:N6    | 2.16                     | 0.71              |
| 19:UP:194:LYS:HE3  | 19:UP:199:ILE:HD13 | 1.73                     | 0.70              |
| 21:UR:247:SER:OG   | 21:UR:584:GLY:O    | 2.09                     | 0.70              |
| 21:UR:430:GLY:HA2  | 21:UR:455:ILE:HD12 | 1.71                     | 0.70              |
| 66:D3:142:G:H22    | 66:D3:173:A:H2     | 1.37                     | 0.70              |
| 8:UE:116:GLN:OE1   | 8:UE:128:GLN:NE2   | 2.24                     | 0.70              |
| 15:UL:666:ALA:HB3  | 15:UL:670:GLY:H    | 1.55                     | 0.70              |
| 16:UM:626:MET:HB3  | 16:UM:631:MET:HB3  | 1.71                     | 0.70              |
| 23:UT:436:PHE:HA   | 23:UT:439:VAL:HG12 | 1.73                     | 0.70              |
| 27:UZ:245:LYS:NZ   | 27:UZ:246:THR:O    | 2.20                     | 0.70              |
| 31:CH:411:PHE:HA   | 31:CH:427:LEU:HD13 | 1.73                     | 0.70              |
| 33:CJ:109:LEU:HD11 | 66:D3:1159:C:H41   | 1.56                     | 0.70              |
| 33:CJ:170:VAL:HA   | 33:CJ:254:PHE:HB3  | 1.73                     | 0.70              |
| 50:DF:145:ASP:OD1  | 50:DF:146:THR:N    | 2.20                     | 0.70              |
| 51:DG:72:ARG:HH12  | 66:D3:419:G:H4'    | 1.55                     | 0.70              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 65:D2:426:G:H21     | 65:D2:428:A:H8      | 1.38                     | 0.70              |
| 66:D3:1072:C:N4     | 66:D3:1073:G:O6     | 2.25                     | 0.70              |
| 3:JA:850:LEU:HD13   | 3:JA:854:VAL:HB     | 1.74                     | 0.70              |
| 11:UH:314:LEU:HA    | 11:UH:321:ILE:HA    | 1.73                     | 0.70              |
| 13:UJ:1458:PHE:HB2  | 13:UJ:1503:LEU:HD21 | 1.73                     | 0.70              |
| 15:UL:536:CYS:HB3   | 15:UL:549:SER:HB3   | 1.73                     | 0.70              |
| 20:UQ:90:LYS:NZ     | 20:UQ:144:VAL:O     | 2.22                     | 0.70              |
| 20:UQ:469:ASN:ND2   | 20:UQ:539:THR:O     | 2.24                     | 0.70              |
| 35:CL:137:LEU:HD23  | 35:CL:166:ARG:HB2   | 1.72                     | 0.70              |
| 65:D2:479:G:N2      | 67:D4:39:C:O2       | 2.20                     | 0.70              |
| 66:D3:1033:C:H2'    | 66:D3:1034:C:H6     | 1.56                     | 0.70              |
| 4:UA:155:SER:OG     | 4:UA:203:GLN:NE2    | 2.23                     | 0.70              |
| 18:UO:398:SER:HB2   | 18:UO:434:ARG:HH22  | 1.56                     | 0.70              |
| 22:US:180:PHE:O     | 22:US:184:TYR:HB2   | 1.91                     | 0.70              |
| 23:UT:1678:MET:HE1  | 23:UT:1690:LEU:HD21 | 1.73                     | 0.70              |
| 24:UU:311:VAL:HG22  | 24:UU:321:GLU:HB3   | 1.71                     | 0.70              |
| 35:CL:74:VAL:CG1    | 35:CL:119:GLU:HA    | 2.20                     | 0.70              |
| 35:CL:184:ARG:NH2   | 66:D3:466:U:OP1     | 2.22                     | 0.70              |
| 37:CN:169:VAL:O     | 37:CN:173:LYS:HB2   | 1.91                     | 0.70              |
| 39:JF:46:ALA:HB3    | 39:JF:207:GLY:HA2   | 1.73                     | 0.70              |
| 39:JF:213:LYS:HZ2   | 39:JF:215:ASN:HB3   | 1.56                     | 0.70              |
| 13:UJ:600:LEU:HD23  | 13:UJ:603:LYS:HE2   | 1.72                     | 0.70              |
| 20:UQ:264:ILE:HA    | 20:UQ:271:LEU:HD13  | 1.74                     | 0.70              |
| 20:UQ:581:GLY:HA2   | 20:UQ:602:PRO:HD2   | 1.72                     | 0.70              |
| 23:UT:522:LEU:HA    | 23:UT:525:ILE:HG12  | 1.72                     | 0.70              |
| 29:CE:225:GLU:HG2   | 29:CE:226:ILE:HD12  | 1.74                     | 0.70              |
| 33:CJ:139:LEU:HB2   | 33:CJ:157:PHE:CE1   | 2.27                     | 0.70              |
| 38:JC:138:PRO:HG2   | 43:JK:464:LEU:HB2   | 1.72                     | 0.70              |
| 39:JF:180:LEU:HD13  | 39:JF:227:LEU:HD23  | 1.74                     | 0.70              |
| 13:UJ:728:GLU:HB3   | 13:UJ:734:ILE:HD13  | 1.73                     | 0.70              |
| 16:UM:542:CYS:O     | 16:UM:546:LYS:N     | 2.24                     | 0.70              |
| 23:UT:1721:ILE:HG13 | 23:UT:1750:SER:HB2  | 1.74                     | 0.70              |
| 35:CL:1154:LYS:NZ   | 67:D4:11:U:OP1      | 2.22                     | 0.70              |
| 37:CN:105:SER:OG    | 37:CN:194:ARG:NH1   | 2.25                     | 0.70              |
| 47:JP:224:SER:HB3   | 47:JP:238:THR:HG22  | 1.73                     | 0.70              |
| 13:UJ:1525:GLU:HA   | 13:UJ:1528:VAL:HG22 | 1.74                     | 0.70              |
| 13:UJ:1616:VAL:HA   | 13:UJ:1619:ARG:HD3  | 1.73                     | 0.70              |
| 22:US:474:HIS:HD2   | 22:US:477:VAL:H     | 1.40                     | 0.70              |
| 49:DE:151:ASP:OD1   | 51:DG:215:ARG:NH2   | 2.25                     | 0.70              |
| 66:D3:164:A:H2'     | 66:D3:165:G:H8      | 1.54                     | 0.70              |
| 1:CB:92:ARG:NH1     | 1:CB:160:ASP:O      | 2.24                     | 0.70              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:UK:161:ARG:NE   | 14:UK:164:ASN:O    | 2.25                     | 0.70              |
| 14:UK:217:ARG:NH2  | 65:D2:260:A:O4'    | 2.25                     | 0.70              |
| 23:UT:84:ASP:HA    | 23:UT:87:ILE:HD12  | 1.74                     | 0.70              |
| 38:JC:221:GLU:HG2  | 38:JC:253:TYR:HE2  | 1.57                     | 0.70              |
| 47:JP:382:ARG:NH2  | 67:D4:34:A:OP1     | 2.23                     | 0.70              |
| 50:DF:53:VAL:HG21  | 50:DF:59:VAL:HA    | 1.73                     | 0.70              |
| 52:DH:144:VAL:HA   | 60:DW:42:GLN:HE21  | 1.55                     | 0.70              |
| 4:UA:120:GLN:HG2   | 4:UA:141:VAL:HG22  | 1.72                     | 0.70              |
| 5:UB:515:HIS:HB3   | 5:UB:518:ILE:HB    | 1.74                     | 0.70              |
| 7:UD:413:ASN:HB3   | 7:UD:415:LYS:HZ3   | 1.57                     | 0.70              |
| 10:UG:430:VAL:HG21 | 32:CI:3:ARG:HE     | 1.57                     | 0.70              |
| 15:UL:400:SER:HB2  | 15:UL:404:LYS:HB2  | 1.72                     | 0.70              |
| 15:UL:802:GLU:OE1  | 15:UL:802:GLU:N    | 2.23                     | 0.70              |
| 16:UM:537:TRP:CD1  | 16:UM:553:GLY:HA2  | 2.27                     | 0.70              |
| 18:UO:496:HIS:HB3  | 18:UO:497:LYS:HZ2  | 1.56                     | 0.70              |
| 23:UT:1780:ARG:NH2 | 23:UT:1860:ASN:OD1 | 2.22                     | 0.70              |
| 54:DJ:152:SER:OG   | 66:D3:766:U:O4     | 2.09                     | 0.70              |
| 66:D3:901:G:N2     | 66:D3:901:G:OP2    | 2.24                     | 0.70              |
| 10:UG:364:ARG:NH2  | 65:D2:316:U:OP1    | 2.25                     | 0.70              |
| 21:UR:139:VAL:HG23 | 21:UR:140:THR:HG23 | 1.73                     | 0.70              |
| 24:UU:638:GLY:O    | 24:UU:656:ASN:ND2  | 2.25                     | 0.70              |
| 35:CL:52:ARG:NH2   | 66:D3:436:A:OP2    | 2.25                     | 0.70              |
| 38:JC:322:HIS:ND1  | 38:JC:328:MET:O    | 2.23                     | 0.70              |
| 46:JO:131:PHE:CD2  | 46:JO:192:LYS:HE3  | 2.26                     | 0.70              |
| 51:DG:13:GLN:NE2   | 66:D3:151:G:N3     | 2.32                     | 0.70              |
| 65:D2:238:G:N1     | 65:D2:240:C:O2     | 2.24                     | 0.70              |
| 8:UE:506:LEU:HD13  | 18:UO:507:MET:HG2  | 1.71                     | 0.69              |
| 18:UO:493:HIS:O    | 18:UO:497:LYS:NZ   | 2.24                     | 0.69              |
| 21:UR:237:ARG:NH1  | 65:D2:279:A:OP2    | 2.25                     | 0.69              |
| 24:UU:307:GLN:NE2  | 29:CE:422:THR:O    | 2.24                     | 0.69              |
| 27:UZ:181:ARG:NH1  | 48:JQ:198:ASP:O    | 2.24                     | 0.69              |
| 38:JC:4:LYS:HE2    | 38:JC:359:ILE:HG22 | 1.74                     | 0.69              |
| 1:CB:205:ARG:HA    | 1:CB:208:ILE:HD12  | 1.73                     | 0.69              |
| 7:UD:277:LYS:NZ    | 21:UR:347:GLY:O    | 2.25                     | 0.69              |
| 13:UJ:652:MET:HG3  | 13:UJ:687:LEU:HD21 | 1.73                     | 0.69              |
| 15:UL:161:SER:HB3  | 15:UL:189:TRP:HZ2  | 1.57                     | 0.69              |
| 16:UM:578:VAL:HG13 | 16:UM:592:SER:HB2  | 1.74                     | 0.69              |
| 23:UT:1560:ARG:NH2 | 23:UT:1622:GLY:O   | 2.23                     | 0.69              |
| 23:UT:1989:ASP:O   | 23:UT:1996:GLN:NE2 | 2.24                     | 0.69              |
| 28:CD:284:TYR:OH   | 29:CE:258:LEU:HD22 | 1.92                     | 0.69              |
| 32:CI:75:GLU:HB2   | 32:CI:94:ILE:HD12  | 1.72                     | 0.69              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 45:JN:301:LYS:NZ   | 66:D3:1033:C:N3     | 2.39                     | 0.69              |
| 51:DG:76:LEU:HD23  | 51:DG:76:LEU:H      | 1.57                     | 0.69              |
| 66:D3:1614:A:N6    | 66:D3:1615:C:N3     | 2.40                     | 0.69              |
| 67:D4:197:U:C5     | 67:D4:198:U:H5      | 2.10                     | 0.69              |
| 6:UC:521:ARG:HH12  | 35:CL:1046:THR:HG23 | 1.58                     | 0.69              |
| 10:UG:141:LYS:HB3  | 13:UJ:20:LEU:HD13   | 1.74                     | 0.69              |
| 13:UJ:626:PHE:O    | 13:UJ:630:TYR:HB2   | 1.91                     | 0.69              |
| 27:UZ:119:TYR:O    | 27:UZ:149:LYS:NZ    | 2.20                     | 0.69              |
| 35:CL:1110:ARG:NH2 | 65:D2:411:A:O3'     | 2.24                     | 0.69              |
| 14:UK:34:TYR:OH    | 35:CL:993:ASP:OD2   | 2.09                     | 0.69              |
| 18:UO:226:ILE:HG12 | 18:UO:239:LEU:HD21  | 1.73                     | 0.69              |
| 18:UO:440:GLU:O    | 18:UO:444:ASN:ND2   | 2.25                     | 0.69              |
| 20:UQ:113:ASN:O    | 20:UQ:133:LYS:NZ    | 2.24                     | 0.69              |
| 20:UQ:246:SER:OG   | 20:UQ:248:GLN:NE2   | 2.25                     | 0.69              |
| 20:UQ:460:PHE:HA   | 20:UQ:467:GLN:HA    | 1.73                     | 0.69              |
| 33:CJ:213:GLY:N    | 34:CK:381:LEU:O     | 2.26                     | 0.69              |
| 45:JN:317:ASN:OD1  | 60:DW:4:SER:OG      | 2.09                     | 0.69              |
| 47:JP:201:ILE:HG23 | 47:JP:215:LEU:HB2   | 1.74                     | 0.69              |
| 66:D3:272:U:O2'    | 66:D3:273:G:O4'     | 2.11                     | 0.69              |
| 66:D3:627:C:N4     | 66:D3:972:G:O6      | 2.19                     | 0.69              |
| 4:UA:576:ARG:HB3   | 32:CI:142:LEU:HD21  | 1.74                     | 0.69              |
| 15:UL:806:MET:HG2  | 15:UL:835:PHE:HZ    | 1.57                     | 0.69              |
| 20:UQ:443:ASN:O    | 20:UQ:447:LYS:N     | 2.25                     | 0.69              |
| 23:UT:267:SER:OG   | 23:UT:313:ARG:NH1   | 2.25                     | 0.69              |
| 23:UT:1903:LEU:HB3 | 23:UT:1914:THR:HG21 | 1.71                     | 0.69              |
| 25:UV:1109:LYS:NZ  | 25:UV:1170:GLY:O    | 2.25                     | 0.69              |
| 47:JP:263:ARG:NH1  | 47:JP:265:ASN:OD1   | 2.25                     | 0.69              |
| 52:DH:34:LEU:HA    | 52:DH:37:GLU:HB2    | 1.74                     | 0.69              |
| 8:UE:87:LEU:O      | 8:UE:96:THR:N       | 2.26                     | 0.69              |
| 11:UH:643:ASP:OD1  | 12:UI:502:ARG:NH2   | 2.20                     | 0.69              |
| 18:UO:177:ILE:HD12 | 18:UO:183:LEU:HB3   | 1.74                     | 0.69              |
| 28:CD:261:GLN:NE2  | 28:CD:262:ASP:O     | 2.25                     | 0.69              |
| 30:CG:20:ILE:HD11  | 30:CG:121:ILE:HD11  | 1.75                     | 0.69              |
| 39:JF:112:VAL:HB   | 39:JF:124:VAL:HB    | 1.74                     | 0.69              |
| 60:DW:82:LYS:NZ    | 66:D3:749:U:OP2     | 2.25                     | 0.69              |
| 24:UU:611:THR:HB   | 24:UU:621:ASP:HB3   | 1.75                     | 0.69              |
| 27:UZ:178:ALA:HB2  | 48:JQ:199:GLU:HG3   | 1.75                     | 0.69              |
| 35:CL:1052:SER:O   | 66:D3:575:C:N4      | 2.25                     | 0.69              |
| 39:JG:121:LEU:HB2  | 39:JG:163:ILE:O     | 1.93                     | 0.69              |
| 42:JJ:204:ARG:NH1  | 42:JJ:250:LEU:O     | 2.24                     | 0.69              |
| 2:DA:68:VAL:HG11   | 2:DA:73:LEU:HD22    | 1.74                     | 0.69              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:DA:175:GLU:OE2    | 2:DA:187:LYS:NZ     | 2.17                     | 0.69              |
| 9:UF:342:TRP:CZ3    | 9:UF:362:THR:HB     | 2.28                     | 0.69              |
| 15:UL:224:SER:OG    | 15:UL:252:SER:O     | 2.10                     | 0.69              |
| 15:UL:333:ARG:NH1   | 15:UL:334:SER:O     | 2.26                     | 0.69              |
| 16:UM:551:SER:HA    | 16:UM:557:VAL:HG22  | 1.74                     | 0.69              |
| 18:UO:256:THR:HG21  | 18:UO:303:LEU:HD12  | 1.74                     | 0.69              |
| 23:UT:1224:LEU:HD23 | 23:UT:1227:ILE:HD11 | 1.73                     | 0.69              |
| 23:UT:1243:ILE:HA   | 23:UT:1246:ILE:HD12 | 1.75                     | 0.69              |
| 24:UU:91:TYR:CE2    | 24:UU:123:ILE:HD13  | 2.27                     | 0.69              |
| 24:UU:91:TYR:HE2    | 24:UU:123:ILE:HD13  | 1.58                     | 0.69              |
| 24:UU:569:VAL:HB    | 24:UU:579:ARG:HB2   | 1.75                     | 0.69              |
| 28:CD:119:ILE:HD11  | 47:JP:155:TYR:HD1   | 1.56                     | 0.69              |
| 30:CF:62:GLU:HA     | 30:CF:65:LEU:HB3    | 1.73                     | 0.69              |
| 33:CJ:212:ALA:O     | 34:CK:383:ARG:NH2   | 2.26                     | 0.69              |
| 35:CL:776:GLN:HA    | 35:CL:780:ILE:HG12  | 1.74                     | 0.69              |
| 50:DF:200:ASN:HD21  | 50:DF:207:THR:HG23  | 1.57                     | 0.69              |
| 53:DI:79:ALA:HB2    | 53:DI:164:ARG:HH11  | 1.57                     | 0.69              |
| 55:DL:132:SER:HB2   | 55:DL:135:VAL:HG12  | 1.74                     | 0.69              |
| 61:DX:95:PHE:HD2    | 61:DX:135:LEU:HD23  | 1.56                     | 0.69              |
| 65:D2:323:A:H2'     | 65:D2:324:U:H4'     | 1.75                     | 0.69              |
| 66:D3:1739:C:H2'    | 66:D3:1740:A:H8     | 1.58                     | 0.69              |
| 5:UB:651:TRP:CD1    | 5:UB:660:ILE:HG21   | 2.28                     | 0.69              |
| 6:UC:521:ARG:NH2    | 66:D3:579:A:O3'     | 2.25                     | 0.69              |
| 14:UK:221:GLN:HA    | 14:UK:224:LEU:HD12  | 1.74                     | 0.69              |
| 15:UL:147:VAL:O     | 15:UL:156:LEU:N     | 2.26                     | 0.69              |
| 25:UV:469:ASP:O     | 25:UV:473:LYS:N     | 2.26                     | 0.69              |
| 35:CL:52:ARG:HH12   | 66:D3:436:A:P       | 2.15                     | 0.69              |
| 49:DE:38:LEU:HD12   | 49:DE:39:ARG:HG2    | 1.73                     | 0.69              |
| 66:D3:231:U:O2'     | 66:D3:233:C:OP2     | 2.11                     | 0.69              |
| 1:CA:297:ARG:HH11   | 1:CA:322:ARG:HG3    | 1.57                     | 0.69              |
| 1:CB:212:LYS:NZ     | 28:CD:259:MET:O     | 2.26                     | 0.69              |
| 20:UQ:255:ASN:ND2   | 65:D2:81:A:OP1      | 2.26                     | 0.69              |
| 20:UQ:433:ARG:HH22  | 20:UQ:703:LYS:HB2   | 1.58                     | 0.69              |
| 24:UU:632:VAL:HG22  | 24:UU:643:THR:HG22  | 1.73                     | 0.69              |
| 30:CF:13:ASP:OD1    | 30:CF:16:LEU:N      | 2.22                     | 0.69              |
| 38:JC:333:ASN:ND2   | 38:JC:335:SER:OG    | 2.26                     | 0.69              |
| 47:JP:248:ASP:OD1   | 47:JP:249:LEU:N     | 2.26                     | 0.69              |
| 53:DI:5:ARG:HH12    | 66:D3:332:U:H1'     | 1.58                     | 0.69              |
| 57:DO:22:SER:HB3    | 57:DO:25:ASP:H      | 1.57                     | 0.69              |
| 6:UC:599:LYS:HD3    | 6:UC:602:LEU:HD12   | 1.74                     | 0.68              |
| 7:UD:616:LYS:NZ     | 13:UJ:628:ASN:OD1   | 2.26                     | 0.68              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 18:UO:280:HIS:HA    | 18:UO:296:TRP:O     | 1.93                     | 0.68              |
| 21:UR:232:LYS:HD2   | 21:UR:554:ASN:HD22  | 1.55                     | 0.68              |
| 23:UT:1801:ASN:ND2  | 66:D3:650:U:OP1     | 2.25                     | 0.68              |
| 25:UV:525:LEU:HB2   | 25:UV:617:LEU:HB2   | 1.74                     | 0.68              |
| 27:UZ:50:ARG:NH2    | 66:D3:1510:U:OP1    | 2.25                     | 0.68              |
| 29:CE:28:LEU:HG     | 29:CE:33:ASP:HB2    | 1.74                     | 0.68              |
| 66:D3:58:U:O2'      | 66:D3:451:A:N3      | 2.25                     | 0.68              |
| 4:UA:524:ARG:NH2    | 4:UA:529:GLU:OE2    | 2.26                     | 0.68              |
| 5:UB:426:THR:HG22   | 5:UB:462:LEU:HD22   | 1.74                     | 0.68              |
| 7:UD:378:TYR:OH     | 7:UD:632:ASN:ND2    | 2.26                     | 0.68              |
| 11:UH:676:TRP:HB2   | 12:UI:486:LEU:HD13  | 1.74                     | 0.68              |
| 13:UJ:82:ASP:OD1    | 13:UJ:83:ARG:N      | 2.26                     | 0.68              |
| 18:UO:259:ASP:OD1   | 18:UO:260:TYR:N     | 2.27                     | 0.68              |
| 20:UQ:225:ILE:O     | 20:UQ:238:SER:HA    | 1.93                     | 0.68              |
| 25:UV:158:VAL:HG21  | 25:UV:237:HIS:HB2   | 1.75                     | 0.68              |
| 28:CD:182:ASP:OD2   | 28:CD:314:ARG:NH1   | 2.25                     | 0.68              |
| 30:CG:7:LYS:H       | 31:CH:463:GLN:HE22  | 1.41                     | 0.68              |
| 51:DG:160:ARG:NE    | 66:D3:66:U:O2       | 2.26                     | 0.68              |
| 2:DA:214:LYS:NZ     | 66:D3:886:U:OP1     | 2.27                     | 0.68              |
| 3:JA:841:ARG:HH12   | 3:JA:858:MET:HG2    | 1.58                     | 0.68              |
| 9:UF:138:LYS:NZ     | 28:CD:84:LEU:HG     | 2.08                     | 0.68              |
| 13:UJ:364:ASN:OD1   | 13:UJ:365:ILE:HD12  | 1.92                     | 0.68              |
| 15:UL:417:TRP:CD1   | 15:UL:424:CYS:HA    | 2.27                     | 0.68              |
| 15:UL:767:GLU:HB3   | 15:UL:771:ARG:NH1   | 2.06                     | 0.68              |
| 23:UT:616:PRO:HD2   | 23:UT:619:LEU:HD12  | 1.75                     | 0.68              |
| 23:UT:1298:LEU:HD22 | 23:UT:1301:ILE:HD13 | 1.75                     | 0.68              |
| 24:UU:208:GLN:NE2   | 24:UU:209:ILE:O     | 2.26                     | 0.68              |
| 25:UV:268:LEU:HB2   | 25:UV:294:LEU:HB2   | 1.75                     | 0.68              |
| 66:D3:75:U:N3       | 66:D3:76:A:N3       | 2.42                     | 0.68              |
| 3:JA:569:PRO:HD3    | 3:JA:583:LEU:HG     | 1.74                     | 0.68              |
| 3:JA:631:SER:O      | 3:JA:721:HIS:ND1    | 2.26                     | 0.68              |
| 6:UC:439:ASP:OD1    | 39:JG:136:ARG:NH1   | 2.23                     | 0.68              |
| 7:UD:187:GLU:OE1    | 30:CF:120:LYS:NZ    | 2.21                     | 0.68              |
| 14:UK:14:ARG:HG2    | 14:UK:15:GLU:H      | 1.56                     | 0.68              |
| 16:UM:535:GLY:O     | 16:UM:552:SER:OG    | 2.11                     | 0.68              |
| 18:UO:248:ARG:NH2   | 18:UO:291:GLN:OE1   | 2.17                     | 0.68              |
| 24:UU:342:TYR:HH    | 24:UU:345:SER:HG    | 1.34                     | 0.68              |
| 27:UZ:209:ILE:HA    | 27:UZ:212:ILE:HD12  | 1.76                     | 0.68              |
| 28:CD:196:LYS:NZ    | 28:CD:211:PRO:O     | 2.27                     | 0.68              |
| 31:CH:166:VAL:H     | 31:CH:175:SER:HB2   | 1.57                     | 0.68              |
| 32:CI:47:TYR:OH     | 32:CI:110:ARG:NH1   | 2.26                     | 0.68              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 36:CM:231:ARG:NH1  | 66:D3:1132:A:O2'    | 2.27                     | 0.68              |
| 38:JC:121:ARG:NH1  | 38:JC:137:ILE:O     | 2.26                     | 0.68              |
| 51:DG:173:PRO:O    | 66:D3:78:A:O2'      | 2.10                     | 0.68              |
| 56:DN:109:LYS:NZ   | 66:D3:976:G:OP1     | 2.27                     | 0.68              |
| 7:UD:767:LYS:HZ2   | 19:UP:214:GLY:H     | 1.40                     | 0.68              |
| 13:UJ:1748:VAL:HA  | 13:UJ:1752:LEU:HD23 | 1.74                     | 0.68              |
| 16:UM:532:HIS:CD2  | 16:UM:533:LYS:H     | 2.11                     | 0.68              |
| 20:UQ:147:SER:OG   | 20:UQ:148:GLU:OE2   | 2.11                     | 0.68              |
| 23:UT:167:VAL:HG22 | 23:UT:204:PRO:HD3   | 1.76                     | 0.68              |
| 23:UT:1405:GLY:O   | 23:UT:1414:GLN:NE2  | 2.27                     | 0.68              |
| 23:UT:1952:SER:HB2 | 23:UT:1995:ARG:HH21 | 1.58                     | 0.68              |
| 25:UV:441:GLN:NE2  | 25:UV:442:PHE:O     | 2.26                     | 0.68              |
| 28:CD:30:ARG:HH22  | 47:JP:99:THR:C      | 1.97                     | 0.68              |
| 29:CE:4:VAL:HG23   | 29:CE:88:ILE:HB     | 1.75                     | 0.68              |
| 31:CH:367:LYS:HG3  | 31:CH:371:ARG:HD2   | 1.76                     | 0.68              |
| 33:CJ:143:HIS:HB2  | 33:CJ:151:SER:HB3   | 1.75                     | 0.68              |
| 35:CL:145:ASN:HA   | 35:CL:177:PHE:HE1   | 1.58                     | 0.68              |
| 37:CN:4:GLU:HG2    | 37:CN:152:PRO:HG3   | 1.74                     | 0.68              |
| 45:JN:271:GLN:HA   | 45:JN:290:SER:HB2   | 1.75                     | 0.68              |
| 47:JP:298:LEU:O    | 47:JP:457:ARG:NH1   | 2.27                     | 0.68              |
| 48:JQ:181:ASP:OD1  | 48:JQ:182:HIS:N     | 2.26                     | 0.68              |
| 53:DI:98:LYS:NZ    | 66:D3:329:G:OP1     | 2.26                     | 0.68              |
| 7:UD:52:SER:HA     | 7:UD:104:TRP:HE3    | 1.56                     | 0.68              |
| 7:UD:249:ARG:NH2   | 7:UD:293:ASN:OD1    | 2.27                     | 0.68              |
| 16:UM:126:ILE:HD11 | 16:UM:140:PHE:HD1   | 1.58                     | 0.68              |
| 18:UO:195:LEU:O    | 18:UO:206:ILE:N     | 2.27                     | 0.68              |
| 26:UX:65:VAL:HG21  | 26:UX:86:MET:HE3    | 1.74                     | 0.68              |
| 35:CL:51:GLU:OE1   | 61:DX:46:SER:OG     | 2.07                     | 0.68              |
| 51:DG:137:ARG:NH1  | 66:D3:144:U:O4      | 2.26                     | 0.68              |
| 1:CB:159:LEU:HD11  | 1:CB:317:VAL:HG21   | 1.74                     | 0.68              |
| 5:UB:644:ASP:OD1   | 5:UB:687:LYS:NZ     | 2.23                     | 0.68              |
| 15:UL:661:TRP:NE1  | 15:UL:677:HIS:HB2   | 2.09                     | 0.68              |
| 23:UT:538:LEU:HD21 | 23:UT:565:LEU:HD22  | 1.75                     | 0.68              |
| 23:UT:1521:ASN:OD1 | 23:UT:1522:GLN:N    | 2.27                     | 0.68              |
| 26:UX:19:THR:HG23  | 26:UX:20:LYS:HD3    | 1.76                     | 0.68              |
| 28:CD:100:ILE:HD11 | 28:CD:105:LEU:HD23  | 1.76                     | 0.68              |
| 44:JM:127:ARG:HA   | 44:JM:130:LEU:HD13  | 1.76                     | 0.68              |
| 51:DG:202:ARG:NH1  | 66:D3:183:U:O2'     | 2.26                     | 0.68              |
| 52:DH:7:LYS:O      | 52:DH:42:GLN:NE2    | 2.26                     | 0.68              |
| 54:DJ:131:GLN:HE21 | 66:D3:513:U:C4'     | 2.06                     | 0.68              |
| 66:D3:390:G:N2     | 66:D3:407:A:N7      | 2.40                     | 0.68              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 66:D3:868:G:H2'     | 66:D3:869:A:H8      | 1.58                     | 0.68              |
| 2:DA:122:GLU:OE2    | 2:DA:123:ALA:N      | 2.27                     | 0.68              |
| 3:JA:547:LYS:NZ     | 3:JA:548:ASN:O      | 2.27                     | 0.68              |
| 5:UB:498:LEU:HD11   | 5:UB:545:VAL:HG11   | 1.75                     | 0.68              |
| 18:UO:91:SER:OG     | 18:UO:137:ASN:OD1   | 2.11                     | 0.68              |
| 23:UT:1022:VAL:HG23 | 23:UT:1023:LEU:HD12 | 1.75                     | 0.68              |
| 24:UU:488:ASN:ND2   | 58:DQ:98:ASP:OD2    | 2.27                     | 0.68              |
| 26:UX:149:LYS:HD3   | 26:UX:170:ILE:HD11  | 1.74                     | 0.68              |
| 30:CF:118:LYS:HA    | 30:CF:121:ILE:HG22  | 1.76                     | 0.68              |
| 39:JG:31:LEU:HD12   | 39:JG:40:ARG:HH21   | 1.59                     | 0.68              |
| 46:JO:195:HIS:HB3   | 46:JO:197:ILE:HG22  | 1.74                     | 0.68              |
| 61:DX:86:PHE:CZ     | 61:DX:120:VAL:HG21  | 2.29                     | 0.68              |
| 65:D2:174:U:H3      | 65:D2:222:G:H1      | 1.39                     | 0.68              |
| 11:UH:673:THR:HG22  | 12:UI:490:GLU:HG3   | 1.75                     | 0.68              |
| 15:UL:201:ILE:H     | 16:UM:660:LYS:HE2   | 1.59                     | 0.68              |
| 16:UM:393:SER:HB3   | 16:UM:406:ALA:HB3   | 1.76                     | 0.68              |
| 20:UQ:578:ASN:ND2   | 65:D2:7:A:N7        | 2.42                     | 0.68              |
| 25:UV:975:LEU:HB2   | 25:UV:1041:VAL:HG12 | 1.76                     | 0.68              |
| 26:UX:84:ARG:NH2    | 60:DW:97:ARG:HH12   | 1.92                     | 0.68              |
| 35:CL:103:GLY:HA3   | 35:CL:358:MET:HE3   | 1.76                     | 0.68              |
| 35:CL:558:ILE:HG23  | 35:CL:562:GLU:OE2   | 1.94                     | 0.68              |
| 35:CL:1157:LYS:NZ   | 67:D4:13:C:OP2      | 2.27                     | 0.68              |
| 4:UA:493:TRP:HA     | 4:UA:517:ASP:HB2    | 1.74                     | 0.68              |
| 15:UL:344:THR:O     | 15:UL:352:GLU:HB2   | 1.93                     | 0.68              |
| 15:UL:624:LEU:HD12  | 15:UL:629:ASN:HB2   | 1.76                     | 0.68              |
| 22:US:381:LYS:HE3   | 22:US:461:SER:HB2   | 1.74                     | 0.68              |
| 23:UT:1012:ARG:HB3  | 53:DI:116:HIS:HA    | 1.76                     | 0.68              |
| 35:CL:137:LEU:HD21  | 35:CL:230:MET:HG2   | 1.76                     | 0.68              |
| 52:DH:102:PRO:O     | 66:D3:810:G:N2      | 2.27                     | 0.68              |
| 1:CA:102:LYS:O      | 44:JM:136:TYR:OH    | 2.11                     | 0.67              |
| 15:UL:338:ILE:HA    | 15:UL:357:THR:HA    | 1.76                     | 0.67              |
| 15:UL:364:TYR:HB3   | 15:UL:383:HIS:HB2   | 1.76                     | 0.67              |
| 15:UL:941:THR:OG1   | 34:CK:464:SER:O     | 2.12                     | 0.67              |
| 18:UO:51:HIS:HB3    | 18:UO:53:HIS:CE1    | 2.29                     | 0.67              |
| 23:UT:1220:LEU:HD22 | 23:UT:1250:ILE:HD13 | 1.76                     | 0.67              |
| 25:UV:793:PRO:HB3   | 37:CN:191:PHE:HE2   | 1.59                     | 0.67              |
| 33:CJ:118:ASN:ND2   | 33:CJ:118:ASN:O     | 2.27                     | 0.67              |
| 8:UE:443:GLN:NE2    | 18:UO:252:ASN:OD1   | 2.27                     | 0.67              |
| 11:UH:31:VAL:HA     | 11:UH:355:LEU:H     | 1.58                     | 0.67              |
| 23:UT:75:GLN:N      | 23:UT:79:GLN:OE1    | 2.26                     | 0.67              |
| 23:UT:1932:GLU:HG3  | 23:UT:1933:ILE:HD12 | 1.74                     | 0.67              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:UV:197:GLN:NE2  | 25:UV:200:GLY:O    | 2.27                     | 0.67              |
| 29:CE:73:GLU:HA    | 29:CE:76:LEU:HG    | 1.75                     | 0.67              |
| 33:CJ:138:ASP:OD2  | 33:CJ:156:HIS:ND1  | 2.26                     | 0.67              |
| 66:D3:1697:G:N2    | 66:D3:1704:U:O2    | 2.28                     | 0.67              |
| 67:D4:106:C:H42    | 67:D4:309:G:H1     | 1.42                     | 0.67              |
| 3:JA:722:TYR:HA    | 3:JA:765:VAL:HG22  | 1.76                     | 0.67              |
| 4:UA:130:ASP:OD1   | 4:UA:131:ARG:N     | 2.27                     | 0.67              |
| 5:UB:434:ILE:O     | 5:UB:438:ASN:ND2   | 2.27                     | 0.67              |
| 7:UD:102:LEU:HD22  | 7:UD:114:LEU:HD11  | 1.77                     | 0.67              |
| 16:UM:439:ALA:HB3  | 16:UM:497:LEU:HD13 | 1.76                     | 0.67              |
| 24:UU:207:ASP:OD1  | 24:UU:208:GLN:N    | 2.26                     | 0.67              |
| 25:UV:751:LYS:HE2  | 25:UV:787:GLU:HA   | 1.74                     | 0.67              |
| 26:UX:187:ASP:OD2  | 54:DJ:53:ARG:NH2   | 2.28                     | 0.67              |
| 28:CD:377:ARG:NH2  | 67:D4:257:A:OP2    | 2.28                     | 0.67              |
| 31:CH:317:ILE:HG12 | 31:CH:319:TYR:HE1  | 1.58                     | 0.67              |
| 38:JC:277:ILE:HG23 | 38:JC:288:LYS:HZ2  | 1.58                     | 0.67              |
| 53:DI:99:ALA:H     | 53:DI:170:SER:HA   | 1.60                     | 0.67              |
| 66:D3:23:G:H1      | 66:D3:603:U:H3     | 1.41                     | 0.67              |
| 66:D3:851:U:H1'    | 66:D3:852:C:H5     | 1.58                     | 0.67              |
| 9:UF:118:LYS:HG2   | 9:UF:153:TYR:CE1   | 2.29                     | 0.67              |
| 10:UG:213:TRP:NE1  | 10:UG:229:ARG:HG3  | 2.09                     | 0.67              |
| 12:UI:500:GLN:OE1  | 18:UO:503:ARG:NH1  | 2.27                     | 0.67              |
| 14:UK:134:THR:HG22 | 19:UP:177:ARG:HB3  | 1.76                     | 0.67              |
| 16:UM:728:ILE:O    | 16:UM:767:HIS:NE2  | 2.15                     | 0.67              |
| 25:UV:761:ARG:HD3  | 25:UV:896:THR:HG22 | 1.75                     | 0.67              |
| 29:CE:16:LYS:NZ    | 29:CE:18:SER:OG    | 2.28                     | 0.67              |
| 29:CE:353:GLY:H    | 29:CE:356:LYS:HD3  | 1.59                     | 0.67              |
| 35:CL:45:ARG:NH1   | 66:D3:28:A:O5'     | 2.27                     | 0.67              |
| 38:JC:23:ARG:HH21  | 38:JC:315:VAL:HG22 | 1.58                     | 0.67              |
| 39:JG:73:HIS:O     | 39:JG:77:LEU:HB2   | 1.94                     | 0.67              |
| 66:D3:1512:G:H2'   | 66:D3:1513:G:C8    | 2.29                     | 0.67              |
| 2:DA:62:LYS:NZ     | 2:DA:89:ASP:O      | 2.26                     | 0.67              |
| 21:UR:400:ILE:HD13 | 21:UR:425:ALA:HB1  | 1.77                     | 0.67              |
| 33:CJ:226:ASN:ND2  | 33:CJ:289:TYR:OH   | 2.28                     | 0.67              |
| 4:UA:647:ALA:HB3   | 10:UG:171:LYS:HD2  | 1.76                     | 0.67              |
| 9:UF:178:VAL:HG23  | 9:UF:181:LEU:HB3   | 1.75                     | 0.67              |
| 13:UJ:1603:MET:HA  | 13:UJ:1606:LYS:HE2 | 1.77                     | 0.67              |
| 31:CH:200:ASP:HB2  | 31:CH:211:LEU:HD11 | 1.76                     | 0.67              |
| 44:JM:50:SER:N     | 44:JM:53:GLN:OE1   | 2.28                     | 0.67              |
| 46:JO:100:LEU:HD11 | 46:JO:113:ALA:HB1  | 1.75                     | 0.67              |
| 53:DI:58:LEU:O     | 53:DI:59:ARG:NH1   | 2.26                     | 0.67              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 54:DJ:37:LYS:NZ     | 66:D3:474:A:O2'     | 2.24                     | 0.67              |
| 2:DA:33:LYS:HD2     | 2:DA:41:ARG:HB3     | 1.76                     | 0.67              |
| 3:JA:163:THR:HG21   | 3:JA:172:TYR:HB2    | 1.75                     | 0.67              |
| 7:UD:366:ASN:O      | 20:UQ:247:SER:OG    | 2.11                     | 0.67              |
| 10:UG:69:GLU:HG3    | 10:UG:70:SER:H      | 1.58                     | 0.67              |
| 10:UG:78:ASN:HD21   | 10:UG:80:LEU:HB3    | 1.60                     | 0.67              |
| 10:UG:283:ASP:OD1   | 10:UG:288:TYR:N     | 2.27                     | 0.67              |
| 13:UJ:128:HIS:HB2   | 13:UJ:155:ILE:HG12  | 1.77                     | 0.67              |
| 16:UM:488:HIS:NE2   | 16:UM:490:HIS:O     | 2.28                     | 0.67              |
| 22:US:470:MET:HE1   | 22:US:485:ALA:HB2   | 1.76                     | 0.67              |
| 29:CE:89:VAL:HG11   | 29:CE:95:ALA:HB2    | 1.76                     | 0.67              |
| 30:CF:50:GLU:OE2    | 30:CF:118:LYS:NZ    | 2.22                     | 0.67              |
| 30:CG:6:PRO:HB2     | 31:CH:465:GLN:HE21  | 1.59                     | 0.67              |
| 53:DI:21:PHE:CD2    | 53:DI:22:ARG:HD3    | 2.30                     | 0.67              |
| 66:D3:918:U:H2'     | 66:D3:919:A:C8      | 2.30                     | 0.67              |
| 3:JA:587:GLN:HB3    | 3:JA:637:ARG:HB3    | 1.77                     | 0.67              |
| 8:UE:212:LEU:HB2    | 8:UE:226:LEU:HB2    | 1.76                     | 0.67              |
| 20:UQ:265:ASP:OD1   | 20:UQ:266:ASN:N     | 2.28                     | 0.67              |
| 20:UQ:443:ASN:O     | 20:UQ:447:LYS:HA    | 1.95                     | 0.67              |
| 20:UQ:779:ILE:HG13  | 20:UQ:780:GLU:H     | 1.59                     | 0.67              |
| 24:UU:422:ALA:O     | 24:UU:423:ARG:NH1   | 2.26                     | 0.67              |
| 35:CL:119:GLU:O     | 35:CL:119:GLU:HG2   | 1.94                     | 0.67              |
| 35:CL:821:LYS:NZ    | 36:CM:79:GLY:O      | 2.28                     | 0.67              |
| 49:DE:126:VAL:HB    | 49:DE:158:ASP:HB2   | 1.75                     | 0.67              |
| 61:DX:95:PHE:CD2    | 61:DX:135:LEU:HD23  | 2.30                     | 0.67              |
| 4:UA:151:SER:HB3    | 4:UA:164:THR:HB     | 1.76                     | 0.67              |
| 1:CB:264:GLN:N      | 1:CB:320:TYR:O      | 2.28                     | 0.67              |
| 23:UT:1811:ILE:HD11 | 23:UT:1875:LEU:HD21 | 1.77                     | 0.67              |
| 25:UV:441:GLN:HE22  | 25:UV:470:LYS:H     | 1.42                     | 0.67              |
| 25:UV:677:ILE:O     | 25:UV:681:ILE:HG13  | 1.95                     | 0.67              |
| 35:CL:861:THR:O     | 35:CL:882:ASN:HB2   | 1.95                     | 0.67              |
| 42:JJ:94:PHE:HA     | 42:JJ:141:THR:O     | 1.94                     | 0.67              |
| 50:DF:37:GLN:HB3    | 58:DQ:53:LEU:HD22   | 1.75                     | 0.67              |
| 56:DN:121:ARG:NH2   | 66:D3:867:G:O3'     | 2.28                     | 0.67              |
| 61:DX:66:SER:H      | 61:DX:69:ARG:HB3    | 1.59                     | 0.67              |
| 10:UG:140:ARG:HE    | 13:UJ:20:LEU:HD11   | 1.59                     | 0.67              |
| 10:UG:329:LEU:HD22  | 10:UG:406:ALA:HB2   | 1.77                     | 0.67              |
| 16:UM:642:GLN:HG3   | 16:UM:644:TRP:HE1   | 1.59                     | 0.67              |
| 23:UT:256:SER:O     | 23:UT:260:HIS:ND1   | 2.28                     | 0.67              |
| 35:CL:289:HIS:HB2   | 35:CL:815:LEU:HD21  | 1.77                     | 0.67              |
| 65:D2:336:G:N2      | 65:D2:389:U:O2      | 2.28                     | 0.67              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:UA:743:PHE:HE2   | 4:UA:770:ILE:HD11  | 1.61                     | 0.66              |
| 7:UD:427:ASN:O     | 7:UD:444:ARG:NH2   | 2.27                     | 0.66              |
| 23:UT:1056:GLN:NE2 | 66:D3:200:A:OP2    | 2.27                     | 0.66              |
| 31:CH:317:ILE:HG12 | 31:CH:319:TYR:CE1  | 2.30                     | 0.66              |
| 33:CJ:101:SER:O    | 33:CJ:116:ARG:NH2  | 2.27                     | 0.66              |
| 37:CN:178:ASP:OD1  | 37:CN:179:TYR:N    | 2.28                     | 0.66              |
| 38:JC:55:PHE:HD2   | 38:JC:58:ALA:H     | 1.40                     | 0.66              |
| 39:JF:116:THR:HG22 | 39:JF:120:ILE:H    | 1.60                     | 0.66              |
| 53:DI:67:TRP:HD1   | 53:DI:70:GLU:HB3   | 1.59                     | 0.66              |
| 65:D2:193:G:H2'    | 65:D2:194:G:H8     | 1.60                     | 0.66              |
| 5:UB:745:LYS:NZ    | 66:D3:1174:C:OP2   | 2.25                     | 0.66              |
| 7:UD:450:VAL:HG13  | 7:UD:465:LEU:HB2   | 1.76                     | 0.66              |
| 8:UE:111:ASP:OD2   | 8:UE:112:LEU:N     | 2.28                     | 0.66              |
| 8:UE:148:LEU:HA    | 8:UE:167:SER:HB3   | 1.78                     | 0.66              |
| 12:UI:435:LEU:HD22 | 12:UI:478:ASN:HD21 | 1.61                     | 0.66              |
| 13:UJ:226:ASN:OD1  | 67:D4:333:U:O2'    | 2.08                     | 0.66              |
| 13:UJ:658:ALA:HB2  | 13:UJ:670:LEU:HD22 | 1.77                     | 0.66              |
| 13:UJ:696:LEU:O    | 13:UJ:699:ARG:NH1  | 2.28                     | 0.66              |
| 21:UR:307:GLN:OE1  | 21:UR:472:GLN:NE2  | 2.28                     | 0.66              |
| 23:UT:1957:GLN:NE2 | 23:UT:1995:ARG:O   | 2.28                     | 0.66              |
| 24:UU:190:LEU:HD13 | 24:UU:200:PHE:HD2  | 1.61                     | 0.66              |
| 25:UV:1100:VAL:HB  | 25:UV:1182:ILE:HB  | 1.77                     | 0.66              |
| 31:CH:300:ALA:HB1  | 31:CH:324:ILE:HD12 | 1.78                     | 0.66              |
| 38:JC:206:PHE:HB2  | 38:JC:216:SER:HB3  | 1.77                     | 0.66              |
| 49:DE:72:VAL:N     | 49:DE:75:LYS:O     | 2.27                     | 0.66              |
| 56:DN:18:TYR:HE2   | 60:DW:56:HIS:CD2   | 2.14                     | 0.66              |
| 3:JA:497:ILE:HG13  | 3:JA:498:LYS:HD3   | 1.77                     | 0.66              |
| 10:UG:116:ILE:HG23 | 10:UG:125:LEU:HD11 | 1.77                     | 0.66              |
| 13:UJ:781:ASN:OD1  | 13:UJ:782:VAL:N    | 2.28                     | 0.66              |
| 23:UT:1253:ASN:ND2 | 23:UT:1255:ASN:OD1 | 2.27                     | 0.66              |
| 35:CL:145:ASN:ND2  | 35:CL:173:HIS:HB3  | 2.10                     | 0.66              |
| 35:CL:819:GLU:O    | 35:CL:852:ARG:NH2  | 2.25                     | 0.66              |
| 35:CL:1123:LYS:HZ2 | 66:D3:487:G:P      | 2.18                     | 0.66              |
| 36:CM:146:VAL:HG12 | 36:CM:174:ILE:HD13 | 1.77                     | 0.66              |
| 38:JC:156:GLY:HA3  | 38:JC:183:VAL:HG11 | 1.78                     | 0.66              |
| 43:JK:485:TRP:HB2  | 43:JK:490:ILE:HD11 | 1.76                     | 0.66              |
| 66:D3:1540:G:N2    | 66:D3:1571:C:O2    | 2.28                     | 0.66              |
| 2:DA:241:GLY:HA3   | 25:UV:656:ARG:HB3  | 1.76                     | 0.66              |
| 5:UB:701:ALA:HA    | 22:US:417:HIS:HB2  | 1.77                     | 0.66              |
| 7:UD:87:GLN:HB3    | 7:UD:378:TYR:CD2   | 2.30                     | 0.66              |
| 13:UJ:304:GLN:O    | 13:UJ:307:LYS:NZ   | 2.24                     | 0.66              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 15:UL:209:GLY:H     | 15:UL:220:THR:HG22 | 1.60                     | 0.66              |
| 20:UQ:108:THR:HG22  | 20:UQ:118:VAL:HG22 | 1.76                     | 0.66              |
| 23:UT:867:LYS:HG3   | 23:UT:892:LEU:HD13 | 1.76                     | 0.66              |
| 24:UU:584:HIS:HE2   | 24:UU:602:SER:HG   | 1.42                     | 0.66              |
| 31:CH:164:GLN:HE22  | 31:CH:528:GLU:HG2  | 1.59                     | 0.66              |
| 65:D2:228:A:H2'     | 65:D2:229:A:C8     | 2.31                     | 0.66              |
| 66:D3:323:A:O2'     | 66:D3:346:G:N2     | 2.29                     | 0.66              |
| 66:D3:894:U:H2'     | 66:D3:895:G:H8     | 1.60                     | 0.66              |
| 10:UG:67:LEU:HB3    | 10:UG:410:ASN:HD22 | 1.60                     | 0.66              |
| 12:UI:435:LEU:HD21  | 12:UI:475:THR:HG22 | 1.78                     | 0.66              |
| 18:UO:502:GLN:O     | 18:UO:505:GLU:HG2  | 1.95                     | 0.66              |
| 23:UT:1228:LEU:HD12 | 23:UT:1271:LEU:HG  | 1.78                     | 0.66              |
| 25:UV:1101:ASP:HB2  | 25:UV:1233:ASN:HB3 | 1.76                     | 0.66              |
| 35:CL:830:ARG:HB2   | 35:CL:880:TYR:CD1  | 2.31                     | 0.66              |
| 47:JP:55:ALA:HA     | 47:JP:379:ALA:HB1  | 1.77                     | 0.66              |
| 58:DQ:66:ARG:HD3    | 65:D2:267:U:O4     | 1.96                     | 0.66              |
| 60:DW:114:GLU:OE1   | 60:DW:117:ARG:NH2  | 2.26                     | 0.66              |
| 65:D2:89:C:H3'      | 65:D2:90:G:H5'     | 1.77                     | 0.66              |
| 65:D2:361:G:N2      | 65:D2:364:A:OP2    | 2.28                     | 0.66              |
| 66:D3:793:A:H2      | 66:D3:796:A:H3'    | 1.61                     | 0.66              |
| 66:D3:1788:G:H2'    | 66:D3:1789:G:H8    | 1.60                     | 0.66              |
| 14:UK:64:TYR:O      | 14:UK:67:MET:HG3   | 1.96                     | 0.66              |
| 14:UK:111:ARG:NE    | 14:UK:212:LYS:HG2  | 2.08                     | 0.66              |
| 23:UT:276:SER:HB2   | 23:UT:320:THR:HG21 | 1.77                     | 0.66              |
| 30:CG:8:ALA:HB3     | 31:CH:465:GLN:HE22 | 1.60                     | 0.66              |
| 31:CH:141:LEU:HD13  | 31:CH:570:GLN:HB3  | 1.76                     | 0.66              |
| 32:CI:62:SER:OG     | 33:CJ:57:ARG:NH1   | 2.28                     | 0.66              |
| 45:JN:257:ALA:O     | 45:JN:260:GLY:O    | 2.14                     | 0.66              |
| 55:DL:47:THR:HG23   | 55:DL:114:ALA:HB1  | 1.76                     | 0.66              |
| 62:DY:124:ARG:NH2   | 66:D3:151:G:N7     | 2.43                     | 0.66              |
| 4:UA:359:ARG:NH1    | 34:CK:484:MET:HB3  | 2.11                     | 0.66              |
| 10:UG:531:HIS:CE1   | 65:D2:365:G:H4'    | 2.30                     | 0.66              |
| 13:UJ:1667:VAL:HG13 | 13:UJ:1710:ALA:HA  | 1.77                     | 0.66              |
| 13:UJ:1746:ARG:NH1  | 23:UT:40:ASP:O     | 2.28                     | 0.66              |
| 15:UL:330:GLN:HE22  | 15:UL:367:ILE:HG21 | 1.61                     | 0.66              |
| 20:UQ:90:LYS:NZ     | 20:UQ:143:ASN:OD1  | 2.29                     | 0.66              |
| 34:CK:332:ALA:HA    | 34:CK:335:ARG:HH11 | 1.60                     | 0.66              |
| 34:CK:343:GLU:CD    | 34:CK:344:GLU:H    | 1.98                     | 0.66              |
| 37:CN:18:PHE:HB2    | 37:CN:35:HIS:HB3   | 1.77                     | 0.66              |
| 37:CN:46:ASN:ND2    | 37:CN:48:ASN:OD1   | 2.29                     | 0.66              |
| 2:DA:199:ASN:HA     | 2:DA:202:LYS:HE3   | 1.77                     | 0.66              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 7:UD:212:ILE:HB     | 7:UD:227:HIS:HB2    | 1.78                     | 0.66              |
| 11:UH:635:PHE:CD2   | 12:UI:492:ILE:HD11  | 2.30                     | 0.66              |
| 13:UJ:1557:ASP:O    | 13:UJ:1571:ARG:NH1  | 2.29                     | 0.66              |
| 22:US:281:LEU:HA    | 22:US:285:ILE:HB    | 1.76                     | 0.66              |
| 22:US:399:ILE:HD11  | 22:US:480:LEU:HB3   | 1.75                     | 0.66              |
| 23:UT:225:GLN:HG3   | 23:UT:228:LEU:H     | 1.60                     | 0.66              |
| 35:CL:775:GLU:OE1   | 35:CL:779:ARG:NH2   | 2.28                     | 0.66              |
| 35:CL:1110:ARG:HE   | 65:D2:411:A:HO2'    | 1.41                     | 0.66              |
| 3:JA:742:PHE:HB3    | 3:JA:762:MET:SD     | 2.36                     | 0.66              |
| 4:UA:148:ASP:OD1    | 4:UA:149:ILE:N      | 2.28                     | 0.66              |
| 4:UA:791:HIS:O      | 4:UA:795:ASN:ND2    | 2.29                     | 0.66              |
| 1:CB:124:SER:OG     | 1:CB:140:GLU:OE2    | 2.14                     | 0.66              |
| 1:CB:251:ARG:NH2    | 7:UD:179:HIS:O      | 2.29                     | 0.66              |
| 5:UB:662:LEU:O      | 5:UB:666:GLN:NE2    | 2.29                     | 0.66              |
| 13:UJ:1606:LYS:HA   | 13:UJ:1609:ILE:HD12 | 1.77                     | 0.66              |
| 20:UQ:141:LEU:HD21  | 20:UQ:144:VAL:HG23  | 1.78                     | 0.66              |
| 20:UQ:426:ARG:NH2   | 65:D2:70:A:OP2      | 2.28                     | 0.66              |
| 23:UT:30:PRO:HA     | 23:UT:33:ASN:HB2    | 1.76                     | 0.66              |
| 25:UV:633:ALA:HA    | 25:UV:664:THR:HA    | 1.78                     | 0.66              |
| 27:UZ:97:PHE:CZ     | 27:UZ:180:LEU:HD11  | 2.30                     | 0.66              |
| 38:JC:357:ASP:OD1   | 38:JC:358:SER:N     | 2.29                     | 0.66              |
| 46:JO:258:ARG:HG3   | 66:D3:629:U:H5''    | 1.77                     | 0.66              |
| 49:DE:182:TYR:HB2   | 49:DE:228:ILE:HD11  | 1.77                     | 0.66              |
| 66:D3:29:U:H2'      | 66:D3:30:G:H8       | 1.59                     | 0.66              |
| 4:UA:570:THR:HG22   | 4:UA:572:LYS:H      | 1.60                     | 0.66              |
| 5:UB:482:GLN:HB2    | 5:UB:486:LYS:NZ     | 2.11                     | 0.66              |
| 10:UG:77:GLU:OE1    | 47:JP:1:MET:N       | 2.26                     | 0.66              |
| 11:UH:670:GLU:O     | 11:UH:673:THR:OG1   | 2.12                     | 0.66              |
| 12:UI:504:GLU:OE2   | 12:UI:507:ARG:NH2   | 2.29                     | 0.66              |
| 15:UL:386:GLU:HB2   | 15:UL:391:ARG:HD3   | 1.78                     | 0.66              |
| 20:UQ:710:LEU:HB3   | 20:UQ:722:LEU:HD22  | 1.78                     | 0.66              |
| 23:UT:1632:LEU:HD23 | 23:UT:1633:PRO:HD3  | 1.78                     | 0.66              |
| 24:UU:510:LEU:HD21  | 24:UU:514:ASN:HA    | 1.78                     | 0.66              |
| 35:CL:125:LEU:HB3   | 35:CL:902:VAL:HG23  | 1.78                     | 0.66              |
| 39:JF:106:LYS:HZ1   | 39:JG:230:TYR:HD1   | 1.43                     | 0.66              |
| 54:DJ:71:PHE:HE2    | 66:D3:762:A:HO2'    | 1.44                     | 0.66              |
| 62:DY:102:LYS:NZ    | 66:D3:444:C:OP1     | 2.29                     | 0.66              |
| 67:D4:197:U:H5      | 67:D4:198:U:H5      | 1.44                     | 0.66              |
| 3:JA:540:LEU:HD23   | 3:JA:585:VAL:HG12   | 1.77                     | 0.65              |
| 4:UA:329:VAL:HB     | 4:UA:339:LEU:HG     | 1.78                     | 0.65              |
| 3:JB:591:GLU:O      | 3:JB:631:SER:HA     | 1.96                     | 0.65              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 5:UB:576:ILE:HD13   | 5:UB:671:TYR:CE1    | 2.32                     | 0.65              |
| 6:UC:544:ILE:O      | 35:CL:193:ARG:NH1   | 2.29                     | 0.65              |
| 8:UE:151:LEU:HD11   | 8:UE:163:LEU:HD12   | 1.78                     | 0.65              |
| 13:UJ:560:ILE:HG13  | 13:UJ:599:PHE:HB3   | 1.78                     | 0.65              |
| 16:UM:173:LYS:HG3   | 16:UM:185:THR:HG22  | 1.78                     | 0.65              |
| 23:UT:1340:SER:O    | 23:UT:1344:TRP:N    | 2.26                     | 0.65              |
| 23:UT:1942:LEU:HD13 | 23:UT:1945:ILE:HD11 | 1.78                     | 0.65              |
| 29:CE:164:ILE:HG22  | 29:CE:301:ALA:HA    | 1.78                     | 0.65              |
| 38:JC:336:ILE:HB    | 38:JC:337:PRO:HD3   | 1.78                     | 0.65              |
| 39:JF:197:ASP:HB2   | 39:JF:200:GLU:HB2   | 1.76                     | 0.65              |
| 45:JN:234:VAL:H     | 45:JN:239:ARG:NH1   | 1.95                     | 0.65              |
| 47:JP:296:ARG:HG3   | 47:JP:458:LYS:HG3   | 1.78                     | 0.65              |
| 49:DE:197:HIS:NE2   | 49:DE:199:GLU:OE2   | 2.27                     | 0.65              |
| 54:DJ:60:LEU:HD21   | 54:DJ:93:LEU:HB3    | 1.77                     | 0.65              |
| 1:CA:231:ARG:NH1    | 28:CD:102:ASP:OD1   | 2.30                     | 0.65              |
| 7:UD:95:LYS:HE3     | 7:UD:426:GLN:HA     | 1.79                     | 0.65              |
| 9:UF:83:LEU:HA      | 9:UF:86:TRP:HE1     | 1.61                     | 0.65              |
| 9:UF:342:TRP:HZ2    | 9:UF:358:LEU:HB3    | 1.60                     | 0.65              |
| 13:UJ:238:LEU:HD23  | 13:UJ:260:ILE:HD11  | 1.78                     | 0.65              |
| 23:UT:261:GLU:O     | 23:UT:264:THR:OG1   | 2.12                     | 0.65              |
| 23:UT:1112:TRP:HA   | 23:UT:1118:LEU:HB3  | 1.78                     | 0.65              |
| 23:UT:1381:LYS:HB3  | 23:UT:1386:GLU:HG3  | 1.78                     | 0.65              |
| 24:UU:45:GLY:HA2    | 65:D2:308:A:O2'     | 1.97                     | 0.65              |
| 42:JJ:217:GLU:OE2   | 42:JJ:224:ILE:N     | 2.29                     | 0.65              |
| 47:JP:443:ASN:OD1   | 47:JP:446:ARG:NH2   | 2.21                     | 0.65              |
| 55:DL:72:THR:O      | 55:DL:88:ARG:NH2    | 2.24                     | 0.65              |
| 66:D3:1505:A:C5     | 66:D3:1506:G:H1'    | 2.31                     | 0.65              |
| 15:UL:299:ARG:HD3   | 15:UL:317:ILE:HG23  | 1.76                     | 0.65              |
| 19:UP:194:LYS:HD2   | 19:UP:199:ILE:HG21  | 1.78                     | 0.65              |
| 20:UQ:730:ASP:O     | 20:UQ:734:VAL:N     | 2.30                     | 0.65              |
| 22:US:196:GLN:HE21  | 22:US:253:PHE:HE1   | 1.42                     | 0.65              |
| 23:UT:1308:LEU:HD21 | 23:UT:1350:THR:HG21 | 1.79                     | 0.65              |
| 51:DG:76:LEU:HB2    | 51:DG:92:ARG:HD3    | 1.78                     | 0.65              |
| 51:DG:132:ARG:HH12  | 66:D3:150:U:H5'     | 1.61                     | 0.65              |
| 52:DH:113:PRO:HB2   | 52:DH:116:ARG:H     | 1.61                     | 0.65              |
| 52:DH:131:PHE:CD1   | 52:DH:132:PRO:HA    | 2.31                     | 0.65              |
| 55:DL:129:ARG:NH1   | 66:D3:335:U:O2'     | 2.29                     | 0.65              |
| 67:D4:16:A:H2'      | 67:D4:17:G:C8       | 2.31                     | 0.65              |
| 3:JA:918:ARG:NH1    | 3:JA:921:SER:OG     | 2.30                     | 0.65              |
| 4:UA:190:HIS:ND1    | 4:UA:210:SER:HB3    | 2.12                     | 0.65              |
| 10:UG:483:ILE:HD11  | 10:UG:516:VAL:HA    | 1.79                     | 0.65              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 13:UJ:1664:LYS:NZ  | 67:D4:145:U:OP2     | 2.30                     | 0.65              |
| 25:UV:173:ASN:ND2  | 66:D3:1700:C:OP2    | 2.29                     | 0.65              |
| 54:DJ:135:ALA:HB2  | 54:DJ:140:ILE:HD13  | 1.77                     | 0.65              |
| 56:DN:67:THR:HG23  | 56:DN:69:ASN:H      | 1.61                     | 0.65              |
| 4:UA:397:LYS:O     | 4:UA:398:ARG:HD3    | 1.96                     | 0.65              |
| 15:UL:49:VAL:HG12  | 15:UL:63:LEU:HB2    | 1.79                     | 0.65              |
| 16:UM:107:ILE:HD11 | 16:UM:147:ILE:HG22  | 1.78                     | 0.65              |
| 16:UM:599:ILE:HB   | 16:UM:613:LEU:HB2   | 1.77                     | 0.65              |
| 20:UQ:250:GLN:N    | 20:UQ:250:GLN:OE1   | 2.29                     | 0.65              |
| 21:UR:232:LYS:HD2  | 21:UR:554:ASN:ND2   | 2.11                     | 0.65              |
| 23:UT:296:GLU:O    | 23:UT:300:GLN:NE2   | 2.29                     | 0.65              |
| 24:UU:232:MET:HB2  | 24:UU:242:ARG:HB2   | 1.79                     | 0.65              |
| 29:CE:158:LYS:HA   | 29:CE:283:ILE:HD13  | 1.78                     | 0.65              |
| 29:CE:309:LEU:HG   | 29:CE:371:LEU:HD21  | 1.76                     | 0.65              |
| 31:CH:455:THR:O    | 31:CH:460:ARG:NH2   | 2.29                     | 0.65              |
| 36:CM:183:ILE:O    | 36:CM:312:ARG:NH1   | 2.29                     | 0.65              |
| 47:JP:290:ASP:OD1  | 47:JP:291:MET:N     | 2.30                     | 0.65              |
| 49:DE:38:LEU:HB3   | 66:D3:298:C:H5'     | 1.79                     | 0.65              |
| 67:D4:202:G:H1     | 67:D4:247:U:H3      | 1.42                     | 0.65              |
| 7:UD:449:LYS:NZ    | 7:UD:450:VAL:O      | 2.30                     | 0.65              |
| 13:UJ:1741:ASP:HB2 | 13:UJ:1744:ILE:HD12 | 1.76                     | 0.65              |
| 15:UL:130:ASP:O    | 15:UL:134:THR:N     | 2.30                     | 0.65              |
| 18:UO:82:ASP:OD1   | 18:UO:83:VAL:N      | 2.30                     | 0.65              |
| 22:US:286:ILE:HA   | 22:US:289:PHE:HB2   | 1.78                     | 0.65              |
| 33:CJ:245:VAL:HG11 | 34:CK:373:ILE:HG21  | 1.77                     | 0.65              |
| 35:CL:187:LYS:HG3  | 35:CL:206:TYR:CE1   | 2.31                     | 0.65              |
| 53:DI:21:PHE:HD2   | 53:DI:22:ARG:HD3    | 1.60                     | 0.65              |
| 54:DJ:59:LEU:HD21  | 54:DJ:72:GLU:HG2    | 1.78                     | 0.65              |
| 56:DN:121:ARG:NH1  | 66:D3:868:G:OP1     | 2.27                     | 0.65              |
| 61:DX:130:VAL:HG13 | 61:DX:135:LEU:HD11  | 1.77                     | 0.65              |
| 65:D2:21:A:H2'     | 65:D2:22:A:H8       | 1.62                     | 0.65              |
| 66:D3:641:G:N2     | 66:D3:693:U:O2      | 2.22                     | 0.65              |
| 2:DA:134:VAL:HG13  | 2:DA:218:LEU:HB2    | 1.76                     | 0.65              |
| 5:UB:433:ILE:HG12  | 5:UB:455:LEU:HD13   | 1.78                     | 0.65              |
| 8:UE:215:TYR:HD1   | 8:UE:222:THR:HA     | 1.60                     | 0.65              |
| 10:UG:333:SER:HB2  | 10:UG:378:VAL:HG11  | 1.78                     | 0.65              |
| 10:UG:431:ARG:NH2  | 67:D4:37:G:N3       | 2.45                     | 0.65              |
| 13:UJ:255:ILE:HD11 | 20:UQ:884:MET:HG2   | 1.77                     | 0.65              |
| 24:UU:366:MET:O    | 24:UU:377:SER:HA    | 1.97                     | 0.65              |
| 33:CJ:181:ASN:OD1  | 33:CJ:182:GLN:N     | 2.30                     | 0.65              |
| 65:D2:409:C:H2'    | 65:D2:410:A:C8      | 2.32                     | 0.65              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 66:D3:54:C:O2      | 66:D3:426:G:N2     | 2.17                     | 0.65              |
| 66:D3:1073:G:H2'   | 66:D3:1074:G:H8    | 1.60                     | 0.65              |
| 3:JA:91:MET:SD     | 3:JA:91:MET:N      | 2.69                     | 0.65              |
| 4:UA:373:ASP:OD1   | 4:UA:374:ILE:N     | 2.28                     | 0.65              |
| 9:UF:16:ASP:OD2    | 10:UG:15:ARG:NH1   | 2.28                     | 0.65              |
| 11:UH:254:GLY:O    | 11:UH:258:PRO:CA   | 2.43                     | 0.65              |
| 14:UK:165:ARG:HH12 | 19:UP:176:PHE:HZ   | 1.45                     | 0.65              |
| 15:UL:341:ALA:HB1  | 15:UL:353:LEU:HD11 | 1.78                     | 0.65              |
| 15:UL:439:LEU:HD12 | 15:UL:440:PRO:HD2  | 1.79                     | 0.65              |
| 23:UT:56:GLU:O     | 62:DY:21:LYS:NZ    | 2.28                     | 0.65              |
| 23:UT:1952:SER:HB2 | 23:UT:1995:ARG:HD2 | 1.78                     | 0.65              |
| 25:UV:1186:ILE:O   | 25:UV:1191:LYS:NZ  | 2.29                     | 0.65              |
| 27:UZ:84:ARG:NH2   | 66:D3:1478:G:H4'   | 2.12                     | 0.65              |
| 30:CF:115:TYR:HA   | 30:CF:118:LYS:HG2  | 1.77                     | 0.65              |
| 31:CH:164:GLN:NE2  | 31:CH:528:GLU:O    | 2.30                     | 0.65              |
| 33:CJ:150:THR:HA   | 33:CJ:167:LEU:O    | 1.97                     | 0.65              |
| 33:CJ:290:LEU:HD11 | 66:D3:563:U:H5'    | 1.78                     | 0.65              |
| 47:JP:180:SER:OG   | 52:DH:147:ASN:ND2  | 2.30                     | 0.65              |
| 3:JA:9:ARG:NH1     | 3:JA:216:VAL:O     | 2.29                     | 0.65              |
| 4:UA:420:ARG:HA    | 34:CK:468:ARG:HH12 | 1.62                     | 0.65              |
| 1:CB:166:PRO:HA    | 1:CB:188:VAL:HA    | 1.79                     | 0.65              |
| 1:CB:237:VAL:HG12  | 1:CB:260:PHE:HB3   | 1.78                     | 0.65              |
| 13:UJ:219:ASN:OD1  | 20:UQ:872:PHE:HB2  | 1.97                     | 0.65              |
| 13:UJ:1555:ALA:O   | 13:UJ:1571:ARG:NH1 | 2.30                     | 0.65              |
| 18:UO:34:GLN:HB2   | 18:UO:71:ARG:HH21  | 1.60                     | 0.65              |
| 35:CL:616:ASP:OD1  | 35:CL:617:THR:N    | 2.30                     | 0.65              |
| 35:CL:1086:MET:HE2 | 65:D2:408:U:H1'    | 1.78                     | 0.65              |
| 51:DG:137:ARG:HH22 | 66:D3:144:U:H5     | 1.45                     | 0.65              |
| 66:D3:161:U:H2'    | 66:D3:162:A:H8     | 1.62                     | 0.65              |
| 66:D3:1050:G:N2    | 66:D3:1051:G:N3    | 2.44                     | 0.65              |
| 1:CA:122:ARG:HD2   | 1:CA:140:GLU:OE2   | 1.96                     | 0.65              |
| 4:UA:491:ALA:HB1   | 4:UA:518:VAL:HG23  | 1.79                     | 0.65              |
| 9:UF:31:LEU:HD11   | 21:UR:27:PHE:CD1   | 2.32                     | 0.65              |
| 10:UG:67:LEU:HB3   | 10:UG:410:ASN:ND2  | 2.12                     | 0.65              |
| 11:UH:313:LYS:O    | 11:UH:322:SER:N    | 2.30                     | 0.65              |
| 12:UI:447:ASN:ND2  | 12:UI:449:GLU:OE2  | 2.30                     | 0.65              |
| 13:UJ:258:HIS:HB3  | 13:UJ:298:THR:HG21 | 1.78                     | 0.65              |
| 14:UK:249:LYS:HD3  | 67:D4:328:A:H3'    | 1.77                     | 0.65              |
| 23:UT:438:GLU:HA   | 23:UT:764:ARG:HH22 | 1.62                     | 0.65              |
| 23:UT:798:PRO:O    | 23:UT:802:ASN:ND2  | 2.30                     | 0.65              |
| 24:UU:583:GLY:HA3  | 24:UU:610:ARG:HH12 | 1.62                     | 0.65              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 33:CJ:92:THR:HG21   | 33:CJ:96:PRO:HB3    | 1.77                     | 0.65              |
| 35:CL:124:ASP:OD1   | 35:CL:126:ASN:ND2   | 2.29                     | 0.65              |
| 35:CL:873:LYS:NZ    | 66:D3:574:G:OP2     | 2.30                     | 0.65              |
| 39:JG:88:ARG:HD2    | 39:JG:91:ILE:HG23   | 1.79                     | 0.65              |
| 42:JJ:210:GLY:HA2   | 42:JJ:213:LYS:HD2   | 1.79                     | 0.65              |
| 50:DF:81:ARG:NH1    | 66:D3:1616:G:OP1    | 2.29                     | 0.65              |
| 50:DF:165:LEU:O     | 50:DF:169:ASN:ND2   | 2.30                     | 0.65              |
| 4:UA:80:ILE:HD11    | 4:UA:89:VAL:HG22    | 1.78                     | 0.64              |
| 4:UA:633:LYS:HE2    | 65:D2:293:U:H5      | 1.62                     | 0.64              |
| 1:CB:91:HIS:HE1     | 14:UK:164:ASN:HA    | 1.61                     | 0.64              |
| 5:UB:703:GLN:HB3    | 22:US:417:HIS:CE1   | 2.32                     | 0.64              |
| 8:UE:89:SER:OG      | 8:UE:92:ALA:O       | 2.13                     | 0.64              |
| 13:UJ:137:LEU:HD11  | 13:UJ:191:LEU:HD21  | 1.78                     | 0.64              |
| 18:UO:5:ARG:HH12    | 65:D2:87:C:P        | 2.19                     | 0.64              |
| 18:UO:278:ASP:OD1   | 22:US:331:ASN:ND2   | 2.30                     | 0.64              |
| 23:UT:251:ALA:HA    | 23:UT:254:ILE:HD12  | 1.78                     | 0.64              |
| 27:UZ:54:PRO:HG3    | 27:UZ:152:TYR:HA    | 1.79                     | 0.64              |
| 32:CI:104:SER:OG    | 65:D2:393:C:OP2     | 2.14                     | 0.64              |
| 39:JF:123:GLU:HB3   | 39:JF:161:LYS:HB3   | 1.79                     | 0.64              |
| 66:D3:329:G:H2'     | 66:D3:330:G:C8      | 2.33                     | 0.64              |
| 66:D3:683:C:H2'     | 66:D3:684:A:H8      | 1.61                     | 0.64              |
| 66:D3:1151:A:H2'    | 66:D3:1152:A:H8     | 1.62                     | 0.64              |
| 10:UG:214:LEU:HD21  | 10:UG:216:TYR:HE1   | 1.63                     | 0.64              |
| 24:UU:738:ASP:OD1   | 42:JJ:269:ARG:NH2   | 2.31                     | 0.64              |
| 25:UV:906:TYR:HE1   | 25:UV:950:ILE:HD11  | 1.62                     | 0.64              |
| 26:UX:91:LEU:HD22   | 54:DJ:54:ARG:HH11   | 1.62                     | 0.64              |
| 32:CI:54:ILE:HD13   | 32:CI:82:LEU:HD21   | 1.79                     | 0.64              |
| 32:CI:131:ILE:HG12  | 32:CI:136:VAL:HG11  | 1.78                     | 0.64              |
| 35:CL:177:PHE:HD2   | 35:CL:183:LEU:HA    | 1.61                     | 0.64              |
| 44:JM:50:SER:OG     | 44:JM:51:LYS:N      | 2.26                     | 0.64              |
| 49:DE:184:THR:N     | 49:DE:224:ASN:O     | 2.21                     | 0.64              |
| 52:DH:80:GLU:HA     | 52:DH:83:LYS:HD2    | 1.80                     | 0.64              |
| 3:JA:827:ARG:HG2    | 3:JA:830:LEU:HD12   | 1.79                     | 0.64              |
| 10:UG:162:ASN:ND2   | 10:UG:429:GLU:OE1   | 2.30                     | 0.64              |
| 23:UT:365:PHE:O     | 23:UT:369:SER:HB3   | 1.96                     | 0.64              |
| 23:UT:969:SER:O     | 23:UT:972:LEU:C     | 2.36                     | 0.64              |
| 23:UT:1211:ILE:HD12 | 23:UT:1216:VAL:HG21 | 1.79                     | 0.64              |
| 24:UU:717:ASP:OD1   | 24:UU:718:LYS:N     | 2.30                     | 0.64              |
| 30:CF:33:LEU:HD11   | 30:CF:100:ALA:HB1   | 1.79                     | 0.64              |
| 36:CM:107:ALA:HB1   | 36:CM:170:VAL:HG11  | 1.79                     | 0.64              |
| 51:DG:52:ILE:HA     | 51:DG:111:LEU:HD13  | 1.79                     | 0.64              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 65:D2:398:A:H2      | 65:D2:460:U:C2      | 2.14                     | 0.64              |
| 10:UG:123:THR:OG1   | 10:UG:140:ARG:NH1   | 2.30                     | 0.64              |
| 13:UJ:214:THR:O     | 13:UJ:218:ILE:HG12  | 1.97                     | 0.64              |
| 14:UK:40:ASP:HA     | 14:UK:43:ARG:HE     | 1.62                     | 0.64              |
| 18:UO:75:LYS:NZ     | 18:UO:111:TYR:O     | 2.25                     | 0.64              |
| 24:UU:511:ASP:OD1   | 24:UU:512:GLY:N     | 2.30                     | 0.64              |
| 24:UU:552:HIS:HD2   | 24:UU:555:SER:H     | 1.44                     | 0.64              |
| 28:CD:237:LEU:HD22  | 28:CD:248:ALA:HB2   | 1.80                     | 0.64              |
| 29:CE:149:ARG:HB3   | 29:CE:154:PHE:CD2   | 2.32                     | 0.64              |
| 2:DA:32:ILE:HG22    | 2:DA:96:LEU:HB2     | 1.77                     | 0.64              |
| 3:JA:541:TYR:O      | 3:JA:637:ARG:NH1    | 2.30                     | 0.64              |
| 3:JA:765:VAL:HB     | 3:JA:774:LEU:HD11   | 1.78                     | 0.64              |
| 35:CL:298:VAL:HA    | 35:CL:793:PHE:CE1   | 2.32                     | 0.64              |
| 38:JC:253:TYR:HE1   | 38:JC:265:ILE:HG23  | 1.60                     | 0.64              |
| 66:D3:952:A:H2'     | 66:D3:953:G:H8      | 1.63                     | 0.64              |
| 7:UD:336:ILE:HD11   | 7:UD:347:LEU:HD12   | 1.80                     | 0.64              |
| 14:UK:108:ARG:HH22  | 67:D4:325:C:P       | 2.20                     | 0.64              |
| 15:UL:14:PHE:HB2    | 15:UL:681:ILE:HB    | 1.79                     | 0.64              |
| 15:UL:658:SER:OG    | 15:UL:678:ASP:N     | 2.30                     | 0.64              |
| 16:UM:559:ILE:HB    | 16:UM:569:LYS:HB2   | 1.79                     | 0.64              |
| 17:UN:338:LEU:HD13  | 17:UN:341:LYS:HE3   | 1.78                     | 0.64              |
| 23:UT:1244:LEU:HD11 | 23:UT:1280:LEU:HD13 | 1.79                     | 0.64              |
| 24:UU:589:THR:HG23  | 24:UU:604:SER:HA    | 1.79                     | 0.64              |
| 27:UZ:24:CYS:HA     | 27:UZ:30:LEU:HB3    | 1.79                     | 0.64              |
| 38:JC:116:HIS:CE1   | 38:JC:126:GLN:HE22  | 2.14                     | 0.64              |
| 38:JC:227:ARG:NH1   | 38:JC:248:SER:OG    | 2.31                     | 0.64              |
| 58:DQ:12:LYS:HE2    | 58:DQ:17:THR:HG22   | 1.78                     | 0.64              |
| 60:DW:82:LYS:O      | 60:DW:86:ILE:HG12   | 1.96                     | 0.64              |
| 65:D2:314:U:O2'     | 65:D2:315:U:OP1     | 2.14                     | 0.64              |
| 1:CA:128:PRO:HA     | 1:CA:136:PRO:HA     | 1.79                     | 0.64              |
| 1:CB:106:LEU:HD21   | 1:CB:156:MET:HG3    | 1.79                     | 0.64              |
| 6:UC:604:ARG:NE     | 26:UX:44:ILE:O      | 2.27                     | 0.64              |
| 13:UJ:559:ASN:ND2   | 13:UJ:595:THR:O     | 2.30                     | 0.64              |
| 20:UQ:229:SER:OG    | 20:UQ:232:ASP:OD1   | 2.14                     | 0.64              |
| 22:US:48:THR:O      | 22:US:52:LEU:N      | 2.30                     | 0.64              |
| 23:UT:878:ASN:HD21  | 23:UT:881:LEU:HD22  | 1.62                     | 0.64              |
| 25:UV:269:ARG:NH1   | 25:UV:271:SER:OG    | 2.31                     | 0.64              |
| 25:UV:523:TYR:HD2   | 25:UV:616:LYS:HB3   | 1.62                     | 0.64              |
| 25:UV:1222:GLU:HB3  | 37:CN:60:LEU:HD21   | 1.80                     | 0.64              |
| 35:CL:618:PHE:CZ    | 36:CM:274:LYS:HE2   | 2.33                     | 0.64              |
| 46:JO:38:GLU:OE2    | 46:JO:86:ARG:NH2    | 2.30                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 50:DF:81:ARG:NH2   | 66:D3:1615:C:OP1   | 2.31                     | 0.64              |
| 52:DH:97:ARG:HE    | 52:DH:98:ILE:H     | 1.44                     | 0.64              |
| 58:DQ:100:GLN:NE2  | 58:DQ:104:GLU:OE1  | 2.30                     | 0.64              |
| 66:D3:75:U:C4      | 66:D3:76:A:H1'     | 2.32                     | 0.64              |
| 66:D3:953:G:H2'    | 66:D3:954:G:H8     | 1.63                     | 0.64              |
| 66:D3:1038:U:O2'   | 66:D3:1039:A:O5'   | 2.15                     | 0.64              |
| 66:D3:1699:G:N2    | 66:D3:1702:A:OP2   | 2.28                     | 0.64              |
| 2:DA:24:PHE:HZ     | 57:DO:39:ILE:HA    | 1.63                     | 0.64              |
| 9:UF:134:ASN:O     | 9:UF:138:LYS:HG2   | 1.97                     | 0.64              |
| 11:UH:569:GLU:O    | 11:UH:572:SER:OG   | 2.15                     | 0.64              |
| 13:UJ:112:ALA:O    | 13:UJ:116:HIS:ND1  | 2.30                     | 0.64              |
| 23:UT:43:GLU:O     | 31:CH:63:ARG:NH2   | 2.29                     | 0.64              |
| 27:UZ:73:LEU:HB3   | 27:UZ:125:VAL:HG23 | 1.80                     | 0.64              |
| 38:JC:14:TYR:HE1   | 38:JC:363:LEU:HD22 | 1.63                     | 0.64              |
| 54:DJ:108:ARG:NH2  | 54:DJ:145:SER:OG   | 2.30                     | 0.64              |
| 3:JA:752:ASN:HD21  | 3:JA:755:THR:HG1   | 1.46                     | 0.64              |
| 1:CB:241:PHE:HD1   | 1:CB:268:VAL:HG13  | 1.62                     | 0.64              |
| 7:UD:76:ILE:HG13   | 7:UD:91:ILE:HB     | 1.78                     | 0.64              |
| 13:UJ:25:ARG:HH12  | 47:JP:16:VAL:HG12  | 1.63                     | 0.64              |
| 15:UL:592:SER:OG   | 15:UL:594:ASP:OD1  | 2.13                     | 0.64              |
| 21:UR:399:LYS:NZ   | 21:UR:401:GLU:OE1  | 2.25                     | 0.64              |
| 24:UU:173:LEU:HD22 | 24:UU:221:ILE:HD11 | 1.80                     | 0.64              |
| 27:UZ:164:ARG:NH1  | 65:D2:257:G:O3'    | 2.29                     | 0.64              |
| 34:CK:366:GLU:HB3  | 34:CK:370:ARG:HH22 | 1.63                     | 0.64              |
| 45:JN:294:ARG:NH2  | 66:D3:7:G:OP2      | 2.31                     | 0.64              |
| 51:DG:138:ALA:HA   | 51:DG:141:ILE:HD12 | 1.79                     | 0.64              |
| 55:DL:65:SER:HB3   | 66:D3:247:A:H2     | 1.63                     | 0.64              |
| 66:D3:1673:G:N2    | 66:D3:1729:C:O2    | 2.31                     | 0.64              |
| 2:DA:180:THR:OG1   | 2:DA:183:GLN:OE1   | 2.11                     | 0.64              |
| 4:UA:514:VAL:HG11  | 4:UA:534:THR:HG21  | 1.80                     | 0.64              |
| 5:UB:554:GLN:OE1   | 5:UB:559:ARG:N     | 2.29                     | 0.64              |
| 8:UE:473:LYS:HG2   | 8:UE:474:PRO:HD2   | 1.80                     | 0.64              |
| 14:UK:116:LYS:O    | 14:UK:119:GLU:HG3  | 1.97                     | 0.64              |
| 15:UL:41:LEU:HB2   | 15:UL:54:ILE:HD11  | 1.79                     | 0.64              |
| 17:UN:299:ASN:HD21 | 66:D3:-7:A:H5'     | 1.62                     | 0.64              |
| 20:UQ:258:TYR:CE2  | 20:UQ:414:ILE:HG12 | 2.33                     | 0.64              |
| 20:UQ:443:ASN:O    | 20:UQ:447:LYS:CA   | 2.46                     | 0.64              |
| 21:UR:148:THR:N    | 21:UR:152:GLU:OE1  | 2.20                     | 0.64              |
| 25:UV:373:ARG:O    | 25:UV:522:LYS:NZ   | 2.31                     | 0.64              |
| 25:UV:586:VAL:O    | 25:UV:611:ASP:N    | 2.24                     | 0.64              |
| 27:UZ:235:ILE:HG21 | 27:UZ:239:ILE:HG22 | 1.80                     | 0.64              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 35:CL:161:HIS:HA    | 61:DX:144:ARG:HH12  | 1.62                     | 0.64              |
| 37:CN:223:LEU:HG    | 37:CN:227:ARG:HH12  | 1.61                     | 0.64              |
| 44:JM:193:GLU:O     | 44:JM:196:GLU:HG3   | 1.98                     | 0.64              |
| 46:JO:255:GLN:NE2   | 46:JO:256:LEU:O     | 2.31                     | 0.64              |
| 50:DF:40:ILE:HG23   | 50:DF:69:PHE:CE2    | 2.32                     | 0.64              |
| 66:D3:891:A:H2'     | 66:D3:892:A:H8      | 1.63                     | 0.64              |
| 23:UT:408:VAL:O     | 23:UT:411:PHE:C     | 2.37                     | 0.63              |
| 31:CH:241:THR:HG21  | 31:CH:285:SER:HA    | 1.80                     | 0.63              |
| 38:JC:192:ASN:HB3   | 43:JK:485:TRP:HZ3   | 1.61                     | 0.63              |
| 45:JN:308:ILE:HG21  | 60:DW:95:PRO:HG3    | 1.80                     | 0.63              |
| 60:DW:35:ILE:O      | 60:DW:39:GLN:HG3    | 1.97                     | 0.63              |
| 1:CB:297:ARG:NH2    | 1:CB:322:ARG:O      | 2.31                     | 0.63              |
| 7:UD:322:ASN:HB3    | 20:UQ:329:ASN:HD22  | 1.63                     | 0.63              |
| 15:UL:414:LEU:HB3   | 15:UL:428:PHE:HB2   | 1.79                     | 0.63              |
| 15:UL:837:ASP:OD1   | 15:UL:882:ARG:NH1   | 2.30                     | 0.63              |
| 20:UQ:388:PRO:HG2   | 20:UQ:781:SER:HB3   | 1.79                     | 0.63              |
| 21:UR:138:LEU:HA    | 21:UR:144:LYS:HB3   | 1.80                     | 0.63              |
| 22:US:350:MET:HG2   | 22:US:355:ARG:HH11  | 1.62                     | 0.63              |
| 23:UT:1951:THR:HG21 | 23:UT:1986:VAL:HG12 | 1.79                     | 0.63              |
| 25:UV:305:PRO:HA    | 25:UV:308:LEU:HB3   | 1.80                     | 0.63              |
| 58:DQ:17:THR:OG1    | 58:DQ:70:THR:OG1    | 2.15                     | 0.63              |
| 66:D3:898:A:N1      | 66:D3:911:U:O2'     | 2.31                     | 0.63              |
| 2:DA:155:TYR:OH     | 66:D3:932:U:OP2     | 2.16                     | 0.63              |
| 10:UG:502:ARG:NH2   | 65:D2:369:G:N7      | 2.36                     | 0.63              |
| 11:UH:678:LEU:HB3   | 12:UI:460:LEU:HD22  | 1.79                     | 0.63              |
| 13:UJ:407:PHE:O     | 13:UJ:410:ILE:O     | 2.15                     | 0.63              |
| 14:UK:142:LYS:HA    | 14:UK:145:GLU:HG2   | 1.81                     | 0.63              |
| 15:UL:861:ILE:HD11  | 16:UM:805:ILE:HG23  | 1.79                     | 0.63              |
| 20:UQ:298:ASP:OD2   | 20:UQ:299:SER:N     | 2.28                     | 0.63              |
| 23:UT:675:SER:HA    | 23:UT:678:TRP:CE3   | 2.34                     | 0.63              |
| 24:UU:97:LYS:HD2    | 24:UU:109:LEU:HD11  | 1.80                     | 0.63              |
| 33:CJ:119:ARG:HD2   | 33:CJ:122:TYR:HB2   | 1.80                     | 0.63              |
| 35:CL:762:LEU:HD13  | 35:CL:765:ASN:HD22  | 1.64                     | 0.63              |
| 46:JO:193:ASN:OD1   | 66:D3:1028:C:N4     | 2.31                     | 0.63              |
| 52:DH:25:VAL:O      | 52:DH:29:ASN:ND2    | 2.27                     | 0.63              |
| 57:DO:41:ARG:NH2    | 66:D3:916:U:H3      | 1.95                     | 0.63              |
| 65:D2:146:G:H2'     | 65:D2:147:C:C6      | 2.32                     | 0.63              |
| 66:D3:279:G:H8      | 66:D3:280:U:H4'     | 1.63                     | 0.63              |
| 10:UG:543:LYS:NZ    | 10:UG:544:ASP:H     | 1.97                     | 0.63              |
| 20:UQ:167:SER:OG    | 65:D2:64:U:OP2      | 2.16                     | 0.63              |
| 33:CJ:287:LYS:NZ    | 33:CJ:288:ASP:O     | 2.31                     | 0.63              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 35:CL:254:HIS:HB2  | 35:CL:257:LEU:HB2   | 1.79                     | 0.63              |
| 35:CL:790:ARG:HG2  | 35:CL:790:ARG:HH11  | 1.61                     | 0.63              |
| 55:DL:123:VAL:HG12 | 55:DL:142:VAL:HA    | 1.79                     | 0.63              |
| 61:DX:43:PHE:CE2   | 61:DX:49:ALA:HB2    | 2.33                     | 0.63              |
| 66:D3:164:A:H2'    | 66:D3:165:G:C8      | 2.32                     | 0.63              |
| 66:D3:640:U:H2'    | 66:D3:641:G:H8      | 1.62                     | 0.63              |
| 67:D4:329:C:H2'    | 67:D4:330:A:H8      | 1.63                     | 0.63              |
| 3:JA:500:PRO:O     | 3:JA:504:THR:OG1    | 2.16                     | 0.63              |
| 4:UA:482:SER:O     | 4:UA:486:SER:N      | 2.31                     | 0.63              |
| 12:UI:412:THR:HA   | 12:UI:451:LEU:HD11  | 1.81                     | 0.63              |
| 12:UI:485:ALA:O    | 12:UI:488:SER:OG    | 2.17                     | 0.63              |
| 18:UO:248:ARG:NH2  | 18:UO:289:ASN:O     | 2.32                     | 0.63              |
| 18:UO:268:MET:SD   | 18:UO:285:ASP:HB3   | 2.39                     | 0.63              |
| 20:UQ:215:VAL:HA   | 20:UQ:218:LYS:HG2   | 1.79                     | 0.63              |
| 22:US:472:HIS:CD2  | 22:US:474:HIS:H     | 2.17                     | 0.63              |
| 25:UV:1096:TYR:HA  | 25:UV:1185:LEU:HD21 | 1.80                     | 0.63              |
| 30:CG:8:ALA:HB3    | 31:CH:465:GLN:NE2   | 2.13                     | 0.63              |
| 38:JC:66:ARG:HB2   | 38:JC:109:ASP:HA    | 1.81                     | 0.63              |
| 40:JH:399:ILE:HA   | 40:JH:409:ALA:HB1   | 1.80                     | 0.63              |
| 45:JN:157:GLN:HG2  | 45:JN:214:ARG:HH21  | 1.64                     | 0.63              |
| 49:DE:191:ARG:HH11 | 49:DE:245:LYS:HD3   | 1.63                     | 0.63              |
| 58:DQ:79:TYR:O     | 58:DQ:82:ARG:HG2    | 1.99                     | 0.63              |
| 61:DX:65:ASN:H     | 61:DX:69:ARG:HG2    | 1.64                     | 0.63              |
| 66:D3:476:U:OP1    | 66:D3:477:A:O2'     | 2.10                     | 0.63              |
| 66:D3:845:G:N7     | 66:D3:846:G:N2      | 2.46                     | 0.63              |
| 4:UA:713:ASP:O     | 4:UA:746:ASN:ND2    | 2.31                     | 0.63              |
| 7:UD:122:VAL:HG11  | 19:UP:192:PRO:HD2   | 1.81                     | 0.63              |
| 16:UM:104:PRO:O    | 16:UM:122:THR:N     | 2.23                     | 0.63              |
| 16:UM:111:ASP:OD1  | 16:UM:112:SER:N     | 2.32                     | 0.63              |
| 20:UQ:144:VAL:HG22 | 20:UQ:153:ILE:HG22  | 1.81                     | 0.63              |
| 20:UQ:483:LYS:HG2  | 20:UQ:487:GLU:HB3   | 1.81                     | 0.63              |
| 21:UR:15:PRO:HB2   | 21:UR:20:GLN:HE21   | 1.63                     | 0.63              |
| 21:UR:427:ASN:OD1  | 21:UR:428:ALA:N     | 2.32                     | 0.63              |
| 23:UT:597:ARG:HG3  | 23:UT:626:GLU:OE2   | 1.98                     | 0.63              |
| 23:UT:1648:GLU:OE2 | 23:UT:1651:ARG:NH1  | 2.32                     | 0.63              |
| 24:UU:154:TYR:OH   | 24:UU:194:ARG:O     | 2.13                     | 0.63              |
| 35:CL:59:VAL:HG21  | 35:CL:61:ARG:CZ     | 2.29                     | 0.63              |
| 52:DH:75:THR:HG23  | 52:DH:76:LYS:HD3    | 1.80                     | 0.63              |
| 66:D3:1140:G:H2'   | 66:D3:1141:G:H8     | 1.64                     | 0.63              |
| 66:D3:1680:G:O4'   | 66:D3:1721:A:N6     | 2.30                     | 0.63              |
| 4:UA:160:PHE:CZ    | 4:UA:183:ALA:HB3    | 2.34                     | 0.63              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 4:UA:303:ASN:HD21   | 4:UA:324:LEU:HD23   | 1.64                     | 0.63              |
| 4:UA:420:ARG:HG3    | 34:CK:468:ARG:NH2   | 2.14                     | 0.63              |
| 1:CB:184:VAL:HG23   | 1:CB:194:VAL:HG11   | 1.80                     | 0.63              |
| 7:UD:476:LYS:N      | 7:UD:489:CYS:O      | 2.32                     | 0.63              |
| 11:UH:524:THR:O     | 11:UH:553:GLN:NE2   | 2.31                     | 0.63              |
| 15:UL:180:THR:HG21  | 15:UL:210:LEU:HD21  | 1.80                     | 0.63              |
| 18:UO:279:GLY:O     | 18:UO:297:LYS:HA    | 1.99                     | 0.63              |
| 23:UT:1711:ASP:OD2  | 23:UT:1762:SER:OG   | 2.16                     | 0.63              |
| 24:UU:366:MET:HG3   | 24:UU:380:LEU:HD11  | 1.80                     | 0.63              |
| 25:UV:412:LEU:HD12  | 25:UV:421:LEU:HD23  | 1.79                     | 0.63              |
| 27:UZ:209:ILE:H     | 27:UZ:209:ILE:HD12  | 1.63                     | 0.63              |
| 32:CI:29:ASP:OD1    | 32:CI:30:THR:N      | 2.31                     | 0.63              |
| 33:CJ:89:ILE:HG23   | 33:CJ:117:LEU:HD13  | 1.81                     | 0.63              |
| 38:JC:17:SER:HG     | 38:JC:340:THR:H     | 1.46                     | 0.63              |
| 38:JC:148:LYS:O     | 43:JK:479:ILE:HD12  | 1.98                     | 0.63              |
| 65:D2:324:U:H2'     | 65:D2:327:A:C8      | 2.34                     | 0.63              |
| 66:D3:1775:U:H3     | 66:D3:1786:G:H1     | 1.45                     | 0.63              |
| 3:JA:35:ASN:O       | 3:JA:39:ASN:ND2     | 2.32                     | 0.63              |
| 3:JA:173:ARG:NH1    | 3:JA:521:ASP:OD2    | 2.30                     | 0.63              |
| 6:UC:608:PHE:HD2    | 26:UX:147:GLN:HE21  | 1.47                     | 0.63              |
| 7:UD:397:SER:O      | 7:UD:421:THR:CA     | 2.35                     | 0.63              |
| 8:UE:115:ASN:ND2    | 8:UE:130:ASP:OD1    | 2.32                     | 0.63              |
| 11:UH:55:TYR:HA     | 11:UH:72:THR:HA     | 1.81                     | 0.63              |
| 20:UQ:277:SER:OG    | 65:D2:82:A:OP2      | 2.15                     | 0.63              |
| 21:UR:435:PHE:CE1   | 21:UR:443:VAL:HG12  | 2.33                     | 0.63              |
| 23:UT:1527:LEU:HD22 | 23:UT:1551:LEU:HD13 | 1.81                     | 0.63              |
| 25:UV:1148:GLN:HA   | 25:UV:1151:LYS:HZ2  | 1.63                     | 0.63              |
| 35:CL:161:HIS:O     | 61:DX:144:ARG:NH1   | 2.31                     | 0.63              |
| 35:CL:1114:GLN:NE2  | 65:D2:412:A:H1'     | 2.14                     | 0.63              |
| 36:CM:282:GLU:OE2   | 36:CM:291:ARG:N     | 2.30                     | 0.63              |
| 66:D3:391:A:H2'     | 66:D3:392:G:C8      | 2.34                     | 0.63              |
| 66:D3:647:G:H1      | 66:D3:687:G:H22     | 1.45                     | 0.63              |
| 66:D3:938:G:C2      | 66:D3:942:G:C2      | 2.87                     | 0.63              |
| 77:EJ:270:THR:H     | 77:EJ:275:MET:HA    | 1.64                     | 0.63              |
| 4:UA:828:ILE:HD11   | 24:UU:929:CYS:SG    | 2.39                     | 0.63              |
| 1:CB:294:ARG:NH2    | 19:UP:182:SER:OG    | 2.32                     | 0.63              |
| 5:UB:712:THR:O      | 5:UB:713:HIS:ND1    | 2.31                     | 0.63              |
| 7:UD:120:SER:OG     | 7:UD:121:THR:N      | 2.31                     | 0.63              |
| 7:UD:347:LEU:HB3    | 7:UD:361:LEU:HD21   | 1.81                     | 0.63              |
| 7:UD:767:LYS:HZ2    | 19:UP:214:GLY:N     | 1.97                     | 0.63              |
| 8:UE:128:GLN:HG3    | 8:UE:137:LEU:HB2    | 1.81                     | 0.63              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 11:UH:636:GLN:OE1  | 20:UQ:605:ASN:ND2   | 2.26                     | 0.63              |
| 13:UJ:304:GLN:HE22 | 13:UJ:347:PHE:H     | 1.46                     | 0.63              |
| 15:UL:162:HIS:O    | 34:CK:522:ARG:NH2   | 2.32                     | 0.63              |
| 15:UL:298:LYS:O    | 15:UL:301:LYS:HG2   | 1.98                     | 0.63              |
| 20:UQ:40:ASP:O     | 20:UQ:42:ARG:N      | 2.31                     | 0.63              |
| 28:CD:323:THR:HA   | 28:CD:391:ASN:ND2   | 2.13                     | 0.63              |
| 31:CH:327:ASP:O    | 31:CH:338:THR:HA    | 1.98                     | 0.63              |
| 34:CK:330:VAL:HG11 | 35:CL:932:LEU:HD12  | 1.81                     | 0.63              |
| 37:CN:63:ASN:OD1   | 37:CN:66:HIS:ND1    | 2.29                     | 0.63              |
| 46:JO:218:GLU:N    | 46:JO:218:GLU:OE2   | 2.32                     | 0.63              |
| 52:DH:38:LEU:HA    | 52:DH:41:LEU:HD13   | 1.80                     | 0.63              |
| 53:DI:191:PHE:O    | 53:DI:194:ARG:HG3   | 1.99                     | 0.63              |
| 62:DY:109:LYS:NZ   | 66:D3:54:C:O3'      | 2.31                     | 0.63              |
| 67:D4:94:A:H61     | 67:D4:322:A:H61     | 1.45                     | 0.63              |
| 78:EK:300:LEU:O    | 78:EK:389:THR:HA    | 1.98                     | 0.63              |
| 2:DA:146:GLN:H     | 2:DA:149:GLN:HE21   | 1.47                     | 0.62              |
| 3:JA:508:PRO:O     | 3:JA:649:TYR:OH     | 2.17                     | 0.62              |
| 5:UB:612:THR:HG23  | 5:UB:614:ILE:H      | 1.63                     | 0.62              |
| 8:UE:23:ALA:HB1    | 21:UR:261:PRO:HG3   | 1.80                     | 0.62              |
| 9:UF:167:ILE:HD11  | 17:UN:327:PHE:CD2   | 2.34                     | 0.62              |
| 14:UK:70:ARG:HH21  | 14:UK:78:LEU:HD22   | 1.64                     | 0.62              |
| 14:UK:147:THR:HB   | 14:UK:150:LYS:HE2   | 1.80                     | 0.62              |
| 15:UL:22:ASN:HD21  | 15:UL:85:LEU:H      | 1.47                     | 0.62              |
| 15:UL:555:VAL:HB   | 15:UL:569:LEU:HB2   | 1.79                     | 0.62              |
| 16:UM:490:HIS:ND1  | 16:UM:512:ASP:OD2   | 2.32                     | 0.62              |
| 17:UN:336:THR:HG22 | 17:UN:338:LEU:H     | 1.64                     | 0.62              |
| 20:UQ:711:ILE:HD13 | 20:UQ:722:LEU:HD13  | 1.81                     | 0.62              |
| 23:UT:443:PRO:O    | 23:UT:449:ARG:NH2   | 2.31                     | 0.62              |
| 23:UT:513:ASN:HA   | 23:UT:516:LYS:HD2   | 1.80                     | 0.62              |
| 25:UV:705:HIS:HA   | 25:UV:708:LEU:HD12  | 1.81                     | 0.62              |
| 28:CD:79:LYS:NZ    | 28:CD:112:GLU:OE2   | 2.32                     | 0.62              |
| 30:CG:7:LYS:HG3    | 31:CH:463:GLN:HE22  | 1.64                     | 0.62              |
| 35:CL:968:THR:HG22 | 35:CL:1001:VAL:HG12 | 1.81                     | 0.62              |
| 38:JC:110:ASP:OD2  | 38:JC:111:TRP:N     | 2.32                     | 0.62              |
| 39:JG:163:ILE:HD12 | 39:JG:170:HIS:CG    | 2.34                     | 0.62              |
| 46:JO:252:PRO:HG3  | 56:DN:112:LYS:HG3   | 1.79                     | 0.62              |
| 66:D3:427:C:O2'    | 66:D3:459:G:N3      | 2.32                     | 0.62              |
| 7:UD:202:ILE:HD11  | 7:UD:267:PHE:HE2    | 1.64                     | 0.62              |
| 16:UM:749:ASN:OD1  | 16:UM:750:ALA:N     | 2.29                     | 0.62              |
| 20:UQ:469:ASN:OD1  | 20:UQ:470:TYR:N     | 2.32                     | 0.62              |
| 23:UT:77:LEU:HA    | 23:UT:80:ILE:HD12   | 1.79                     | 0.62              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 31:CH:504:ASN:HB2   | 31:CH:506:ARG:CZ    | 2.29                     | 0.62              |
| 35:CL:91:ARG:HH22   | 35:CL:214:ARG:NE    | 1.97                     | 0.62              |
| 35:CL:921:GLU:CD    | 36:CM:365:LYS:HD2   | 2.20                     | 0.62              |
| 36:CM:67:ILE:HG12   | 36:CM:74:VAL:HG22   | 1.81                     | 0.62              |
| 38:JC:59:SER:OG     | 38:JC:333:ASN:N     | 2.31                     | 0.62              |
| 52:DH:56:LYS:HB3    | 52:DH:88:ARG:NH1    | 2.13                     | 0.62              |
| 53:DI:52:ASN:ND2    | 66:D3:333:A:OP1     | 2.32                     | 0.62              |
| 66:D3:139:C:N4      | 66:D3:175:G:N3      | 2.45                     | 0.62              |
| 66:D3:552:G:N1      | 66:D3:587:C:O2      | 2.32                     | 0.62              |
| 1:CA:195:TYR:HD1    | 1:CA:218:ILE:HG12   | 1.63                     | 0.62              |
| 1:CA:222:GLU:OE2    | 1:CA:229:LYS:HD2    | 1.99                     | 0.62              |
| 2:DA:223:PHE:HE2    | 2:DA:228:LEU:HD12   | 1.64                     | 0.62              |
| 3:JA:144:GLY:HA3    | 3:JA:476:TYR:HB3    | 1.81                     | 0.62              |
| 7:UD:271:THR:HG22   | 7:UD:272:LEU:N      | 2.12                     | 0.62              |
| 10:UG:329:LEU:HD13  | 10:UG:406:ALA:HA    | 1.81                     | 0.62              |
| 14:UK:120:LYS:NZ    | 67:D4:320:G:OP1     | 2.27                     | 0.62              |
| 15:UL:299:ARG:HA    | 15:UL:302:ARG:HD2   | 1.81                     | 0.62              |
| 20:UQ:357:ILE:HD12  | 20:UQ:371:PHE:CD1   | 2.34                     | 0.62              |
| 23:UT:1763:LEU:HA   | 23:UT:1766:PHE:HE2  | 1.62                     | 0.62              |
| 24:UU:613:ASP:HB2   | 24:UU:620:ILE:HD13  | 1.81                     | 0.62              |
| 25:UV:1163:LEU:HD11 | 25:UV:1182:ILE:HG22 | 1.80                     | 0.62              |
| 26:UX:100:ASP:OD1   | 26:UX:127:ARG:NH2   | 2.32                     | 0.62              |
| 33:CJ:82:GLY:H      | 33:CJ:83:ILE:HD12   | 1.63                     | 0.62              |
| 36:CM:55:LEU:HB2    | 36:CM:88:HIS:CE1    | 2.34                     | 0.62              |
| 38:JC:51:GLN:NE2    | 38:JC:90:SER:OG     | 2.25                     | 0.62              |
| 39:JF:99:LEU:HD21   | 39:JF:238:CYS:HB2   | 1.80                     | 0.62              |
| 66:D3:1115:U:H2'    | 66:D3:1116:A:H8     | 1.65                     | 0.62              |
| 66:D3:1511:U:H2'    | 66:D3:1512:G:C8     | 2.34                     | 0.62              |
| 4:UA:518:VAL:HG12   | 4:UA:534:THR:HG22   | 1.81                     | 0.62              |
| 4:UA:656:ARG:NH1    | 10:UG:210:GLU:OE1   | 2.32                     | 0.62              |
| 6:UC:541:ASN:OD1    | 6:UC:542:TYR:N      | 2.32                     | 0.62              |
| 13:UJ:1581:LYS:NZ   | 13:UJ:1584:GLU:OE2  | 2.26                     | 0.62              |
| 23:UT:689:TYR:CE2   | 23:UT:785:ILE:HG12  | 2.34                     | 0.62              |
| 23:UT:1893:GLU:HA   | 23:UT:1896:ILE:HD12 | 1.81                     | 0.62              |
| 24:UU:308:PRO:HB2   | 24:UU:324:PHE:HB2   | 1.80                     | 0.62              |
| 28:CD:196:LYS:HA    | 28:CD:216:PHE:CZ    | 2.33                     | 0.62              |
| 29:CE:14:LEU:HD23   | 29:CE:45:ALA:HB3    | 1.82                     | 0.62              |
| 31:CH:140:LEU:HD11  | 31:CH:537:PHE:HD2   | 1.63                     | 0.62              |
| 47:JP:440:ARG:HG3   | 66:D3:1069:A:H5''   | 1.82                     | 0.62              |
| 52:DH:162:ILE:HA    | 52:DH:165:LYS:HD2   | 1.82                     | 0.62              |
| 53:DI:10:LYS:NZ     | 66:D3:323:A:OP2     | 2.23                     | 0.62              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 53:DI:175:GLN:NE2   | 66:D3:332:U:OP2     | 2.27                     | 0.62              |
| 60:DW:57:ARG:HB3    | 66:D3:863:A:H4'     | 1.82                     | 0.62              |
| 66:D3:1629:G:N1     | 66:D3:1637:C:O2     | 2.32                     | 0.62              |
| 67:D4:205:G:N2      | 67:D4:206:C:N3      | 2.47                     | 0.62              |
| 5:UB:422:LEU:HD22   | 5:UB:466:TYR:CD2    | 2.34                     | 0.62              |
| 7:UD:343:GLY:O      | 7:UD:682:THR:OG1    | 2.13                     | 0.62              |
| 16:UM:226:ASN:HD22  | 16:UM:230:LYS:HG3   | 1.63                     | 0.62              |
| 16:UM:403:ILE:HG13  | 16:UM:415:TRP:HB2   | 1.81                     | 0.62              |
| 23:UT:103:LEU:HD22  | 23:UT:135:LEU:HD11  | 1.82                     | 0.62              |
| 23:UT:322:VAL:HA    | 23:UT:330:ILE:HD11  | 1.81                     | 0.62              |
| 35:CL:791:ILE:HD12  | 35:CL:793:PHE:CZ    | 2.34                     | 0.62              |
| 35:CL:934:LEU:HD12  | 35:CL:1003:LEU:HD22 | 1.82                     | 0.62              |
| 35:CL:1110:ARG:NE   | 65:D2:411:A:O2'     | 2.23                     | 0.62              |
| 36:CM:249:SER:O     | 36:CM:253:GLY:CA    | 2.48                     | 0.62              |
| 49:DE:200:ARG:NH2   | 66:D3:246:G:OP2     | 2.33                     | 0.62              |
| 51:DG:46:LYS:HB2    | 51:DG:119:GLN:HE22  | 1.65                     | 0.62              |
| 52:DH:5:GLN:NE2     | 52:DH:18:LEU:O      | 2.31                     | 0.62              |
| 66:D3:365:G:H1      | 66:D3:377:G:H1'     | 1.63                     | 0.62              |
| 2:DA:175:GLU:HG2    | 2:DA:193:ILE:HD11   | 1.82                     | 0.62              |
| 7:UD:758:ASN:O      | 7:UD:763:HIS:ND1    | 2.31                     | 0.62              |
| 9:UF:368:THR:HA     | 9:UF:371:ILE:HD12   | 1.82                     | 0.62              |
| 10:UG:348:SER:OG    | 10:UG:350:ASP:OD1   | 2.12                     | 0.62              |
| 13:UJ:1655:LEU:HD23 | 13:UJ:1666:LEU:HD13 | 1.81                     | 0.62              |
| 16:UM:415:TRP:CZ2   | 16:UM:426:ILE:HD13  | 2.34                     | 0.62              |
| 16:UM:602:TRP:HB3   | 16:UM:609:CYS:HA    | 1.82                     | 0.62              |
| 20:UQ:36:ARG:HH22   | 20:UQ:90:LYS:HD2    | 1.65                     | 0.62              |
| 24:UU:853:ASN:OD1   | 24:UU:854:SER:N     | 2.32                     | 0.62              |
| 25:UV:508:SER:HA    | 25:UV:512:LEU:HD13  | 1.80                     | 0.62              |
| 36:CM:267:ILE:HG22  | 36:CM:270:GLU:H     | 1.63                     | 0.62              |
| 2:DA:105:PHE:CD2    | 2:DA:213:ARG:HA     | 2.34                     | 0.62              |
| 1:CB:184:VAL:HA     | 1:CB:187:VAL:HG12   | 1.82                     | 0.62              |
| 7:UD:571:THR:HG21   | 7:UD:632:ASN:HB3    | 1.82                     | 0.62              |
| 10:UG:67:LEU:HD13   | 10:UG:410:ASN:HD21  | 1.64                     | 0.62              |
| 11:UH:635:PHE:HD2   | 12:UI:492:ILE:HD11  | 1.64                     | 0.62              |
| 13:UJ:242:SER:HB3   | 13:UJ:261:LEU:HD21  | 1.81                     | 0.62              |
| 13:UJ:1723:LEU:HA   | 13:UJ:1726:LEU:HG   | 1.80                     | 0.62              |
| 15:UL:363:GLU:HG2   | 15:UL:381:LYS:HD2   | 1.80                     | 0.62              |
| 16:UM:457:ALA:HB3   | 16:UM:494:ILE:HD13  | 1.81                     | 0.62              |
| 20:UQ:362:GLU:HB3   | 20:UQ:454:ILE:HD11  | 1.81                     | 0.62              |
| 21:UR:557:THR:HG23  | 21:UR:559:GLY:H     | 1.64                     | 0.62              |
| 23:UT:1733:LYS:NZ   | 23:UT:1745:ILE:O    | 2.22                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:UV:959:LEU:HD23 | 25:UV:962:LEU:HD12 | 1.81                     | 0.62              |
| 34:CK:429:GLU:HA   | 34:CK:432:LYS:HD2  | 1.82                     | 0.62              |
| 34:CK:534:ARG:NH1  | 66:D3:1628:U:OP2   | 2.23                     | 0.62              |
| 35:CL:69:PRO:HB3   | 35:CL:114:ARG:HG3  | 1.81                     | 0.62              |
| 65:D2:94:A:H2'     | 65:D2:95:A:H8      | 1.63                     | 0.62              |
| 65:D2:133:U:H2'    | 65:D2:134:A:C8     | 2.35                     | 0.62              |
| 68:EA:162:U:H5'    | 79:EN:224:GLY:HA3  | 1.81                     | 0.62              |
| 4:UA:666:ARG:HA    | 4:UA:666:ARG:NE    | 2.14                     | 0.62              |
| 1:CB:218:ILE:HD11  | 29:CE:144:ALA:HB3  | 1.82                     | 0.62              |
| 7:UD:294:TYR:OH    | 7:UD:310:ASN:ND2   | 2.32                     | 0.62              |
| 8:UE:53:LEU:HD11   | 8:UE:60:VAL:HG13   | 1.81                     | 0.62              |
| 13:UJ:98:ILE:HG21  | 13:UJ:131:ASN:ND2  | 2.14                     | 0.62              |
| 13:UJ:106:SER:HB2  | 13:UJ:138:SER:HB2  | 1.82                     | 0.62              |
| 21:UR:168:PHE:CE1  | 24:UU:218:LEU:HD11 | 2.35                     | 0.62              |
| 22:US:321:ASN:HA   | 22:US:361:LEU:HD21 | 1.82                     | 0.62              |
| 23:UT:462:ARG:NH2  | 23:UT:463:ASP:OD1  | 2.33                     | 0.62              |
| 25:UV:762:TYR:HE2  | 25:UV:900:GLU:HG2  | 1.64                     | 0.62              |
| 32:CI:78:LEU:HD23  | 32:CI:97:LEU:HD21  | 1.81                     | 0.62              |
| 32:CI:161:VAL:O    | 32:CI:164:SER:OG   | 2.06                     | 0.62              |
| 50:DF:117:THR:HG22 | 50:DF:191:ALA:HA   | 1.82                     | 0.62              |
| 53:DI:32:GLN:O     | 53:DI:56:ARG:NH1   | 2.32                     | 0.62              |
| 65:D2:2:U:H2'      | 65:D2:3:G:C8       | 2.35                     | 0.62              |
| 65:D2:468:A:H61    | 67:D4:49:C:N4      | 1.96                     | 0.62              |
| 66:D3:52:U:H2'     | 66:D3:53:G:H8      | 1.64                     | 0.62              |
| 66:D3:158:U:H2'    | 66:D3:160:C:H5''   | 1.82                     | 0.62              |
| 79:EN:436:GLU:O    | 79:EN:440:LEU:N    | 2.32                     | 0.62              |
| 6:UC:608:PHE:HA    | 26:UX:147:GLN:HE21 | 1.64                     | 0.62              |
| 7:UD:302:ARG:HG2   | 7:UD:332:ASP:HA    | 1.81                     | 0.62              |
| 7:UD:532:ASN:OD1   | 7:UD:546:GLY:N     | 2.33                     | 0.62              |
| 7:UD:594:PHE:HA    | 7:UD:611:LEU:HA    | 1.80                     | 0.62              |
| 10:UG:287:TYR:CE1  | 10:UG:304:ARG:HD2  | 2.35                     | 0.62              |
| 11:UH:272:PHE:HA   | 11:UH:280:GLN:H    | 1.65                     | 0.62              |
| 12:UI:499:ILE:HA   | 12:UI:502:ARG:CD   | 2.29                     | 0.62              |
| 13:UJ:111:LEU:O    | 13:UJ:114:THR:OG1  | 2.14                     | 0.62              |
| 16:UM:8:LYS:O      | 16:UM:644:TRP:HA   | 1.99                     | 0.62              |
| 16:UM:732:ASN:HD22 | 16:UM:735:GLN:HE22 | 1.46                     | 0.62              |
| 16:UM:788:TYR:OH   | 34:CK:496:TYR:O    | 2.18                     | 0.62              |
| 21:UR:426:VAL:HG21 | 21:UR:458:ILE:HG13 | 1.82                     | 0.62              |
| 24:UU:902:ASN:HB3  | 24:UU:905:ILE:HG12 | 1.81                     | 0.62              |
| 25:UV:434:LEU:N    | 25:UV:485:TYR:OH   | 2.31                     | 0.62              |
| 25:UV:577:ARG:NH2  | 25:UV:629:THR:OG1  | 2.33                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:UV:785:GLU:OE1  | 25:UV:785:GLU:N    | 2.33                     | 0.62              |
| 25:UV:1058:LEU:HG  | 25:UV:1059:PRO:HD3 | 1.81                     | 0.62              |
| 29:CE:286:ASN:N    | 29:CE:374:ASP:OD2  | 2.32                     | 0.62              |
| 36:CM:206:ASN:HA   | 36:CM:209:ILE:HG12 | 1.82                     | 0.62              |
| 36:CM:260:ASP:OD1  | 36:CM:261:ILE:N    | 2.31                     | 0.62              |
| 38:JC:92:LYS:HG3   | 38:JC:93:PHE:HD1   | 1.64                     | 0.62              |
| 38:JC:96:HIS:ND1   | 66:D3:392:G:O2'    | 2.28                     | 0.62              |
| 53:DI:35:ASN:O     | 53:DI:37:LYS:NZ    | 2.28                     | 0.62              |
| 56:DN:87:ASP:OD1   | 56:DN:88:LEU:N     | 2.32                     | 0.62              |
| 65:D2:94:A:H2'     | 65:D2:95:A:C8      | 2.35                     | 0.62              |
| 65:D2:180:G:N2     | 65:D2:217:C:O2     | 2.17                     | 0.62              |
| 65:D2:387:C:N3     | 65:D2:388:C:N4     | 2.47                     | 0.62              |
| 66:D3:1123:C:O2    | 67:D4:2:U:N3       | 2.32                     | 0.62              |
| 4:UA:148:ASP:HB3   | 4:UA:166:LYS:HE2   | 1.81                     | 0.62              |
| 4:UA:222:LYS:HA    | 4:UA:246:TYR:HB2   | 1.82                     | 0.62              |
| 4:UA:385:GLU:HB2   | 4:UA:414:TRP:HH2   | 1.64                     | 0.62              |
| 4:UA:718:ASP:OD1   | 4:UA:719:VAL:N     | 2.33                     | 0.62              |
| 16:UM:801:GLU:OE1  | 24:UU:931:GLY:N    | 2.32                     | 0.62              |
| 18:UO:257:CYS:HB3  | 18:UO:275:SER:HB3  | 1.82                     | 0.62              |
| 20:UQ:616:SER:OG   | 20:UQ:618:ASP:OD1  | 2.12                     | 0.62              |
| 22:US:167:LYS:O    | 22:US:272:GLN:NE2  | 2.33                     | 0.62              |
| 22:US:329:ARG:HA   | 22:US:329:ARG:HH11 | 1.65                     | 0.62              |
| 24:UU:126:ASP:OD1  | 24:UU:142:LYS:HD2  | 1.99                     | 0.62              |
| 25:UV:326:LEU:HD12 | 25:UV:327:PRO:HD2  | 1.82                     | 0.62              |
| 25:UV:1107:GLY:HA2 | 25:UV:1178:ASP:HB3 | 1.80                     | 0.62              |
| 27:UZ:250:THR:HG23 | 66:D3:1498:G:H5'   | 1.82                     | 0.62              |
| 33:CJ:235:GLN:HB3  | 33:CJ:250:VAL:O    | 2.00                     | 0.62              |
| 35:CL:830:ARG:HB2  | 35:CL:880:TYR:HD1  | 1.62                     | 0.62              |
| 67:D4:67:G:H2'     | 67:D4:68:A:H8      | 1.64                     | 0.62              |
| 1:CB:251:ARG:HH21  | 7:UD:178:GLU:HB2   | 1.63                     | 0.61              |
| 11:UH:631:SER:O    | 11:UH:634:LEU:HG   | 2.01                     | 0.61              |
| 13:UJ:1653:ASN:OD1 | 13:UJ:1656:SER:OG  | 2.18                     | 0.61              |
| 16:UM:516:LYS:HB3  | 16:UM:525:LEU:HD11 | 1.82                     | 0.61              |
| 22:US:276:SER:HA   | 22:US:279:LEU:HD12 | 1.81                     | 0.61              |
| 23:UT:498:ILE:HD11 | 23:UT:540:THR:HG21 | 1.82                     | 0.61              |
| 29:CE:318:GLN:OE1  | 67:D4:325:C:N4     | 2.21                     | 0.61              |
| 31:CH:308:SER:OG   | 31:CH:311:GLN:OE1  | 2.10                     | 0.61              |
| 33:CJ:21:GLN:O     | 33:CJ:24:GLN:NE2   | 2.32                     | 0.61              |
| 33:CJ:59:ASP:HA    | 33:CJ:62:LEU:HG    | 1.81                     | 0.61              |
| 35:CL:140:LEU:HG   | 35:CL:142:ILE:HD11 | 1.80                     | 0.61              |
| 35:CL:562:GLU:HG2  | 35:CL:565:ARG:NE   | 2.15                     | 0.61              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 35:CL:841:THR:HG23 | 35:CL:859:ILE:HA    | 1.80                     | 0.61              |
| 35:CL:866:ARG:NH2  | 61:DX:59:ILE:O      | 2.32                     | 0.61              |
| 66:D3:1502:G:N2    | 66:D3:1505:A:OP2    | 2.33                     | 0.61              |
| 6:UC:562:ARG:HB3   | 54:DJ:37:LYS:HB3    | 1.82                     | 0.61              |
| 10:UG:134:VAL:HG23 | 10:UG:148:LEU:HB2   | 1.81                     | 0.61              |
| 21:UR:143:THR:O    | 21:UR:146:LEU:N     | 2.32                     | 0.61              |
| 23:UT:459:LEU:HD22 | 23:UT:462:ARG:HH11  | 1.64                     | 0.61              |
| 23:UT:492:GLN:NE2  | 23:UT:495:GLU:OE1   | 2.32                     | 0.61              |
| 23:UT:864:ASP:HA   | 23:UT:867:LYS:HE2   | 1.82                     | 0.61              |
| 23:UT:1546:GLN:O   | 23:UT:1549:VAL:HG12 | 2.00                     | 0.61              |
| 25:UV:355:GLN:HB3  | 25:UV:414:HIS:CE1   | 2.35                     | 0.61              |
| 27:UZ:55:ARG:NH2   | 48:JQ:189:PRO:O     | 2.32                     | 0.61              |
| 28:CD:180:LEU:HD21 | 29:CE:183:ARG:HG2   | 1.81                     | 0.61              |
| 35:CL:832:HIS:N    | 35:CL:914:ALA:O     | 2.27                     | 0.61              |
| 37:CN:63:ASN:H     | 37:CN:66:HIS:HB2    | 1.65                     | 0.61              |
| 38:JC:15:GLN:HG3   | 38:JC:341:TYR:HE1   | 1.63                     | 0.61              |
| 44:JM:124:ILE:HG23 | 44:JM:141:TRP:HZ3   | 1.65                     | 0.61              |
| 60:DW:72:CYS:HB2   | 60:DW:129:VAL:HG12  | 1.82                     | 0.61              |
| 65:D2:93:A:H2'     | 65:D2:94:A:H8       | 1.65                     | 0.61              |
| 66:D3:1775:U:H2'   | 66:D3:1776:A:C8     | 2.34                     | 0.61              |
| 67:D4:78:G:H2'     | 67:D4:79:G:H8       | 1.65                     | 0.61              |
| 3:JA:545:HIS:HB2   | 3:JA:637:ARG:NH1    | 2.15                     | 0.61              |
| 3:JA:563:LYS:NZ    | 3:JA:564:LEU:O      | 2.33                     | 0.61              |
| 6:UC:599:LYS:NZ    | 44:JM:138:LYS:O     | 2.26                     | 0.61              |
| 8:UE:60:VAL:HG12   | 8:UE:80:MET:HG2     | 1.82                     | 0.61              |
| 8:UE:103:ASN:ND2   | 8:UE:127:TYR:OH     | 2.34                     | 0.61              |
| 13:UJ:1668:LYS:NZ  | 67:D4:145:U:O4      | 2.33                     | 0.61              |
| 14:UK:143:MET:HE3  | 19:UP:171:VAL:HG12  | 1.82                     | 0.61              |
| 14:UK:207:ARG:HH21 | 14:UK:211:LEU:HD21  | 1.65                     | 0.61              |
| 16:UM:217:ASP:OD1  | 16:UM:218:ASP:N     | 2.31                     | 0.61              |
| 18:UO:273:ILE:HG22 | 18:UO:283:VAL:HG22  | 1.82                     | 0.61              |
| 18:UO:411:LYS:NZ   | 18:UO:452:ASP:OD1   | 2.33                     | 0.61              |
| 21:UR:545:HIS:HB2  | 21:UR:552:PHE:CZ    | 2.35                     | 0.61              |
| 23:UT:27:LYS:NZ    | 23:UT:29:GLU:HB2    | 2.15                     | 0.61              |
| 23:UT:1265:TYR:CZ  | 23:UT:1298:LEU:HD21 | 2.35                     | 0.61              |
| 35:CL:828:ARG:NH1  | 61:DX:94:ASN:O      | 2.32                     | 0.61              |
| 36:CM:249:SER:O    | 36:CM:253:GLY:HA2   | 2.00                     | 0.61              |
| 49:DE:65:LEU:HD23  | 49:DE:70:VAL:HG21   | 1.81                     | 0.61              |
| 54:DJ:143:ILE:HG12 | 66:D3:767:U:N3      | 2.16                     | 0.61              |
| 66:D3:1775:U:O2    | 66:D3:1786:G:N2     | 2.28                     | 0.61              |
| 5:UB:625:GLU:O     | 5:UB:627:HIS:ND1    | 2.32                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:UB:640:MET:SD    | 5:UB:680:LYS:HD3   | 2.40                     | 0.61              |
| 10:UG:267:LEU:HD23 | 10:UG:444:LEU:HB2  | 1.82                     | 0.61              |
| 10:UG:283:ASP:CG   | 10:UG:287:TYR:H    | 2.04                     | 0.61              |
| 10:UG:389:LEU:HD23 | 10:UG:402:ILE:HA   | 1.81                     | 0.61              |
| 11:UH:561:LEU:HB3  | 11:UH:566:LEU:HD21 | 1.82                     | 0.61              |
| 16:UM:241:GLN:NE2  | 16:UM:260:THR:OG1  | 2.33                     | 0.61              |
| 18:UO:25:ARG:NH2   | 65:D2:100:G:N7     | 2.49                     | 0.61              |
| 18:UO:97:CYS:HB2   | 18:UO:140:LEU:HD11 | 1.81                     | 0.61              |
| 18:UO:427:VAL:HG23 | 18:UO:428:ARG:H    | 1.66                     | 0.61              |
| 21:UR:424:ILE:HG23 | 21:UR:434:GLU:HG2  | 1.80                     | 0.61              |
| 23:UT:408:VAL:O    | 23:UT:411:PHE:O    | 2.18                     | 0.61              |
| 25:UV:381:HIS:NE2  | 25:UV:478:THR:O    | 2.34                     | 0.61              |
| 25:UV:723:ASN:OD1  | 25:UV:724:LEU:N    | 2.33                     | 0.61              |
| 28:CD:169:LYS:NZ   | 28:CD:391:ASN:O    | 2.33                     | 0.61              |
| 38:JC:63:LYS:NZ    | 38:JC:105:THR:OG1  | 2.30                     | 0.61              |
| 51:DG:7:TYR:HD2    | 51:DG:10:ASN:HB2   | 1.65                     | 0.61              |
| 67:D4:23:U:O2'     | 67:D4:26:C:N4      | 2.28                     | 0.61              |
| 1:CA:178:GLY:HA3   | 1:CA:210:MET:SD    | 2.41                     | 0.61              |
| 4:UA:349:ASN:HA    | 4:UA:682:THR:HG21  | 1.82                     | 0.61              |
| 4:UA:533:SER:OG    | 4:UA:580:PHE:O     | 2.18                     | 0.61              |
| 4:UA:844:TYR:OH    | 15:UL:896:ASP:OD1  | 2.13                     | 0.61              |
| 1:CB:231:ARG:HA    | 1:CB:260:PHE:CZ    | 2.36                     | 0.61              |
| 5:UB:485:TYR:HD2   | 5:UB:486:LYS:HD3   | 1.64                     | 0.61              |
| 16:UM:270:ILE:HG22 | 16:UM:277:VAL:HG22 | 1.82                     | 0.61              |
| 18:UO:395:PHE:HZ   | 65:D2:86:C:H5      | 1.47                     | 0.61              |
| 20:UQ:180:ASP:OD2  | 20:UQ:181:ALA:N    | 2.34                     | 0.61              |
| 20:UQ:884:MET:N    | 20:UQ:884:MET:SD   | 2.72                     | 0.61              |
| 21:UR:168:PHE:CD1  | 24:UU:218:LEU:HD11 | 2.35                     | 0.61              |
| 23:UT:790:GLU:HG3  | 23:UT:841:ILE:HD12 | 1.82                     | 0.61              |
| 23:UT:971:ARG:NH1  | 23:UT:996:ARG:O    | 2.34                     | 0.61              |
| 23:UT:1242:LYS:HA  | 23:UT:1245:LYS:HE2 | 1.82                     | 0.61              |
| 25:UV:1156:LYS:HG3 | 25:UV:1157:TYR:HD1 | 1.64                     | 0.61              |
| 35:CL:939:TYR:HB3  | 35:CL:949:LYS:HD2  | 1.81                     | 0.61              |
| 37:CN:92:GLU:O     | 37:CN:121:ARG:NH2  | 2.25                     | 0.61              |
| 57:DO:52:ARG:HE    | 66:D3:905:A:H3'    | 1.64                     | 0.61              |
| 65:D2:193:G:H2'    | 65:D2:194:G:C8     | 2.35                     | 0.61              |
| 66:D3:586:G:O2'    | 66:D3:587:C:OP1    | 2.17                     | 0.61              |
| 7:UD:579:ARG:NH1   | 7:UD:644:SER:OG    | 2.32                     | 0.61              |
| 7:UD:586:THR:O     | 7:UD:589:ASN:N     | 2.33                     | 0.61              |
| 9:UF:91:ARG:O      | 9:UF:95:ILE:HG12   | 2.00                     | 0.61              |
| 10:UG:126:LEU:HB2  | 10:UG:159:TYR:CE2  | 2.35                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:UI:425:ASN:ND2  | 12:UI:463:LYS:HG3  | 2.15                     | 0.61              |
| 13:UJ:1499:ILE:HA  | 13:UJ:1502:LYS:HD2 | 1.82                     | 0.61              |
| 13:UJ:1602:ASP:OD1 | 13:UJ:1606:LYS:NZ  | 2.26                     | 0.61              |
| 14:UK:203:GLN:HA   | 14:UK:206:GLN:HG2  | 1.80                     | 0.61              |
| 23:UT:656:LYS:NZ   | 23:UT:692:ASP:OD1  | 2.31                     | 0.61              |
| 32:CI:36:TYR:CE1   | 32:CI:108:ARG:HB3  | 2.35                     | 0.61              |
| 35:CL:762:LEU:HA   | 35:CL:765:ASN:HD22 | 1.65                     | 0.61              |
| 53:DI:81:VAL:HA    | 53:DI:102:VAL:HG12 | 1.82                     | 0.61              |
| 66:D3:1073:G:H2'   | 66:D3:1074:G:C8    | 2.34                     | 0.61              |
| 2:DA:36:SER:HA     | 2:DA:41:ARG:HH12   | 1.65                     | 0.61              |
| 9:UF:320:ILE:HD11  | 9:UF:338:VAL:HG11  | 1.83                     | 0.61              |
| 14:UK:108:ARG:NH2  | 67:D4:325:C:OP2    | 2.32                     | 0.61              |
| 14:UK:117:LYS:NZ   | 14:UK:204:HIS:HE1  | 1.98                     | 0.61              |
| 16:UM:435:ALA:HB1  | 16:UM:459:ASN:HB3  | 1.81                     | 0.61              |
| 20:UQ:363:ASN:ND2  | 20:UQ:368:ASP:OD2  | 2.34                     | 0.61              |
| 28:CD:34:VAL:O     | 28:CD:37:GLN:HG2   | 2.00                     | 0.61              |
| 32:CI:71:ARG:HE    | 33:CJ:61:SER:HB2   | 1.64                     | 0.61              |
| 36:CM:339:LEU:HD12 | 36:CM:350:MET:HG3  | 1.82                     | 0.61              |
| 44:JM:135:HIS:CE1  | 66:D3:487:G:C2     | 2.88                     | 0.61              |
| 50:DF:84:LYS:NZ    | 66:D3:1613:U:O5'   | 2.23                     | 0.61              |
| 52:DH:70:PHE:O     | 52:DH:74:GLN:HB2   | 1.99                     | 0.61              |
| 66:D3:328:A:H2'    | 66:D3:329:G:H8     | 1.64                     | 0.61              |
| 3:JA:887:ALA:HA    | 3:JA:891:GLN:HB3   | 1.83                     | 0.61              |
| 7:UD:739:LYS:HB2   | 7:UD:740:PRO:HD3   | 1.81                     | 0.61              |
| 8:UE:128:GLN:HB3   | 8:UE:138:GLN:HG2   | 1.82                     | 0.61              |
| 13:UJ:336:LEU:HD11 | 13:UJ:348:ILE:HD11 | 1.82                     | 0.61              |
| 13:UJ:626:PHE:O    | 13:UJ:630:TYR:CB   | 2.49                     | 0.61              |
| 13:UJ:1613:MET:O   | 13:UJ:1619:ARG:NH2 | 2.26                     | 0.61              |
| 16:UM:348:PRO:HD2  | 16:UM:419:GLU:HG3  | 1.82                     | 0.61              |
| 20:UQ:318:GLU:HG2  | 20:UQ:320:VAL:HG12 | 1.82                     | 0.61              |
| 20:UQ:430:LYS:NZ   | 65:D2:69:U:OP2     | 2.34                     | 0.61              |
| 20:UQ:447:LYS:HZ3  | 20:UQ:770:TYR:HB2  | 1.66                     | 0.61              |
| 20:UQ:510:TYR:HE1  | 20:UQ:527:HIS:HB3  | 1.64                     | 0.61              |
| 20:UQ:663:LYS:HE3  | 20:UQ:712:THR:HA   | 1.82                     | 0.61              |
| 24:UU:223:LEU:HB2  | 24:UU:231:ILE:HG13 | 1.81                     | 0.61              |
| 24:UU:877:ASN:HB2  | 24:UU:881:TYR:CE2  | 2.36                     | 0.61              |
| 25:UV:755:PRO:HA   | 25:UV:782:VAL:HG12 | 1.82                     | 0.61              |
| 25:UV:1135:ASN:OD1 | 25:UV:1137:ASN:ND2 | 2.33                     | 0.61              |
| 28:CD:12:PRO:HG2   | 28:CD:151:GLN:HG2  | 1.82                     | 0.61              |
| 31:CH:326:GLU:HG3  | 31:CH:341:ALA:HB2  | 1.83                     | 0.61              |
| 36:CM:109:PHE:HA   | 36:CM:361:ASN:ND2  | 2.15                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:JC:23:ARG:NE    | 38:JC:314:SER:O    | 2.33                     | 0.61              |
| 38:JC:296:ILE:HG12 | 38:JC:298:LYS:HE2  | 1.81                     | 0.61              |
| 42:JJ:105:ARG:NH2  | 42:JJ:162:PHE:O    | 2.32                     | 0.61              |
| 54:DJ:93:LEU:HA    | 54:DJ:96:VAL:HG12  | 1.82                     | 0.61              |
| 60:DW:56:HIS:O     | 66:D3:861:U:O2'    | 2.18                     | 0.61              |
| 66:D3:939:A:H2'    | 66:D3:940:A:C8     | 2.36                     | 0.61              |
| 3:JA:790:SER:HA    | 3:JA:794:HIS:HA    | 1.81                     | 0.61              |
| 4:UA:420:ARG:NH2   | 66:D3:1633:A:O2'   | 2.33                     | 0.61              |
| 7:UD:250:THR:OG1   | 7:UD:252:GLN:OE1   | 2.16                     | 0.61              |
| 7:UD:476:LYS:NZ    | 7:UD:493:ASP:OD1   | 2.33                     | 0.61              |
| 13:UJ:1523:ARG:HD2 | 67:D4:140:C:H2'    | 1.82                     | 0.61              |
| 15:UL:134:THR:HB   | 15:UL:150:LEU:HB2  | 1.81                     | 0.61              |
| 16:UM:180:ARG:NH1  | 66:D3:1778:G:OP1   | 2.34                     | 0.61              |
| 22:US:350:MET:HA   | 22:US:355:ARG:NH1  | 2.16                     | 0.61              |
| 23:UT:631:THR:OG1  | 23:UT:634:ASN:OD1  | 2.18                     | 0.61              |
| 23:UT:1523:TYR:O   | 23:UT:1527:LEU:HG  | 2.01                     | 0.61              |
| 25:UV:556:ILE:H    | 25:UV:556:ILE:HD12 | 1.66                     | 0.61              |
| 25:UV:698:ASN:H    | 25:UV:702:LYS:HZ3  | 1.48                     | 0.61              |
| 28:CD:213:ASN:OD1  | 28:CD:214:TYR:N    | 2.34                     | 0.61              |
| 38:JC:275:LYS:N    | 38:JC:291:THR:O    | 2.29                     | 0.61              |
| 47:JP:313:PHE:CE1  | 47:JP:320:ILE:HG12 | 2.36                     | 0.61              |
| 60:DW:11:LEU:HD21  | 60:DW:37:PHE:CE1   | 2.36                     | 0.61              |
| 60:DW:50:PHE:HB3   | 60:DW:63:VAL:HA    | 1.83                     | 0.61              |
| 66:D3:391:A:H2'    | 66:D3:392:G:H8     | 1.64                     | 0.61              |
| 78:EK:81:ALA:HB1   | 78:EK:82:PRO:HA    | 1.83                     | 0.61              |
| 1:CA:142:ARG:HH21  | 1:CA:183:HIS:CD2   | 2.19                     | 0.61              |
| 1:CA:283:GLU:HB3   | 26:UX:150:CYS:SG   | 2.40                     | 0.61              |
| 3:JA:139:ILE:O     | 3:JA:475:ARG:NH2   | 2.30                     | 0.61              |
| 4:UA:705:SER:OG    | 4:UA:706:THR:N     | 2.34                     | 0.61              |
| 7:UD:485:LYS:HE3   | 7:UD:497:ILE:HG22  | 1.83                     | 0.61              |
| 8:UE:281:ILE:HG12  | 8:UE:291:ILE:HD11  | 1.83                     | 0.61              |
| 11:UH:656:GLU:O    | 11:UH:659:THR:OG1  | 2.16                     | 0.61              |
| 18:UO:75:LYS:HD3   | 18:UO:111:TYR:HA   | 1.81                     | 0.61              |
| 20:UQ:386:ASN:OD1  | 20:UQ:387:GLY:N    | 2.32                     | 0.61              |
| 20:UQ:768:TRP:CZ3  | 20:UQ:770:TYR:HA   | 2.35                     | 0.61              |
| 23:UT:15:ARG:NH1   | 66:D3:82:U:OP1     | 2.30                     | 0.61              |
| 23:UT:591:LEU:O    | 23:UT:597:ARG:NH2  | 2.33                     | 0.61              |
| 24:UU:173:LEU:HD21 | 24:UU:219:ASP:HA   | 1.83                     | 0.61              |
| 24:UU:279:ASP:OD1  | 24:UU:280:ARG:NH1  | 2.34                     | 0.61              |
| 25:UV:304:GLU:H    | 25:UV:307:LYS:HE3  | 1.66                     | 0.61              |
| 25:UV:1063:ARG:NH2 | 25:UV:1095:ASP:OD2 | 2.33                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:CF:65:LEU:O     | 30:CF:68:PRO:HD2   | 2.01                     | 0.61              |
| 55:DL:66:ILE:HD11  | 55:DL:126:GLY:HA3  | 1.83                     | 0.61              |
| 56:DN:30:SER:O     | 56:DN:34:ILE:HG12  | 2.01                     | 0.61              |
| 56:DN:100:LYS:HE2  | 56:DN:104:ARG:HH12 | 1.65                     | 0.61              |
| 66:D3:23:G:N2      | 66:D3:603:U:O2     | 2.34                     | 0.61              |
| 66:D3:1151:A:H2'   | 66:D3:1152:A:C8    | 2.34                     | 0.61              |
| 4:UA:341:GLN:HE21  | 4:UA:378:PHE:HB3   | 1.65                     | 0.60              |
| 10:UG:466:LEU:O    | 10:UG:469:THR:OG1  | 2.17                     | 0.60              |
| 14:UK:71:LYS:O     | 14:UK:79:ILE:HG12  | 2.01                     | 0.60              |
| 16:UM:161:TRP:HB3  | 16:UM:177:LEU:HD22 | 1.82                     | 0.60              |
| 16:UM:300:SER:HB2  | 16:UM:316:VAL:HG22 | 1.83                     | 0.60              |
| 16:UM:314:ILE:HA   | 16:UM:330:THR:HG23 | 1.83                     | 0.60              |
| 20:UQ:507:MET:HG2  | 20:UQ:532:TRP:HB2  | 1.82                     | 0.60              |
| 23:UT:796:ILE:HA   | 23:UT:799:PHE:HD2  | 1.66                     | 0.60              |
| 23:UT:864:ASP:OD1  | 23:UT:865:VAL:N    | 2.33                     | 0.60              |
| 23:UT:1519:SER:O   | 23:UT:1523:TYR:CB  | 2.47                     | 0.60              |
| 24:UU:117:ASN:OD1  | 24:UU:118:VAL:N    | 2.34                     | 0.60              |
| 25:UV:1204:VAL:HA  | 25:UV:1214:LEU:HA  | 1.82                     | 0.60              |
| 26:UX:91:LEU:HD13  | 54:DJ:54:ARG:NH1   | 2.16                     | 0.60              |
| 29:CE:339:TYR:HE1  | 29:CE:357:GLY:HA2  | 1.65                     | 0.60              |
| 33:CJ:166:SER:HB2  | 66:D3:1597:A:N3    | 2.16                     | 0.60              |
| 35:CL:1144:LYS:HA  | 35:CL:1147:GLU:OE2 | 2.01                     | 0.60              |
| 38:JC:205:GLU:OE1  | 38:JC:217:LYS:NZ   | 2.33                     | 0.60              |
| 46:JO:208:GLU:O    | 46:JO:212:ARG:HG2  | 2.01                     | 0.60              |
| 49:DE:134:LYS:N    | 66:D3:253:A:OP1    | 2.34                     | 0.60              |
| 50:DF:184:PHE:O    | 50:DF:185:ARG:NH1  | 2.31                     | 0.60              |
| 62:DY:110:GLN:HB3  | 62:DY:114:ARG:NH1  | 2.16                     | 0.60              |
| 2:DA:205:PHE:CE2   | 66:D3:1065:A:H4'   | 2.36                     | 0.60              |
| 4:UA:308:VAL:HG22  | 4:UA:319:PHE:CD1   | 2.35                     | 0.60              |
| 4:UA:420:ARG:HG3   | 34:CK:468:ARG:CZ   | 2.31                     | 0.60              |
| 3:JB:790:SER:HA    | 3:JB:794:HIS:HA    | 1.82                     | 0.60              |
| 7:UD:474:SER:OG    | 7:UD:490:SER:OG    | 2.03                     | 0.60              |
| 7:UD:488:ILE:O     | 7:UD:495:VAL:HA    | 2.01                     | 0.60              |
| 9:UF:166:ASN:HD22  | 9:UF:169:GLN:NE2   | 1.99                     | 0.60              |
| 15:UL:24:VAL:HB    | 15:UL:42:ILE:HB    | 1.82                     | 0.60              |
| 15:UL:279:LYS:NZ   | 66:D3:1739:C:OP1   | 2.34                     | 0.60              |
| 15:UL:617:SER:HB3  | 15:UL:635:LYS:HD3  | 1.82                     | 0.60              |
| 20:UQ:20:PRO:HA    | 20:UQ:48:PHE:HA    | 1.82                     | 0.60              |
| 20:UQ:561:LEU:HD12 | 20:UQ:562:PRO:HD2  | 1.82                     | 0.60              |
| 25:UV:252:LEU:HB3  | 25:UV:270:ILE:HD11 | 1.81                     | 0.60              |
| 32:CI:36:TYR:HE1   | 32:CI:108:ARG:HB3  | 1.66                     | 0.60              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 33:CJ:121:ASN:ND2   | 66:D3:1585:U:OP2    | 2.24                     | 0.60              |
| 35:CL:1123:LYS:NZ   | 66:D3:486:G:O3'     | 2.33                     | 0.60              |
| 37:CN:259:ARG:O     | 37:CN:263:ARG:HG2   | 2.01                     | 0.60              |
| 38:JC:140:PHE:O     | 38:JC:158:SER:N     | 2.34                     | 0.60              |
| 39:JG:17:LYS:NZ     | 39:JG:18:ALA:O      | 2.33                     | 0.60              |
| 39:JG:154:ASN:OD1   | 39:JG:155:SER:N     | 2.34                     | 0.60              |
| 50:DF:47:SER:OG     | 50:DF:48:PHE:N      | 2.33                     | 0.60              |
| 65:D2:215:U:H2'     | 65:D2:216:U:H6      | 1.65                     | 0.60              |
| 66:D3:1670:G:O2'    | 66:D3:1731:A:N6     | 2.34                     | 0.60              |
| 1:CA:120:GLU:N      | 1:CA:120:GLU:OE1    | 2.32                     | 0.60              |
| 3:JA:473:PRO:HD2    | 3:JA:478:PRO:HG3    | 1.83                     | 0.60              |
| 4:UA:185:THR:OG1    | 4:UA:186:THR:N      | 2.34                     | 0.60              |
| 4:UA:608:ASN:HD22   | 24:UU:513:MET:HG3   | 1.65                     | 0.60              |
| 5:UB:613:ILE:HG13   | 5:UB:615:PRO:HD3    | 1.84                     | 0.60              |
| 7:UD:548:GLY:HA2    | 7:UD:570:ILE:HG12   | 1.84                     | 0.60              |
| 9:UF:297:ASP:OD1    | 9:UF:298:SER:N      | 2.33                     | 0.60              |
| 13:UJ:1380:LEU:HD11 | 13:UJ:1400:ILE:HG12 | 1.82                     | 0.60              |
| 18:UO:125:HIS:NE2   | 39:JG:19:LEU:O      | 2.33                     | 0.60              |
| 20:UQ:660:GLN:HG2   | 20:UQ:661:THR:HG23  | 1.82                     | 0.60              |
| 23:UT:1279:ASN:HA   | 23:UT:1282:VAL:HG22 | 1.81                     | 0.60              |
| 24:UU:631:ASN:HB2   | 24:UU:644:THR:HG22  | 1.83                     | 0.60              |
| 33:CJ:53:GLN:HG3    | 45:JN:215:LEU:HD21  | 1.82                     | 0.60              |
| 42:JJ:199:SER:HA    | 42:JJ:202:ILE:HD12  | 1.83                     | 0.60              |
| 44:JM:197:LYS:O     | 44:JM:200:SER:OG    | 2.17                     | 0.60              |
| 46:JO:137:ARG:NE    | 66:D3:1027:A:OP1    | 2.35                     | 0.60              |
| 66:D3:329:G:H2'     | 66:D3:330:G:H8      | 1.66                     | 0.60              |
| 9:UF:113:TYR:CD2    | 9:UF:132:ILE:HD12   | 2.35                     | 0.60              |
| 11:UH:598:GLU:HA    | 11:UH:601:LYS:HE2   | 1.83                     | 0.60              |
| 11:UH:599:MET:HE3   | 11:UH:644:SER:HB3   | 1.84                     | 0.60              |
| 12:UI:505:MET:SD    | 18:UO:507:MET:HB2   | 2.41                     | 0.60              |
| 18:UO:378:LYS:HD2   | 21:UR:292:GLY:HA3   | 1.82                     | 0.60              |
| 18:UO:500:GLU:HA    | 18:UO:503:ARG:CG    | 2.31                     | 0.60              |
| 21:UR:349:GLU:OE2   | 21:UR:353:ARG:NH1   | 2.34                     | 0.60              |
| 23:UT:935:VAL:HG21  | 23:UT:945:ARG:HH21  | 1.66                     | 0.60              |
| 23:UT:1289:ILE:HD13 | 23:UT:1305:VAL:HG21 | 1.81                     | 0.60              |
| 23:UT:1761:ILE:O    | 23:UT:1803:ASN:ND2  | 2.29                     | 0.60              |
| 23:UT:1948:SER:OG   | 23:UT:1950:SER:O    | 2.15                     | 0.60              |
| 25:UV:676:PRO:HB2   | 25:UV:678:ILE:HG12  | 1.82                     | 0.60              |
| 27:UZ:27:ASN:HB3    | 27:UZ:30:LEU:HB2    | 1.82                     | 0.60              |
| 35:CL:1033:ARG:HB2  | 35:CL:1038:ILE:HD11 | 1.82                     | 0.60              |
| 39:JG:55:ILE:HD11   | 39:JG:76:LEU:HD13   | 1.83                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 44:JM:213:ARG:NH1  | 66:D3:1492:A:OP1   | 2.34                     | 0.60              |
| 50:DF:100:ASN:OD1  | 50:DF:101:GLY:N    | 2.32                     | 0.60              |
| 66:D3:162:A:H3'    | 66:D3:163:G:N2     | 2.16                     | 0.60              |
| 4:UA:62:ASP:OD2    | 4:UA:104:PHE:N     | 2.34                     | 0.60              |
| 1:CB:169:LYS:HG2   | 1:CB:193:VAL:HG12  | 1.84                     | 0.60              |
| 5:UB:607:THR:N     | 5:UB:610:ARG:HE    | 1.99                     | 0.60              |
| 8:UE:542:ALA:HA    | 11:UH:677:ASN:HD21 | 1.64                     | 0.60              |
| 10:UG:325:SER:OG   | 10:UG:406:ALA:O    | 2.18                     | 0.60              |
| 13:UJ:171:GLU:OE1  | 13:UJ:172:LYS:HB2  | 2.01                     | 0.60              |
| 13:UJ:671:LEU:HD13 | 13:UJ:719:SER:HB2  | 1.83                     | 0.60              |
| 13:UJ:1511:ARG:HG3 | 13:UJ:1525:GLU:OE2 | 2.01                     | 0.60              |
| 13:UJ:1581:LYS:O   | 13:UJ:1585:ASN:ND2 | 2.35                     | 0.60              |
| 16:UM:662:GLN:O    | 16:UM:665:GLN:HG2  | 2.01                     | 0.60              |
| 23:UT:1203:VAL:O   | 23:UT:1206:THR:OG1 | 2.13                     | 0.60              |
| 23:UT:1738:TYR:HD1 | 66:D3:803:A:C4     | 2.18                     | 0.60              |
| 24:UU:227:THR:OG1  | 24:UU:229:GLU:OE1  | 2.16                     | 0.60              |
| 27:UZ:87:LEU:O     | 27:UZ:93:THR:OG1   | 2.19                     | 0.60              |
| 30:CF:115:TYR:CD1  | 30:CF:118:LYS:HD3  | 2.37                     | 0.60              |
| 35:CL:72:VAL:HA    | 35:CL:137:LEU:O    | 2.02                     | 0.60              |
| 47:JP:276:ASN:ND2  | 66:D3:-7:A:H61     | 1.99                     | 0.60              |
| 53:DI:64:ASN:O     | 53:DI:180:ASP:HA   | 2.01                     | 0.60              |
| 54:DJ:114:TYR:HE1  | 54:DJ:121:SER:HA   | 1.66                     | 0.60              |
| 65:D2:236:C:N4     | 65:D2:237:A:N1     | 2.49                     | 0.60              |
| 66:D3:629:U:H2'    | 66:D3:630:A:H8     | 1.67                     | 0.60              |
| 66:D3:880:C:H2'    | 66:D3:881:A:C8     | 2.36                     | 0.60              |
| 66:D3:1060:U:H2'   | 66:D3:1061:A:O4'   | 2.02                     | 0.60              |
| 66:D3:1671:A:H3'   | 66:D3:1672:G:H8    | 1.67                     | 0.60              |
| 1:CA:100:ARG:HB3   | 44:JM:124:ILE:HD11 | 1.83                     | 0.60              |
| 4:UA:389:SER:O     | 4:UA:406:SER:HB2   | 2.01                     | 0.60              |
| 7:UD:210:ILE:HD12  | 7:UD:265:TRP:CZ3   | 2.37                     | 0.60              |
| 10:UG:180:GLU:OE2  | 26:UX:15:ARG:NH1   | 2.34                     | 0.60              |
| 10:UG:290:ALA:HB3  | 10:UG:324:ILE:HD11 | 1.83                     | 0.60              |
| 20:UQ:311:TYR:OH   | 21:UR:394:TRP:O    | 2.19                     | 0.60              |
| 20:UQ:375:ASN:HB2  | 20:UQ:382:LYS:HE2  | 1.82                     | 0.60              |
| 22:US:215:ASN:HB3  | 22:US:218:LYS:HD3  | 1.83                     | 0.60              |
| 23:UT:497:ILE:HA   | 23:UT:500:LEU:HD12 | 1.83                     | 0.60              |
| 23:UT:1127:PHE:HB3 | 23:UT:1130:ALA:HB3 | 1.82                     | 0.60              |
| 26:UX:90:LEU:HD11  | 26:UX:182:ILE:HD11 | 1.82                     | 0.60              |
| 26:UX:91:LEU:HG    | 54:DJ:53:ARG:HG2   | 1.84                     | 0.60              |
| 65:D2:300:C:H2'    | 65:D2:301:U:H6     | 1.66                     | 0.60              |
| 66:D3:1158:C:N4    | 66:D3:1582:U:H5    | 1.99                     | 0.60              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 66:D3:1162:C:O2    | 66:D3:1616:G:N2     | 2.34                     | 0.60              |
| 66:D3:1579:U:H2'   | 66:D3:1580:C:H6     | 1.66                     | 0.60              |
| 6:UC:538:ARG:HB3   | 35:CL:150:MET:HE1   | 1.84                     | 0.60              |
| 16:UM:30:LYS:HA    | 16:UM:45:LEU:C      | 2.20                     | 0.60              |
| 23:UT:558:TRP:HD1  | 23:UT:561:LEU:HD12  | 1.67                     | 0.60              |
| 23:UT:1662:SER:O   | 23:UT:1665:LEU:C    | 2.39                     | 0.60              |
| 27:UZ:226:LYS:HD2  | 27:UZ:229:ARG:HH21  | 1.66                     | 0.60              |
| 29:CE:204:ALA:O    | 29:CE:208:ILE:HD12  | 2.02                     | 0.60              |
| 32:CI:136:VAL:O    | 32:CI:142:LEU:HB2   | 2.02                     | 0.60              |
| 35:CL:300:GLN:HB2  | 35:CL:792:VAL:HG12  | 1.84                     | 0.60              |
| 35:CL:753:LEU:HG   | 35:CL:757:LYS:NZ    | 2.16                     | 0.60              |
| 38:JC:227:ARG:NH1  | 38:JC:230:GLN:OE1   | 2.34                     | 0.60              |
| 66:D3:1679:G:H2'   | 66:D3:1722:A:N6     | 2.17                     | 0.60              |
| 67:D4:43:C:H2'     | 67:D4:44:U:H6       | 1.67                     | 0.60              |
| 67:D4:54:C:N4      | 67:D4:55:A:N7       | 2.49                     | 0.60              |
| 3:JA:95:GLU:HA     | 3:JA:98:ILE:HG12    | 1.84                     | 0.60              |
| 3:JA:160:GLN:NE2   | 3:JA:172:TYR:O      | 2.33                     | 0.60              |
| 3:JA:483:GLU:O     | 3:JA:487:ASN:ND2    | 2.34                     | 0.60              |
| 4:UA:775:LEU:O     | 4:UA:778:ILE:HG22   | 2.01                     | 0.60              |
| 3:JB:752:ASN:O     | 3:JB:756:GLY:N      | 2.34                     | 0.60              |
| 8:UE:473:LYS:HZ2   | 8:UE:475:ALA:HB3    | 1.66                     | 0.60              |
| 8:UE:545:ALA:HB3   | 11:UH:677:ASN:ND2   | 2.17                     | 0.60              |
| 9:UF:186:VAL:HG21  | 9:UF:319:TYR:HE2    | 1.67                     | 0.60              |
| 9:UF:198:ASN:HA    | 9:UF:201:LYS:HD3    | 1.83                     | 0.60              |
| 11:UH:541:LEU:HD23 | 11:UH:565:GLU:HB3   | 1.84                     | 0.60              |
| 13:UJ:267:ALA:O    | 13:UJ:268:LEU:HD23  | 2.01                     | 0.60              |
| 13:UJ:616:PRO:O    | 13:UJ:620:GLU:HG2   | 2.02                     | 0.60              |
| 14:UK:118:LEU:HD13 | 14:UK:204:HIS:HB2   | 1.84                     | 0.60              |
| 15:UL:299:ARG:CZ   | 15:UL:324:PHE:HB2   | 2.31                     | 0.60              |
| 17:UN:299:ASN:HA   | 17:UN:302:VAL:HG12  | 1.83                     | 0.60              |
| 18:UO:168:THR:OG1  | 18:UO:194:ARG:NH1   | 2.35                     | 0.60              |
| 20:UQ:433:ARG:HA   | 20:UQ:701:VAL:HA    | 1.83                     | 0.60              |
| 21:UR:408:CYS:SG   | 21:UR:409:ILE:N     | 2.75                     | 0.60              |
| 23:UT:1958:MET:HA  | 23:UT:1998:LEU:HD23 | 1.82                     | 0.60              |
| 24:UU:257:ARG:NH1  | 24:UU:261:SER:HB2   | 2.17                     | 0.60              |
| 24:UU:506:THR:OG1  | 24:UU:547:THR:O     | 2.19                     | 0.60              |
| 27:UZ:179:GLN:O    | 27:UZ:183:ILE:HG12  | 2.01                     | 0.60              |
| 28:CD:304:SER:O    | 28:CD:308:GLY:N     | 2.35                     | 0.60              |
| 53:DI:50:GLY:HA2   | 66:D3:397:A:H4'     | 1.84                     | 0.60              |
| 55:DL:125:VAL:HG12 | 55:DL:139:VAL:HG12  | 1.83                     | 0.60              |
| 66:D3:1617:U:O4    | 66:D3:1618:C:N4     | 2.34                     | 0.60              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 4:UA:536:LYS:HD2   | 32:CI:182:PHE:CZ    | 2.37                     | 0.60              |
| 4:UA:608:ASN:ND2   | 24:UU:513:MET:HG3   | 2.17                     | 0.60              |
| 5:UB:444:ASN:O     | 5:UB:448:PHE:N      | 2.31                     | 0.60              |
| 5:UB:799:TYR:HH    | 61:DX:42:PRO:N      | 1.99                     | 0.60              |
| 7:UD:46:ILE:HG21   | 7:UD:350:GLY:HA3    | 1.83                     | 0.60              |
| 8:UE:440:ILE:HD11  | 8:UE:452:LEU:HD11   | 1.83                     | 0.60              |
| 13:UJ:1691:ILE:O   | 13:UJ:1695:MET:HG3  | 2.01                     | 0.60              |
| 15:UL:410:SER:HB2  | 15:UL:432:TYR:CE2   | 2.37                     | 0.60              |
| 16:UM:85:LEU:HB2   | 16:UM:101:ILE:HD11  | 1.84                     | 0.60              |
| 20:UQ:38:SER:HB2   | 20:UQ:43:ASN:HB2    | 1.84                     | 0.60              |
| 23:UT:292:LEU:HG   | 23:UT:293:PRO:HD3   | 1.83                     | 0.60              |
| 23:UT:1681:LEU:HB2 | 23:UT:1690:LEU:HD12 | 1.84                     | 0.60              |
| 28:CD:270:ASN:OD1  | 28:CD:271:VAL:N     | 2.35                     | 0.60              |
| 38:JC:357:ASP:O    | 38:JC:361:GLU:HG3   | 2.01                     | 0.60              |
| 65:D2:350:A:H2'    | 65:D2:351:A:H8      | 1.66                     | 0.60              |
| 66:D3:1130:G:H21   | 66:D3:1138:A:H62    | 1.50                     | 0.60              |
| 77:EJ:276:THR:HA   | 77:EJ:283:THR:HA    | 1.83                     | 0.60              |
| 4:UA:440:PRO:HG3   | 4:UA:483:GLN:HG2    | 1.84                     | 0.60              |
| 4:UA:593:VAL:HG13  | 4:UA:686:PHE:CE2    | 2.37                     | 0.60              |
| 1:CB:201:HIS:O     | 1:CB:204:GLY:N      | 2.34                     | 0.60              |
| 7:UD:568:ASN:OD1   | 7:UD:569:PHE:N      | 2.35                     | 0.60              |
| 11:UH:576:ARG:HG3  | 11:UH:578:LEU:HG    | 1.84                     | 0.60              |
| 22:US:181:THR:HG1  | 22:US:225:HIS:CE1   | 2.20                     | 0.60              |
| 24:UU:135:ASN:ND2  | 24:UU:165:GLY:O     | 2.33                     | 0.60              |
| 25:UV:143:GLU:HA   | 25:UV:176:PHE:O     | 2.01                     | 0.60              |
| 27:UZ:34:LYS:HG3   | 27:UZ:203:TYR:HE1   | 1.66                     | 0.60              |
| 28:CD:263:ILE:HG13 | 28:CD:264:SER:H     | 1.67                     | 0.60              |
| 32:CI:13:LEU:O     | 32:CI:15:LYS:N      | 2.35                     | 0.60              |
| 32:CI:94:ILE:HG23  | 33:CJ:58:TYR:HB3    | 1.83                     | 0.60              |
| 33:CJ:88:ILE:HG13  | 33:CJ:138:ASP:HB2   | 1.83                     | 0.60              |
| 35:CL:170:VAL:HG12 | 35:CL:205:PHE:HB2   | 1.84                     | 0.60              |
| 36:CM:142:GLU:O    | 36:CM:147:ARG:NH2   | 2.35                     | 0.60              |
| 46:JO:113:ALA:O    | 46:JO:116:ILE:HG22  | 2.02                     | 0.60              |
| 47:JP:444:GLU:OE1  | 47:JP:448:ARG:NH2   | 2.33                     | 0.60              |
| 53:DI:76:THR:OG1   | 53:DI:105:ASP:OD1   | 2.19                     | 0.60              |
| 58:DQ:52:LEU:HD13  | 58:DQ:60:PHE:HD2    | 1.65                     | 0.60              |
| 66:D3:67:A:O2'     | 66:D3:69:G:OP1      | 2.19                     | 0.60              |
| 66:D3:1688:U:H2'   | 66:D3:1689:A:C8     | 2.37                     | 0.60              |
| 77:EJ:154:GLU:HA   | 77:EJ:202:ARG:HA    | 1.82                     | 0.60              |
| 3:JA:748:ARG:HH22  | 3:JA:752:ASN:HB3    | 1.67                     | 0.59              |
| 1:CB:198:GLU:OE2   | 1:CB:200:SER:N      | 2.26                     | 0.59              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 6:UC:494:TYR:HA    | 6:UC:497:GLN:NE2    | 2.17                     | 0.59              |
| 9:UF:145:ASP:OD1   | 44:JM:67:THR:OG1    | 2.19                     | 0.59              |
| 13:UJ:76:GLU:OE1   | 13:UJ:76:GLU:N      | 2.28                     | 0.59              |
| 13:UJ:286:LEU:O    | 13:UJ:326:LYS:NZ    | 2.31                     | 0.59              |
| 13:UJ:1671:GLY:HA3 | 13:UJ:1713:LEU:HD22 | 1.82                     | 0.59              |
| 15:UL:10:GLN:OE1   | 15:UL:682:ARG:NH1   | 2.33                     | 0.59              |
| 16:UM:265:ALA:HA   | 16:UM:290:ILE:HG13  | 1.84                     | 0.59              |
| 16:UM:745:ASP:OD2  | 34:CK:508:ARG:NH1   | 2.35                     | 0.59              |
| 17:UN:306:ARG:NH2  | 66:D3:-5:G:OP2      | 2.35                     | 0.59              |
| 18:UO:43:THR:O     | 18:UO:304:SER:OG    | 2.19                     | 0.59              |
| 24:UU:392:ARG:NH2  | 67:D4:64:A:OP2      | 2.35                     | 0.59              |
| 25:UV:538:ASN:OD1  | 25:UV:541:THR:OG1   | 2.20                     | 0.59              |
| 29:CE:298:ARG:HB3  | 29:CE:341:LEU:HD21  | 1.84                     | 0.59              |
| 33:CJ:74:ASP:OD2   | 33:CJ:201:ARG:NH1   | 2.34                     | 0.59              |
| 33:CJ:282:ARG:NH1  | 66:D3:560:U:H5      | 1.99                     | 0.59              |
| 35:CL:632:LYS:HA   | 35:CL:635:PHE:HB3   | 1.84                     | 0.59              |
| 38:JC:146:TYR:HA   | 38:JC:152:ASP:O     | 2.02                     | 0.59              |
| 44:JM:184:ASN:HB3  | 44:JM:185:LYS:HZ2   | 1.67                     | 0.59              |
| 46:JO:250:PRO:HG3  | 56:DN:106:ARG:HG3   | 1.84                     | 0.59              |
| 46:JO:273:LYS:O    | 46:JO:276:LYS:HG2   | 2.01                     | 0.59              |
| 47:JP:321:VAL:HG23 | 47:JP:356:TYR:CE2   | 2.36                     | 0.59              |
| 47:JP:436:SER:OG   | 47:JP:437:ILE:N     | 2.34                     | 0.59              |
| 61:DX:137:LYS:NZ   | 66:D3:548:G:OP2     | 2.35                     | 0.59              |
| 71:ED:246:ALA:HA   | 71:ED:276:CYS:HA    | 1.84                     | 0.59              |
| 3:JA:79:LYS:HA     | 3:JA:82:LYS:HG2     | 1.83                     | 0.59              |
| 1:CB:163:PHE:HB3   | 1:CB:239:CYS:SG     | 2.42                     | 0.59              |
| 5:UB:707:PRO:HD2   | 39:JF:229:ASN:ND2   | 2.17                     | 0.59              |
| 7:UD:104:TRP:HA    | 7:UD:113:ARG:O      | 2.02                     | 0.59              |
| 8:UE:209:ASP:OD1   | 8:UE:210:ARG:N      | 2.35                     | 0.59              |
| 13:UJ:205:THR:HB   | 13:UJ:210:LEU:HD21  | 1.84                     | 0.59              |
| 16:UM:592:SER:HB3  | 16:UM:602:TRP:HH2   | 1.66                     | 0.59              |
| 18:UO:53:HIS:H     | 18:UO:53:HIS:HD1    | 1.50                     | 0.59              |
| 18:UO:426:LYS:HG3  | 18:UO:429:VAL:HG21  | 1.84                     | 0.59              |
| 23:UT:953:LEU:HD12 | 23:UT:961:ILE:HG12  | 1.83                     | 0.59              |
| 24:UU:24:PHE:HB3   | 24:UU:654:TRP:HB3   | 1.83                     | 0.59              |
| 25:UV:921:ASP:OD2  | 25:UV:1172:ASN:ND2  | 2.35                     | 0.59              |
| 27:UZ:119:TYR:CE1  | 27:UZ:149:LYS:HD2   | 2.37                     | 0.59              |
| 27:UZ:246:THR:H    | 27:UZ:249:SER:HG    | 1.50                     | 0.59              |
| 30:CG:94:SER:HB3   | 30:CG:95:ARG:NH1    | 2.17                     | 0.59              |
| 36:CM:191:ILE:HB   | 36:CM:223:VAL:HG22  | 1.85                     | 0.59              |
| 39:JF:243:HIS:ND1  | 39:JG:240:LYS:HE2   | 2.18                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:JG:54:LYS:NZ    | 39:JG:56:SER:OG    | 2.35                     | 0.59              |
| 49:DE:212:ASP:OD1  | 49:DE:216:ASN:N    | 2.35                     | 0.59              |
| 56:DN:92:ILE:HD13  | 56:DN:122:ILE:HD11 | 1.84                     | 0.59              |
| 66:D3:1497:U:N3    | 66:D3:1511:U:H1'   | 2.17                     | 0.59              |
| 66:D3:1781:A:H3'   | 66:D3:1782:A:H8    | 1.66                     | 0.59              |
| 1:CA:306:LEU:O     | 1:CA:306:LEU:HD12  | 2.03                     | 0.59              |
| 4:UA:800:LYS:HG3   | 24:UU:928:PHE:CE2  | 2.37                     | 0.59              |
| 3:JB:619:SER:HA    | 3:JB:623:GLN:HA    | 1.83                     | 0.59              |
| 6:UC:434:PHE:HA    | 39:JG:132:ARG:HH12 | 1.67                     | 0.59              |
| 7:UD:561:LYS:HZ3   | 7:UD:563:LEU:HA    | 1.67                     | 0.59              |
| 10:UG:102:LYS:NZ   | 10:UG:387:GLU:OE2  | 2.33                     | 0.59              |
| 10:UG:357:SER:HA   | 10:UG:364:ARG:HD3  | 1.83                     | 0.59              |
| 10:UG:477:ALA:HA   | 10:UG:515:ARG:HH22 | 1.68                     | 0.59              |
| 15:UL:549:SER:HB2  | 15:UL:579:ILE:HD11 | 1.84                     | 0.59              |
| 15:UL:629:ASN:HB3  | 15:UL:641:TYR:HE1  | 1.67                     | 0.59              |
| 15:UL:897:ASP:HA   | 16:UM:761:ARG:HH21 | 1.67                     | 0.59              |
| 18:UO:5:ARG:N      | 20:UQ:336:ARG:HH12 | 2.00                     | 0.59              |
| 20:UQ:527:HIS:CE1  | 20:UQ:556:PRO:HB3  | 2.38                     | 0.59              |
| 21:UR:227:LEU:O    | 21:UR:593:HIS:NE2  | 2.36                     | 0.59              |
| 21:UR:358:PHE:HA   | 21:UR:376:LEU:O    | 2.02                     | 0.59              |
| 23:UT:480:TYR:O    | 23:UT:484:ILE:HG12 | 2.01                     | 0.59              |
| 23:UT:673:ARG:NH2  | 23:UT:773:LEU:HB3  | 2.17                     | 0.59              |
| 23:UT:723:GLY:HA3  | 23:UT:751:SER:HB2  | 1.83                     | 0.59              |
| 23:UT:1841:GLU:O   | 23:UT:1844:ASP:N   | 2.34                     | 0.59              |
| 24:UU:502:LYS:O    | 24:UU:503:ARG:NH1  | 2.35                     | 0.59              |
| 33:CJ:211:ASN:OD1  | 33:CJ:212:ALA:N    | 2.27                     | 0.59              |
| 35:CL:1138:ARG:NH1 | 66:D3:492:A:OP2    | 2.34                     | 0.59              |
| 38:JC:125:PHE:HB2  | 38:JC:132:HIS:HB2  | 1.84                     | 0.59              |
| 38:JC:195:LEU:O    | 38:JC:206:PHE:HA   | 2.03                     | 0.59              |
| 51:DG:2:LYS:NZ     | 66:D3:154:G:OP1    | 2.29                     | 0.59              |
| 1:CB:181:VAL:HG21  | 1:CB:196:ALA:HB2   | 1.84                     | 0.59              |
| 8:UE:167:SER:O     | 8:UE:168:HIS:ND1   | 2.35                     | 0.59              |
| 12:UI:499:ILE:HA   | 12:UI:502:ARG:HD3  | 1.85                     | 0.59              |
| 13:UJ:1712:LYS:NZ  | 13:UJ:1751:GLY:HA3 | 2.17                     | 0.59              |
| 16:UM:585:ASN:O    | 16:UM:587:GLN:NE2  | 2.34                     | 0.59              |
| 16:UM:660:LYS:NZ   | 16:UM:664:GLU:OE2  | 2.35                     | 0.59              |
| 18:UO:500:GLU:HA   | 18:UO:503:ARG:HG2  | 1.84                     | 0.59              |
| 19:UP:198:ILE:O    | 19:UP:201:SER:OG   | 2.18                     | 0.59              |
| 20:UQ:293:LEU:HD12 | 20:UQ:324:TRP:CZ3  | 2.38                     | 0.59              |
| 20:UQ:704:ASN:O    | 20:UQ:704:ASN:ND2  | 2.32                     | 0.59              |
| 21:UR:312:ILE:HD11 | 21:UR:326:LEU:HD11 | 1.85                     | 0.59              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 21:UR:384:ILE:HG21  | 21:UR:423:LEU:HD11  | 1.84                     | 0.59              |
| 23:UT:550:GLU:OE1   | 23:UT:588:ASN:ND2   | 2.32                     | 0.59              |
| 23:UT:1278:ARG:HG3  | 23:UT:1315:ARG:HG2  | 1.84                     | 0.59              |
| 23:UT:1635:ILE:HG13 | 23:UT:1636:LEU:HD22 | 1.84                     | 0.59              |
| 25:UV:589:LYS:O     | 25:UV:609:ASN:ND2   | 2.34                     | 0.59              |
| 30:CG:30:LEU:O      | 30:CG:31:ARG:HG2    | 2.03                     | 0.59              |
| 36:CM:269:GLU:N     | 36:CM:269:GLU:OE1   | 2.35                     | 0.59              |
| 47:JP:189:ARG:NH2   | 47:JP:229:GLN:OE1   | 2.36                     | 0.59              |
| 55:DL:11:ARG:NH1    | 66:D3:342:C:OP1     | 2.35                     | 0.59              |
| 66:D3:870:C:H2'     | 66:D3:871:G:H8      | 1.68                     | 0.59              |
| 4:UA:388:SER:OG     | 4:UA:389:SER:N      | 2.35                     | 0.59              |
| 8:UE:543:LEU:HD11   | 18:UO:463:VAL:HG23  | 1.85                     | 0.59              |
| 14:UK:146:PHE:O     | 19:UP:173:ARG:NH1   | 2.33                     | 0.59              |
| 14:UK:201:VAL:HA    | 14:UK:204:HIS:HD2   | 1.66                     | 0.59              |
| 16:UM:418:ASN:HB3   | 16:UM:420:ASN:OD1   | 2.01                     | 0.59              |
| 16:UM:465:LYS:H     | 16:UM:486:THR:HG23  | 1.68                     | 0.59              |
| 21:UR:165:ARG:NE    | 24:UU:218:LEU:HD23  | 2.18                     | 0.59              |
| 23:UT:262:ALA:O     | 23:UT:267:SER:OG    | 2.21                     | 0.59              |
| 25:UV:299:PRO:HD2   | 25:UV:302:VAL:HG11  | 1.85                     | 0.59              |
| 31:CH:488:ILE:HD11  | 31:CH:496:LEU:HB3   | 1.85                     | 0.59              |
| 39:JF:90:ASP:OD1    | 39:JF:91:ILE:N      | 2.32                     | 0.59              |
| 55:DL:57:LYS:HE3    | 66:D3:326:G:H5''    | 1.85                     | 0.59              |
| 55:DL:101:GLU:OE1   | 55:DL:103:ARG:NH1   | 2.35                     | 0.59              |
| 65:D2:93:A:H2'      | 65:D2:94:A:C8       | 2.38                     | 0.59              |
| 66:D3:202:A:H2'     | 66:D3:203:U:H4'     | 1.84                     | 0.59              |
| 66:D3:540:G:N2      | 66:D3:542:A:N7      | 2.51                     | 0.59              |
| 79:EN:870:ILE:O     | 79:EN:873:SER:CB    | 2.51                     | 0.59              |
| 5:UB:600:LEU:O      | 5:UB:675:TYR:OH     | 2.21                     | 0.59              |
| 5:UB:620:SER:O      | 5:UB:624:THR:OG1    | 2.15                     | 0.59              |
| 9:UF:102:LYS:NZ     | 65:D2:482:A:OP2     | 2.34                     | 0.59              |
| 10:UG:46:LEU:HD22   | 17:UN:859:ARG:HD2   | 1.84                     | 0.59              |
| 14:UK:82:ARG:NH2    | 35:CL:1087:LYS:O    | 2.35                     | 0.59              |
| 21:UR:570:PHE:CD2   | 21:UR:577:LEU:HD13  | 2.37                     | 0.59              |
| 23:UT:1458:GLN:HB3  | 23:UT:1462:ARG:HH22 | 1.66                     | 0.59              |
| 26:UX:63:TYR:CD2    | 26:UX:90:LEU:HD23   | 2.37                     | 0.59              |
| 30:CG:7:LYS:HB3     | 30:CG:65:LEU:HD21   | 1.85                     | 0.59              |
| 33:CJ:257:ARG:HH11  | 33:CJ:277:LEU:HD11  | 1.66                     | 0.59              |
| 39:JG:43:VAL:HB     | 39:JG:112:VAL:HG12  | 1.85                     | 0.59              |
| 51:DG:10:ASN:ND2    | 51:DG:127:THR:O     | 2.20                     | 0.59              |
| 62:DY:98:GLU:OE1    | 62:DY:99:LYS:N      | 2.36                     | 0.59              |
| 66:D3:145:A:O2'     | 66:D3:146:U:O5'     | 2.21                     | 0.59              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 66:D3:312:A:N6      | 66:D3:352:A:H1'     | 2.16                     | 0.59              |
| 66:D3:358:U:H2'     | 66:D3:360:A:C8      | 2.38                     | 0.59              |
| 66:D3:656:G:O2'     | 66:D3:678:A:N1      | 2.35                     | 0.59              |
| 66:D3:950:C:H2'     | 66:D3:951:A:H8      | 1.68                     | 0.59              |
| 71:ED:177:ARG:HA    | 71:ED:187:VAL:HA    | 1.82                     | 0.59              |
| 3:JA:743:VAL:HG11   | 3:JA:814:LEU:HD11   | 1.83                     | 0.59              |
| 7:UD:355:THR:OG1    | 7:UD:372:MET:O      | 2.13                     | 0.59              |
| 8:UE:72:ASP:OD1     | 8:UE:73:THR:N       | 2.35                     | 0.59              |
| 9:UF:73:ARG:NH2     | 21:UR:13:PRO:O      | 2.36                     | 0.59              |
| 9:UF:138:LYS:HZ2    | 28:CD:84:LEU:HG     | 1.68                     | 0.59              |
| 13:UJ:716:PHE:O     | 13:UJ:719:SER:OG    | 2.18                     | 0.59              |
| 16:UM:662:GLN:NE2   | 16:UM:666:GLU:OE2   | 2.35                     | 0.59              |
| 21:UR:317:ARG:HH12  | 65:D2:233:G:N2      | 1.98                     | 0.59              |
| 23:UT:1314:SER:HA   | 23:UT:1320:ASP:HB2  | 1.83                     | 0.59              |
| 25:UV:400:LEU:HD23  | 25:UV:425:VAL:HG12  | 1.85                     | 0.59              |
| 27:UZ:56:ILE:HD11   | 48:JQ:192:ALA:HA    | 1.83                     | 0.59              |
| 27:UZ:130:ARG:HG2   | 48:JQ:184:TYR:HE2   | 1.66                     | 0.59              |
| 27:UZ:148:LYS:NZ    | 66:D3:1512:G:OP1    | 2.30                     | 0.59              |
| 32:CI:24:ASP:O      | 32:CI:26:GLY:N      | 2.34                     | 0.59              |
| 35:CL:833:ARG:HG3   | 35:CL:834:TRP:CD1   | 2.37                     | 0.59              |
| 46:JO:142:ARG:NH1   | 46:JO:168:GLY:O     | 2.36                     | 0.59              |
| 65:D2:329:A:N6      | 65:D2:385:A:C4      | 2.70                     | 0.59              |
| 66:D3:49:C:OP2      | 66:D3:425:A:N6      | 2.35                     | 0.59              |
| 66:D3:1171:A:H2'    | 66:D3:1172:G:H8     | 1.67                     | 0.59              |
| 7:UD:449:LYS:NZ     | 7:UD:465:LEU:O      | 2.32                     | 0.59              |
| 9:UF:111:ALA:HB1    | 44:JM:73:ALA:HB2    | 1.83                     | 0.59              |
| 12:UI:419:PHE:O     | 12:UI:422:THR:OG1   | 2.16                     | 0.59              |
| 13:UJ:1591:THR:O    | 13:UJ:1595:THR:HG23 | 2.02                     | 0.59              |
| 15:UL:161:SER:O     | 15:UL:187:LYS:NZ    | 2.36                     | 0.59              |
| 16:UM:288:LEU:HB3   | 16:UM:306:LEU:HD12  | 1.84                     | 0.59              |
| 18:UO:108:TYR:HA    | 18:UO:117:LEU:HB3   | 1.84                     | 0.59              |
| 20:UQ:89:VAL:HG11   | 20:UQ:141:LEU:HD22  | 1.84                     | 0.59              |
| 20:UQ:534:LYS:HD3   | 20:UQ:541:TRP:CE2   | 2.37                     | 0.59              |
| 23:UT:322:VAL:O     | 23:UT:368:ASN:ND2   | 2.35                     | 0.59              |
| 23:UT:476:LEU:O     | 23:UT:518:MET:HE1   | 2.03                     | 0.59              |
| 23:UT:1261:ILE:HG21 | 23:UT:1295:VAL:HG21 | 1.85                     | 0.59              |
| 23:UT:1379:ASN:HB3  | 23:UT:1428:THR:HA   | 1.83                     | 0.59              |
| 23:UT:1922:ILE:HB   | 23:UT:1934:PHE:CE1  | 2.38                     | 0.59              |
| 25:UV:493:GLY:O     | 25:UV:497:ARG:HG2   | 2.03                     | 0.59              |
| 25:UV:685:ALA:HA    | 25:UV:688:LYS:HG2   | 1.85                     | 0.59              |
| 35:CL:878:HIS:O     | 66:D3:572:C:N4      | 2.36                     | 0.59              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 36:CM:109:PHE:HA    | 36:CM:361:ASN:HD21  | 1.67                     | 0.59              |
| 44:JM:153:ILE:O     | 44:JM:154:GLU:HG2   | 2.02                     | 0.59              |
| 45:JN:240:ARG:O     | 45:JN:243:ILE:HG22  | 2.03                     | 0.59              |
| 50:DF:113:ILE:HD13  | 50:DF:190:ILE:HD11  | 1.85                     | 0.59              |
| 61:DX:89:ASN:O      | 61:DX:92:CYS:N      | 2.35                     | 0.59              |
| 66:D3:457:G:H2'     | 66:D3:458:G:H8      | 1.68                     | 0.59              |
| 66:D3:1776:A:H2'    | 66:D3:1777:G:C8     | 2.37                     | 0.59              |
| 3:JA:70:ARG:HH12    | 66:D3:415:C:P       | 2.26                     | 0.59              |
| 3:JA:563:LYS:N      | 3:JA:587:GLN:HE22   | 2.01                     | 0.59              |
| 1:CB:228:GLN:O      | 1:CB:231:ARG:N      | 2.35                     | 0.59              |
| 1:CB:230:TYR:HD1    | 1:CB:234:ILE:HD12   | 1.67                     | 0.59              |
| 3:JB:119:TYR:N      | 3:JB:141:THR:O      | 2.32                     | 0.59              |
| 7:UD:762:PHE:O      | 7:UD:765:LYS:NZ     | 2.23                     | 0.59              |
| 8:UE:336:ASN:O      | 18:UO:373:ILE:HD12  | 2.03                     | 0.59              |
| 8:UE:444:ALA:O      | 8:UE:447:SER:O      | 2.21                     | 0.59              |
| 13:UJ:128:HIS:CD2   | 13:UJ:129:VAL:HG13  | 2.37                     | 0.59              |
| 14:UK:18:GLN:OE1    | 14:UK:19:LEU:N      | 2.35                     | 0.59              |
| 15:UL:476:ILE:HG22  | 15:UL:492:SER:HB3   | 1.83                     | 0.59              |
| 15:UL:912:TRP:CD2   | 16:UM:779:VAL:HG21  | 2.38                     | 0.59              |
| 16:UM:517:ILE:O     | 16:UM:526:GLU:N     | 2.35                     | 0.59              |
| 20:UQ:306:SER:HA    | 20:UQ:346:VAL:HG11  | 1.85                     | 0.59              |
| 22:US:466:LEU:HD23  | 22:US:469:LEU:HD12  | 1.84                     | 0.59              |
| 23:UT:841:ILE:HG22  | 23:UT:876:TYR:HE1   | 1.67                     | 0.59              |
| 23:UT:1275:PHE:O    | 23:UT:1281:ARG:NH1  | 2.32                     | 0.59              |
| 23:UT:1742:VAL:HB   | 23:UT:1745:ILE:HD12 | 1.83                     | 0.59              |
| 23:UT:1758:ALA:HB3  | 23:UT:1799:GLY:HA3  | 1.85                     | 0.59              |
| 25:UV:215:GLU:OE1   | 25:UV:223:ARG:NH1   | 2.33                     | 0.59              |
| 25:UV:444:SER:N     | 25:UV:471:SER:OG    | 2.32                     | 0.59              |
| 25:UV:623:GLU:N     | 25:UV:623:GLU:OE1   | 2.35                     | 0.59              |
| 29:CE:285:PRO:HG3   | 29:CE:382:ASP:HA    | 1.84                     | 0.59              |
| 35:CL:559:SER:OG    | 35:CL:561:GLU:OE1   | 2.19                     | 0.59              |
| 38:JC:51:GLN:NE2    | 51:DG:76:LEU:HD21   | 2.17                     | 0.59              |
| 39:JF:104:ILE:N     | 39:JF:246:GLU:OE2   | 2.34                     | 0.59              |
| 47:JP:420:PRO:HD2   | 47:JP:423:ILE:HD12  | 1.85                     | 0.59              |
| 52:DH:24:PHE:HA     | 52:DH:27:LEU:HD12   | 1.85                     | 0.59              |
| 52:DH:102:PRO:HG2   | 66:D3:810:G:C2      | 2.37                     | 0.59              |
| 3:JA:567:LEU:HD22   | 3:JA:653:ALA:HB2    | 1.84                     | 0.59              |
| 13:UJ:1423:LEU:HD22 | 13:UJ:1456:VAL:HG12 | 1.84                     | 0.59              |
| 13:UJ:1666:LEU:O    | 13:UJ:1670:ILE:HD12 | 2.03                     | 0.59              |
| 15:UL:161:SER:O     | 15:UL:163:LYS:NZ    | 2.36                     | 0.59              |
| 15:UL:229:TRP:HB3   | 15:UL:242:LEU:HD11  | 1.85                     | 0.59              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 15:UL:888:ARG:NH2   | 16:UM:807:ASP:OD1   | 2.30                     | 0.59              |
| 20:UQ:657:SER:HB3   | 20:UQ:675:ARG:NH2   | 2.18                     | 0.59              |
| 23:UT:1548:ILE:HD13 | 23:UT:1551:LEU:HD21 | 1.85                     | 0.59              |
| 23:UT:1696:TYR:HA   | 23:UT:1699:LYS:HZ3  | 1.68                     | 0.59              |
| 24:UU:35:ASN:ND2    | 24:UU:53:CYS:SG     | 2.71                     | 0.59              |
| 25:UV:580:TYR:HB2   | 25:UV:618:ILE:HB    | 1.84                     | 0.59              |
| 28:CD:297:HIS:HA    | 28:CD:301:PRO:HB3   | 1.85                     | 0.59              |
| 29:CE:145:HIS:HB3   | 29:CE:149:ARG:CZ    | 2.33                     | 0.59              |
| 35:CL:252:LEU:O     | 35:CL:268:LYS:CB    | 2.47                     | 0.59              |
| 51:DG:57:ASP:OD1    | 51:DG:61:PHE:N      | 2.35                     | 0.59              |
| 54:DJ:121:SER:O     | 54:DJ:124:HIS:N     | 2.36                     | 0.59              |
| 66:D3:524:U:H2'     | 66:D3:525:A:H5''    | 1.85                     | 0.59              |
| 66:D3:951:A:H2'     | 66:D3:952:A:H8      | 1.67                     | 0.59              |
| 66:D3:1657:U:H4'    | 66:D3:1658:G:O5'    | 2.02                     | 0.59              |
| 3:JA:182:ALA:HB1    | 3:JA:185:ASN:HB2    | 1.84                     | 0.58              |
| 7:UD:739:LYS:H      | 7:UD:739:LYS:HD2    | 1.68                     | 0.58              |
| 9:UF:138:LYS:HZ3    | 28:CD:85:ASN:HA     | 1.66                     | 0.58              |
| 9:UF:183:TYR:CZ     | 9:UF:322:LEU:HD12   | 2.37                     | 0.58              |
| 9:UF:285:TYR:O      | 9:UF:288:LYS:HG3    | 2.02                     | 0.58              |
| 13:UJ:1708:ILE:HG23 | 13:UJ:1752:LEU:HD21 | 1.85                     | 0.58              |
| 23:UT:262:ALA:HB1   | 23:UT:272:VAL:HG12  | 1.84                     | 0.58              |
| 23:UT:1732:GLU:OE2  | 66:D3:803:A:N6      | 2.35                     | 0.58              |
| 23:UT:1763:LEU:HD22 | 23:UT:1810:SER:HB2  | 1.84                     | 0.58              |
| 23:UT:1900:ARG:O    | 23:UT:1903:LEU:HG   | 2.03                     | 0.58              |
| 24:UU:28:ARG:NH1    | 24:UU:383:ASP:OD2   | 2.36                     | 0.58              |
| 24:UU:91:TYR:CE2    | 24:UU:123:ILE:HG21  | 2.38                     | 0.58              |
| 25:UV:1227:GLY:O    | 25:UV:1231:VAL:N    | 2.35                     | 0.58              |
| 31:CH:68:LYS:O      | 31:CH:71:LEU:N      | 2.36                     | 0.58              |
| 34:CK:330:VAL:HG13  | 35:CL:934:LEU:HD23  | 1.85                     | 0.58              |
| 34:CK:473:THR:O     | 34:CK:477:GLU:HG2   | 2.03                     | 0.58              |
| 35:CL:91:ARG:NH2    | 35:CL:214:ARG:HE    | 2.01                     | 0.58              |
| 56:DN:99:ARG:NH2    | 56:DN:141:TYR:OH    | 2.35                     | 0.58              |
| 66:D3:161:U:H2'     | 66:D3:162:A:C8      | 2.38                     | 0.58              |
| 66:D3:1202:A:N6     | 66:D3:1210:C:O2'    | 2.36                     | 0.58              |
| 79:EN:647:HIS:O     | 79:EN:651:GLN:N     | 2.31                     | 0.58              |
| 1:CA:178:GLY:HA2    | 1:CA:181:VAL:HB     | 1.84                     | 0.58              |
| 3:JA:752:ASN:ND2    | 3:JA:755:THR:OG1    | 2.24                     | 0.58              |
| 5:UB:647:ILE:HA     | 5:UB:651:TRP:CE3    | 2.37                     | 0.58              |
| 6:UC:509:ARG:HH11   | 66:D3:1504:G:P      | 2.26                     | 0.58              |
| 9:UF:118:LYS:HG2    | 9:UF:153:TYR:CZ     | 2.38                     | 0.58              |
| 13:UJ:636:ASP:OD2   | 13:UJ:639:ARG:NH1   | 2.35                     | 0.58              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 15:UL:53:ASP:OD1   | 15:UL:54:ILE:N      | 2.36                     | 0.58              |
| 15:UL:474:ALA:N    | 15:UL:494:ASP:OD2   | 2.37                     | 0.58              |
| 20:UQ:313:LEU:HD22 | 20:UQ:321:MET:SD    | 2.44                     | 0.58              |
| 22:US:350:MET:CE   | 22:US:386:LEU:HB3   | 2.33                     | 0.58              |
| 23:UT:194:GLU:HG2  | 23:UT:238:GLU:HG2   | 1.84                     | 0.58              |
| 25:UV:552:ARG:O    | 25:UV:556:ILE:HA    | 2.03                     | 0.58              |
| 25:UV:1097:ASP:H   | 25:UV:1185:LEU:HD23 | 1.69                     | 0.58              |
| 29:CE:314:ALA:N    | 30:CF:38:ASN:OD1    | 2.34                     | 0.58              |
| 38:JC:98:ASP:OD1   | 38:JC:99:ALA:N      | 2.36                     | 0.58              |
| 38:JC:162:LEU:HB2  | 38:JC:176:PHE:HB2   | 1.85                     | 0.58              |
| 38:JC:363:LEU:HA   | 38:JC:366:LYS:HE2   | 1.85                     | 0.58              |
| 39:JF:140:LEU:O    | 39:JF:143:GLN:NE2   | 2.36                     | 0.58              |
| 42:JJ:174:LEU:HD13 | 42:JJ:180:LEU:HB2   | 1.85                     | 0.58              |
| 66:D3:1666:U:H2'   | 66:D3:1667:A:C8     | 2.37                     | 0.58              |
| 66:D3:1697:G:H2'   | 66:D3:1698:G:H8     | 1.65                     | 0.58              |
| 79:EN:325:PRO:O    | 79:EN:553:GLY:N     | 2.35                     | 0.58              |
| 1:CA:263:ASP:OD1   | 1:CA:264:GLN:N      | 2.37                     | 0.58              |
| 3:JA:195:ASN:ND2   | 3:JA:197:ASN:OD1    | 2.36                     | 0.58              |
| 3:JA:904:LEU:HD21  | 3:JA:908:GLN:HB2    | 1.85                     | 0.58              |
| 7:UD:626:TRP:HH2   | 7:UD:657:ILE:HD11   | 1.68                     | 0.58              |
| 8:UE:109:ASP:OD1   | 8:UE:150:LYS:HA     | 2.03                     | 0.58              |
| 8:UE:513:LEU:HA    | 8:UE:516:ILE:HG22   | 1.85                     | 0.58              |
| 9:UF:144:VAL:HG11  | 9:UF:178:VAL:HG21   | 1.85                     | 0.58              |
| 11:UH:596:LYS:HD3  | 11:UH:600:LYS:HZ3   | 1.67                     | 0.58              |
| 12:UI:501:GLY:O    | 12:UI:505:MET:HG2   | 2.03                     | 0.58              |
| 13:UJ:381:ARG:HH12 | 20:UQ:853:ILE:HG13  | 1.68                     | 0.58              |
| 18:UO:372:HIS:N    | 21:UR:287:SER:OG    | 2.28                     | 0.58              |
| 21:UR:456:THR:HG23 | 21:UR:457:LYS:HG2   | 1.85                     | 0.58              |
| 22:US:349:LEU:HD23 | 22:US:355:ARG:NH1   | 2.18                     | 0.58              |
| 23:UT:1155:ASP:HB2 | 23:UT:1201:LEU:HD12 | 1.85                     | 0.58              |
| 24:UU:101:TYR:CD1  | 24:UU:106:GLU:HA    | 2.38                     | 0.58              |
| 24:UU:332:SER:O    | 24:UU:334:ASP:N     | 2.35                     | 0.58              |
| 25:UV:913:VAL:O    | 25:UV:917:LYS:HG2   | 2.03                     | 0.58              |
| 29:CE:277:SER:OG   | 29:CE:293:GLU:OE1   | 2.17                     | 0.58              |
| 31:CH:240:LEU:HD11 | 31:CH:256:ARG:HG2   | 1.85                     | 0.58              |
| 50:DF:23:VAL:HG12  | 58:DQ:58:ASP:HB3    | 1.86                     | 0.58              |
| 51:DG:193:LEU:O    | 51:DG:197:ASN:ND2   | 2.36                     | 0.58              |
| 52:DH:29:ASN:HA    | 52:DH:35:LYS:NZ     | 2.19                     | 0.58              |
| 52:DH:141:ARG:NH1  | 52:DH:141:ARG:HB2   | 2.17                     | 0.58              |
| 66:D3:390:G:H1     | 66:D3:407:A:N6      | 1.96                     | 0.58              |
| 66:D3:1114:G:H2'   | 66:D3:1115:U:C6     | 2.38                     | 0.58              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 10:UG:283:ASP:OD2  | 10:UG:285:SER:OG    | 2.16                     | 0.58              |
| 15:UL:41:LEU:O     | 15:UL:51:ILE:HA     | 2.03                     | 0.58              |
| 15:UL:269:THR:OG1  | 15:UL:286:ILE:O     | 2.18                     | 0.58              |
| 15:UL:426:ARG:HD3  | 15:UL:459:LEU:HD13  | 1.85                     | 0.58              |
| 15:UL:672:VAL:HB   | 15:UL:684:TRP:HB2   | 1.85                     | 0.58              |
| 16:UM:601:ILE:O    | 16:UM:610:LEU:N     | 2.35                     | 0.58              |
| 20:UQ:453:HIS:HB3  | 20:UQ:456:ALA:O     | 2.03                     | 0.58              |
| 24:UU:229:GLU:OE2  | 24:UU:245:LYS:NZ    | 2.37                     | 0.58              |
| 25:UV:177:ASN:ND2  | 25:UV:212:GLU:OE2   | 2.37                     | 0.58              |
| 26:UX:99:THR:OG1   | 26:UX:101:CYS:SG    | 2.51                     | 0.58              |
| 28:CD:174:ILE:HD11 | 28:CD:295:LYS:HB3   | 1.85                     | 0.58              |
| 33:CJ:109:LEU:HD21 | 66:D3:1159:C:N4     | 2.18                     | 0.58              |
| 33:CJ:126:ASN:HD22 | 58:DQ:123:ARG:HH12  | 1.50                     | 0.58              |
| 34:CK:366:GLU:HB3  | 34:CK:370:ARG:HH12  | 1.68                     | 0.58              |
| 66:D3:924:A:H2'    | 66:D3:925:G:C8      | 2.39                     | 0.58              |
| 66:D3:1654:G:H2'   | 66:D3:1655:A:H8     | 1.67                     | 0.58              |
| 3:JA:183:ARG:NH1   | 3:JA:557:SER:O      | 2.36                     | 0.58              |
| 1:CB:211:ALA:HB1   | 29:CE:145:HIS:HE2   | 1.69                     | 0.58              |
| 7:UD:741:LEU:HA    | 7:UD:756:GLU:HA     | 1.84                     | 0.58              |
| 10:UG:216:TYR:CD2  | 10:UG:261:PRO:HB3   | 2.39                     | 0.58              |
| 15:UL:920:PHE:HB2  | 15:UL:926:GLN:HG2   | 1.84                     | 0.58              |
| 16:UM:88:PHE:HB2   | 16:UM:95:VAL:HG12   | 1.84                     | 0.58              |
| 18:UO:136:ASP:OD1  | 18:UO:137:ASN:N     | 2.37                     | 0.58              |
| 18:UO:275:SER:OG   | 18:UO:302:VAL:O     | 2.22                     | 0.58              |
| 22:US:345:ILE:HD11 | 22:US:382:LYS:HD3   | 1.85                     | 0.58              |
| 23:UT:1011:LEU:HA  | 53:DI:115:ALA:HB1   | 1.85                     | 0.58              |
| 23:UT:1383:ASN:HB3 | 23:UT:1386:GLU:HG2  | 1.86                     | 0.58              |
| 23:UT:1718:VAL:HA  | 23:UT:1721:ILE:HG22 | 1.85                     | 0.58              |
| 25:UV:1205:LYS:NZ  | 25:UV:1214:LEU:O    | 2.36                     | 0.58              |
| 27:UZ:17:LEU:O     | 27:UZ:21:ILE:HG12   | 2.03                     | 0.58              |
| 35:CL:210:VAL:O    | 35:CL:210:VAL:HG13  | 2.03                     | 0.58              |
| 37:CN:208:ASP:N    | 37:CN:212:PHE:O     | 2.35                     | 0.58              |
| 38:JC:258:ARG:HB3  | 43:JK:497:LEU:HD23  | 1.84                     | 0.58              |
| 39:JG:56:SER:HA    | 39:JG:63:ASP:N      | 2.18                     | 0.58              |
| 55:DL:122:ILE:HG23 | 55:DL:143:SER:HB2   | 1.85                     | 0.58              |
| 66:D3:91:G:H2'     | 66:D3:92:A:C8       | 2.38                     | 0.58              |
| 66:D3:273:G:H1     | 66:D3:283:U:H3      | 1.49                     | 0.58              |
| 66:D3:972:G:H2'    | 66:D3:973:A:C8      | 2.39                     | 0.58              |
| 66:D3:1776:A:H2'   | 66:D3:1777:G:H8     | 1.68                     | 0.58              |
| 67:D4:68:A:H2'     | 67:D4:69:A:C8       | 2.34                     | 0.58              |
| 3:JA:142:VAL:O     | 3:JA:475:ARG:NH2    | 2.36                     | 0.58              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 6:UC:608:PHE:HD2   | 26:UX:147:GLN:NE2   | 2.02                     | 0.58              |
| 20:UQ:211:MET:HA   | 20:UQ:224:SER:O     | 2.03                     | 0.58              |
| 20:UQ:317:TRP:HA   | 20:UQ:340:ILE:HG23  | 1.85                     | 0.58              |
| 20:UQ:583:LYS:HG2  | 20:UQ:599:ILE:HG22  | 1.86                     | 0.58              |
| 23:UT:1063:SER:HA  | 23:UT:1108:LEU:HD13 | 1.85                     | 0.58              |
| 24:UU:353:PRO:HA   | 24:UU:370:SER:HB2   | 1.84                     | 0.58              |
| 25:UV:356:THR:HG23 | 25:UV:359:PHE:HB2   | 1.86                     | 0.58              |
| 27:UZ:77:LYS:NZ    | 65:D2:253:U:O2'     | 2.37                     | 0.58              |
| 28:CD:82:LEU:HB3   | 28:CD:113:PHE:HE2   | 1.67                     | 0.58              |
| 28:CD:197:GLU:OE1  | 29:CE:165:GLN:NE2   | 2.37                     | 0.58              |
| 29:CE:405:ASP:OD2  | 29:CE:407:ARG:NH2   | 2.36                     | 0.58              |
| 35:CL:135:ALA:O    | 35:CL:238:ARG:NH2   | 2.36                     | 0.58              |
| 38:JC:316:ASP:O    | 38:JC:333:ASN:ND2   | 2.32                     | 0.58              |
| 44:JM:70:ASP:O     | 44:JM:74:ASN:ND2    | 2.36                     | 0.58              |
| 47:JP:48:THR:HG21  | 47:JP:410:ILE:HG23  | 1.86                     | 0.58              |
| 52:DH:169:PHE:HB3  | 52:DH:183:PHE:CE2   | 2.39                     | 0.58              |
| 65:D2:481:U:O2'    | 65:D2:482:A:OP2     | 2.21                     | 0.58              |
| 66:D3:639:U:O2'    | 66:D3:640:U:O5'     | 2.21                     | 0.58              |
| 66:D3:655:G:N2     | 66:D3:679:U:O4'     | 2.37                     | 0.58              |
| 66:D3:955:A:H2'    | 66:D3:956:C:O4'     | 2.03                     | 0.58              |
| 66:D3:1739:C:H2'   | 66:D3:1740:A:C8     | 2.38                     | 0.58              |
| 1:CA:264:GLN:CA    | 1:CA:320:TYR:O      | 2.48                     | 0.58              |
| 3:JA:12:SER:O      | 3:JA:16:ASN:ND2     | 2.36                     | 0.58              |
| 4:UA:633:LYS:HE2   | 65:D2:293:U:C5      | 2.39                     | 0.58              |
| 1:CB:292:LYS:NZ    | 7:UD:138:ASP:O      | 2.36                     | 0.58              |
| 7:UD:529:ASN:HA    | 7:UD:545:ARG:HH21   | 1.68                     | 0.58              |
| 8:UE:48:GLU:OE1    | 8:UE:48:GLU:N       | 2.36                     | 0.58              |
| 10:UG:449:ILE:HG23 | 17:UN:842:TYR:HB3   | 1.86                     | 0.58              |
| 13:UJ:304:GLN:NE2  | 13:UJ:347:PHE:H     | 2.01                     | 0.58              |
| 14:UK:215:GLN:NE2  | 14:UK:219:ASP:OD2   | 2.35                     | 0.58              |
| 15:UL:142:ASP:N    | 15:UL:142:ASP:OD1   | 2.37                     | 0.58              |
| 15:UL:188:LEU:HB3  | 15:UL:198:GLU:HB2   | 1.85                     | 0.58              |
| 15:UL:940:GLY:HA2  | 34:CK:465:LEU:HD23  | 1.85                     | 0.58              |
| 18:UO:301:PRO:HG2  | 18:UO:323:SER:HB2   | 1.84                     | 0.58              |
| 20:UQ:528:ILE:HD12 | 20:UQ:548:ILE:HG12  | 1.84                     | 0.58              |
| 20:UQ:885:ASP:OD1  | 20:UQ:886:THR:N     | 2.37                     | 0.58              |
| 22:US:222:LEU:HA   | 22:US:225:HIS:HE1   | 1.68                     | 0.58              |
| 23:UT:922:MET:HA   | 23:UT:925:VAL:HB    | 1.84                     | 0.58              |
| 25:UV:127:PHE:HD1  | 25:UV:283:TYR:HB3   | 1.69                     | 0.58              |
| 27:UZ:173:PRO:HA   | 27:UZ:176:VAL:HG22  | 1.85                     | 0.58              |
| 35:CL:629:ASP:HA   | 35:CL:632:LYS:HE2   | 1.85                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 42:JJ:168:LEU:O    | 42:JJ:172:ILE:HG12 | 2.04                     | 0.58              |
| 49:DE:47:PHE:HD2   | 49:DE:48:LEU:HD22  | 1.69                     | 0.58              |
| 51:DG:185:GLN:HA   | 51:DG:188:ARG:NE   | 2.18                     | 0.58              |
| 52:DH:62:VAL:HG11  | 52:DH:70:PHE:HE2   | 1.68                     | 0.58              |
| 62:DY:89:TYR:CG    | 66:D3:525:A:H4'    | 2.38                     | 0.58              |
| 66:D3:114:C:N4     | 66:D3:245:U:O2     | 2.37                     | 0.58              |
| 66:D3:635:A:H2'    | 66:D3:636:A:C8     | 2.37                     | 0.58              |
| 2:DA:31:ASP:OD2    | 2:DA:32:ILE:N      | 2.37                     | 0.58              |
| 1:CB:292:LYS:HZ3   | 7:UD:138:ASP:HB3   | 1.69                     | 0.58              |
| 14:UK:63:TYR:HE2   | 14:UK:65:HIS:CE1   | 2.22                     | 0.58              |
| 15:UL:183:ASP:O    | 15:UL:185:MET:N    | 2.36                     | 0.58              |
| 15:UL:258:LYS:HZ3  | 15:UL:259:ILE:H    | 1.52                     | 0.58              |
| 15:UL:905:LEU:HG   | 16:UM:782:VAL:HG23 | 1.86                     | 0.58              |
| 18:UO:428:ARG:NH2  | 20:UQ:518:ASP:O    | 2.31                     | 0.58              |
| 23:UT:259:LEU:HD23 | 23:UT:263:LEU:HD23 | 1.86                     | 0.58              |
| 25:UV:524:ASP:H    | 25:UV:618:ILE:HD13 | 1.66                     | 0.58              |
| 25:UV:1188:PRO:HA  | 25:UV:1191:LYS:HB2 | 1.86                     | 0.58              |
| 31:CH:323:ASP:OD1  | 31:CH:324:ILE:N    | 2.33                     | 0.58              |
| 33:CJ:268:ASN:HD22 | 33:CJ:271:ALA:HB2  | 1.69                     | 0.58              |
| 35:CL:99:ASN:OD1   | 35:CL:100:ASP:N    | 2.37                     | 0.58              |
| 36:CM:172:SER:HB3  | 36:CM:174:ILE:HD11 | 1.84                     | 0.58              |
| 36:CM:192:THR:HG22 | 36:CM:248:GLN:NE2  | 2.19                     | 0.58              |
| 39:JG:120:ILE:H    | 39:JG:120:ILE:HD12 | 1.69                     | 0.58              |
| 45:JN:224:HIS:HE2  | 67:D4:15:U:P       | 2.26                     | 0.58              |
| 51:DG:31:ARG:HG2   | 51:DG:100:ALA:HB1  | 1.86                     | 0.58              |
| 53:DI:5:ARG:HB3    | 53:DI:28:GLU:HB2   | 1.86                     | 0.58              |
| 53:DI:113:PHE:O    | 53:DI:117:TYR:HB2  | 2.04                     | 0.58              |
| 65:D2:352:U:H3'    | 65:D2:353:A:H8     | 1.67                     | 0.58              |
| 3:JA:107:TYR:HB2   | 3:JA:110:GLU:HG2   | 1.86                     | 0.58              |
| 1:CB:305:THR:OG1   | 14:UK:132:ASN:N    | 2.36                     | 0.58              |
| 8:UE:489:ALA:HB1   | 18:UO:16:LEU:HD11  | 1.86                     | 0.58              |
| 10:UG:212:GLY:O    | 10:UG:230:THR:OG1  | 2.17                     | 0.58              |
| 13:UJ:25:ARG:HH22  | 47:JP:11:ASP:HA    | 1.67                     | 0.58              |
| 13:UJ:308:GLY:HA2  | 21:UR:225:SER:HB3  | 1.86                     | 0.58              |
| 14:UK:100:LYS:HE3  | 35:CL:1094:TYR:HE1 | 1.69                     | 0.58              |
| 15:UL:17:ILE:HG23  | 15:UL:52:TRP:HZ2   | 1.69                     | 0.58              |
| 17:UN:336:THR:HB   | 17:UN:339:GLN:HG2  | 1.86                     | 0.58              |
| 19:UP:185:GLN:HA   | 19:UP:188:LYS:NZ   | 2.19                     | 0.58              |
| 20:UQ:19:LYS:NZ    | 20:UQ:366:ASN:HD21 | 2.01                     | 0.58              |
| 20:UQ:55:TYR:CZ    | 20:UQ:385:ILE:HD12 | 2.39                     | 0.58              |
| 23:UT:262:ALA:O    | 23:UT:313:ARG:NH1  | 2.37                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:UT:597:ARG:HH12 | 23:UT:668:GLY:HA3  | 1.69                     | 0.58              |
| 23:UT:653:LYS:NZ   | 23:UT:654:THR:O    | 2.36                     | 0.58              |
| 23:UT:1716:MET:HA  | 23:UT:1719:LYS:HE2 | 1.86                     | 0.58              |
| 24:UU:934:ALA:O    | 24:UU:938:THR:HG22 | 2.04                     | 0.58              |
| 25:UV:141:TRP:CD1  | 25:UV:178:TYR:HB3  | 2.38                     | 0.58              |
| 25:UV:166:LYS:HE2  | 25:UV:597:ARG:HD2  | 1.84                     | 0.58              |
| 29:CE:227:LEU:HD12 | 29:CE:228:PRO:HD2  | 1.85                     | 0.58              |
| 33:CJ:189:LEU:HB3  | 33:CJ:191:PHE:CE1  | 2.38                     | 0.58              |
| 39:JG:76:LEU:HD23  | 39:JG:76:LEU:H     | 1.68                     | 0.58              |
| 42:JJ:184:THR:HA   | 42:JJ:231:ILE:O    | 2.04                     | 0.58              |
| 55:DL:37:ASN:HA    | 55:DL:44:THR:HG21  | 1.86                     | 0.58              |
| 66:D3:389:G:H2'    | 66:D3:390:G:C8     | 2.38                     | 0.58              |
| 70:EC:15:ASP:O     | 78:EK:40:TYR:CB    | 2.52                     | 0.58              |
| 1:CB:191:GLU:OE1   | 1:CB:191:GLU:N     | 2.32                     | 0.58              |
| 7:UD:550:VAL:HG13  | 7:UD:563:LEU:HB2   | 1.86                     | 0.58              |
| 8:UE:75:ALA:HA     | 8:UE:90:VAL:HG13   | 1.85                     | 0.58              |
| 8:UE:88:TYR:HB2    | 8:UE:95:VAL:HG12   | 1.84                     | 0.58              |
| 8:UE:215:TYR:CD1   | 8:UE:222:THR:HA    | 2.37                     | 0.58              |
| 13:UJ:157:LEU:HD12 | 13:UJ:165:SER:HA   | 1.86                     | 0.58              |
| 14:UK:184:ILE:HD12 | 65:D2:427:A:H5'    | 1.86                     | 0.58              |
| 18:UO:233:ASN:HD22 | 18:UO:247:GLU:HB3  | 1.67                     | 0.58              |
| 18:UO:482:GLU:HA   | 18:UO:485:ILE:HD12 | 1.86                     | 0.58              |
| 20:UQ:386:ASN:HD21 | 20:UQ:458:GLN:HE21 | 1.52                     | 0.58              |
| 21:UR:141:ASN:HD22 | 65:D2:307:C:H5'    | 1.69                     | 0.58              |
| 22:US:224:ASN:O    | 22:US:284:ARG:NH2  | 2.25                     | 0.58              |
| 25:UV:765:LEU:HD21 | 25:UV:917:LYS:HB2  | 1.85                     | 0.58              |
| 32:CI:7:HIS:ND1    | 67:D4:34:A:C5      | 2.68                     | 0.58              |
| 33:CJ:281:ILE:HD11 | 66:D3:562:G:C4     | 2.39                     | 0.58              |
| 35:CL:52:ARG:HH22  | 66:D3:436:A:P      | 2.27                     | 0.58              |
| 38:JC:55:PHE:CE2   | 38:JC:57:GLU:HB2   | 2.38                     | 0.58              |
| 38:JC:83:VAL:O     | 38:JC:92:LYS:N     | 2.36                     | 0.58              |
| 45:JN:209:ARG:NH2  | 65:D2:337:G:OP1    | 2.37                     | 0.58              |
| 45:JN:226:ASP:OD1  | 45:JN:227:LYS:N    | 2.37                     | 0.58              |
| 46:JO:116:ILE:HD13 | 46:JO:174:MET:HG3  | 1.85                     | 0.58              |
| 50:DF:200:ASN:ND2  | 50:DF:207:THR:HG23 | 2.19                     | 0.58              |
| 51:DG:74:LYS:HA    | 51:DG:96:SER:HA    | 1.85                     | 0.58              |
| 52:DH:27:LEU:O     | 52:DH:31:SER:HB3   | 2.03                     | 0.58              |
| 65:D2:101:G:H3'    | 65:D2:103:G:H21    | 1.69                     | 0.58              |
| 65:D2:218:U:H2'    | 65:D2:219:U:C6     | 2.39                     | 0.58              |
| 66:D3:1033:C:H2'   | 66:D3:1034:C:C6    | 2.38                     | 0.58              |
| 66:D3:1615:C:H5''  | 66:D3:1616:G:O4'   | 2.03                     | 0.58              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:CB:233:LEU:HD21   | 29:CE:144:ALA:HB2  | 1.85                     | 0.57              |
| 5:UB:639:VAL:O      | 5:UB:642:SER:OG    | 2.17                     | 0.57              |
| 10:UG:178:ASP:OD1   | 10:UG:179:HIS:N    | 2.36                     | 0.57              |
| 13:UJ:1680:VAL:HG23 | 13:UJ:1683:HIS:HB2 | 1.86                     | 0.57              |
| 14:UK:16:ARG:NH2    | 66:D3:556:A:N7     | 2.52                     | 0.57              |
| 14:UK:16:ARG:NH2    | 66:D3:575:C:N3     | 2.52                     | 0.57              |
| 15:UL:87:ALA:HB2    | 15:UL:94:LEU:HD13  | 1.84                     | 0.57              |
| 20:UQ:503:ASP:OD2   | 20:UQ:504:GLY:N    | 2.36                     | 0.57              |
| 22:US:362:MET:HG3   | 22:US:401:PHE:CZ   | 2.39                     | 0.57              |
| 22:US:490:LYS:HE2   | 22:US:493:TYR:CE1  | 2.38                     | 0.57              |
| 23:UT:687:ASN:OD1   | 23:UT:688:VAL:N    | 2.37                     | 0.57              |
| 23:UT:1736:GLU:N    | 23:UT:1736:GLU:OE2 | 2.34                     | 0.57              |
| 24:UU:242:ARG:HH21  | 24:UU:244:ILE:HD11 | 1.69                     | 0.57              |
| 24:UU:853:ASN:HB3   | 24:UU:860:GLU:HG3  | 1.84                     | 0.57              |
| 26:UX:96:PRO:HG2    | 26:UX:125:ILE:HD13 | 1.86                     | 0.57              |
| 30:CG:33:LEU:HD13   | 30:CG:102:ILE:HD13 | 1.86                     | 0.57              |
| 35:CL:210:VAL:HG11  | 82:CL:2001:GTP:H2' | 1.86                     | 0.57              |
| 35:CL:831:ARG:HH21  | 35:CL:838:ILE:HG22 | 1.69                     | 0.57              |
| 40:JH:317:PHE:O     | 40:JH:322:LEU:N    | 2.28                     | 0.57              |
| 47:JP:276:ASN:HD21  | 66:D3:-7:A:H61     | 1.52                     | 0.57              |
| 50:DF:98:MET:HB3    | 50:DF:110:ALA:HB2  | 1.86                     | 0.57              |
| 51:DG:194:LYS:HA    | 51:DG:197:ASN:HD21 | 1.69                     | 0.57              |
| 79:EN:642:ASN:O     | 79:EN:646:TYR:N    | 2.33                     | 0.57              |
| 3:JA:511:SER:O      | 3:JA:652:ARG:NH1   | 2.37                     | 0.57              |
| 3:JA:545:HIS:HB2    | 3:JA:637:ARG:HH12  | 1.67                     | 0.57              |
| 4:UA:11:LEU:HD23    | 4:UA:701:LEU:HD22  | 1.85                     | 0.57              |
| 7:UD:121:THR:OG1    | 7:UD:142:GLY:O     | 2.19                     | 0.57              |
| 7:UD:269:PHE:HD2    | 21:UR:443:VAL:HG23 | 1.69                     | 0.57              |
| 13:UJ:1586:LEU:C    | 13:UJ:1587:ARG:HD3 | 2.25                     | 0.57              |
| 14:UK:28:LEU:HD11   | 35:CL:969:VAL:HG11 | 1.86                     | 0.57              |
| 14:UK:247:GLN:NE2   | 14:UK:248:ARG:O    | 2.38                     | 0.57              |
| 15:UL:75:ARG:HE     | 15:UL:76:GLY:H     | 1.51                     | 0.57              |
| 15:UL:181:SER:OG    | 15:UL:183:ASP:OD1  | 2.22                     | 0.57              |
| 15:UL:633:CYS:HB2   | 15:UL:660:VAL:HG11 | 1.85                     | 0.57              |
| 17:UN:832:ASN:HD21  | 17:UN:834:LYS:NZ   | 2.02                     | 0.57              |
| 20:UQ:391:VAL:O     | 20:UQ:438:THR:OG1  | 2.11                     | 0.57              |
| 20:UQ:437:THR:HG22  | 20:UQ:709:ARG:NE   | 2.19                     | 0.57              |
| 22:US:452:ASP:OD2   | 22:US:455:LEU:HD13 | 2.03                     | 0.57              |
| 23:UT:1463:GLN:NE2  | 23:UT:1463:GLN:O   | 2.36                     | 0.57              |
| 24:UU:666:ARG:HG2   | 24:UU:667:THR:H    | 1.68                     | 0.57              |
| 25:UV:197:GLN:OE1   | 25:UV:367:ARG:NH2  | 2.37                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:CE:366:LYS:HB3  | 29:CE:390:SER:OG   | 2.04                     | 0.57              |
| 31:CH:134:ARG:NH1  | 31:CH:535:GLU:OE1  | 2.37                     | 0.57              |
| 35:CL:750:TRP:CE3  | 61:DX:77:ILE:HG23  | 2.39                     | 0.57              |
| 45:JN:286:ARG:NE   | 65:D2:337:G:O2'    | 2.37                     | 0.57              |
| 50:DF:52:GLU:HG3   | 50:DF:54:LYS:HG2   | 1.84                     | 0.57              |
| 66:D3:1684:U:H2'   | 66:D3:1685:G:H8    | 1.69                     | 0.57              |
| 3:JA:23:ARG:NH2    | 3:JA:480:ASP:OD2   | 2.37                     | 0.57              |
| 4:UA:564:PHE:HB3   | 4:UA:624:ASN:ND2   | 2.19                     | 0.57              |
| 6:UC:602:LEU:HD11  | 66:D3:498:G:H5''   | 1.86                     | 0.57              |
| 7:UD:69:ILE:HD11   | 7:UD:356:LEU:HD13  | 1.86                     | 0.57              |
| 7:UD:336:ILE:HD12  | 7:UD:348:VAL:O     | 2.04                     | 0.57              |
| 13:UJ:148:PHE:HA   | 13:UJ:151:ILE:HG22 | 1.87                     | 0.57              |
| 13:UJ:745:TYR:CE2  | 13:UJ:747:GLN:HG3  | 2.39                     | 0.57              |
| 15:UL:337:LYS:HB3  | 15:UL:358:SER:HB3  | 1.87                     | 0.57              |
| 15:UL:915:ARG:HG3  | 15:UL:916:HIS:CD2  | 2.39                     | 0.57              |
| 16:UM:84:LEU:HD13  | 16:UM:86:LYS:NZ    | 2.19                     | 0.57              |
| 16:UM:104:PRO:HG2  | 16:UM:122:THR:HB   | 1.86                     | 0.57              |
| 18:UO:5:ARG:NH1    | 65:D2:86:C:O2'     | 2.37                     | 0.57              |
| 20:UQ:17:GLY:HA3   | 20:UQ:51:GLN:HE21  | 1.69                     | 0.57              |
| 20:UQ:612:SER:OG   | 20:UQ:662:VAL:HG22 | 2.05                     | 0.57              |
| 22:US:383:LEU:O    | 22:US:387:THR:HG23 | 2.03                     | 0.57              |
| 23:UT:978:PHE:HE2  | 23:UT:1024:GLN:HG3 | 1.68                     | 0.57              |
| 25:UV:304:GLU:HB3  | 25:UV:307:LYS:HG3  | 1.86                     | 0.57              |
| 25:UV:461:GLY:O    | 25:UV:463:GLN:NE2  | 2.37                     | 0.57              |
| 26:UX:65:VAL:HG11  | 26:UX:86:MET:CE    | 2.35                     | 0.57              |
| 29:CE:167:ILE:HD11 | 29:CE:298:ARG:HG2  | 1.86                     | 0.57              |
| 33:CJ:258:LEU:HD23 | 33:CJ:259:PHE:N    | 2.19                     | 0.57              |
| 35:CL:63:PRO:HG2   | 35:CL:68:PRO:HD3   | 1.85                     | 0.57              |
| 46:JO:47:LYS:O     | 46:JO:50:GLU:HB3   | 2.05                     | 0.57              |
| 46:JO:259:LYS:NZ   | 66:D3:631:G:OP1    | 2.37                     | 0.57              |
| 47:JP:187:SER:HA   | 47:JP:194:PHE:HA   | 1.84                     | 0.57              |
| 55:DL:73:GLY:HA3   | 55:DL:86:ILE:HD12  | 1.86                     | 0.57              |
| 62:DY:104:SER:OG   | 62:DY:107:GLN:OE1  | 2.21                     | 0.57              |
| 1:CA:219:PRO:HB2   | 1:CA:221:ILE:HD11  | 1.87                     | 0.57              |
| 3:JA:721:HIS:O     | 3:JA:769:ARG:NH1   | 2.38                     | 0.57              |
| 10:UG:333:SER:O    | 10:UG:333:SER:OG   | 2.22                     | 0.57              |
| 13:UJ:16:ALA:HA    | 13:UJ:24:ARG:HH22  | 1.68                     | 0.57              |
| 13:UJ:712:ASN:HB3  | 13:UJ:715:HIS:HB2  | 1.87                     | 0.57              |
| 14:UK:18:GLN:HB2   | 14:UK:28:LEU:H     | 1.69                     | 0.57              |
| 14:UK:202:LYS:NZ   | 14:UK:206:GLN:OE1  | 2.38                     | 0.57              |
| 15:UL:447:LEU:O    | 15:UL:454:LEU:HD12 | 2.05                     | 0.57              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 16:UM:104:PRO:HB3  | 57:DO:72:LYS:HZ1    | 1.69                     | 0.57              |
| 17:UN:294:GLU:O    | 17:UN:297:LYS:HG2   | 2.05                     | 0.57              |
| 20:UQ:80:GLN:HE22  | 20:UQ:86:GLU:HB2    | 1.70                     | 0.57              |
| 20:UQ:254:TYR:OH   | 65:D2:63:G:N7       | 2.37                     | 0.57              |
| 20:UQ:297:ILE:HG22 | 20:UQ:485:ARG:HH22  | 1.68                     | 0.57              |
| 20:UQ:387:GLY:O    | 20:UQ:389:LEU:HG    | 2.03                     | 0.57              |
| 21:UR:17:GLU:HA    | 21:UR:20:GLN:OE1    | 2.03                     | 0.57              |
| 21:UR:249:SER:N    | 21:UR:269:ASP:OD2   | 2.37                     | 0.57              |
| 23:UT:1345:LEU:HG  | 23:UT:1346:PRO:HD3  | 1.85                     | 0.57              |
| 23:UT:1716:MET:SD  | 23:UT:1716:MET:N    | 2.73                     | 0.57              |
| 27:UZ:203:TYR:CD2  | 27:UZ:206:LYS:HG2   | 2.40                     | 0.57              |
| 47:JP:226:LYS:HD2  | 47:JP:267:ILE:O     | 2.03                     | 0.57              |
| 51:DG:87:ARG:NH1   | 66:D3:159:U:O2      | 2.37                     | 0.57              |
| 53:DI:175:GLN:NE2  | 66:D3:331:A:OP2     | 2.32                     | 0.57              |
| 65:D2:350:A:H2'    | 65:D2:351:A:C8      | 2.39                     | 0.57              |
| 1:CA:301:LEU:H     | 1:CA:318:GLY:HA2    | 1.68                     | 0.57              |
| 2:DA:59:ASP:OD1    | 2:DA:60:ALA:N       | 2.36                     | 0.57              |
| 7:UD:363:SER:HB2   | 7:UD:366:ASN:HB2    | 1.87                     | 0.57              |
| 9:UF:23:LEU:HD23   | 9:UF:23:LEU:H       | 1.69                     | 0.57              |
| 11:UH:532:PHE:CE2  | 11:UH:536:ARG:HB2   | 2.40                     | 0.57              |
| 13:UJ:1404:PHE:HD2 | 13:UJ:1422:VAL:HG13 | 1.70                     | 0.57              |
| 13:UJ:1458:PHE:HA  | 13:UJ:1503:LEU:HD11 | 1.86                     | 0.57              |
| 13:UJ:1510:PHE:O   | 13:UJ:1514:SER:HB3  | 2.04                     | 0.57              |
| 13:UJ:1662:ILE:HA  | 13:UJ:1665:TYR:HD2  | 1.70                     | 0.57              |
| 13:UJ:1733:ILE:HA  | 13:UJ:1736:LEU:HD12 | 1.87                     | 0.57              |
| 15:UL:260:GLU:HB3  | 15:UL:273:TYR:CE1   | 2.40                     | 0.57              |
| 15:UL:643:ASP:HB2  | 15:UL:650:ILE:HD11  | 1.86                     | 0.57              |
| 17:UN:831:ILE:O    | 17:UN:831:ILE:HG13  | 2.05                     | 0.57              |
| 18:UO:149:THR:HG23 | 18:UO:164:LEU:HB3   | 1.86                     | 0.57              |
| 18:UO:275:SER:OG   | 18:UO:302:VAL:HG13  | 2.03                     | 0.57              |
| 24:UU:610:ARG:HE   | 24:UU:673:PHE:HE2   | 1.52                     | 0.57              |
| 31:CH:289:ARG:NE   | 31:CH:332:ALA:O     | 2.37                     | 0.57              |
| 33:CJ:212:ALA:HA   | 34:CK:381:LEU:HB3   | 1.87                     | 0.57              |
| 35:CL:628:VAL:HG21 | 36:CM:218:ASN:HB3   | 1.87                     | 0.57              |
| 35:CL:877:GLU:O    | 35:CL:878:HIS:ND1   | 2.37                     | 0.57              |
| 36:CM:119:LYS:HG2  | 36:CM:165:GLU:OE1   | 2.04                     | 0.57              |
| 38:JC:290:VAL:O    | 38:JC:297:ALA:HA    | 2.04                     | 0.57              |
| 50:DF:76:ARG:NH2   | 58:DQ:122:ARG:HE    | 2.01                     | 0.57              |
| 50:DF:81:ARG:HA    | 66:D3:1615:C:C5     | 2.40                     | 0.57              |
| 57:DO:20:TYR:HB3   | 57:DO:27:PHE:HD2    | 1.68                     | 0.57              |
| 65:D2:117:G:H2'    | 65:D2:118:A:H8      | 1.69                     | 0.57              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 65:D2:470:U:H3      | 67:D4:48:A:N6      | 1.96                     | 0.57              |
| 66:D3:777:C:H5'     | 66:D3:778:G:H21    | 1.69                     | 0.57              |
| 73:EF:202:ALA:O     | 73:EF:206:SER:N    | 2.35                     | 0.57              |
| 79:EN:863:MET:O     | 79:EN:867:LYS:N    | 2.37                     | 0.57              |
| 2:DA:223:PHE:CE2    | 2:DA:228:LEU:HD12  | 2.40                     | 0.57              |
| 3:JA:837:PHE:HA     | 3:JA:840:LYS:HG2   | 1.86                     | 0.57              |
| 3:JA:916:ILE:HA     | 3:JA:919:LYS:HD2   | 1.87                     | 0.57              |
| 4:UA:438:VAL:HG12   | 4:UA:445:VAL:HG22  | 1.87                     | 0.57              |
| 4:UA:587:PHE:CE2    | 4:UA:688:PRO:HA    | 2.36                     | 0.57              |
| 7:UD:576:ASN:HD21   | 7:UD:646:LEU:HD21  | 1.70                     | 0.57              |
| 8:UE:346:HIS:HB2    | 65:D2:150:G:C2     | 2.39                     | 0.57              |
| 12:UI:414:PRO:HA    | 12:UI:417:LYS:HE3  | 1.85                     | 0.57              |
| 13:UJ:315:LEU:HD12  | 13:UJ:316:PRO:HD2  | 1.85                     | 0.57              |
| 13:UJ:414:LEU:HD13  | 13:UJ:417:LYS:HD2  | 1.87                     | 0.57              |
| 14:UK:217:ARG:NH2   | 65:D2:260:A:C8     | 2.68                     | 0.57              |
| 14:UK:250:ARG:HG3   | 14:UK:250:ARG:HH21 | 1.70                     | 0.57              |
| 15:UL:639:VAL:HB    | 15:UL:653:LEU:HB2  | 1.87                     | 0.57              |
| 15:UL:923:GLU:OE1   | 42:JJ:264:ARG:NH2  | 2.37                     | 0.57              |
| 18:UO:413:LEU:O     | 18:UO:416:THR:HG22 | 2.04                     | 0.57              |
| 18:UO:423:LYS:NZ    | 20:UQ:475:SER:O    | 2.30                     | 0.57              |
| 23:UT:1273:LYS:HE2  | 23:UT:1349:PHE:HB2 | 1.87                     | 0.57              |
| 23:UT:1781:ILE:HG23 | 23:UT:1785:ASN:HB2 | 1.87                     | 0.57              |
| 25:UV:204:ASP:OD1   | 25:UV:205:THR:N    | 2.37                     | 0.57              |
| 28:CD:15:TYR:HE2    | 28:CD:78:LEU:HB2   | 1.69                     | 0.57              |
| 33:CJ:189:LEU:HB3   | 33:CJ:191:PHE:HE1  | 1.70                     | 0.57              |
| 35:CL:58:MET:SD     | 66:D3:434:G:N1     | 2.77                     | 0.57              |
| 35:CL:65:ASP:OD2    | 35:CL:784:LYS:NZ   | 2.38                     | 0.57              |
| 35:CL:105:ILE:HG23  | 35:CL:117:PHE:HB2  | 1.86                     | 0.57              |
| 49:DE:57:ASN:OD1    | 49:DE:58:GLY:N     | 2.38                     | 0.57              |
| 54:DJ:36:LEU:HD23   | 54:DJ:41:GLU:HB3   | 1.87                     | 0.57              |
| 79:EN:794:LEU:O     | 79:EN:798:ASN:N    | 2.35                     | 0.57              |
| 2:DA:36:SER:HA      | 2:DA:41:ARG:NH1    | 2.20                     | 0.57              |
| 2:DA:71:ALA:HB2     | 2:DA:80:SER:HA     | 1.87                     | 0.57              |
| 2:DA:138:PHE:O      | 2:DA:213:ARG:N     | 2.37                     | 0.57              |
| 3:JA:173:ARG:HH22   | 3:JA:183:ARG:HG2   | 1.70                     | 0.57              |
| 4:UA:631:ASN:ND2    | 65:D2:294:U:OP1    | 2.38                     | 0.57              |
| 4:UA:759:PRO:O      | 4:UA:763:ILE:HG13  | 2.05                     | 0.57              |
| 10:UG:274:ARG:HB2   | 10:UG:295:ASP:OD2  | 2.04                     | 0.57              |
| 14:UK:116:LYS:HD3   | 67:D4:323:G:O5'    | 2.05                     | 0.57              |
| 18:UO:274:ALA:O     | 18:UO:281:VAL:HA   | 2.04                     | 0.57              |
| 23:UT:641:ARG:O     | 23:UT:645:VAL:HG23 | 2.04                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:UT:1743:LYS:HA  | 23:UT:1746:LYS:HG2 | 1.85                     | 0.57              |
| 25:UV:141:TRP:HE3  | 25:UV:144:LYS:HZ3  | 1.52                     | 0.57              |
| 29:CE:347:LEU:HD13 | 29:CE:350:GLN:HE22 | 1.68                     | 0.57              |
| 33:CJ:53:GLN:CG    | 45:JN:215:LEU:HD21 | 2.35                     | 0.57              |
| 33:CJ:211:ASN:CG   | 33:CJ:212:ALA:H    | 2.08                     | 0.57              |
| 35:CL:286:THR:H    | 35:CL:298:VAL:HG12 | 1.68                     | 0.57              |
| 35:CL:567:TRP:CH2  | 36:CM:315:LYS:HD2  | 2.40                     | 0.57              |
| 38:JC:238:ASN:OD1  | 38:JC:239:ASP:N    | 2.38                     | 0.57              |
| 52:DH:102:PRO:HB3  | 52:DH:109:VAL:HG21 | 1.87                     | 0.57              |
| 60:DW:90:THR:HG22  | 60:DW:102:VAL:HG21 | 1.87                     | 0.57              |
| 66:D3:0:U:H4'      | 66:D3:1:U:O5'      | 2.05                     | 0.57              |
| 66:D3:1575:G:C6    | 66:D3:1576:A:C6    | 2.93                     | 0.57              |
| 4:UA:202:ASP:O     | 4:UA:204:GLU:N     | 2.35                     | 0.57              |
| 1:CB:110:ASN:HA    | 1:CB:186:ASP:OD1   | 2.05                     | 0.57              |
| 1:CB:227:PRO:HA    | 1:CB:230:TYR:CE2   | 2.40                     | 0.57              |
| 3:JB:752:ASN:N     | 3:JB:757:GLU:O     | 2.38                     | 0.57              |
| 7:UD:395:SER:OG    | 7:UD:396:GLU:N     | 2.38                     | 0.57              |
| 13:UJ:1553:ARG:O   | 13:UJ:1557:ASP:HB2 | 2.05                     | 0.57              |
| 14:UK:213:GLN:HE22 | 14:UK:217:ARG:HH11 | 1.53                     | 0.57              |
| 17:UN:338:LEU:O    | 17:UN:342:VAL:HG22 | 2.04                     | 0.57              |
| 20:UQ:34:ILE:HD11  | 20:UQ:90:LYS:HA    | 1.87                     | 0.57              |
| 20:UQ:319:LYS:HD3  | 20:UQ:339:GLY:H    | 1.70                     | 0.57              |
| 22:US:502:ASN:N    | 22:US:505:SER:OG   | 2.36                     | 0.57              |
| 23:UT:874:LEU:HD11 | 23:UT:885:ARG:HB3  | 1.87                     | 0.57              |
| 23:UT:947:ILE:HG21 | 66:D3:257:A:H5'    | 1.87                     | 0.57              |
| 23:UT:1611:PRO:HA  | 23:UT:1614:GLU:OE1 | 2.05                     | 0.57              |
| 30:CF:23:VAL:HA    | 30:CF:26:GLN:NE2   | 2.18                     | 0.57              |
| 31:CH:409:ASP:OD1  | 31:CH:412:HIS:N    | 2.24                     | 0.57              |
| 32:CI:71:ARG:NE    | 33:CJ:61:SER:HB2   | 2.19                     | 0.57              |
| 32:CI:93:LYS:O     | 32:CI:96:ASP:N     | 2.37                     | 0.57              |
| 35:CL:631:ILE:HD11 | 36:CM:283:ILE:HG22 | 1.86                     | 0.57              |
| 35:CL:878:HIS:HB2  | 66:D3:572:C:N3     | 2.20                     | 0.57              |
| 37:CN:144:TYR:OH   | 37:CN:156:PHE:N    | 2.27                     | 0.57              |
| 38:JC:94:ASP:OD1   | 38:JC:95:ARG:N     | 2.38                     | 0.57              |
| 46:JO:91:PRO:O     | 46:JO:94:ILE:HG22  | 2.05                     | 0.57              |
| 55:DL:109:VAL:HG22 | 55:DL:137:PHE:HB2  | 1.87                     | 0.57              |
| 60:DW:75:ILE:HG22  | 60:DW:77:PRO:HD2   | 1.87                     | 0.57              |
| 60:DW:111:MET:HE1  | 60:DW:116:ALA:HA   | 1.87                     | 0.57              |
| 65:D2:123:C:H3'    | 65:D2:124:A:C8     | 2.39                     | 0.57              |
| 65:D2:192:G:H2'    | 65:D2:193:G:C8     | 2.39                     | 0.57              |
| 66:D3:1614:A:H2'   | 66:D3:1615:C:H5'   | 1.87                     | 0.57              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 67:D4:53:U:H2'      | 67:D4:54:C:C6       | 2.39                     | 0.57              |
| 1:CA:111:MET:HE1    | 1:CA:190:PRO:HG3    | 1.87                     | 0.57              |
| 3:JA:60:LYS:HD2     | 3:JA:61:LYS:N       | 2.20                     | 0.57              |
| 4:UA:524:ARG:NH2    | 4:UA:526:ASP:OD1    | 2.38                     | 0.57              |
| 13:UJ:48:ILE:HD11   | 13:UJ:123:ARG:NH1   | 2.19                     | 0.57              |
| 13:UJ:1705:LEU:HD21 | 13:UJ:1744:ILE:HG12 | 1.87                     | 0.57              |
| 14:UK:65:HIS:CD2    | 67:D4:55:A:H2       | 2.23                     | 0.57              |
| 15:UL:17:ILE:HG23   | 15:UL:52:TRP:CZ2    | 2.39                     | 0.57              |
| 16:UM:281:THR:HA    | 16:UM:327:ILE:HB    | 1.87                     | 0.57              |
| 16:UM:416:ARG:CZ    | 16:UM:418:ASN:HD21  | 2.18                     | 0.57              |
| 21:UR:218:TYR:OH    | 24:UU:283:ARG:NH1   | 2.38                     | 0.57              |
| 21:UR:317:ARG:HH22  | 65:D2:233:G:N2      | 2.02                     | 0.57              |
| 23:UT:229:TYR:OH    | 23:UT:273:SER:OG    | 2.20                     | 0.57              |
| 23:UT:468:ALA:HB3   | 23:UT:503:ARG:HH22  | 1.69                     | 0.57              |
| 24:UU:616:THR:HG23  | 24:UU:618:GLY:H     | 1.69                     | 0.57              |
| 25:UV:1065:THR:O    | 25:UV:1069:LYS:HG2  | 2.04                     | 0.57              |
| 29:CE:323:GLU:OE2   | 29:CE:324:LYS:HG3   | 2.05                     | 0.57              |
| 30:CG:95:ARG:NH1    | 31:CH:551:ARG:H     | 1.99                     | 0.57              |
| 31:CH:199:TYR:CD1   | 31:CH:210:LYS:HA    | 2.40                     | 0.57              |
| 37:CN:80:THR:HB     | 37:CN:136:ASN:HB3   | 1.86                     | 0.57              |
| 38:JC:317:ILE:HA    | 38:JC:333:ASN:HB3   | 1.86                     | 0.57              |
| 51:DG:48:TYR:OH     | 51:DG:119:GLN:O     | 2.19                     | 0.57              |
| 56:DN:29:SER:HB3    | 56:DN:32:SER:HB3    | 1.87                     | 0.57              |
| 65:D2:158:G:H2'     | 65:D2:159:A:C8      | 2.39                     | 0.57              |
| 2:DA:135:LEU:HD12   | 2:DA:217:LEU:HA     | 1.86                     | 0.57              |
| 4:UA:345:PHE:HE2    | 4:UA:677:PRO:HG2    | 1.68                     | 0.57              |
| 4:UA:512:ILE:HG12   | 4:UA:547:ALA:HB1    | 1.85                     | 0.57              |
| 12:UI:498:GLY:O     | 12:UI:502:ARG:HG3   | 2.05                     | 0.57              |
| 14:UK:59:ASN:OD1    | 33:CJ:3:ARG:NH1     | 2.35                     | 0.57              |
| 15:UL:258:LYS:NZ    | 15:UL:259:ILE:H     | 2.02                     | 0.57              |
| 15:UL:284:PHE:HA    | 15:UL:329:PHE:H     | 1.70                     | 0.57              |
| 18:UO:357:PHE:O     | 18:UO:360:MET:HB3   | 2.05                     | 0.57              |
| 20:UQ:875:MET:O     | 20:UQ:879:ILE:HB    | 2.05                     | 0.57              |
| 21:UR:401:GLU:HG3   | 21:UR:402:GLY:H     | 1.70                     | 0.57              |
| 21:UR:561:PRO:O     | 21:UR:587:ARG:NH1   | 2.38                     | 0.57              |
| 22:US:352:VAL:HG22  | 22:US:353:LYS:H     | 1.70                     | 0.57              |
| 23:UT:99:ASP:O      | 23:UT:103:LEU:HG    | 2.05                     | 0.57              |
| 24:UU:228:GLY:HA2   | 24:UU:246:ILE:O     | 1.96                     | 0.57              |
| 33:CJ:212:ALA:C     | 34:CK:383:ARG:HH21  | 2.07                     | 0.57              |
| 35:CL:299:ALA:HB3   | 35:CL:792:VAL:O     | 2.05                     | 0.57              |
| 38:JC:198:GLY:HA3   | 38:JC:234:THR:HG21  | 1.87                     | 0.57              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 47:JP:276:ASN:HB3  | 47:JP:288:TYR:CE1   | 2.39                     | 0.57              |
| 60:DW:18:GLU:HG2   | 60:DW:69:LEU:HD23   | 1.87                     | 0.57              |
| 65:D2:362:C:H2'    | 65:D2:363:A:O4'     | 2.05                     | 0.57              |
| 66:D3:306:U:H2'    | 66:D3:307:G:C8      | 2.40                     | 0.57              |
| 66:D3:487:G:N2     | 66:D3:488:G:C4      | 2.73                     | 0.57              |
| 1:CA:225:ARG:HA    | 1:CA:252:ILE:HD11   | 1.87                     | 0.56              |
| 1:CA:314:CYS:SG    | 1:CA:315:ILE:N      | 2.78                     | 0.56              |
| 3:JA:63:LEU:HB3    | 3:JA:66:PHE:CE1     | 2.40                     | 0.56              |
| 4:UA:272:THR:C     | 4:UA:273:ARG:HD3    | 2.25                     | 0.56              |
| 7:UD:196:LYS:NZ    | 7:UD:246:TYR:OH     | 2.32                     | 0.56              |
| 8:UE:120:ILE:HG12  | 8:UE:151:LEU:HD22   | 1.85                     | 0.56              |
| 9:UF:126:TYR:HE1   | 9:UF:158:HIS:CD2    | 2.23                     | 0.56              |
| 10:UG:386:PHE:O    | 47:JP:8:ARG:NH2     | 2.37                     | 0.56              |
| 13:UJ:75:SER:O     | 13:UJ:78:SER:N      | 2.37                     | 0.56              |
| 16:UM:364:ILE:HB   | 16:UM:382:GLU:HB2   | 1.86                     | 0.56              |
| 20:UQ:320:VAL:HG23 | 20:UQ:335:PRO:HA    | 1.87                     | 0.56              |
| 20:UQ:608:SER:HB3  | 20:UQ:626:PHE:CE1   | 2.40                     | 0.56              |
| 21:UR:129:ASP:HA   | 21:UR:132:LYS:HG2   | 1.86                     | 0.56              |
| 23:UT:948:ALA:O    | 23:UT:952:VAL:HG23  | 2.05                     | 0.56              |
| 23:UT:1326:SER:HA  | 23:UT:1329:LYS:HE2  | 1.87                     | 0.56              |
| 23:UT:1758:ALA:HB1 | 23:UT:1800:LEU:HD22 | 1.86                     | 0.56              |
| 25:UV:649:TRP:HB2  | 25:UV:653:SER:HB2   | 1.88                     | 0.56              |
| 26:UX:128:LEU:HD11 | 26:UX:144:ARG:NH1   | 2.19                     | 0.56              |
| 35:CL:161:HIS:CE1  | 35:CL:916:THR:HG21  | 2.40                     | 0.56              |
| 35:CL:548:ASN:HB3  | 35:CL:551:LYS:HG2   | 1.87                     | 0.56              |
| 47:JP:445:ARG:NH2  | 47:JP:445:ARG:HB2   | 2.20                     | 0.56              |
| 50:DF:100:ASN:ND2  | 66:D3:1473:U:O2     | 2.34                     | 0.56              |
| 50:DF:185:ARG:NH1  | 50:DF:185:ARG:HA    | 2.20                     | 0.56              |
| 55:DL:95:PRO:O     | 55:DL:98:ASN:ND2    | 2.37                     | 0.56              |
| 65:D2:21:A:H2'     | 65:D2:22:A:C8       | 2.40                     | 0.56              |
| 65:D2:180:G:H2'    | 65:D2:181:A:C8      | 2.40                     | 0.56              |
| 4:UA:93:PHE:HE1    | 65:D2:297:U:C5      | 2.23                     | 0.56              |
| 1:CB:321:MET:O     | 1:CB:323:SER:OG     | 2.18                     | 0.56              |
| 7:UD:139:CYS:SG    | 7:UD:144:ILE:HD11   | 2.46                     | 0.56              |
| 8:UE:469:ILE:HB    | 8:UE:508:ILE:HD12   | 1.87                     | 0.56              |
| 9:UF:182:TRP:NE1   | 9:UF:281:LEU:HD21   | 2.19                     | 0.56              |
| 18:UO:7:ARG:HH12   | 18:UO:383:ARG:HG2   | 1.69                     | 0.56              |
| 18:UO:449:GLY:O    | 18:UO:455:SER:OG    | 2.13                     | 0.56              |
| 20:UQ:744:ILE:HG21 | 20:UQ:753:LYS:HD3   | 1.87                     | 0.56              |
| 22:US:472:HIS:HD2  | 22:US:474:HIS:H     | 1.52                     | 0.56              |
| 23:UT:219:LEU:HD21 | 23:UT:270:ARG:HG3   | 1.88                     | 0.56              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 23:UT:524:LYS:NZ    | 23:UT:553:ASN:O     | 2.35                     | 0.56              |
| 23:UT:1405:GLY:HA3  | 23:UT:1417:TYR:CZ   | 2.40                     | 0.56              |
| 23:UT:1857:ILE:HG22 | 47:JP:172:LEU:HD22  | 1.88                     | 0.56              |
| 25:UV:921:ASP:HB2   | 25:UV:926:LEU:HD22  | 1.88                     | 0.56              |
| 28:CD:194:ARG:HH12  | 29:CE:165:GLN:HE22  | 1.51                     | 0.56              |
| 35:CL:71:ILE:HD11   | 35:CL:276:HIS:NE2   | 2.19                     | 0.56              |
| 37:CN:136:ASN:HA    | 37:CN:139:ASN:HD21  | 1.70                     | 0.56              |
| 47:JP:66:HIS:N      | 47:JP:370:GLY:O     | 2.32                     | 0.56              |
| 51:DG:14:LYS:HD2    | 51:DG:123:GLY:HA3   | 1.87                     | 0.56              |
| 51:DG:201:GLN:NE2   | 66:D3:125:U:OP1     | 2.38                     | 0.56              |
| 53:DI:195:ARG:HH12  | 55:DL:12:ALA:HA     | 1.70                     | 0.56              |
| 60:DW:81:VAL:HB     | 60:DW:125:ILE:HD11  | 1.87                     | 0.56              |
| 61:DX:92:CYS:SG     | 61:DX:136:TRP:HB2   | 2.46                     | 0.56              |
| 61:DX:109:ARG:HH22  | 61:DX:119:GLY:H     | 1.52                     | 0.56              |
| 67:D4:32:G:H2'      | 67:D4:33:A:H5''     | 1.87                     | 0.56              |
| 3:JA:104:ARG:NH2    | 3:JA:105:TYR:O      | 2.39                     | 0.56              |
| 4:UA:166:LYS:C      | 4:UA:168:LEU:H      | 2.09                     | 0.56              |
| 4:UA:287:TYR:CE1    | 4:UA:294:LEU:HG     | 2.41                     | 0.56              |
| 4:UA:337:TYR:HE1    | 24:UU:746:PRO:HB3   | 1.69                     | 0.56              |
| 10:UG:198:PHE:CE2   | 10:UG:200:PRO:HA    | 2.40                     | 0.56              |
| 11:UH:552:LYS:HE3   | 11:UH:576:ARG:NH1   | 2.21                     | 0.56              |
| 12:UI:413:GLU:HB3   | 12:UI:416:ILE:HG12  | 1.86                     | 0.56              |
| 13:UJ:67:ALA:O      | 13:UJ:70:SER:OG     | 2.17                     | 0.56              |
| 13:UJ:129:VAL:HG23  | 13:UJ:130:LYS:HG2   | 1.87                     | 0.56              |
| 13:UJ:348:ILE:HD13  | 13:UJ:373:ILE:HG21  | 1.87                     | 0.56              |
| 13:UJ:377:ARG:O     | 13:UJ:381:ARG:HG3   | 2.04                     | 0.56              |
| 15:UL:382:THR:O     | 15:UL:383:HIS:C     | 2.44                     | 0.56              |
| 15:UL:559:PHE:O     | 15:UL:563:MET:N     | 2.34                     | 0.56              |
| 16:UM:720:PHE:HB3   | 16:UM:724:LEU:HD23  | 1.86                     | 0.56              |
| 18:UO:234:PHE:CE1   | 18:UO:248:ARG:HB2   | 2.41                     | 0.56              |
| 20:UQ:497:ASP:OD2   | 20:UQ:498:LEU:N     | 2.38                     | 0.56              |
| 21:UR:480:ARG:O     | 21:UR:496:ARG:HG2   | 2.04                     | 0.56              |
| 22:US:463:LEU:HD13  | 22:US:466:LEU:HD12  | 1.87                     | 0.56              |
| 22:US:480:LEU:O     | 22:US:483:ILE:HG22  | 2.06                     | 0.56              |
| 23:UT:844:VAL:HG11  | 23:UT:850:LEU:HD12  | 1.87                     | 0.56              |
| 23:UT:1660:LYS:HA   | 23:UT:1663:ILE:HG22 | 1.87                     | 0.56              |
| 23:UT:1722:MET:HA   | 23:UT:1725:ILE:HG22 | 1.87                     | 0.56              |
| 24:UU:387:GLN:NE2   | 65:D2:291:G:H21     | 2.03                     | 0.56              |
| 25:UV:726:SER:HB2   | 25:UV:768:PRO:HG2   | 1.85                     | 0.56              |
| 26:UX:10:PHE:HE2    | 32:CI:133:GLN:HG2   | 1.71                     | 0.56              |
| 28:CD:95:ASN:OD1    | 28:CD:96:ILE:N      | 2.38                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:CE:383:SER:OG   | 29:CE:385:ASP:OD2  | 2.22                     | 0.56              |
| 30:CG:18:GLN:NE2   | 31:CH:400:GLY:HA2  | 2.19                     | 0.56              |
| 30:CG:54:MET:HB2   | 30:CG:64:LEU:HD12  | 1.86                     | 0.56              |
| 31:CH:409:ASP:CG   | 31:CH:411:PHE:H    | 2.08                     | 0.56              |
| 36:CM:105:TYR:HE2  | 36:CM:296:LEU:HA   | 1.69                     | 0.56              |
| 37:CN:18:PHE:O     | 37:CN:35:HIS:N     | 2.38                     | 0.56              |
| 38:JC:221:GLU:HG2  | 38:JC:253:TYR:CE2  | 2.40                     | 0.56              |
| 44:JM:127:ARG:HD2  | 44:JM:136:TYR:CZ   | 2.40                     | 0.56              |
| 50:DF:113:ILE:O    | 50:DF:117:THR:HG23 | 2.05                     | 0.56              |
| 52:DH:96:ARG:CZ    | 52:DH:124:LYS:HG2  | 2.35                     | 0.56              |
| 52:DH:97:ARG:HH21  | 52:DH:98:ILE:HG12  | 1.70                     | 0.56              |
| 53:DI:67:TRP:CD1   | 53:DI:70:GLU:HB3   | 2.40                     | 0.56              |
| 65:D2:198:A:H3'    | 65:D2:199:A:H8     | 1.69                     | 0.56              |
| 66:D3:488:G:C5     | 66:D3:489:C:C4     | 2.93                     | 0.56              |
| 66:D3:1683:C:O2'   | 66:D3:1684:U:O5'   | 2.20                     | 0.56              |
| 75:EH:5:ILE:N      | 75:EH:40:GLY:O     | 2.38                     | 0.56              |
| 77:EJ:158:VAL:O    | 77:EJ:189:SER:N    | 2.37                     | 0.56              |
| 3:JA:789:LEU:HD22  | 3:JA:890:LEU:HB3   | 1.86                     | 0.56              |
| 10:UG:157:ALA:HB2  | 10:UG:168:VAL:HG12 | 1.85                     | 0.56              |
| 16:UM:557:VAL:HG23 | 16:UM:578:VAL:HG21 | 1.86                     | 0.56              |
| 16:UM:779:VAL:HA   | 16:UM:782:VAL:HG12 | 1.87                     | 0.56              |
| 18:UO:100:ASP:OD1  | 18:UO:101:ALA:N    | 2.35                     | 0.56              |
| 23:UT:122:LEU:HA   | 23:UT:125:TYR:HB3  | 1.87                     | 0.56              |
| 23:UT:212:VAL:HG21 | 23:UT:258:LEU:HD13 | 1.88                     | 0.56              |
| 23:UT:715:TYR:CG   | 23:UT:762:ILE:HD11 | 2.41                     | 0.56              |
| 23:UT:1362:ALA:O   | 23:UT:1366:ASN:ND2 | 2.38                     | 0.56              |
| 24:UU:183:VAL:HG23 | 24:UU:188:VAL:HG22 | 1.87                     | 0.56              |
| 28:CD:156:HIS:O    | 28:CD:159:SER:OG   | 2.20                     | 0.56              |
| 30:CF:21:LEU:HA    | 30:CF:24:VAL:HG12  | 1.88                     | 0.56              |
| 30:CG:10:PRO:HG3   | 30:CG:125:LEU:HD21 | 1.88                     | 0.56              |
| 35:CL:140:LEU:HD11 | 35:CL:152:THR:HG23 | 1.87                     | 0.56              |
| 36:CM:249:SER:O    | 36:CM:253:GLY:N    | 2.39                     | 0.56              |
| 46:JO:219:ASP:OD1  | 46:JO:220:TRP:N    | 2.39                     | 0.56              |
| 47:JP:228:ASN:ND2  | 47:JP:231:GLU:O    | 2.34                     | 0.56              |
| 47:JP:330:ARG:NH1  | 47:JP:339:SER:OG   | 2.37                     | 0.56              |
| 56:DN:100:LYS:HG2  | 56:DN:104:ARG:NH2  | 2.18                     | 0.56              |
| 57:DO:42:VAL:HG22  | 57:DO:67:VAL:HG23  | 1.88                     | 0.56              |
| 79:EN:419:CYS:O    | 79:EN:423:ALA:N    | 2.37                     | 0.56              |
| 3:JA:59:TYR:OH     | 66:D3:416:A:N1     | 2.38                     | 0.56              |
| 1:CB:146:PRO:HA    | 1:CB:152:ALA:HB3   | 1.88                     | 0.56              |
| 1:CB:294:ARG:NH2   | 19:UP:187:SER:OG   | 2.27                     | 0.56              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 5:UB:451:THR:O     | 5:UB:455:LEU:HG     | 2.05                     | 0.56              |
| 6:UC:560:ASN:CG    | 6:UC:561:SER:H      | 2.08                     | 0.56              |
| 7:UD:635:GLY:HA3   | 7:UD:649:TRP:CE2    | 2.41                     | 0.56              |
| 12:UI:497:LEU:HD12 | 18:UO:502:GLN:OE1   | 2.05                     | 0.56              |
| 13:UJ:359:ASP:OD1  | 13:UJ:361:SER:OG    | 2.12                     | 0.56              |
| 13:UJ:718:ARG:HA   | 13:UJ:721:VAL:HG22  | 1.87                     | 0.56              |
| 13:UJ:1653:ASN:O   | 13:UJ:1656:SER:OG   | 2.24                     | 0.56              |
| 15:UL:15:GLY:O     | 15:UL:360:ASN:ND2   | 2.38                     | 0.56              |
| 15:UL:137:ILE:HD12 | 15:UL:147:VAL:HG22  | 1.88                     | 0.56              |
| 18:UO:92:ASP:O     | 18:UO:94:LYS:NZ     | 2.39                     | 0.56              |
| 20:UQ:73:LEU:HD23  | 20:UQ:129:PRO:HG2   | 1.87                     | 0.56              |
| 20:UQ:143:ASN:OD1  | 20:UQ:144:VAL:N     | 2.39                     | 0.56              |
| 22:US:289:PHE:HZ   | 22:US:295:LEU:HD23  | 1.71                     | 0.56              |
| 23:UT:1374:PHE:O   | 23:UT:1378:ILE:HG13 | 2.06                     | 0.56              |
| 23:UT:1406:LEU:HG  | 23:UT:1487:PRO:HB2  | 1.87                     | 0.56              |
| 25:UV:1087:LEU:O   | 25:UV:1090:THR:OG1  | 2.21                     | 0.56              |
| 27:UZ:56:ILE:HG22  | 27:UZ:188:SER:HB3   | 1.88                     | 0.56              |
| 35:CL:849:LEU:HD11 | 35:CL:890:CYS:SG    | 2.46                     | 0.56              |
| 45:JN:263:VAL:HG11 | 46:JO:142:ARG:NE    | 2.21                     | 0.56              |
| 46:JO:91:PRO:HB2   | 57:DO:102:LEU:HD21  | 1.87                     | 0.56              |
| 51:DG:67:VAL:O     | 51:DG:100:ALA:HB2   | 2.04                     | 0.56              |
| 53:DI:87:ASN:HD21  | 66:D3:341:A:H4'     | 1.70                     | 0.56              |
| 65:D2:137:C:H2'    | 65:D2:138:U:C6      | 2.41                     | 0.56              |
| 65:D2:462:G:O6     | 67:D4:55:A:N6       | 2.39                     | 0.56              |
| 66:D3:480:G:N2     | 66:D3:509:G:N3      | 2.54                     | 0.56              |
| 79:EN:810:PRO:O    | 79:EN:816:ILE:N     | 2.38                     | 0.56              |
| 5:UB:460:LYS:O     | 5:UB:463:SER:OG     | 2.19                     | 0.56              |
| 5:UB:482:GLN:HB2   | 5:UB:486:LYS:HZ3    | 1.71                     | 0.56              |
| 9:UF:152:LYS:HD3   | 44:JM:65:LEU:CD1    | 2.36                     | 0.56              |
| 13:UJ:779:SER:HA   | 13:UJ:788:THR:HG21  | 1.88                     | 0.56              |
| 13:UJ:1595:THR:HA  | 13:UJ:1598:LEU:HG   | 1.88                     | 0.56              |
| 16:UM:655:GLU:HA   | 16:UM:658:LYS:HG2   | 1.87                     | 0.56              |
| 18:UO:366:TYR:CE2  | 18:UO:368:GLY:HA2   | 2.40                     | 0.56              |
| 20:UQ:868:ASN:ND2  | 67:D4:76:U:O2'      | 2.39                     | 0.56              |
| 22:US:190:ASP:OD1  | 22:US:191:ILE:N     | 2.38                     | 0.56              |
| 22:US:399:ILE:HG13 | 22:US:400:PRO:HD3   | 1.88                     | 0.56              |
| 23:UT:1614:GLU:HG3 | 23:UT:1661:ILE:HG22 | 1.88                     | 0.56              |
| 24:UU:263:HIS:HD2  | 24:UU:277:ASP:HA    | 1.70                     | 0.56              |
| 24:UU:589:THR:OG1  | 24:UU:590:ALA:N     | 2.38                     | 0.56              |
| 25:UV:423:LYS:HE3  | 25:UV:499:LEU:HB3   | 1.88                     | 0.56              |
| 33:CJ:173:ARG:HA   | 33:CJ:176:ILE:HD12  | 1.86                     | 0.56              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 46:JO:68:ASN:HD21  | 46:JO:87:LYS:HB2    | 1.69                     | 0.56              |
| 50:DF:142:PRO:HG3  | 50:DF:170:GLN:HG2   | 1.88                     | 0.56              |
| 60:DW:26:LEU:HD23  | 60:DW:27:ILE:N      | 2.20                     | 0.56              |
| 60:DW:66:ASN:OD1   | 60:DW:67:GLY:N      | 2.37                     | 0.56              |
| 66:D3:188:A:H62    | 66:D3:197:A:H1'     | 1.71                     | 0.56              |
| 66:D3:793:A:C2     | 66:D3:796:A:H3'     | 2.41                     | 0.56              |
| 70:EC:162:SER:HA   | 70:EC:186:THR:HA    | 1.87                     | 0.56              |
| 3:JA:522:THR:O     | 3:JA:525:SER:OG     | 2.21                     | 0.56              |
| 4:UA:653:LEU:HD11  | 65:D2:331:U:N3      | 2.20                     | 0.56              |
| 1:CB:277:ASP:OD2   | 1:CB:280:VAL:N      | 2.18                     | 0.56              |
| 5:UB:392:LYS:O     | 5:UB:395:ASP:C      | 2.43                     | 0.56              |
| 5:UB:660:ILE:HA    | 22:US:388:LEU:HD21  | 1.88                     | 0.56              |
| 8:UE:82:ASN:HB3    | 8:UE:84:GLU:HG2     | 1.86                     | 0.56              |
| 10:UG:548:GLU:OE1  | 37:CN:185:HIS:ND1   | 2.34                     | 0.56              |
| 13:UJ:721:VAL:O    | 13:UJ:755:ARG:NE    | 2.37                     | 0.56              |
| 16:UM:271:ASP:OD1  | 16:UM:272:SER:N     | 2.39                     | 0.56              |
| 17:UN:311:LEU:O    | 17:UN:884:MET:HB2   | 2.06                     | 0.56              |
| 20:UQ:364:ASN:ND2  | 20:UQ:409:LYS:O     | 2.39                     | 0.56              |
| 20:UQ:849:ASP:O    | 20:UQ:853:ILE:HD12  | 2.05                     | 0.56              |
| 23:UT:731:SER:OG   | 23:UT:732:SER:N     | 2.38                     | 0.56              |
| 23:UT:801:TYR:HA   | 23:UT:853:HIS:CE1   | 2.41                     | 0.56              |
| 23:UT:1482:SER:O   | 23:UT:1486:ILE:HG12 | 2.06                     | 0.56              |
| 23:UT:1726:PHE:CE2 | 23:UT:1776:LEU:HD22 | 2.40                     | 0.56              |
| 24:UU:669:ASP:OD1  | 24:UU:670:GLU:N     | 2.38                     | 0.56              |
| 28:CD:286:ARG:NH1  | 28:CD:290:ASP:OD2   | 2.39                     | 0.56              |
| 35:CL:90:VAL:O     | 35:CL:94:THR:HG22   | 2.05                     | 0.56              |
| 44:JM:124:ILE:HG23 | 44:JM:141:TRP:CZ3   | 2.40                     | 0.56              |
| 49:DE:32:SER:OG    | 49:DE:33:ALA:N      | 2.38                     | 0.56              |
| 54:DJ:50:SER:O     | 54:DJ:54:ARG:HG2    | 2.05                     | 0.56              |
| 58:DQ:69:VAL:HG11  | 58:DQ:81:ILE:CG1    | 2.35                     | 0.56              |
| 62:DY:53:ASP:HB3   | 62:DY:96:LEU:HD11   | 1.87                     | 0.56              |
| 65:D2:426:G:C2     | 65:D2:428:A:H5''    | 2.41                     | 0.56              |
| 66:D3:31:C:O2'     | 66:D3:547:U:OP1     | 2.24                     | 0.56              |
| 66:D3:104:A:N6     | 66:D3:307:G:H2'     | 2.20                     | 0.56              |
| 66:D3:829:A:H4'    | 66:D3:830:U:H5'     | 1.88                     | 0.56              |
| 7:UD:162:ASN:HB2   | 7:UD:164:THR:HG22   | 1.87                     | 0.56              |
| 7:UD:475:THR:HG22  | 7:UD:488:ILE:HG23   | 1.87                     | 0.56              |
| 8:UE:111:ASP:OD1   | 8:UE:153:ILE:HG12   | 2.05                     | 0.56              |
| 9:UF:155:TYR:HE1   | 9:UF:161:PHE:CZ     | 2.24                     | 0.56              |
| 10:UG:168:VAL:HG22 | 10:UG:177:TYR:HE2   | 1.71                     | 0.56              |
| 13:UJ:413:ASP:OD1  | 13:UJ:413:ASP:N     | 2.38                     | 0.56              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 15:UL:88:HIS:CD2    | 15:UL:91:THR:HG23  | 2.41                     | 0.56              |
| 16:UM:280:ARG:O     | 16:UM:327:ILE:N    | 2.28                     | 0.56              |
| 16:UM:787:PRO:HG3   | 34:CK:495:ILE:HD11 | 1.87                     | 0.56              |
| 22:US:185:TYR:O     | 22:US:192:GLN:NE2  | 2.38                     | 0.56              |
| 22:US:208:TYR:HD1   | 22:US:211:LEU:HD21 | 1.70                     | 0.56              |
| 22:US:349:LEU:HD23  | 22:US:355:ARG:CZ   | 2.36                     | 0.56              |
| 23:UT:91:LEU:HD21   | 23:UT:109:LEU:HD11 | 1.86                     | 0.56              |
| 23:UT:453:PHE:CE1   | 23:UT:488:TYR:HB3  | 2.40                     | 0.56              |
| 23:UT:745:HIS:O     | 23:UT:749:LYS:HG2  | 2.05                     | 0.56              |
| 24:UU:731:MET:HG2   | 24:UU:883:THR:HG21 | 1.87                     | 0.56              |
| 25:UV:870:ALA:O     | 25:UV:875:LYS:NZ   | 2.39                     | 0.56              |
| 27:UZ:90:ASP:O      | 27:UZ:91:GLU:HG3   | 2.06                     | 0.56              |
| 31:CH:328:ILE:HA    | 31:CH:337:VAL:O    | 2.06                     | 0.56              |
| 35:CL:269:VAL:HG21  | 35:CL:796:VAL:HG11 | 1.87                     | 0.56              |
| 35:CL:799:GLU:HA    | 35:CL:802:LYS:HG2  | 1.87                     | 0.56              |
| 38:JC:64:VAL:O      | 38:JC:66:ARG:NH1   | 2.39                     | 0.56              |
| 38:JC:297:ALA:HB3   | 38:JC:311:MET:HE3  | 1.88                     | 0.56              |
| 45:JN:329:ILE:HD11  | 60:DW:89:TRP:CH2   | 2.40                     | 0.56              |
| 49:DE:178:GLY:H     | 49:DE:195:ILE:HG13 | 1.70                     | 0.56              |
| 51:DG:5:ILE:HD11    | 51:DG:113:ILE:HG13 | 1.87                     | 0.56              |
| 66:D3:1274:C:H2'    | 66:D3:1275:A:C8    | 2.41                     | 0.56              |
| 66:D3:1644:C:H2'    | 66:D3:1645:G:H8    | 1.71                     | 0.56              |
| 4:UA:265:CYS:SG     | 4:UA:308:VAL:HG23  | 2.46                     | 0.56              |
| 5:UB:515:HIS:H      | 5:UB:519:THR:HG23  | 1.71                     | 0.56              |
| 7:UD:147:ILE:HD11   | 7:UD:156:LEU:HD13  | 1.87                     | 0.56              |
| 7:UD:468:ASP:HA     | 7:UD:471:LEU:HD12  | 1.88                     | 0.56              |
| 9:UF:33:MET:O       | 9:UF:37:THR:HG23   | 2.06                     | 0.56              |
| 10:UG:475:ASN:OD1   | 10:UG:478:LYS:HE2  | 2.05                     | 0.56              |
| 10:UG:493:LYS:O     | 10:UG:498:ARG:NH2  | 2.38                     | 0.56              |
| 13:UJ:778:SER:O     | 13:UJ:782:VAL:HG22 | 2.06                     | 0.56              |
| 14:UK:22:ARG:NH1    | 35:CL:937:PHE:CG   | 2.74                     | 0.56              |
| 14:UK:208:GLU:O     | 14:UK:212:LYS:HG3  | 2.06                     | 0.56              |
| 15:UL:98:TYR:HE2    | 15:UL:104:LYS:HD2  | 1.71                     | 0.56              |
| 15:UL:201:ILE:HB    | 16:UM:660:LYS:HD3  | 1.88                     | 0.56              |
| 20:UQ:484:VAL:HG23  | 20:UQ:485:ARG:H    | 1.70                     | 0.56              |
| 23:UT:264:THR:O     | 23:UT:267:SER:OG   | 2.21                     | 0.56              |
| 23:UT:1402:ILE:HG13 | 23:UT:1417:TYR:HD1 | 1.70                     | 0.56              |
| 23:UT:1665:LEU:HD12 | 23:UT:1669:TYR:CD2 | 2.40                     | 0.56              |
| 23:UT:1889:VAL:HA   | 23:UT:1892:LEU:HG  | 1.88                     | 0.56              |
| 23:UT:1999:ALA:O    | 23:UT:2003:LEU:HG  | 2.06                     | 0.56              |
| 24:UU:376:TRP:CH2   | 24:UU:388:GLU:HB2  | 2.41                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:UV:547:PHE:O    | 25:UV:552:ARG:NH1  | 2.39                     | 0.56              |
| 31:CH:256:ARG:HA   | 31:CH:282:GLU:HB3  | 1.87                     | 0.56              |
| 46:JO:59:ASP:HB3   | 46:JO:110:PHE:CZ   | 2.41                     | 0.56              |
| 49:DE:201:HIS:ND1  | 49:DE:205:PHE:O    | 2.39                     | 0.56              |
| 53:DI:34:ALA:HB2   | 53:DI:56:ARG:HD3   | 1.88                     | 0.56              |
| 65:D2:182:G:H2'    | 65:D2:183:A:H8     | 1.70                     | 0.56              |
| 65:D2:341:G:N2     | 65:D2:386:A:N7     | 2.54                     | 0.56              |
| 66:D3:1684:U:H2'   | 66:D3:1685:G:C8    | 2.41                     | 0.56              |
| 2:DA:8:ARG:NH2     | 66:D3:908:U:OP2    | 2.38                     | 0.56              |
| 2:DA:24:PHE:CZ     | 57:DO:39:ILE:HA    | 2.41                     | 0.56              |
| 4:UA:172:ILE:HG23  | 4:UA:187:PHE:HE2   | 1.71                     | 0.56              |
| 5:UB:706:LYS:HD2   | 39:JF:229:ASN:OD1  | 2.06                     | 0.56              |
| 8:UE:116:GLN:HB3   | 8:UE:128:GLN:HE22  | 1.71                     | 0.56              |
| 9:UF:166:ASN:HA    | 9:UF:169:GLN:NE2   | 2.21                     | 0.56              |
| 13:UJ:411:ASN:OD1  | 13:UJ:414:LEU:HD23 | 2.06                     | 0.56              |
| 13:UJ:491:TYR:O    | 13:UJ:495:LEU:HG   | 2.06                     | 0.56              |
| 14:UK:66:ALA:HB3   | 35:CL:1079:PHE:HZ  | 1.70                     | 0.56              |
| 20:UQ:533:THR:HG23 | 20:UQ:544:LYS:HB2  | 1.88                     | 0.56              |
| 21:UR:400:ILE:HG21 | 21:UR:425:ALA:HB3  | 1.87                     | 0.56              |
| 23:UT:638:LEU:O    | 23:UT:642:ILE:HG12 | 2.06                     | 0.56              |
| 23:UT:893:ASP:OD1  | 23:UT:894:ASP:N    | 2.39                     | 0.56              |
| 25:UV:713:LEU:O    | 25:UV:716:SER:OG   | 2.19                     | 0.56              |
| 27:UZ:40:ILE:HG12  | 27:UZ:242:ILE:HG13 | 1.86                     | 0.56              |
| 28:CD:73:LEU:HD23  | 28:CD:73:LEU:H     | 1.71                     | 0.56              |
| 32:CI:93:LYS:O     | 32:CI:96:ASP:HB2   | 2.06                     | 0.56              |
| 35:CL:312:PHE:C    | 35:CL:316:LYS:HZ2  | 2.09                     | 0.56              |
| 47:JP:58:PHE:HE2   | 67:D4:31:G:C4      | 2.24                     | 0.56              |
| 55:DL:110:HIS:ND1  | 55:DL:138:ASN:OD1  | 2.25                     | 0.56              |
| 57:DO:40:ALA:HB3   | 57:DO:67:VAL:HG13  | 1.88                     | 0.56              |
| 66:D3:474:A:H2'    | 66:D3:474:A:N3     | 2.20                     | 0.56              |
| 76:EI:318:ARG:O    | 76:EI:322:ALA:N    | 2.38                     | 0.56              |
| 1:CA:85:LYS:NZ     | 44:JM:171:SER:O    | 2.28                     | 0.55              |
| 1:CA:212:LYS:NZ    | 28:CD:160:ARG:HD3  | 2.21                     | 0.55              |
| 2:DA:89:ASP:OD2    | 2:DA:90:GLU:N      | 2.38                     | 0.55              |
| 3:JA:731:GLN:O     | 3:JA:735:LYS:HG2   | 2.06                     | 0.55              |
| 1:CB:228:GLN:O     | 1:CB:231:ARG:HD3   | 2.05                     | 0.55              |
| 5:UB:488:ASN:HD22  | 5:UB:491:ASP:HB2   | 1.71                     | 0.55              |
| 7:UD:381:ASN:HA    | 7:UD:394:TRP:CZ2   | 2.41                     | 0.55              |
| 9:UF:12:ILE:HD13   | 10:UG:66:LEU:HD21  | 1.88                     | 0.55              |
| 14:UK:140:ARG:NH1  | 19:UP:166:LEU:O    | 2.39                     | 0.55              |
| 15:UL:167:THR:HG1  | 15:UL:208:TRP:HD1  | 1.55                     | 0.55              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 16:UM:130:ASP:HB3  | 16:UM:133:ASN:O     | 2.06                     | 0.55              |
| 16:UM:265:ALA:HB2  | 16:UM:288:LEU:HB2   | 1.88                     | 0.55              |
| 21:UR:278:ASP:HB2  | 21:UR:281:THR:H     | 1.70                     | 0.55              |
| 23:UT:492:GLN:HE22 | 23:UT:495:GLU:HB2   | 1.70                     | 0.55              |
| 23:UT:978:PHE:CE2  | 23:UT:1024:GLN:HG3  | 2.40                     | 0.55              |
| 23:UT:1421:LEU:HA  | 23:UT:1424:MET:SD   | 2.47                     | 0.55              |
| 24:UU:131:SER:HB3  | 24:UU:170:LEU:HD11  | 1.87                     | 0.55              |
| 25:UV:195:ILE:HD13 | 25:UV:364:VAL:HG23  | 1.88                     | 0.55              |
| 25:UV:654:SER:OG   | 25:UV:666:CYS:SG    | 2.60                     | 0.55              |
| 25:UV:654:SER:N    | 25:UV:666:CYS:O     | 2.39                     | 0.55              |
| 31:CH:241:THR:HG23 | 31:CH:286:LEU:HD12  | 1.89                     | 0.55              |
| 31:CH:304:ILE:HG13 | 31:CH:318:LEU:HB2   | 1.88                     | 0.55              |
| 34:CK:367:ASP:OD1  | 34:CK:370:ARG:NH1   | 2.39                     | 0.55              |
| 39:JF:47:MET:O     | 39:JF:117:SER:OG    | 2.22                     | 0.55              |
| 66:D3:322:G:H1'    | 66:D3:323:A:C8      | 2.41                     | 0.55              |
| 66:D3:689:G:H2'    | 66:D3:690:G:H8      | 1.72                     | 0.55              |
| 71:ED:158:SER:O    | 71:ED:162:SER:N     | 2.40                     | 0.55              |
| 1:CA:120:GLU:OE2   | 1:CA:142:ARG:HD2    | 2.06                     | 0.55              |
| 3:JA:522:THR:HG21  | 3:JA:706:PRO:HG2    | 1.86                     | 0.55              |
| 7:UD:51:PHE:CE1    | 7:UD:67:LEU:HB3     | 2.42                     | 0.55              |
| 7:UD:330:GLY:H     | 7:UD:353:GLU:CD     | 2.09                     | 0.55              |
| 7:UD:563:LEU:O     | 13:UJ:639:ARG:NH1   | 2.40                     | 0.55              |
| 10:UG:517:GLN:NE2  | 10:UG:521:ASP:OD2   | 2.39                     | 0.55              |
| 11:UH:549:ARG:HH22 | 11:UH:552:LYS:HD2   | 1.70                     | 0.55              |
| 11:UH:671:ARG:NH2  | 12:UI:450:ASN:OD1   | 2.34                     | 0.55              |
| 13:UJ:695:TYR:HE1  | 13:UJ:702:TRP:HB3   | 1.71                     | 0.55              |
| 14:UK:117:LYS:HZ2  | 14:UK:204:HIS:HE1   | 1.53                     | 0.55              |
| 18:UO:189:TYR:OH   | 22:US:370:HIS:O     | 2.24                     | 0.55              |
| 20:UQ:872:PHE:HD1  | 20:UQ:875:MET:HE1   | 1.71                     | 0.55              |
| 22:US:377:ALA:HA   | 22:US:380:ILE:HD12  | 1.87                     | 0.55              |
| 23:UT:1119:TYR:HE2 | 23:UT:1157:ILE:HG13 | 1.71                     | 0.55              |
| 23:UT:1292:GLY:HA2 | 23:UT:1298:LEU:HD12 | 1.88                     | 0.55              |
| 28:CD:121:ASN:O    | 28:CD:125:GLN:HG2   | 2.06                     | 0.55              |
| 30:CG:95:ARG:CZ    | 31:CH:551:ARG:HD3   | 2.37                     | 0.55              |
| 35:CL:303:LYS:HE3  | 35:CL:787:SER:HB2   | 1.89                     | 0.55              |
| 38:JC:171:ARG:CZ   | 43:JK:468:VAL:HA    | 2.36                     | 0.55              |
| 38:JC:236:PHE:HA   | 38:JC:243:PHE:HA    | 1.86                     | 0.55              |
| 47:JP:66:HIS:CD2   | 47:JP:70:VAL:HG22   | 2.41                     | 0.55              |
| 55:DL:49:ILE:HG13  | 55:DL:50:GLU:HG2    | 1.87                     | 0.55              |
| 66:D3:10:G:C2      | 67:D4:22:A:C2       | 2.94                     | 0.55              |
| 66:D3:782:U:H4'    | 66:D3:783:G:OP2     | 2.06                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:JA:894:ASN:O     | 3:JA:897:THR:OG1   | 2.17                     | 0.55              |
| 4:UA:799:ILE:HD13  | 4:UA:824:ILE:HG23  | 1.87                     | 0.55              |
| 1:CB:198:GLU:OE2   | 1:CB:199:PHE:N     | 2.35                     | 0.55              |
| 1:CB:264:GLN:CA    | 1:CB:320:TYR:O     | 2.55                     | 0.55              |
| 9:UF:57:ILE:HD13   | 9:UF:96:TYR:CZ     | 2.41                     | 0.55              |
| 10:UG:548:GLU:O    | 10:UG:551:SER:OG   | 2.13                     | 0.55              |
| 13:UJ:759:ILE:O    | 13:UJ:763:LEU:HB2  | 2.06                     | 0.55              |
| 15:UL:98:TYR:HB2   | 15:UL:102:VAL:HG23 | 1.89                     | 0.55              |
| 15:UL:262:ILE:O    | 15:UL:270:SER:OG   | 2.24                     | 0.55              |
| 15:UL:901:ASN:ND2  | 16:UM:760:ILE:HG23 | 2.21                     | 0.55              |
| 16:UM:159:LYS:HD2  | 16:UM:160:ILE:HG23 | 1.88                     | 0.55              |
| 18:UO:117:LEU:HD21 | 50:DF:124:LEU:HD11 | 1.88                     | 0.55              |
| 20:UQ:820:ASP:OD1  | 20:UQ:821:ILE:N    | 2.38                     | 0.55              |
| 21:UR:458:ILE:HD13 | 21:UR:484:VAL:HA   | 1.88                     | 0.55              |
| 23:UT:45:SER:O     | 23:UT:48:LEU:N     | 2.39                     | 0.55              |
| 23:UT:145:SER:HA   | 23:UT:148:PHE:CD1  | 2.42                     | 0.55              |
| 23:UT:862:ASN:HB3  | 23:UT:865:VAL:HG22 | 1.88                     | 0.55              |
| 24:UU:392:ARG:HE   | 24:UU:449:ARG:NH2  | 2.03                     | 0.55              |
| 25:UV:238:HIS:HA   | 25:UV:241:ILE:HD12 | 1.89                     | 0.55              |
| 25:UV:1162:ILE:HB  | 25:UV:1185:LEU:HB2 | 1.88                     | 0.55              |
| 25:UV:1221:HIS:CE1 | 37:CN:22:ASP:HA    | 2.41                     | 0.55              |
| 27:UZ:65:PHE:HD1   | 27:UZ:70:LEU:HD11  | 1.70                     | 0.55              |
| 31:CH:278:ASP:OD1  | 31:CH:279:ARG:N    | 2.40                     | 0.55              |
| 33:CJ:1:MET:O      | 33:CJ:4:ARG:N      | 2.38                     | 0.55              |
| 38:JC:282:ASN:ND2  | 38:JC:287:ASN:OD1  | 2.37                     | 0.55              |
| 47:JP:73:ILE:HD11  | 47:JP:366:GLY:HA3  | 1.89                     | 0.55              |
| 47:JP:327:LYS:HE3  | 47:JP:349:GLN:HA   | 1.87                     | 0.55              |
| 47:JP:402:GLU:OE1  | 47:JP:405:ARG:NH2  | 2.40                     | 0.55              |
| 49:DE:6:LYS:NZ     | 66:D3:383:G:OP1    | 2.39                     | 0.55              |
| 49:DE:75:LYS:NZ    | 66:D3:123:G:OP1    | 2.25                     | 0.55              |
| 49:DE:79:ASP:CG    | 49:DE:81:THR:H     | 2.10                     | 0.55              |
| 65:D2:428:A:H2'    | 65:D2:429:A:H8     | 1.71                     | 0.55              |
| 66:D3:551:G:O6     | 66:D3:587:C:N4     | 2.38                     | 0.55              |
| 66:D3:804:A:H2'    | 66:D3:805:U:C6     | 2.40                     | 0.55              |
| 66:D3:1170:G:C2    | 66:D3:1171:A:C8    | 2.95                     | 0.55              |
| 67:D4:4:G:H2'      | 67:D4:5:A:H8       | 1.72                     | 0.55              |
| 3:JA:748:ARG:HE    | 3:JA:759:THR:HG22  | 1.71                     | 0.55              |
| 3:JA:822:ASN:HB3   | 3:JA:869:ASP:HB2   | 1.89                     | 0.55              |
| 4:UA:604:TYR:HD1   | 4:UA:611:LEU:HA    | 1.72                     | 0.55              |
| 5:UB:510:THR:HG23  | 5:UB:518:ILE:HG21  | 1.87                     | 0.55              |
| 8:UE:142:ILE:HD11  | 8:UE:145:CYS:SG    | 2.46                     | 0.55              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 10:UG:138:ASP:O    | 10:UG:140:ARG:N     | 2.40                     | 0.55              |
| 13:UJ:176:ALA:O    | 13:UJ:180:ILE:HG13  | 2.07                     | 0.55              |
| 14:UK:40:ASP:OD2   | 14:UK:43:ARG:NH1    | 2.39                     | 0.55              |
| 15:UL:435:THR:OG1  | 15:UL:477:TRP:O     | 2.25                     | 0.55              |
| 15:UL:566:TYR:CD2  | 15:UL:567:LEU:HB2   | 2.41                     | 0.55              |
| 18:UO:260:TYR:HE1  | 18:UO:270:SER:HB3   | 1.70                     | 0.55              |
| 21:UR:257:HIS:CD2  | 21:UR:258:PRO:HD2   | 2.42                     | 0.55              |
| 23:UT:706:LEU:HB3  | 23:UT:707:PRO:HD3   | 1.88                     | 0.55              |
| 23:UT:1617:VAL:HA  | 23:UT:1620:VAL:HG12 | 1.88                     | 0.55              |
| 23:UT:1631:PHE:O   | 23:UT:1634:SER:OG   | 2.23                     | 0.55              |
| 24:UU:168:VAL:HB   | 24:UU:183:VAL:HG13  | 1.88                     | 0.55              |
| 24:UU:401:ARG:HD2  | 65:D2:278:G:O2'     | 2.05                     | 0.55              |
| 25:UV:254:LEU:HD13 | 25:UV:270:ILE:HB    | 1.87                     | 0.55              |
| 25:UV:855:LEU:HD12 | 25:UV:889:TYR:CD2   | 2.37                     | 0.55              |
| 27:UZ:128:ASP:OD1  | 27:UZ:130:ARG:NH1   | 2.39                     | 0.55              |
| 27:UZ:204:ILE:HG13 | 27:UZ:205:GLN:OE1   | 2.06                     | 0.55              |
| 28:CD:281:LEU:HD22 | 29:CE:265:PHE:HZ    | 1.71                     | 0.55              |
| 32:CI:28:ARG:NH1   | 65:D2:393:C:O4'     | 2.39                     | 0.55              |
| 36:CM:230:TRP:O    | 36:CM:235:SER:OG    | 2.13                     | 0.55              |
| 47:JP:326:ASP:O    | 47:JP:328:SER:N     | 2.38                     | 0.55              |
| 56:DN:105:ASN:OD1  | 66:D3:879:G:O2'     | 2.25                     | 0.55              |
| 60:DW:118:ARG:HH21 | 60:DW:119:LYS:NZ    | 2.03                     | 0.55              |
| 65:D2:182:G:H2'    | 65:D2:183:A:C8      | 2.41                     | 0.55              |
| 65:D2:205:C:H2'    | 65:D2:206:A:C8      | 2.42                     | 0.55              |
| 66:D3:31:C:O2'     | 66:D3:547:U:H5''    | 2.07                     | 0.55              |
| 66:D3:237:C:O2'    | 66:D3:239:C:OP2     | 2.23                     | 0.55              |
| 66:D3:866:G:C2     | 66:D3:867:G:C8      | 2.94                     | 0.55              |
| 66:D3:1590:G:N2    | 66:D3:1591:C:N3     | 2.54                     | 0.55              |
| 3:JA:57:TRP:NE1    | 3:JA:125:GLN:OE1    | 2.39                     | 0.55              |
| 3:JA:825:LEU:HD12  | 3:JA:830:LEU:HD21   | 1.88                     | 0.55              |
| 3:JA:913:PHE:HA    | 3:JA:916:ILE:HD12   | 1.87                     | 0.55              |
| 3:JB:567:LEU:O     | 3:JB:583:LEU:N      | 2.24                     | 0.55              |
| 8:UE:259:PRO:HG2   | 8:UE:260:LEU:HD12   | 1.89                     | 0.55              |
| 9:UF:197:ILE:HD12  | 9:UF:200:ARG:HH21   | 1.72                     | 0.55              |
| 11:UH:558:CYS:H    | 11:UH:585:ARG:NH1   | 1.99                     | 0.55              |
| 13:UJ:550:TYR:O    | 13:UJ:553:SER:C     | 2.44                     | 0.55              |
| 13:UJ:1704:LYS:O   | 13:UJ:1708:ILE:HG13 | 2.07                     | 0.55              |
| 16:UM:498:SER:HB2  | 16:UM:539:VAL:HG13  | 1.87                     | 0.55              |
| 20:UQ:850:GLU:HA   | 20:UQ:853:ILE:HD13  | 1.89                     | 0.55              |
| 22:US:341:LEU:O    | 22:US:344:ILE:HG22  | 2.06                     | 0.55              |
| 23:UT:1101:GLN:HA  | 23:UT:1143:LYS:HE3  | 1.88                     | 0.55              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 24:UU:50:ILE:HD13  | 24:UU:311:VAL:HG11  | 1.89                     | 0.55              |
| 25:UV:177:ASN:HD21 | 25:UV:179:LYS:HG2   | 1.71                     | 0.55              |
| 26:UX:62:PRO:HB3   | 26:UX:93:LYS:HB3    | 1.87                     | 0.55              |
| 26:UX:178:HIS:ND1  | 66:D3:370:A:N1      | 2.55                     | 0.55              |
| 28:CD:24:GLN:HE21  | 28:CD:123:LEU:HD12  | 1.71                     | 0.55              |
| 29:CE:88:ILE:HG22  | 29:CE:117:TYR:HE1   | 1.72                     | 0.55              |
| 29:CE:191:HIS:HD1  | 29:CE:247:ILE:HG12  | 1.71                     | 0.55              |
| 31:CH:452:SER:HB3  | 31:CH:460:ARG:HA    | 1.88                     | 0.55              |
| 33:CJ:191:PHE:CD2  | 33:CJ:203:VAL:HG23  | 2.42                     | 0.55              |
| 34:CK:347:PHE:HD1  | 34:CK:348:ASP:O     | 1.90                     | 0.55              |
| 35:CL:128:MET:HE3  | 35:CL:155:PHE:HB2   | 1.88                     | 0.55              |
| 37:CN:64:ILE:HA    | 37:CN:67:MET:SD     | 2.46                     | 0.55              |
| 39:JF:94:GLN:HA    | 39:JF:97:LEU:HD12   | 1.87                     | 0.55              |
| 47:JP:66:HIS:HE1   | 47:JP:93:LYS:HG3    | 1.72                     | 0.55              |
| 47:JP:217:TRP:HZ2  | 47:JP:465:VAL:HG11  | 1.71                     | 0.55              |
| 56:DN:117:LEU:O    | 56:DN:120:SER:OG    | 2.22                     | 0.55              |
| 60:DW:36:LYS:HA    | 60:DW:39:GLN:OE1    | 2.06                     | 0.55              |
| 65:D2:465:G:H2'    | 65:D2:466:A:H8      | 1.72                     | 0.55              |
| 66:D3:390:G:H2'    | 66:D3:391:A:C8      | 2.42                     | 0.55              |
| 66:D3:1038:U:H2'   | 66:D3:1039:A:C8     | 2.41                     | 0.55              |
| 66:D3:1164:G:H2'   | 66:D3:1165:G:C8     | 2.41                     | 0.55              |
| 1:CA:202:ARG:HH22  | 30:CG:68:PRO:HB2    | 1.71                     | 0.55              |
| 2:DA:144:ARG:HD3   | 2:DA:208:GLN:HB3    | 1.89                     | 0.55              |
| 5:UB:784:ILE:O     | 5:UB:787:THR:HG22   | 2.06                     | 0.55              |
| 8:UE:108:LYS:HE2   | 8:UE:122:SER:HB2    | 1.89                     | 0.55              |
| 8:UE:548:ASP:OD1   | 18:UO:488:LYS:HE2   | 2.06                     | 0.55              |
| 13:UJ:1516:PHE:HB2 | 13:UJ:1521:ILE:HD11 | 1.89                     | 0.55              |
| 15:UL:565:PHE:O    | 36:CM:207:ARG:NH1   | 2.38                     | 0.55              |
| 22:US:165:ASP:N    | 22:US:171:ALA:O     | 2.38                     | 0.55              |
| 23:UT:746:ILE:HA   | 23:UT:749:LYS:HE2   | 1.89                     | 0.55              |
| 23:UT:1358:LYS:O   | 23:UT:1364:ARG:NH1  | 2.40                     | 0.55              |
| 24:UU:501:HIS:NE2  | 24:UU:519:SER:OG    | 2.36                     | 0.55              |
| 25:UV:699:GLU:HA   | 25:UV:702:LYS:HD2   | 1.88                     | 0.55              |
| 26:UX:65:VAL:HG11  | 26:UX:86:MET:HE1    | 1.88                     | 0.55              |
| 28:CD:219:LEU:O    | 28:CD:223:ILE:HG22  | 2.06                     | 0.55              |
| 33:CJ:279:ARG:NH2  | 35:CL:975:GLU:OE2   | 2.26                     | 0.55              |
| 35:CL:154:GLU:CD   | 35:CL:912:ARG:HH21  | 2.09                     | 0.55              |
| 37:CN:219:ASN:ND2  | 66:D3:1057:U:O2     | 2.36                     | 0.55              |
| 39:JF:41:MET:SD    | 39:JF:202:ILE:HG23  | 2.46                     | 0.55              |
| 39:JF:246:GLU:HG2  | 39:JF:251:ILE:HD12  | 1.89                     | 0.55              |
| 47:JP:304:HIS:CE1  | 47:JP:324:SER:HB3   | 2.41                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 55:DL:85:VAL:HA    | 55:DL:108:PRO:HA   | 1.89                     | 0.55              |
| 66:D3:880:C:H2'    | 66:D3:881:A:H8     | 1.72                     | 0.55              |
| 4:UA:73:ILE:CD1    | 4:UA:102:VAL:HG21  | 2.36                     | 0.55              |
| 4:UA:620:ASN:OD1   | 4:UA:621:MET:N     | 2.40                     | 0.55              |
| 1:CB:286:PHE:CZ    | 1:CB:314:CYS:HB3   | 2.42                     | 0.55              |
| 5:UB:529:LEU:HD11  | 5:UB:567:PHE:CG    | 2.42                     | 0.55              |
| 8:UE:8:SER:HB2     | 8:UE:17:LEU:HD21   | 1.89                     | 0.55              |
| 9:UF:121:GLY:HA2   | 9:UF:124:THR:HB    | 1.89                     | 0.55              |
| 10:UG:77:GLU:OE2   | 47:JP:2:LYS:N      | 2.40                     | 0.55              |
| 10:UG:228:LEU:HD23 | 10:UG:259:TRP:CE3  | 2.42                     | 0.55              |
| 12:UI:462:LEU:HB3  | 12:UI:463:LYS:HE2  | 1.89                     | 0.55              |
| 13:UJ:535:ALA:HB3  | 13:UJ:540:LYS:HE3  | 1.88                     | 0.55              |
| 15:UL:8:PHE:CZ     | 15:UL:686:GLU:HB3  | 2.41                     | 0.55              |
| 20:UQ:174:TYR:CD1  | 20:UQ:189:HIS:HA   | 2.41                     | 0.55              |
| 20:UQ:623:PHE:CE1  | 20:UQ:632:ILE:HD13 | 2.42                     | 0.55              |
| 20:UQ:779:ILE:HG13 | 20:UQ:780:GLU:N    | 2.21                     | 0.55              |
| 22:US:386:LEU:O    | 22:US:389:GLU:C    | 2.45                     | 0.55              |
| 23:UT:930:PHE:HD1  | 23:UT:964:PHE:HE1  | 1.53                     | 0.55              |
| 23:UT:1140:GLN:O   | 23:UT:1188:LYS:NZ  | 2.31                     | 0.55              |
| 28:CD:277:ARG:CZ   | 29:CE:264:GLU:HB3  | 2.36                     | 0.55              |
| 29:CE:280:MET:HA   | 29:CE:283:ILE:HG22 | 1.88                     | 0.55              |
| 35:CL:555:MET:O    | 36:CM:327:ARG:NH2  | 2.39                     | 0.55              |
| 38:JC:64:VAL:H     | 38:JC:321:GLU:CD   | 2.09                     | 0.55              |
| 39:JG:89:PRO:O     | 39:JG:92:THR:OG1   | 2.17                     | 0.55              |
| 39:JG:198:ASP:OD1  | 39:JG:199:ASP:N    | 2.37                     | 0.55              |
| 42:JJ:142:ASN:HB2  | 42:JJ:145:PHE:HB3  | 1.89                     | 0.55              |
| 50:DF:146:THR:OG1  | 50:DF:157:ARG:HB3  | 2.06                     | 0.55              |
| 53:DI:27:PHE:O     | 66:D3:333:A:N6     | 2.40                     | 0.55              |
| 54:DJ:82:ARG:HE    | 54:DJ:149:ARG:HE   | 1.54                     | 0.55              |
| 56:DN:69:ASN:HB3   | 56:DN:73:ARG:HB3   | 1.88                     | 0.55              |
| 65:D2:300:C:H2'    | 65:D2:301:U:C6     | 2.41                     | 0.55              |
| 66:D3:209:U:H2'    | 66:D3:210:A:C8     | 2.42                     | 0.55              |
| 66:D3:336:G:H3'    | 66:D3:338:C:H5     | 1.70                     | 0.55              |
| 66:D3:693:U:H2'    | 66:D3:695:U:H3'    | 1.89                     | 0.55              |
| 66:D3:972:G:H2'    | 66:D3:973:A:H8     | 1.71                     | 0.55              |
| 66:D3:1788:G:H2'   | 66:D3:1789:G:C8    | 2.42                     | 0.55              |
| 79:EN:921:GLU:O    | 79:EN:925:ASN:N    | 2.40                     | 0.55              |
| 2:DA:33:LYS:HB3    | 2:DA:97:LEU:HD23   | 1.88                     | 0.55              |
| 3:JA:871:MET:HA    | 3:JA:874:SER:HB2   | 1.88                     | 0.55              |
| 4:UA:25:ASP:OD1    | 4:UA:26:GLY:N      | 2.40                     | 0.55              |
| 4:UA:376:SER:O     | 4:UA:378:PHE:N     | 2.40                     | 0.55              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 6:UC:521:ARG:NH1   | 35:CL:1046:THR:HG23 | 2.20                     | 0.55              |
| 7:UD:202:ILE:HD11  | 7:UD:267:PHE:CE2    | 2.42                     | 0.55              |
| 7:UD:522:SER:HA    | 7:UD:528:ILE:HD11   | 1.89                     | 0.55              |
| 8:UE:546:ARG:NH1   | 11:UH:681:THR:OG1   | 2.39                     | 0.55              |
| 9:UF:2:SER:OG      | 9:UF:3:LYS:N        | 2.39                     | 0.55              |
| 10:UG:161:GLN:HE22 | 32:CI:18:PHE:HE2    | 1.55                     | 0.55              |
| 10:UG:198:PHE:HE2  | 10:UG:200:PRO:HA    | 1.72                     | 0.55              |
| 10:UG:288:TYR:HB2  | 10:UG:345:LEU:HD23  | 1.89                     | 0.55              |
| 16:UM:560:TRP:HE1  | 16:UM:567:VAL:HG12  | 1.72                     | 0.55              |
| 16:UM:647:CYS:SG   | 16:UM:650:GLN:NE2   | 2.80                     | 0.55              |
| 21:UR:159:HIS:HB3  | 21:UR:163:ARG:HH21  | 1.72                     | 0.55              |
| 21:UR:164:LEU:CD2  | 24:UU:175:THR:HG22  | 2.36                     | 0.55              |
| 22:US:229:CYS:HB2  | 22:US:253:PHE:CE2   | 2.41                     | 0.55              |
| 23:UT:316:LYS:O    | 23:UT:319:THR:OG1   | 2.23                     | 0.55              |
| 23:UT:393:PHE:CZ   | 23:UT:397:PHE:HE2   | 2.25                     | 0.55              |
| 23:UT:863:THR:HG22 | 23:UT:867:LYS:NZ    | 2.22                     | 0.55              |
| 24:UU:168:VAL:N    | 24:UU:183:VAL:O     | 2.30                     | 0.55              |
| 24:UU:591:PHE:HA   | 24:UU:601:VAL:O     | 2.06                     | 0.55              |
| 24:UU:889:PHE:O    | 24:UU:893:GLY:N     | 2.38                     | 0.55              |
| 25:UV:114:VAL:HG22 | 25:UV:195:ILE:HB    | 1.88                     | 0.55              |
| 25:UV:180:LYS:HD3  | 25:UV:181:PRO:HD2   | 1.89                     | 0.55              |
| 25:UV:439:HIS:CE1  | 25:UV:460:GLU:HB2   | 2.41                     | 0.55              |
| 44:JM:172:THR:HG22 | 44:JM:175:GLU:HG2   | 1.89                     | 0.55              |
| 56:DN:20:ARG:HH22  | 66:D3:862:A:P       | 2.30                     | 0.55              |
| 60:DW:55:ASP:HB2   | 60:DW:57:ARG:HH11   | 1.72                     | 0.55              |
| 65:D2:221:U:H2'    | 65:D2:222:G:C8      | 2.41                     | 0.55              |
| 66:D3:930:A:H5'    | 66:D3:931:C:OP2     | 2.06                     | 0.55              |
| 66:D3:1592:A:H2'   | 66:D3:1593:A:C8     | 2.41                     | 0.55              |
| 71:ED:243:LEU:N    | 71:ED:282:VAL:O     | 2.37                     | 0.55              |
| 79:EN:465:LEU:O    | 79:EN:469:ARG:N     | 2.39                     | 0.55              |
| 2:DA:97:LEU:HB3    | 2:DA:232:HIS:CE1    | 2.41                     | 0.55              |
| 3:JA:524:PHE:HZ    | 3:JA:556:MET:HG3    | 1.72                     | 0.55              |
| 3:JA:894:ASN:HB3   | 3:JA:897:THR:HG23   | 1.87                     | 0.55              |
| 1:CB:159:LEU:HD22  | 1:CB:162:LEU:HB2    | 1.88                     | 0.55              |
| 1:CB:227:PRO:HA    | 1:CB:230:TYR:CZ     | 2.42                     | 0.55              |
| 7:UD:309:GLN:HB2   | 7:UD:320:TRP:CZ3    | 2.42                     | 0.55              |
| 7:UD:385:ASN:HD21  | 7:UD:387:GLU:HB2    | 1.71                     | 0.55              |
| 7:UD:569:PHE:O     | 7:UD:586:THR:OG1    | 2.15                     | 0.55              |
| 11:UH:610:PHE:O    | 11:UH:614:ILE:HG12  | 2.07                     | 0.55              |
| 13:UJ:1682:GLU:OE1 | 13:UJ:1682:GLU:N    | 2.34                     | 0.55              |
| 21:UR:257:HIS:CG   | 21:UR:258:PRO:HD2   | 2.41                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 21:UR:258:PRO:HB3  | 21:UR:469:PRO:HG2  | 1.89                     | 0.55              |
| 24:UU:594:SER:OG   | 24:UU:596:GLU:HG2  | 2.07                     | 0.55              |
| 25:UV:366:GLY:HA2  | 25:UV:422:PHE:HE1  | 1.70                     | 0.55              |
| 25:UV:708:LEU:HD21 | 25:UV:954:LEU:HD21 | 1.88                     | 0.55              |
| 27:UZ:57:ILE:O     | 27:UZ:186:ASN:HB2  | 2.07                     | 0.55              |
| 29:CE:338:LYS:HG3  | 29:CE:339:TYR:CD1  | 2.41                     | 0.55              |
| 35:CL:776:GLN:HG2  | 35:CL:781:GLU:HG3  | 1.89                     | 0.55              |
| 35:CL:833:ARG:CZ   | 35:CL:834:TRP:HE1  | 2.20                     | 0.55              |
| 38:JC:153:LEU:HD23 | 38:JC:167:LEU:HD11 | 1.88                     | 0.55              |
| 39:JF:161:LYS:HG2  | 39:JF:163:ILE:HG23 | 1.88                     | 0.55              |
| 42:JJ:248:VAL:HA   | 42:JJ:251:ILE:HG12 | 1.87                     | 0.55              |
| 47:JP:276:ASN:CG   | 66:D3:-7:A:H61     | 2.10                     | 0.55              |
| 50:DF:72:HIS:CG    | 50:DF:72:HIS:O     | 2.59                     | 0.55              |
| 66:D3:32:U:O2'     | 66:D3:546:U:O2'    | 2.24                     | 0.55              |
| 66:D3:759:U:H5     | 66:D3:761:G:H21    | 1.54                     | 0.55              |
| 66:D3:760:A:C5     | 66:D3:761:G:H1'    | 2.41                     | 0.55              |
| 67:D4:150:A:H61    | 67:D4:163:U:H3     | 1.55                     | 0.55              |
| 1:CB:236:MET:HG3   | 29:CE:122:GLU:HA   | 1.89                     | 0.55              |
| 7:UD:49:LEU:HB2    | 7:UD:337:CYS:SG    | 2.47                     | 0.55              |
| 15:UL:19:SER:OG    | 15:UL:20:ASN:N     | 2.40                     | 0.55              |
| 16:UM:337:HIS:HA   | 16:UM:363:ARG:HH22 | 1.72                     | 0.55              |
| 18:UO:455:SER:O    | 18:UO:459:VAL:HG12 | 2.06                     | 0.55              |
| 20:UQ:154:LEU:HD11 | 20:UQ:171:TYR:HB3  | 1.88                     | 0.55              |
| 20:UQ:401:GLN:HB2  | 20:UQ:412:ASN:HD21 | 1.71                     | 0.55              |
| 23:UT:725:ASN:OD1  | 23:UT:747:TRP:NE1  | 2.39                     | 0.55              |
| 23:UT:1673:VAL:HA  | 23:UT:1676:GLU:OE1 | 2.07                     | 0.55              |
| 25:UV:688:LYS:HE2  | 25:UV:689:HIS:CD2  | 2.42                     | 0.55              |
| 29:CE:250:THR:O    | 29:CE:254:ASN:ND2  | 2.40                     | 0.55              |
| 31:CH:492:TRP:CD1  | 31:CH:556:VAL:HG21 | 2.42                     | 0.55              |
| 32:CI:81:LYS:NZ    | 34:CK:449:ASP:OD1  | 2.32                     | 0.55              |
| 32:CI:113:VAL:HG22 | 32:CI:124:ILE:HD11 | 1.88                     | 0.55              |
| 34:CK:524:ASP:OD1  | 34:CK:527:ARG:NE   | 2.31                     | 0.55              |
| 35:CL:760:LYS:O    | 35:CL:763:GLU:HG3  | 2.06                     | 0.55              |
| 38:JC:185:HIS:ND1  | 38:JC:234:THR:OG1  | 2.40                     | 0.55              |
| 44:JM:203:LYS:O    | 44:JM:206:TYR:N    | 2.40                     | 0.55              |
| 46:JO:273:LYS:HA   | 46:JO:276:LYS:HD3  | 1.88                     | 0.55              |
| 47:JP:146:LYS:HB3  | 47:JP:148:TRP:NE1  | 2.22                     | 0.55              |
| 50:DF:35:GLN:O     | 50:DF:38:THR:OG1   | 2.18                     | 0.55              |
| 51:DG:46:LYS:N     | 51:DG:119:GLN:OE1  | 2.34                     | 0.55              |
| 56:DN:96:VAL:HG22  | 56:DN:146:ALA:HB1  | 1.89                     | 0.55              |
| 57:DO:42:VAL:HG23  | 57:DO:63:ALA:HB1   | 1.88                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 65:D2:191:U:H2'    | 65:D2:192:G:C8     | 2.42                     | 0.55              |
| 66:D3:322:G:O6     | 66:D3:344:A:N6     | 2.39                     | 0.55              |
| 66:D3:542:A:O2'    | 66:D3:543:C:H2'    | 2.07                     | 0.55              |
| 66:D3:1062:A:O2'   | 66:D3:1063:U:O5'   | 2.25                     | 0.55              |
| 3:JA:70:ARG:NH1    | 66:D3:415:C:OP1    | 2.37                     | 0.54              |
| 3:JA:75:ASN:HA     | 3:JA:78:LYS:NZ     | 2.18                     | 0.54              |
| 4:UA:405:SER:CB    | 4:UA:436:LEU:HD23  | 2.36                     | 0.54              |
| 1:CB:144:TRP:HZ3   | 1:CB:155:ILE:HG13  | 1.71                     | 0.54              |
| 7:UD:265:TRP:CD1   | 7:UD:272:LEU:HA    | 2.39                     | 0.54              |
| 7:UD:363:SER:O     | 7:UD:367:GLY:N     | 2.23                     | 0.54              |
| 7:UD:574:HIS:CE1   | 7:UD:637:PHE:HA    | 2.41                     | 0.54              |
| 9:UF:166:ASN:HA    | 9:UF:169:GLN:HE21  | 1.70                     | 0.54              |
| 10:UG:140:ARG:HE   | 13:UJ:20:LEU:CD1   | 2.20                     | 0.54              |
| 13:UJ:193:THR:HG21 | 13:UJ:237:ILE:HG23 | 1.90                     | 0.54              |
| 15:UL:197:ILE:O    | 16:UM:671:ASN:ND2  | 2.32                     | 0.54              |
| 16:UM:337:HIS:HA   | 16:UM:363:ARG:HH12 | 1.72                     | 0.54              |
| 20:UQ:152:ARG:HE   | 20:UQ:231:PHE:HA   | 1.72                     | 0.54              |
| 20:UQ:472:TYR:CD2  | 20:UQ:478:ASN:HB3  | 2.42                     | 0.54              |
| 23:UT:172:LEU:HD23 | 23:UT:176:LEU:HD23 | 1.88                     | 0.54              |
| 23:UT:920:VAL:HG13 | 23:UT:921:VAL:HG13 | 1.89                     | 0.54              |
| 24:UU:141:LYS:HE2  | 24:UU:154:TYR:CD1  | 2.43                     | 0.54              |
| 24:UU:370:SER:O    | 24:UU:373:ARG:N    | 2.40                     | 0.54              |
| 24:UU:840:PHE:HB3  | 24:UU:844:ALA:HB3  | 1.89                     | 0.54              |
| 29:CE:322:ALA:H    | 29:CE:340:GLY:HA2  | 1.71                     | 0.54              |
| 33:CJ:100:LEU:HD22 | 33:CJ:144:GLU:HB3  | 1.89                     | 0.54              |
| 34:CK:341:LEU:HD11 | 35:CL:956:MET:CB   | 2.37                     | 0.54              |
| 38:JC:59:SER:N     | 38:JC:333:ASN:O    | 2.40                     | 0.54              |
| 38:JC:101:ASN:ND2  | 38:JC:104:PHE:HB3  | 2.22                     | 0.54              |
| 46:JO:92:ALA:HB3   | 57:DO:103:ARG:HE   | 1.72                     | 0.54              |
| 51:DG:171:LYS:NZ   | 66:D3:68:A:OP2     | 2.40                     | 0.54              |
| 54:DJ:89:ASP:OD1   | 54:DJ:90:LYS:N     | 2.40                     | 0.54              |
| 65:D2:83:U:O2'     | 65:D2:84:G:OP2     | 2.24                     | 0.54              |
| 65:D2:410:A:H2'    | 65:D2:411:A:C8     | 2.43                     | 0.54              |
| 66:D3:94:U:H2'     | 66:D3:95:G:O4'     | 2.06                     | 0.54              |
| 66:D3:592:A:N7     | 66:D3:593:U:N3     | 2.54                     | 0.54              |
| 69:EB:107:ILE:O    | 69:EB:111:SER:N    | 2.37                     | 0.54              |
| 79:EN:684:VAL:HA   | 79:EN:766:SER:HA   | 1.89                     | 0.54              |
| 4:UA:335:GLU:O     | 24:UU:745:LYS:HG2  | 2.05                     | 0.54              |
| 4:UA:400:GLN:O     | 4:UA:416:LEU:HB2   | 2.07                     | 0.54              |
| 1:CB:179:THR:O     | 1:CB:182:SER:OG    | 2.20                     | 0.54              |
| 1:CB:241:PHE:CD1   | 1:CB:268:VAL:HG13  | 2.42                     | 0.54              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 8:UE:461:ASP:O     | 8:UE:465:ILE:HG12   | 2.07                     | 0.54              |
| 11:UH:182:THR:HA   | 11:UH:206:LEU:HA    | 1.89                     | 0.54              |
| 13:UJ:65:LYS:NZ    | 21:UR:45:ILE:HB     | 2.23                     | 0.54              |
| 15:UL:299:ARG:NH2  | 15:UL:320:SER:OG    | 2.40                     | 0.54              |
| 15:UL:662:ALA:HB3  | 15:UL:675:SER:HB3   | 1.88                     | 0.54              |
| 16:UM:771:LYS:O    | 16:UM:775:ILE:HG12  | 2.07                     | 0.54              |
| 18:UO:5:ARG:CZ     | 18:UO:393:ASN:HD21  | 2.20                     | 0.54              |
| 18:UO:125:HIS:HB3  | 18:UO:145:ASP:HB2   | 1.88                     | 0.54              |
| 18:UO:418:LEU:HD12 | 18:UO:462:TRP:CE2   | 2.43                     | 0.54              |
| 20:UQ:33:ASN:HD22  | 20:UQ:345:GLN:HE22  | 1.53                     | 0.54              |
| 22:US:258:GLU:OE1  | 22:US:289:PHE:HA    | 2.07                     | 0.54              |
| 23:UT:1938:ALA:O   | 23:UT:1942:LEU:HD23 | 2.07                     | 0.54              |
| 25:UV:363:THR:HA   | 25:UV:393:PHE:HE2   | 1.72                     | 0.54              |
| 25:UV:1086:ASN:O   | 25:UV:1090:THR:HG23 | 2.08                     | 0.54              |
| 27:UZ:74:LEU:HD12  | 27:UZ:97:PHE:CZ     | 2.43                     | 0.54              |
| 29:CE:180:TYR:HB3  | 29:CE:262:ILE:HD11  | 1.90                     | 0.54              |
| 31:CH:203:ASP:OD2  | 31:CH:206:LYS:N     | 2.27                     | 0.54              |
| 32:CI:85:MET:SD    | 34:CK:448:LEU:HD22  | 2.47                     | 0.54              |
| 34:CK:538:LYS:HG2  | 66:D3:1628:U:C4     | 2.42                     | 0.54              |
| 35:CL:267:ARG:HD2  | 35:CL:801:VAL:HG11  | 1.88                     | 0.54              |
| 35:CL:948:ILE:HB   | 35:CL:987:TYR:CZ    | 2.42                     | 0.54              |
| 39:JF:49:SER:N     | 39:JF:209:MET:HE3   | 2.23                     | 0.54              |
| 50:DF:34:GLN:O     | 50:DF:37:GLN:HG3    | 2.07                     | 0.54              |
| 50:DF:80:LYS:HG3   | 50:DF:81:ARG:H      | 1.72                     | 0.54              |
| 57:DO:123:SER:OG   | 66:D3:886:U:H1'     | 2.07                     | 0.54              |
| 58:DQ:5:PRO:HG2    | 58:DQ:24:ALA:HB3    | 1.89                     | 0.54              |
| 61:DX:70:LYS:O     | 61:DX:87:VAL:HG12   | 2.06                     | 0.54              |
| 65:D2:312:U:O2'    | 65:D2:313:A:H5'     | 2.07                     | 0.54              |
| 66:D3:629:U:H2'    | 66:D3:630:A:C8      | 2.42                     | 0.54              |
| 66:D3:683:C:H2'    | 66:D3:684:A:C8      | 2.40                     | 0.54              |
| 66:D3:1164:G:H2'   | 66:D3:1165:G:H8     | 1.72                     | 0.54              |
| 77:EJ:159:GLU:HA   | 77:EJ:188:PHE:HA    | 1.89                     | 0.54              |
| 4:UA:495:LYS:HA    | 4:UA:516:SER:O      | 2.08                     | 0.54              |
| 4:UA:531:ALA:HB2   | 4:UA:585:TYR:OH     | 2.07                     | 0.54              |
| 4:UA:575:GLU:OE1   | 32:CI:163:ASN:HB3   | 2.07                     | 0.54              |
| 5:UB:445:VAL:HG23  | 5:UB:449:LYS:HB3    | 1.89                     | 0.54              |
| 6:UC:596:THR:HG22  | 44:JM:137:LYS:HG3   | 1.87                     | 0.54              |
| 7:UD:104:TRP:HE1   | 7:UD:114:LEU:HD13   | 1.72                     | 0.54              |
| 7:UD:265:TRP:HE1   | 7:UD:272:LEU:HD12   | 1.72                     | 0.54              |
| 8:UE:143:ASN:OD1   | 8:UE:144:ASN:N      | 2.41                     | 0.54              |
| 9:UF:172:LEU:HD12  | 9:UF:182:TRP:CZ2    | 2.43                     | 0.54              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 13:UJ:279:MET:HG2  | 13:UJ:299:ILE:HG12  | 1.89                     | 0.54              |
| 13:UJ:1517:ASP:O   | 13:UJ:1521:ILE:HG12 | 2.07                     | 0.54              |
| 14:UK:162:SER:HA   | 14:UK:165:ARG:HH21  | 1.71                     | 0.54              |
| 15:UL:672:VAL:O    | 15:UL:683:ILE:HA    | 2.08                     | 0.54              |
| 19:UP:208:ARG:HG2  | 19:UP:210:ALA:H     | 1.72                     | 0.54              |
| 20:UQ:437:THR:C    | 20:UQ:709:ARG:HH21  | 2.11                     | 0.54              |
| 20:UQ:534:LYS:HG3  | 20:UQ:535:ASN:O     | 2.08                     | 0.54              |
| 21:UR:400:ILE:HD11 | 21:UR:404:ILE:HG23  | 1.88                     | 0.54              |
| 22:US:317:ILE:HG23 | 22:US:358:PHE:HD1   | 1.71                     | 0.54              |
| 23:UT:260:HIS:O    | 23:UT:264:THR:HG23  | 2.08                     | 0.54              |
| 23:UT:884:TYR:HE2  | 23:UT:917:ASP:HB3   | 1.71                     | 0.54              |
| 23:UT:1002:ASN:HA  | 23:UT:1005:ASN:HD21 | 1.72                     | 0.54              |
| 23:UT:1508:GLN:HG2 | 23:UT:1547:LEU:HD22 | 1.89                     | 0.54              |
| 31:CH:425:TRP:CH2  | 31:CH:432:PRO:HG3   | 2.42                     | 0.54              |
| 31:CH:437:ARG:O    | 31:CH:439:ALA:N     | 2.32                     | 0.54              |
| 35:CL:246:ALA:HB3  | 35:CL:810:ILE:HG13  | 1.88                     | 0.54              |
| 35:CL:628:VAL:O    | 35:CL:631:ILE:HG22  | 2.07                     | 0.54              |
| 37:CN:257:PHE:N    | 37:CN:261:GLN:OE1   | 2.39                     | 0.54              |
| 38:JC:255:TYR:HD1  | 38:JC:262:PRO:HA    | 1.72                     | 0.54              |
| 51:DG:79:LYS:HD3   | 51:DG:90:GLY:H      | 1.72                     | 0.54              |
| 58:DQ:42:GLU:HG2   | 58:DQ:45:ARG:NH2    | 2.19                     | 0.54              |
| 66:D3:248:U:C4     | 66:D3:250:C:H1'     | 2.42                     | 0.54              |
| 66:D3:1465:C:C2    | 66:D3:1466:G:C8     | 2.95                     | 0.54              |
| 66:D3:1484:G:O2'   | 66:D3:1606:C:O2'    | 2.24                     | 0.54              |
| 4:UA:6:LYS:NZ      | 4:UA:51:GLU:OE1     | 2.40                     | 0.54              |
| 4:UA:524:ARG:HG3   | 4:UA:585:TYR:CD2    | 2.42                     | 0.54              |
| 7:UD:689:ASN:HD22  | 7:UD:689:ASN:C      | 2.10                     | 0.54              |
| 7:UD:760:LEU:HD23  | 7:UD:760:LEU:H      | 1.71                     | 0.54              |
| 8:UE:213:ASN:ND2   | 8:UE:215:TYR:OH     | 2.38                     | 0.54              |
| 13:UJ:250:SER:HB2  | 13:UJ:253:CYS:SG    | 2.47                     | 0.54              |
| 16:UM:278:LEU:HD12 | 16:UM:279:LYS:HB2   | 1.90                     | 0.54              |
| 16:UM:401:LEU:HA   | 16:UM:417:TYR:HB3   | 1.88                     | 0.54              |
| 18:UO:127:THR:HA   | 18:UO:144:SER:HA    | 1.89                     | 0.54              |
| 18:UO:479:VAL:O    | 18:UO:483:LEU:HG    | 2.08                     | 0.54              |
| 20:UQ:24:ASN:OD1   | 20:UQ:25:LEU:N      | 2.41                     | 0.54              |
| 20:UQ:345:GLN:OE1  | 20:UQ:345:GLN:N     | 2.40                     | 0.54              |
| 23:UT:398:GLN:CD   | 23:UT:746:ILE:HG21  | 2.27                     | 0.54              |
| 23:UT:974:TYR:CG   | 23:UT:1024:GLN:HB3  | 2.43                     | 0.54              |
| 23:UT:1178:CYS:HA  | 23:UT:1181:ILE:HG22 | 1.87                     | 0.54              |
| 23:UT:1724:ASN:HA  | 23:UT:1729:ALA:HB3  | 1.90                     | 0.54              |
| 23:UT:1940:LYS:O   | 23:UT:1944:ILE:HG12 | 2.07                     | 0.54              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 25:UV:140:ASP:HB3  | 25:UV:178:TYR:O     | 2.08                     | 0.54              |
| 25:UV:765:LEU:O    | 25:UV:914:ARG:NH2   | 2.25                     | 0.54              |
| 25:UV:1202:CYS:SG  | 25:UV:1203:ASN:N    | 2.80                     | 0.54              |
| 31:CH:359:PHE:HB3  | 31:CH:425:TRP:CZ3   | 2.43                     | 0.54              |
| 33:CJ:139:LEU:HD22 | 33:CJ:157:PHE:HZ    | 1.73                     | 0.54              |
| 36:CM:145:GLY:HA2  | 36:CM:147:ARG:HH22  | 1.72                     | 0.54              |
| 47:JP:270:ASN:HA   | 47:JP:313:PHE:HD2   | 1.72                     | 0.54              |
| 50:DF:183:ALA:HB2  | 50:DF:193:THR:HG21  | 1.90                     | 0.54              |
| 52:DH:131:PHE:CG   | 52:DH:132:PRO:HA    | 2.43                     | 0.54              |
| 58:DQ:4:VAL:HG21   | 58:DQ:23:LYS:HE3    | 1.89                     | 0.54              |
| 66:D3:863:A:C5     | 66:D3:865:A:C8      | 2.95                     | 0.54              |
| 66:D3:868:G:H2'    | 66:D3:869:A:C8      | 2.40                     | 0.54              |
| 73:EF:259:VAL:O    | 73:EF:263:GLU:N     | 2.32                     | 0.54              |
| 3:JA:76:LYS:HA     | 3:JA:79:LYS:HZ2     | 1.72                     | 0.54              |
| 3:JA:82:LYS:CE     | 62:DY:114:ARG:HG3   | 2.38                     | 0.54              |
| 1:CB:294:ARG:HE    | 19:UP:181:LEU:HD23  | 1.71                     | 0.54              |
| 5:UB:281:LYS:HA    | 40:JH:383:PRO:HA    | 1.90                     | 0.54              |
| 5:UB:453:ASN:HA    | 5:UB:456:ILE:HD12   | 1.88                     | 0.54              |
| 7:UD:157:SER:HB3   | 7:UD:195:TRP:HZ2    | 1.73                     | 0.54              |
| 11:UH:542:SER:HA   | 11:UH:545:ARG:HD2   | 1.89                     | 0.54              |
| 12:UI:417:LYS:HG2  | 12:UI:455:TRP:CZ2   | 2.41                     | 0.54              |
| 13:UJ:1358:CYS:HA  | 13:UJ:1361:VAL:HG12 | 1.90                     | 0.54              |
| 15:UL:281:ILE:HB   | 15:UL:332:ILE:HB    | 1.89                     | 0.54              |
| 15:UL:357:THR:OG1  | 15:UL:361:THR:OG1   | 1.99                     | 0.54              |
| 16:UM:248:PHE:HB3  | 16:UM:256:ARG:CZ    | 2.37                     | 0.54              |
| 20:UQ:604:PHE:HB3  | 20:UQ:606:HIS:CD2   | 2.43                     | 0.54              |
| 20:UQ:769:ASN:HB3  | 20:UQ:773:ASP:OD1   | 2.07                     | 0.54              |
| 20:UQ:780:GLU:O    | 20:UQ:782:THR:N     | 2.38                     | 0.54              |
| 21:UR:128:SER:O    | 21:UR:132:LYS:HE3   | 2.08                     | 0.54              |
| 22:US:395:ILE:HA   | 22:US:398:VAL:HG12  | 1.89                     | 0.54              |
| 23:UT:439:VAL:HA   | 23:UT:442:LYS:HE2   | 1.90                     | 0.54              |
| 23:UT:992:LYS:O    | 23:UT:996:ARG:HG2   | 2.07                     | 0.54              |
| 24:UU:50:ILE:HD11  | 24:UU:311:VAL:HG21  | 1.89                     | 0.54              |
| 25:UV:218:ASP:OD2  | 25:UV:227:LYS:NZ    | 2.35                     | 0.54              |
| 25:UV:858:ARG:HA   | 25:UV:861:ILE:HD12  | 1.88                     | 0.54              |
| 27:UZ:226:LYS:HA   | 27:UZ:229:ARG:HH21  | 1.72                     | 0.54              |
| 29:CE:39:LEU:HD23  | 29:CE:43:LYS:HD2    | 1.90                     | 0.54              |
| 31:CH:440:HIS:CG   | 31:CH:491:SER:HG    | 2.25                     | 0.54              |
| 34:CK:480:GLN:NE2  | 34:CK:482:LEU:HB2   | 2.19                     | 0.54              |
| 36:CM:46:LYS:N     | 36:CM:49:GLU:OE1    | 2.41                     | 0.54              |
| 38:JC:151:CYS:HB2  | 38:JC:167:LEU:HB2   | 1.88                     | 0.54              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 38:JC:349:SER:OG   | 38:JC:353:CYS:SG    | 2.53                     | 0.54              |
| 39:JF:218:ASP:HA   | 39:JF:221:VAL:HG12  | 1.90                     | 0.54              |
| 42:JJ:196:ASP:OD1  | 42:JJ:197:HIS:N     | 2.40                     | 0.54              |
| 49:DE:124:GLY:HA2  | 49:DE:142:HIS:HE1   | 1.73                     | 0.54              |
| 51:DG:7:TYR:CD2    | 51:DG:10:ASN:HB2    | 2.43                     | 0.54              |
| 52:DH:97:ARG:NH1   | 66:D3:693:U:O2'     | 2.41                     | 0.54              |
| 52:DH:103:SER:OG   | 52:DH:104:ARG:N     | 2.40                     | 0.54              |
| 58:DQ:13:LYS:HG3   | 58:DQ:14:LYS:H      | 1.73                     | 0.54              |
| 66:D3:1745:G:H2'   | 66:D3:1746:A:O4'    | 2.07                     | 0.54              |
| 75:EH:84:TYR:N     | 75:EH:97:LEU:O      | 2.36                     | 0.54              |
| 79:EN:86:GLU:HA    | 79:EN:120:ARG:HA    | 1.89                     | 0.54              |
| 3:JA:82:LYS:HE2    | 62:DY:114:ARG:HG3   | 1.90                     | 0.54              |
| 3:JA:906:SER:OG    | 3:JA:907:ASN:N      | 2.39                     | 0.54              |
| 4:UA:440:PRO:HB3   | 4:UA:483:GLN:NE2    | 2.22                     | 0.54              |
| 4:UA:586:SER:OG    | 4:UA:587:PHE:N      | 2.41                     | 0.54              |
| 3:JB:748:ARG:N     | 3:JB:759:THR:O      | 2.32                     | 0.54              |
| 7:UD:83:ASN:ND2    | 7:UD:587:ALA:O      | 2.40                     | 0.54              |
| 7:UD:525:VAL:HG11  | 7:UD:528:ILE:HG23   | 1.90                     | 0.54              |
| 10:UG:373:PHE:HZ   | 10:UG:392:VAL:HG21  | 1.73                     | 0.54              |
| 11:UH:293:TYR:HA   | 11:UH:304:GLN:HA    | 1.88                     | 0.54              |
| 13:UJ:741:LEU:HD21 | 13:UJ:752:ALA:HB3   | 1.89                     | 0.54              |
| 14:UK:77:LEU:HD11  | 35:CL:1071:LYS:NZ   | 2.23                     | 0.54              |
| 20:UQ:476:GLY:H    | 20:UQ:478:ASN:HD21  | 1.56                     | 0.54              |
| 20:UQ:877:ASP:O    | 20:UQ:880:GLN:NE2   | 2.31                     | 0.54              |
| 21:UR:319:ARG:HD3  | 21:UR:353:ARG:NH1   | 2.21                     | 0.54              |
| 23:UT:299:TYR:O    | 23:UT:303:ASN:ND2   | 2.40                     | 0.54              |
| 23:UT:465:PHE:CE2  | 23:UT:482:ARG:HB3   | 2.43                     | 0.54              |
| 23:UT:719:LEU:O    | 23:UT:754:ASN:ND2   | 2.41                     | 0.54              |
| 23:UT:849:GLU:OE2  | 23:UT:853:HIS:NE2   | 2.41                     | 0.54              |
| 23:UT:1394:LEU:HG  | 23:UT:1398:LEU:HD12 | 1.89                     | 0.54              |
| 25:UV:167:PRO:HD3  | 25:UV:226:HIS:CE1   | 2.43                     | 0.54              |
| 25:UV:528:ASP:OD2  | 25:UV:614:ARG:NE    | 2.41                     | 0.54              |
| 29:CE:58:GLU:OE2   | 29:CE:147:ILE:HA    | 2.07                     | 0.54              |
| 29:CE:75:LEU:O     | 29:CE:79:ILE:HG23   | 2.07                     | 0.54              |
| 32:CI:61:LEU:HD23  | 32:CI:64:LEU:HD12   | 1.89                     | 0.54              |
| 34:CK:426:LEU:O    | 34:CK:427:SER:OG    | 2.22                     | 0.54              |
| 35:CL:107:VAL:HG22 | 35:CL:354:ILE:HG22  | 1.90                     | 0.54              |
| 35:CL:879:THR:HB   | 66:D3:572:C:C4      | 2.42                     | 0.54              |
| 36:CM:182:GLU:OE2  | 36:CM:184:ASP:N     | 2.33                     | 0.54              |
| 38:JC:83:VAL:HG12  | 38:JC:92:LYS:HB3    | 1.89                     | 0.54              |
| 39:JG:192:TYR:O    | 39:JG:196:LEU:HG    | 2.08                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:JP:278:VAL:HG13 | 47:JP:313:PHE:HZ   | 1.71                     | 0.54              |
| 50:DF:200:ASN:HA   | 50:DF:203:LYS:NZ   | 2.22                     | 0.54              |
| 52:DH:121:VAL:O    | 52:DH:125:ILE:HD12 | 2.06                     | 0.54              |
| 54:DJ:110:GLN:HG3  | 54:DJ:111:THR:H    | 1.72                     | 0.54              |
| 55:DL:99:ARG:NE    | 55:DL:100:TYR:O    | 2.40                     | 0.54              |
| 57:DO:68:ALA:O     | 57:DO:72:LYS:HG2   | 2.08                     | 0.54              |
| 66:D3:486:G:H4'    | 66:D3:487:G:H5'    | 1.90                     | 0.54              |
| 66:D3:500:C:O2'    | 66:D3:501:U:O5'    | 2.24                     | 0.54              |
| 67:D4:14:A:H3'     | 67:D4:15:U:C6      | 2.43                     | 0.54              |
| 1:CA:189:GLY:O     | 1:CA:216:ASN:ND2   | 2.41                     | 0.54              |
| 3:JA:533:PHE:HE1   | 3:JA:579:ILE:HG13  | 1.73                     | 0.54              |
| 4:UA:220:PHE:CE1   | 4:UA:247:SER:HA    | 2.42                     | 0.54              |
| 4:UA:689:THR:O     | 4:UA:819:THR:OG1   | 2.24                     | 0.54              |
| 5:UB:700:LEU:HD12  | 22:US:463:LEU:H    | 1.73                     | 0.54              |
| 5:UB:716:LYS:HZ1   | 39:JG:153:VAL:HA   | 1.71                     | 0.54              |
| 9:UF:94:PHE:HE1    | 9:UF:98:ARG:HH11   | 1.53                     | 0.54              |
| 9:UF:96:TYR:HD1    | 9:UF:113:TYR:HB2   | 1.73                     | 0.54              |
| 12:UI:429:HIS:HA   | 12:UI:432:LYS:HE2  | 1.90                     | 0.54              |
| 13:UJ:712:ASN:OD1  | 13:UJ:714:GLU:HG3  | 2.07                     | 0.54              |
| 14:UK:161:ARG:CZ   | 14:UK:164:ASN:HB3  | 2.38                     | 0.54              |
| 14:UK:247:GLN:HE22 | 21:UR:515:THR:HB   | 1.71                     | 0.54              |
| 15:UL:273:TYR:HE2  | 15:UL:275:GLN:HB2  | 1.71                     | 0.54              |
| 15:UL:629:ASN:HB3  | 15:UL:641:TYR:CE1  | 2.43                     | 0.54              |
| 18:UO:96:LEU:HD23  | 18:UO:108:TYR:O    | 2.07                     | 0.54              |
| 20:UQ:401:GLN:O    | 20:UQ:412:ASN:ND2  | 2.41                     | 0.54              |
| 20:UQ:471:GLN:NE2  | 20:UQ:541:TRP:H    | 2.02                     | 0.54              |
| 23:UT:523:LEU:HD22 | 23:UT:561:LEU:HD11 | 1.90                     | 0.54              |
| 23:UT:754:ASN:OD1  | 23:UT:755:THR:N    | 2.39                     | 0.54              |
| 23:UT:783:LEU:HD11 | 23:UT:830:VAL:HB   | 1.89                     | 0.54              |
| 23:UT:906:THR:HB   | 53:DI:77:ARG:HH22  | 1.73                     | 0.54              |
| 25:UV:213:LEU:O    | 25:UV:227:LYS:NZ   | 2.37                     | 0.54              |
| 29:CE:171:ASP:OD1  | 29:CE:298:ARG:NH2  | 2.41                     | 0.54              |
| 31:CH:198:LYS:NZ   | 31:CH:266:GLU:O    | 2.40                     | 0.54              |
| 37:CN:151:HIS:CE1  | 37:CN:153:ASN:HB3  | 2.42                     | 0.54              |
| 39:JG:73:HIS:N     | 39:JG:74:GLN:OE1   | 2.41                     | 0.54              |
| 49:DE:125:LYS:HB2  | 49:DE:226:PHE:CE1  | 2.42                     | 0.54              |
| 52:DH:31:SER:CB    | 52:DH:34:LEU:HB3   | 2.38                     | 0.54              |
| 60:DW:78:ARG:NH1   | 66:D3:805:U:O2'    | 2.40                     | 0.54              |
| 61:DX:95:PHE:CE2   | 61:DX:135:LEU:HB3  | 2.43                     | 0.54              |
| 66:D3:933:A:H2'    | 66:D3:933:A:N3     | 2.23                     | 0.54              |
| 66:D3:956:C:O3'    | 66:D3:1047:G:N2    | 2.41                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:DA:148:ASN:O     | 66:D3:1066:C:O2'   | 2.26                     | 0.54              |
| 3:JA:54:SER:O      | 3:JA:120:GLY:N     | 2.40                     | 0.54              |
| 3:JA:904:LEU:HD23  | 3:JA:909:THR:HG23  | 1.89                     | 0.54              |
| 1:CB:218:ILE:HD13  | 29:CE:141:LEU:HA   | 1.90                     | 0.54              |
| 7:UD:368:ASN:O     | 7:UD:679:LEU:HD11  | 2.08                     | 0.54              |
| 8:UE:363:VAL:HG12  | 20:UQ:546:LYS:HB3  | 1.90                     | 0.54              |
| 8:UE:465:ILE:HD12  | 8:UE:501:TRP:CZ2   | 2.43                     | 0.54              |
| 9:UF:182:TRP:CD1   | 9:UF:281:LEU:HD21  | 2.42                     | 0.54              |
| 11:UH:305:VAL:HA   | 11:UH:311:VAL:HA   | 1.90                     | 0.54              |
| 13:UJ:18:VAL:O     | 13:UJ:20:LEU:N     | 2.41                     | 0.54              |
| 14:UK:30:LYS:NZ    | 66:D3:556:A:OP2    | 2.33                     | 0.54              |
| 15:UL:554:THR:OG1  | 15:UL:569:LEU:O    | 2.23                     | 0.54              |
| 15:UL:642:TRP:CZ3  | 15:UL:649:CYS:HB3  | 2.42                     | 0.54              |
| 16:UM:415:TRP:HA   | 16:UM:425:ASP:O    | 2.07                     | 0.54              |
| 16:UM:455:LEU:HD11 | 16:UM:463:ILE:HD12 | 1.90                     | 0.54              |
| 17:UN:295:VAL:HG21 | 47:JP:291:MET:CE   | 2.37                     | 0.54              |
| 21:UR:130:ASP:OD2  | 24:UU:179:LYS:NZ   | 2.29                     | 0.54              |
| 23:UT:1272:PHE:CE1 | 23:UT:1281:ARG:HD2 | 2.43                     | 0.54              |
| 28:CD:8:LEU:HB2    | 28:CD:98:LEU:HD11  | 1.89                     | 0.54              |
| 31:CH:137:GLY:HA3  | 31:CH:500:LYS:HE2  | 1.89                     | 0.54              |
| 35:CL:968:THR:OG1  | 35:CL:972:ILE:HG12 | 2.08                     | 0.54              |
| 39:JF:104:ILE:HB   | 39:JF:246:GLU:HG2  | 1.89                     | 0.54              |
| 39:JG:151:ARG:HB3  | 39:JG:155:SER:HA   | 1.90                     | 0.54              |
| 42:JJ:246:SER:O    | 42:JJ:249:SER:OG   | 2.24                     | 0.54              |
| 46:JO:252:PRO:HB3  | 56:DN:116:ILE:HD11 | 1.88                     | 0.54              |
| 47:JP:17:LYS:NZ    | 47:JP:20:GLN:HB2   | 2.22                     | 0.54              |
| 56:DN:105:ASN:HD21 | 66:D3:879:G:H1'    | 1.73                     | 0.54              |
| 65:D2:117:G:H2'    | 65:D2:118:A:C8     | 2.43                     | 0.54              |
| 66:D3:50:C:H41     | 66:D3:425:A:H8     | 1.56                     | 0.54              |
| 66:D3:1579:U:H2'   | 66:D3:1580:C:C6    | 2.43                     | 0.54              |
| 7:UD:87:GLN:HB3    | 7:UD:378:TYR:HD2   | 1.73                     | 0.54              |
| 8:UE:153:ILE:HG22  | 8:UE:163:LEU:HB2   | 1.90                     | 0.54              |
| 8:UE:348:LYS:NZ    | 18:UO:3:THR:OG1    | 2.41                     | 0.54              |
| 11:UH:562:PRO:O    | 11:UH:566:LEU:HD23 | 2.07                     | 0.54              |
| 14:UK:22:ARG:HH12  | 35:CL:937:PHE:HB3  | 1.72                     | 0.54              |
| 14:UK:200:GLN:HA   | 14:UK:203:GLN:NE2  | 2.22                     | 0.54              |
| 15:UL:415:LYS:HB3  | 15:UL:417:TRP:NE1  | 2.22                     | 0.54              |
| 16:UM:127:ILE:HG23 | 16:UM:136:ILE:HG23 | 1.90                     | 0.54              |
| 18:UO:288:ASP:O    | 18:UO:291:GLN:HG2  | 2.08                     | 0.54              |
| 21:UR:142:LYS:NZ   | 29:CE:430:ASP:OD2  | 2.41                     | 0.54              |
| 23:UT:461:ILE:HG13 | 23:UT:486:PHE:CZ   | 2.43                     | 0.54              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 23:UT:1057:GLN:HA  | 23:UT:1060:LYS:HG2  | 1.90                     | 0.54              |
| 23:UT:1471:GLU:O   | 23:UT:1517:HIS:NE2  | 2.41                     | 0.54              |
| 29:CE:3:TYR:CG     | 29:CE:14:LEU:HD21   | 2.43                     | 0.54              |
| 29:CE:4:VAL:O      | 29:CE:14:LEU:HA     | 2.07                     | 0.54              |
| 30:CG:28:ALA:HB2   | 30:CG:33:LEU:HD23   | 1.90                     | 0.54              |
| 31:CH:488:ILE:HG13 | 31:CH:524:ILE:HD13  | 1.89                     | 0.54              |
| 35:CL:765:ASN:OD1  | 36:CM:308:ILE:HG12  | 2.08                     | 0.54              |
| 35:CL:769:TYR:HA   | 35:CL:776:GLN:NE2   | 2.23                     | 0.54              |
| 35:CL:824:ILE:HD12 | 35:CL:926:ILE:HG12  | 1.90                     | 0.54              |
| 35:CL:963:GLY:N    | 35:CL:976:ILE:O     | 2.41                     | 0.54              |
| 50:DF:184:PHE:HD2  | 50:DF:185:ARG:HG2   | 1.72                     | 0.54              |
| 65:D2:8:A:C6       | 65:D2:9:G:H1'       | 2.43                     | 0.54              |
| 65:D2:410:A:H2'    | 65:D2:411:A:H8      | 1.72                     | 0.54              |
| 66:D3:65:A:O2'     | 66:D3:67:A:OP1      | 2.21                     | 0.54              |
| 66:D3:144:U:O2'    | 66:D3:145:A:H5'     | 2.08                     | 0.54              |
| 66:D3:503:G:O2'    | 66:D3:504:U:H5'     | 2.07                     | 0.54              |
| 66:D3:1573:A:H4'   | 66:D3:1574:G:O5'    | 2.08                     | 0.54              |
| 66:D3:1644:C:H2'   | 66:D3:1645:G:C8     | 2.42                     | 0.54              |
| 2:DA:50:LYS:HD3    | 2:DA:52:THR:N       | 2.21                     | 0.54              |
| 3:JA:160:GLN:O     | 3:JA:163:THR:OG1    | 2.22                     | 0.54              |
| 7:UD:485:LYS:HD2   | 7:UD:499:ASP:HA     | 1.90                     | 0.54              |
| 10:UG:178:ASP:HB3  | 10:UG:182:THR:HB    | 1.89                     | 0.54              |
| 11:UH:599:MET:HE1  | 11:UH:640:LEU:C     | 2.29                     | 0.54              |
| 13:UJ:119:GLU:HA   | 13:UJ:122:VAL:HG12  | 1.89                     | 0.54              |
| 14:UK:213:GLN:O    | 14:UK:217:ARG:HG2   | 2.06                     | 0.54              |
| 16:UM:630:ASP:HB3  | 16:UM:646:ASP:HB2   | 1.90                     | 0.54              |
| 16:UM:804:TYR:HD2  | 24:UU:928:PHE:HA    | 1.73                     | 0.54              |
| 18:UO:133:HIS:HB3  | 18:UO:136:ASP:O     | 2.07                     | 0.54              |
| 18:UO:164:LEU:HD21 | 18:UO:196:TYR:CG    | 2.43                     | 0.54              |
| 18:UO:232:ASN:HA   | 18:UO:254:ALA:HA    | 1.89                     | 0.54              |
| 21:UR:129:ASP:OD1  | 21:UR:130:ASP:N     | 2.41                     | 0.54              |
| 21:UR:388:HIS:HB2  | 21:UR:395:LEU:HG    | 1.89                     | 0.54              |
| 21:UR:496:ARG:HH11 | 21:UR:496:ARG:HG3   | 1.73                     | 0.54              |
| 22:US:301:ASP:OD2  | 22:US:302:SER:N     | 2.41                     | 0.54              |
| 23:UT:714:ASP:OD2  | 23:UT:715:TYR:N     | 2.40                     | 0.54              |
| 23:UT:1119:TYR:HA  | 23:UT:1122:LEU:HD12 | 1.90                     | 0.54              |
| 23:UT:1636:LEU:HA  | 23:UT:1639:ILE:HG22 | 1.90                     | 0.54              |
| 24:UU:141:LYS:HG3  | 24:UU:154:TYR:HB2   | 1.89                     | 0.54              |
| 27:UZ:41:ASN:HA    | 27:UZ:195:ASN:O     | 2.08                     | 0.54              |
| 28:CD:34:VAL:HG23  | 28:CD:37:GLN:NE2    | 2.23                     | 0.54              |
| 28:CD:297:HIS:NE2  | 28:CD:309:GLU:OE2   | 2.41                     | 0.54              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 29:CE:380:ARG:HG3   | 29:CE:382:ASP:H     | 1.73                     | 0.54              |
| 31:CH:337:VAL:HG11  | 31:CH:407:MET:HG3   | 1.90                     | 0.54              |
| 35:CL:775:GLU:HA    | 35:CL:779:ARG:NH2   | 2.22                     | 0.54              |
| 38:JC:250:GLY:HA2   | 38:JC:274:ILE:HG23  | 1.89                     | 0.54              |
| 45:JN:226:ASP:OD1   | 45:JN:227:LYS:NZ    | 2.41                     | 0.54              |
| 49:DE:182:TYR:CE2   | 49:DE:190:GLY:HA2   | 2.43                     | 0.54              |
| 51:DG:85:ARG:HH22   | 51:DG:87:ARG:NH1    | 2.05                     | 0.54              |
| 56:DN:33:VAL:O      | 56:DN:37:ILE:HG12   | 2.07                     | 0.54              |
| 60:DW:107:SER:OG    | 66:D3:802:G:N2      | 2.41                     | 0.54              |
| 61:DX:90:ASP:O      | 61:DX:93:LEU:HB3    | 2.08                     | 0.54              |
| 65:D2:140:U:H2'     | 65:D2:143:A:H2      | 1.72                     | 0.54              |
| 65:D2:192:G:H2'     | 65:D2:193:G:H8      | 1.72                     | 0.54              |
| 66:D3:97:C:H1'      | 66:D3:426:G:H5'     | 1.90                     | 0.54              |
| 66:D3:647:G:H22     | 66:D3:687:G:H22     | 1.56                     | 0.54              |
| 1:CA:172:TYR:CD1    | 1:CA:175:ALA:HB2    | 2.43                     | 0.53              |
| 1:CB:144:TRP:CD1    | 1:CB:183:HIS:ND1    | 2.76                     | 0.53              |
| 7:UD:45:THR:OG1     | 7:UD:352:VAL:HA     | 2.08                     | 0.53              |
| 8:UE:166:ALA:HB1    | 8:UE:191:VAL:HG21   | 1.90                     | 0.53              |
| 9:UF:60:GLU:OE2     | 9:UF:88:ILE:HG23    | 2.08                     | 0.53              |
| 10:UG:129:GLY:N     | 10:UG:133:HIS:O     | 2.37                     | 0.53              |
| 11:UH:558:CYS:O     | 11:UH:585:ARG:NH1   | 2.41                     | 0.53              |
| 13:UJ:286:LEU:HD11  | 13:UJ:292:LYS:HA    | 1.90                     | 0.53              |
| 13:UJ:699:ARG:HH21  | 13:UJ:744:ASP:HB2   | 1.73                     | 0.53              |
| 13:UJ:1380:LEU:HD22 | 13:UJ:1403:LEU:HD13 | 1.90                     | 0.53              |
| 13:UJ:1418:ASN:OD1  | 13:UJ:1419:ILE:HD12 | 2.08                     | 0.53              |
| 14:UK:14:ARG:NE     | 66:D3:583:C:O2'     | 2.39                     | 0.53              |
| 14:UK:156:SER:HB2   | 65:D2:205:C:O2'     | 2.08                     | 0.53              |
| 18:UO:173:THR:OG1   | 18:UO:216:GLU:O     | 2.25                     | 0.53              |
| 18:UO:365:GLU:HA    | 18:UO:367:GLN:HE22  | 1.73                     | 0.53              |
| 20:UQ:197:ILE:HB    | 20:UQ:211:MET:HE3   | 1.90                     | 0.53              |
| 20:UQ:259:VAL:HA    | 20:UQ:275:PHE:HD1   | 1.73                     | 0.53              |
| 23:UT:327:GLY:N     | 23:UT:368:ASN:OD1   | 2.42                     | 0.53              |
| 23:UT:625:ILE:HD11  | 23:UT:641:ARG:HB2   | 1.89                     | 0.53              |
| 23:UT:1662:SER:O    | 23:UT:1665:LEU:O    | 2.26                     | 0.53              |
| 24:UU:503:ARG:CZ    | 24:UU:503:ARG:HA    | 2.37                     | 0.53              |
| 31:CH:438:ILE:O     | 31:CH:441:GLY:N     | 2.39                     | 0.53              |
| 33:CJ:97:SER:OG     | 33:CJ:144:GLU:OE1   | 2.25                     | 0.53              |
| 35:CL:92:ARG:NH2    | 35:CL:221:LEU:HD11  | 2.16                     | 0.53              |
| 38:JC:256:ASP:HB2   | 38:JC:259:THR:HG22  | 1.90                     | 0.53              |
| 39:JF:116:THR:HG23  | 39:JF:118:ARG:H     | 1.73                     | 0.53              |
| 42:JJ:93:LYS:HB3    | 42:JJ:143:PRO:HB3   | 1.90                     | 0.53              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 54:DJ:127:VAL:O     | 54:DJ:131:GLN:CB    | 2.55                     | 0.53              |
| 55:DL:104:HIS:ND1   | 66:D3:351:C:O2      | 2.41                     | 0.53              |
| 66:D3:823:G:H2'     | 66:D3:824:G:C8      | 2.43                     | 0.53              |
| 66:D3:1603:U:H2'    | 66:D3:1604:U:C6     | 2.36                     | 0.53              |
| 78:EK:136:CYS:CA    | 78:EK:145:PHE:CB    | 2.85                     | 0.53              |
| 2:DA:27:LYS:HD3     | 2:DA:49:ASN:HA      | 1.89                     | 0.53              |
| 7:UD:121:THR:HG23   | 7:UD:138:ASP:OD2    | 2.08                     | 0.53              |
| 7:UD:612:THR:HG22   | 7:UD:614:TRP:H      | 1.73                     | 0.53              |
| 8:UE:154:VAL:HG21   | 8:UE:162:GLN:HG2    | 1.91                     | 0.53              |
| 8:UE:444:ALA:O      | 8:UE:447:SER:C      | 2.46                     | 0.53              |
| 9:UF:342:TRP:HH2    | 9:UF:359:TYR:HA     | 1.73                     | 0.53              |
| 13:UJ:306:LEU:O     | 13:UJ:307:LYS:HD3   | 2.07                     | 0.53              |
| 13:UJ:1652:VAL:O    | 13:UJ:1694:HIS:NE2  | 2.41                     | 0.53              |
| 16:UM:602:TRP:HA    | 16:UM:610:LEU:H     | 1.73                     | 0.53              |
| 20:UQ:207:LEU:HD23  | 20:UQ:229:SER:HA    | 1.89                     | 0.53              |
| 21:UR:351:THR:O     | 21:UR:380:ASN:ND2   | 2.41                     | 0.53              |
| 23:UT:27:LYS:NZ     | 23:UT:32:ARG:HB2    | 2.23                     | 0.53              |
| 23:UT:1113:ALA:HB1  | 23:UT:1157:ILE:HB   | 1.89                     | 0.53              |
| 23:UT:1811:ILE:HG21 | 23:UT:1879:VAL:HG21 | 1.90                     | 0.53              |
| 23:UT:1888:THR:HG22 | 23:UT:1890:SER:H    | 1.73                     | 0.53              |
| 23:UT:1896:ILE:HD13 | 23:UT:1929:GLU:HG2  | 1.89                     | 0.53              |
| 23:UT:2000:PHE:HB3  | 23:UT:2004:LYS:HZ3  | 1.73                     | 0.53              |
| 24:UU:552:HIS:NE2   | 24:UU:554:SER:HB2   | 2.23                     | 0.53              |
| 24:UU:621:ASP:HA    | 24:UU:668:ILE:HD11  | 1.90                     | 0.53              |
| 25:UV:584:GLU:HB3   | 25:UV:614:ARG:HB2   | 1.91                     | 0.53              |
| 27:UZ:150:LEU:HD12  | 27:UZ:151:PRO:HD2   | 1.90                     | 0.53              |
| 28:CD:176:GLN:O     | 28:CD:180:LEU:HD23  | 2.08                     | 0.53              |
| 28:CD:284:TYR:OH    | 29:CE:258:LEU:N     | 2.41                     | 0.53              |
| 28:CD:326:SER:HG    | 28:CD:392:TYR:HE2   | 1.56                     | 0.53              |
| 30:CF:20:ILE:O      | 30:CF:23:VAL:HG12   | 2.08                     | 0.53              |
| 33:CJ:275:TRP:CG    | 33:CJ:276:GLN:N     | 2.76                     | 0.53              |
| 39:JG:167:ILE:H     | 39:JG:167:ILE:HD12  | 1.73                     | 0.53              |
| 47:JP:313:PHE:HE1   | 47:JP:320:ILE:HG12  | 1.71                     | 0.53              |
| 49:DE:42:LEU:HD21   | 49:DE:47:PHE:HB2    | 1.90                     | 0.53              |
| 51:DG:51:LYS:HB3    | 51:DG:112:VAL:HG13  | 1.89                     | 0.53              |
| 53:DI:152:ILE:HD12  | 53:DI:156:VAL:HG23  | 1.89                     | 0.53              |
| 62:DY:12:VAL:HA     | 62:DY:23:PHE:HB3    | 1.90                     | 0.53              |
| 62:DY:51:GLU:OE1    | 62:DY:54:ALA:N      | 2.41                     | 0.53              |
| 65:D2:472:A:H2'     | 65:D2:473:A:H8      | 1.73                     | 0.53              |
| 66:D3:105:A:H62     | 66:D3:308:C:N4      | 2.05                     | 0.53              |
| 66:D3:387:A:N7      | 66:D3:402:C:H5''    | 2.23                     | 0.53              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 66:D3:635:A:H2'     | 66:D3:636:A:H8      | 1.73                     | 0.53              |
| 67:D4:201:C:H2'     | 67:D4:202:G:C8      | 2.43                     | 0.53              |
| 4:UA:778:ILE:O      | 4:UA:782:ILE:HG12   | 2.08                     | 0.53              |
| 7:UD:88:GLU:OE1     | 7:UD:527:TYR:OH     | 2.20                     | 0.53              |
| 7:UD:170:ILE:HG22   | 7:UD:177:LEU:HD21   | 1.90                     | 0.53              |
| 7:UD:338:ALA:HB1    | 7:UD:361:LEU:HD11   | 1.89                     | 0.53              |
| 8:UE:119:CYS:SG     | 8:UE:127:TYR:HB2    | 2.48                     | 0.53              |
| 8:UE:168:HIS:CD2    | 24:UU:646:VAL:HG11  | 2.42                     | 0.53              |
| 10:UG:203:TYR:HE2   | 10:UG:433:LEU:HD23  | 1.74                     | 0.53              |
| 13:UJ:1623:ILE:HD12 | 13:UJ:1626:LEU:HD21 | 1.90                     | 0.53              |
| 14:UK:24:ARG:HG3    | 14:UK:25:TYR:H      | 1.74                     | 0.53              |
| 16:UM:801:GLU:OE1   | 24:UU:930:MET:HB3   | 2.08                     | 0.53              |
| 17:UN:301:ILE:HD12  | 17:UN:897:PRO:HD2   | 1.90                     | 0.53              |
| 18:UO:403:ASN:HA    | 18:UO:406:VAL:HG13  | 1.91                     | 0.53              |
| 18:UO:488:LYS:HZ2   | 18:UO:492:ARG:HG3   | 1.73                     | 0.53              |
| 20:UQ:582:LEU:HD21  | 20:UQ:624:HIS:CE1   | 2.43                     | 0.53              |
| 23:UT:1083:TYR:CE2  | 23:UT:1125:ASP:HB2  | 2.43                     | 0.53              |
| 23:UT:1236:GLN:HG3  | 23:UT:1238:ASN:H    | 1.73                     | 0.53              |
| 23:UT:1606:ILE:O    | 23:UT:1610:MET:HE2  | 2.07                     | 0.53              |
| 25:UV:1227:GLY:HA3  | 25:UV:1231:VAL:HG23 | 1.88                     | 0.53              |
| 29:CE:312:SER:OG    | 29:CE:316:THR:OG1   | 2.24                     | 0.53              |
| 33:CJ:227:ARG:HH11  | 33:CJ:227:ARG:HG3   | 1.72                     | 0.53              |
| 35:CL:769:TYR:HB3   | 35:CL:777:ARG:CZ    | 2.39                     | 0.53              |
| 36:CM:155:LYS:HG3   | 36:CM:164:GLY:HA2   | 1.90                     | 0.53              |
| 36:CM:335:THR:HG22  | 36:CM:354:ILE:HD11  | 1.90                     | 0.53              |
| 42:JJ:186:GLU:HB2   | 42:JJ:189:ASP:HB2   | 1.88                     | 0.53              |
| 49:DE:172:PHE:HE2   | 49:DE:174:LYS:HE3   | 1.74                     | 0.53              |
| 58:DQ:97:VAL:HG12   | 58:DQ:98:ASP:N      | 2.23                     | 0.53              |
| 62:DY:111:LYS:HA    | 62:DY:114:ARG:NE    | 2.24                     | 0.53              |
| 66:D3:328:A:H2'     | 66:D3:329:G:C8      | 2.44                     | 0.53              |
| 66:D3:1208:A:H2'    | 66:D3:1209:C:O4'    | 2.08                     | 0.53              |
| 2:DA:216:LYS:NZ     | 66:D3:885:G:OP1     | 2.36                     | 0.53              |
| 5:UB:573:LEU:HD13   | 5:UB:591:ILE:HG13   | 1.91                     | 0.53              |
| 11:UH:257:SER:C     | 11:UH:259:ILE:H     | 2.08                     | 0.53              |
| 16:UM:129:VAL:HG23  | 16:UM:135:TYR:C     | 2.29                     | 0.53              |
| 23:UT:867:LYS:HD3   | 23:UT:892:LEU:HD22  | 1.91                     | 0.53              |
| 23:UT:1014:ASN:ND2  | 53:DI:114:GLU:HB3   | 2.23                     | 0.53              |
| 23:UT:1277:GLU:HB3  | 23:UT:1280:LEU:HB2  | 1.89                     | 0.53              |
| 24:UU:35:ASN:HD22   | 24:UU:55:GLY:N      | 1.98                     | 0.53              |
| 24:UU:285:HIS:CD2   | 24:UU:339:PRO:HB3   | 2.43                     | 0.53              |
| 25:UV:169:PRO:HA    | 25:UV:172:THR:HG22  | 1.90                     | 0.53              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 25:UV:577:ARG:HA   | 25:UV:623:GLU:HG2   | 1.89                     | 0.53              |
| 25:UV:586:VAL:HB   | 25:UV:612:PHE:O     | 2.09                     | 0.53              |
| 29:CE:230:GLU:O    | 29:CE:234:ARG:HG2   | 2.08                     | 0.53              |
| 35:CL:256:GLU:HA   | 35:CL:259:GLU:CD    | 2.29                     | 0.53              |
| 35:CL:620:LYS:HA   | 35:CL:623:LYS:HG2   | 1.91                     | 0.53              |
| 35:CL:1107:LYS:HD2 | 65:D2:412:A:H5''    | 1.91                     | 0.53              |
| 39:JF:151:ARG:HG3  | 39:JF:158:LYS:HA    | 1.89                     | 0.53              |
| 47:JP:290:ASP:OD2  | 66:D3:-7:A:N6       | 2.37                     | 0.53              |
| 51:DG:85:ARG:HG2   | 51:DG:86:PRO:HD2    | 1.90                     | 0.53              |
| 56:DN:61:THR:HG22  | 56:DN:66:ILE:HD11   | 1.90                     | 0.53              |
| 58:DQ:63:ILE:HG21  | 58:DQ:92:TYR:CE2    | 2.43                     | 0.53              |
| 65:D2:446:U:H2'    | 65:D2:447:G:C8      | 2.44                     | 0.53              |
| 66:D3:473:A:H62    | 66:D3:474:A:H62     | 1.55                     | 0.53              |
| 69:EB:207:GLU:O    | 69:EB:211:LYS:N     | 2.39                     | 0.53              |
| 78:EK:568:VAL:O    | 78:EK:625:SER:HA    | 2.08                     | 0.53              |
| 3:JA:23:ARG:HG2    | 3:JA:145:GLY:H      | 1.73                     | 0.53              |
| 4:UA:54:HIS:ND1    | 4:UA:74:ASP:HB3     | 2.22                     | 0.53              |
| 4:UA:558:ASP:OD2   | 4:UA:611:LEU:HD13   | 2.09                     | 0.53              |
| 7:UD:240:LEU:HD11  | 7:UD:242:TRP:CE2    | 2.43                     | 0.53              |
| 8:UE:523:LEU:HB2   | 8:UE:527:HIS:HE2    | 1.73                     | 0.53              |
| 9:UF:133:TYR:CD2   | 9:UF:150:CYS:HB2    | 2.43                     | 0.53              |
| 11:UH:588:GLN:HG2  | 20:UQ:606:HIS:CD2   | 2.44                     | 0.53              |
| 13:UJ:152:LEU:HD11 | 13:UJ:157:LEU:HD11  | 1.91                     | 0.53              |
| 13:UJ:314:GLN:HG3  | 13:UJ:353:ARG:HB3   | 1.91                     | 0.53              |
| 13:UJ:1533:ASN:O   | 13:UJ:1537:LEU:HG   | 2.08                     | 0.53              |
| 13:UJ:1737:LEU:HG  | 23:UT:31:ALA:HB1    | 1.90                     | 0.53              |
| 15:UL:588:ILE:HG13 | 15:UL:602:LEU:HG    | 1.89                     | 0.53              |
| 23:UT:57:ILE:HA    | 62:DY:21:LYS:HZ3    | 1.74                     | 0.53              |
| 23:UT:1218:SER:O   | 23:UT:1221:ILE:HG12 | 2.08                     | 0.53              |
| 23:UT:1912:ILE:HA  | 23:UT:1958:MET:HE3  | 1.90                     | 0.53              |
| 24:UU:581:LEU:HD23 | 24:UU:612:TRP:CD2   | 2.44                     | 0.53              |
| 25:UV:138:ILE:HD12 | 25:UV:238:HIS:HB3   | 1.91                     | 0.53              |
| 25:UV:858:ARG:HH11 | 25:UV:861:ILE:HD13  | 1.74                     | 0.53              |
| 26:UX:132:HIS:CD2  | 26:UX:140:CYS:SG    | 2.99                     | 0.53              |
| 31:CH:59:PRO:O     | 31:CH:63:ARG:HG3    | 2.07                     | 0.53              |
| 31:CH:155:ASN:OD1  | 31:CH:156:ASN:N     | 2.42                     | 0.53              |
| 35:CL:151:GLU:HG3  | 35:CL:912:ARG:NH2   | 2.21                     | 0.53              |
| 35:CL:948:ILE:HB   | 35:CL:987:TYR:CE2   | 2.44                     | 0.53              |
| 36:CM:291:ARG:HG2  | 36:CM:317:GLN:HG2   | 1.89                     | 0.53              |
| 38:JC:167:LEU:HD23 | 43:JK:476:GLU:HB3   | 1.90                     | 0.53              |
| 38:JC:276:LYS:HG3  | 38:JC:278:ILE:HG12  | 1.90                     | 0.53              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 65:D2:266:U:H4'     | 65:D2:267:U:H2'     | 1.88                     | 0.53              |
| 66:D3:144:U:H3      | 66:D3:171:A:H61     | 1.57                     | 0.53              |
| 66:D3:539:G:H1'     | 66:D3:540:G:C2      | 2.44                     | 0.53              |
| 66:D3:1510:U:H2'    | 66:D3:1511:U:O4'    | 2.08                     | 0.53              |
| 71:ED:40:ARG:N      | 71:ED:44:ARG:O      | 2.40                     | 0.53              |
| 2:DA:117:TRP:CZ3    | 2:DA:152:ARG:HD3    | 2.44                     | 0.53              |
| 4:UA:114:ALA:HB2    | 4:UA:152:LEU:HD11   | 1.91                     | 0.53              |
| 4:UA:473:GLU:O      | 4:UA:494:ASP:HB2    | 2.09                     | 0.53              |
| 8:UE:438:THR:OG1    | 8:UE:468:THR:HA     | 2.08                     | 0.53              |
| 8:UE:495:GLN:O      | 8:UE:499:ASN:N      | 2.36                     | 0.53              |
| 8:UE:514:VAL:HG13   | 18:UO:511:LEU:HD12  | 1.91                     | 0.53              |
| 9:UF:41:HIS:NE2     | 47:JP:21:GLU:O      | 2.40                     | 0.53              |
| 11:UH:667:GLU:HA    | 11:UH:670:GLU:OE2   | 2.09                     | 0.53              |
| 13:UJ:1445:ILE:HD12 | 13:UJ:1483:SER:HB2  | 1.91                     | 0.53              |
| 15:UL:140:SER:OG    | 15:UL:142:ASP:OD1   | 2.26                     | 0.53              |
| 16:UM:336:ASN:OD1   | 16:UM:337:HIS:N     | 2.42                     | 0.53              |
| 18:UO:257:CYS:SG    | 18:UO:305:CYS:N     | 2.77                     | 0.53              |
| 20:UQ:447:LYS:NZ    | 20:UQ:769:ASN:OD1   | 2.23                     | 0.53              |
| 22:US:317:ILE:HG23  | 22:US:358:PHE:CD1   | 2.44                     | 0.53              |
| 23:UT:670:LEU:HD11  | 23:UT:777:GLN:HB3   | 1.90                     | 0.53              |
| 23:UT:1477:LYS:HD2  | 23:UT:1480:SER:H    | 1.72                     | 0.53              |
| 23:UT:1515:ALA:HB3  | 23:UT:1554:PRO:HG2  | 1.89                     | 0.53              |
| 23:UT:1701:MET:HG3  | 23:UT:1705:LEU:HD23 | 1.90                     | 0.53              |
| 25:UV:100:SER:O     | 25:UV:104:LYS:HG2   | 2.09                     | 0.53              |
| 25:UV:258:TYR:HA    | 25:UV:266:PRO:HA    | 1.90                     | 0.53              |
| 25:UV:1160:SER:HA   | 25:UV:1187:LYS:HD2  | 1.90                     | 0.53              |
| 28:CD:25:ASP:OD1    | 28:CD:25:ASP:N      | 2.39                     | 0.53              |
| 31:CH:171:THR:HG22  | 31:CH:173:GLU:OE1   | 2.08                     | 0.53              |
| 35:CL:553:ILE:HG12  | 36:CM:323:ILE:HD12  | 1.91                     | 0.53              |
| 37:CN:86:GLU:H      | 37:CN:127:LYS:HB3   | 1.73                     | 0.53              |
| 38:JC:141:GLY:HA2   | 38:JC:157:ALA:HA    | 1.91                     | 0.53              |
| 39:JF:115:GLN:HE21  | 39:JF:119:GLY:HA2   | 1.74                     | 0.53              |
| 49:DE:238:LEU:HD23  | 49:DE:242:LYS:HA    | 1.90                     | 0.53              |
| 56:DN:38:VAL:O      | 56:DN:42:ARG:HG2    | 2.09                     | 0.53              |
| 56:DN:124:ARG:HH21  | 66:D3:628:G:P       | 2.31                     | 0.53              |
| 61:DX:134:ALA:HB1   | 61:DX:139:LYS:HB2   | 1.91                     | 0.53              |
| 66:D3:891:A:H2'     | 66:D3:892:A:C8      | 2.42                     | 0.53              |
| 66:D3:1706:C:H2'    | 66:D3:1707:A:C8     | 2.43                     | 0.53              |
| 1:CA:287:ALA:HA     | 26:UX:148:HIS:CE1   | 2.43                     | 0.53              |
| 4:UA:420:ARG:HG3    | 34:CK:468:ARG:NH1   | 2.24                     | 0.53              |
| 9:UF:57:ILE:HG21    | 9:UF:96:TYR:OH      | 2.09                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:UI:445:PRO:HG2  | 12:UI:446:TRP:CD1  | 2.44                     | 0.53              |
| 14:UK:165:ARG:NH1  | 19:UP:176:PHE:HZ   | 2.06                     | 0.53              |
| 15:UL:449:THR:OG1  | 15:UL:451:ASN:O    | 2.24                     | 0.53              |
| 16:UM:97:ARG:HD3   | 16:UM:134:GLY:H    | 1.74                     | 0.53              |
| 16:UM:151:LYS:O    | 16:UM:163:LEU:HD12 | 2.09                     | 0.53              |
| 16:UM:239:VAL:HG12 | 16:UM:241:GLN:HG2  | 1.90                     | 0.53              |
| 18:UO:488:LYS:HA   | 18:UO:491:VAL:HG22 | 1.91                     | 0.53              |
| 20:UQ:296:HIS:CE1  | 20:UQ:314:SER:HG   | 2.26                     | 0.53              |
| 23:UT:280:MET:SD   | 23:UT:281:ASN:ND2  | 2.81                     | 0.53              |
| 25:UV:369:TRP:HE3  | 25:UV:370:LEU:HD22 | 1.73                     | 0.53              |
| 25:UV:469:ASP:OD1  | 25:UV:471:SER:OG   | 2.25                     | 0.53              |
| 32:CI:83:TYR:O     | 32:CI:86:GLY:N     | 2.39                     | 0.53              |
| 37:CN:261:GLN:O    | 37:CN:265:ARG:HG2  | 2.09                     | 0.53              |
| 38:JC:202:ASN:HD21 | 38:JC:228:PRO:HA   | 1.73                     | 0.53              |
| 38:JC:227:ARG:HE   | 38:JC:230:GLN:HE22 | 1.53                     | 0.53              |
| 39:JG:114:ILE:HB   | 39:JG:122:ILE:HB   | 1.91                     | 0.53              |
| 47:JP:460:GLN:OE1  | 47:JP:460:GLN:N    | 2.34                     | 0.53              |
| 50:DF:53:VAL:CG2   | 50:DF:59:VAL:HA    | 2.39                     | 0.53              |
| 51:DG:56:ASN:HD22  | 66:D3:154:G:H1'    | 1.73                     | 0.53              |
| 51:DG:174:LYS:HG2  | 66:D3:78:A:C2      | 2.44                     | 0.53              |
| 55:DL:57:LYS:HD3   | 55:DL:131:ILE:HG21 | 1.91                     | 0.53              |
| 62:DY:81:GLU:HA    | 62:DY:84:LYS:HG2   | 1.91                     | 0.53              |
| 65:D2:426:G:N3     | 65:D2:428:A:H5''   | 2.24                     | 0.53              |
| 66:D3:450:U:H2'    | 66:D3:451:A:C8     | 2.44                     | 0.53              |
| 66:D3:568:G:C2     | 66:D3:569:C:N3     | 2.77                     | 0.53              |
| 66:D3:1063:U:O2'   | 66:D3:1064:G:O5'   | 2.24                     | 0.53              |
| 66:D3:1704:U:H2'   | 66:D3:1705:C:C6    | 2.44                     | 0.53              |
| 67:D4:172:U:H2'    | 67:D4:173:A:C8     | 2.44                     | 0.53              |
| 79:EN:489:ILE:O    | 79:EN:493:GLU:N    | 2.40                     | 0.53              |
| 3:JA:112:GLU:HG3   | 3:JA:137:ARG:HH22  | 1.73                     | 0.53              |
| 4:UA:617:VAL:HG11  | 4:UA:681:VAL:HG21  | 1.91                     | 0.53              |
| 5:UB:675:TYR:HB3   | 5:UB:677:ASP:OD1   | 2.09                     | 0.53              |
| 7:UD:590:LYS:HD2   | 7:UD:592:TYR:CZ    | 2.44                     | 0.53              |
| 10:UG:230:THR:HG22 | 10:UG:259:TRP:CZ2  | 2.43                     | 0.53              |
| 13:UJ:259:THR:O    | 13:UJ:262:VAL:HG12 | 2.09                     | 0.53              |
| 14:UK:58:ARG:NH2   | 35:CL:1076:GLU:OE1 | 2.42                     | 0.53              |
| 14:UK:220:ALA:O    | 14:UK:224:LEU:HG   | 2.09                     | 0.53              |
| 15:UL:129:PHE:HA   | 15:UL:135:ARG:O    | 2.08                     | 0.53              |
| 16:UM:15:ILE:HD11  | 16:UM:43:ILE:HD11  | 1.90                     | 0.53              |
| 16:UM:16:TYR:CE2   | 16:UM:35:PRO:HD2   | 2.44                     | 0.53              |
| 16:UM:64:ILE:HA    | 16:UM:80:SER:HA    | 1.91                     | 0.53              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 16:UM:494:ILE:HA   | 16:UM:510:SER:HB2   | 1.91                     | 0.53              |
| 16:UM:518:TRP:HA   | 16:UM:526:GLU:H     | 1.73                     | 0.53              |
| 18:UO:51:HIS:O     | 18:UO:53:HIS:N      | 2.41                     | 0.53              |
| 22:US:509:ALA:O    | 22:US:512:SER:OG    | 2.26                     | 0.53              |
| 23:UT:13:ARG:HH12  | 62:DY:84:LYS:C      | 2.12                     | 0.53              |
| 23:UT:294:VAL:HA   | 23:UT:297:VAL:HG22  | 1.91                     | 0.53              |
| 23:UT:558:TRP:CD1  | 23:UT:561:LEU:HD12  | 2.44                     | 0.53              |
| 23:UT:1502:ASN:HA  | 23:UT:1505:ASN:ND2  | 2.24                     | 0.53              |
| 23:UT:1524:LYS:HE3 | 23:UT:1590:LEU:HD11 | 1.91                     | 0.53              |
| 23:UT:1537:LYS:HG3 | 23:UT:1541:MET:HE1  | 1.90                     | 0.53              |
| 24:UU:459:ASP:OD2  | 24:UU:483:SER:OG    | 2.26                     | 0.53              |
| 25:UV:961:VAL:O    | 25:UV:965:ILE:HG12  | 2.08                     | 0.53              |
| 27:UZ:110:PHE:CD2  | 27:UZ:118:LEU:HD11  | 2.44                     | 0.53              |
| 29:CE:21:LYS:O     | 29:CE:25:SER:OG     | 2.22                     | 0.53              |
| 35:CL:892:PRO:HB3  | 35:CL:920:GLU:O     | 2.09                     | 0.53              |
| 36:CM:200:VAL:HG12 | 36:CM:201:SER:N     | 2.22                     | 0.53              |
| 38:JC:154:TYR:OH   | 38:JC:188:ILE:HB    | 2.08                     | 0.53              |
| 49:DE:175:PHE:HE2  | 49:DE:198:LYS:HD2   | 1.74                     | 0.53              |
| 50:DF:157:ARG:HB2  | 50:DF:224:ASN:ND2   | 2.23                     | 0.53              |
| 65:D2:407:A:C6     | 65:D2:450:G:N2      | 2.77                     | 0.53              |
| 66:D3:290:G:H2'    | 66:D3:291:G:C8      | 2.44                     | 0.53              |
| 66:D3:480:G:H22    | 66:D3:509:G:H1'     | 1.74                     | 0.53              |
| 66:D3:1066:C:H2'   | 66:D3:1067:C:C6     | 2.44                     | 0.53              |
| 66:D3:1542:G:N7    | 66:D3:1569:A:N6     | 2.54                     | 0.53              |
| 66:D3:1621:U:H2'   | 66:D3:1622:G:C8     | 2.44                     | 0.53              |
| 3:JA:896:ASP:O     | 3:JA:900:LYS:HG2    | 2.08                     | 0.53              |
| 5:UB:515:HIS:CE1   | 5:UB:517:VAL:HG22   | 2.44                     | 0.53              |
| 7:UD:455:PRO:HA    | 7:UD:460:LEU:HG     | 1.90                     | 0.53              |
| 8:UE:121:ASP:OD2   | 8:UE:123:SER:OG     | 2.25                     | 0.53              |
| 9:UF:278:MET:CE    | 9:UF:316:SER:HB3    | 2.39                     | 0.53              |
| 13:UJ:135:LEU:HD21 | 13:UJ:151:ILE:HD11  | 1.90                     | 0.53              |
| 15:UL:262:ILE:HB   | 15:UL:343:TRP:CD1   | 2.43                     | 0.53              |
| 16:UM:719:ILE:O    | 16:UM:758:ARG:NH2   | 2.41                     | 0.53              |
| 16:UM:757:GLN:HA   | 16:UM:760:ILE:HG22  | 1.91                     | 0.53              |
| 17:UN:309:ASP:O    | 17:UN:310:HIS:ND1   | 2.41                     | 0.53              |
| 20:UQ:375:ASN:ND2  | 21:UR:340:GLU:OE2   | 2.38                     | 0.53              |
| 20:UQ:631:GLN:HG2  | 20:UQ:652:GLU:HG2   | 1.91                     | 0.53              |
| 20:UQ:868:ASN:OD1  | 20:UQ:871:SER:HB2   | 2.09                     | 0.53              |
| 22:US:498:PHE:HA   | 22:US:501:TRP:HE1   | 1.74                     | 0.53              |
| 23:UT:237:THR:O    | 23:UT:241:THR:HG22  | 2.09                     | 0.53              |
| 23:UT:726:LYS:HE3  | 23:UT:729:TRP:HA    | 1.89                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:UU:530:ASP:HB2  | 24:UU:537:LEU:HD21 | 1.90                     | 0.53              |
| 29:CE:302:HIS:CG   | 29:CE:320:LEU:HD21 | 2.44                     | 0.53              |
| 31:CH:457:GLU:HA   | 31:CH:460:ARG:HG3  | 1.91                     | 0.53              |
| 31:CH:488:ILE:HG21 | 31:CH:524:ILE:HG21 | 1.90                     | 0.53              |
| 35:CL:114:ARG:NH1  | 35:CL:306:ASP:OD2  | 2.35                     | 0.53              |
| 35:CL:275:LEU:O    | 35:CL:276:HIS:ND1  | 2.42                     | 0.53              |
| 44:JM:132:PRO:HD3  | 44:JM:186:TYR:CE2  | 2.43                     | 0.53              |
| 46:JO:258:ARG:NH1  | 56:DN:127:ARG:HH22 | 2.07                     | 0.53              |
| 46:JO:261:ASP:O    | 46:JO:265:GLU:HG2  | 2.09                     | 0.53              |
| 47:JP:112:LEU:H    | 47:JP:112:LEU:HD12 | 1.74                     | 0.53              |
| 50:DF:207:THR:HA   | 50:DF:212:LYS:NZ   | 2.24                     | 0.53              |
| 51:DG:31:ARG:NH2   | 51:DG:66:GLY:H     | 2.06                     | 0.53              |
| 65:D2:6:A:N6       | 65:D2:8:A:N3       | 2.57                     | 0.53              |
| 66:D3:628:G:N1     | 66:D3:970:A:OP2    | 2.33                     | 0.53              |
| 66:D3:950:C:H2'    | 66:D3:951:A:C8     | 2.44                     | 0.53              |
| 75:EH:204:THR:O    | 75:EH:208:TYR:N    | 2.41                     | 0.53              |
| 79:EN:771:GLY:HA2  | 79:EN:807:VAL:HA   | 1.91                     | 0.53              |
| 3:JA:722:TYR:HB2   | 3:JA:763:LEU:HD11  | 1.91                     | 0.53              |
| 3:JA:748:ARG:NE    | 3:JA:759:THR:H     | 2.07                     | 0.53              |
| 8:UE:191:VAL:HG12  | 8:UE:206:ALA:HB2   | 1.90                     | 0.53              |
| 9:UF:168:PHE:O     | 9:UF:172:LEU:HD23  | 2.08                     | 0.53              |
| 10:UG:141:LYS:HE2  | 13:UJ:20:LEU:HD22  | 1.91                     | 0.53              |
| 10:UG:246:VAL:HG13 | 10:UG:248:HIS:HE1  | 1.74                     | 0.53              |
| 10:UG:430:VAL:HG11 | 32:CI:3:ARG:HH21   | 1.73                     | 0.53              |
| 11:UH:655:LEU:O    | 11:UH:659:THR:HG23 | 2.08                     | 0.53              |
| 13:UJ:16:ALA:O     | 13:UJ:24:ARG:NH2   | 2.42                     | 0.53              |
| 13:UJ:44:ASP:OD1   | 47:JP:17:LYS:HB3   | 2.09                     | 0.53              |
| 16:UM:40:ILE:HD11  | 16:UM:64:ILE:HG12  | 1.91                     | 0.53              |
| 16:UM:347:GLY:HA2  | 16:UM:417:TYR:HE1  | 1.74                     | 0.53              |
| 16:UM:522:ASN:HB3  | 16:UM:524:GLU:HG2  | 1.91                     | 0.53              |
| 17:UN:859:ARG:HA   | 17:UN:862:ARG:HG3  | 1.91                     | 0.53              |
| 18:UO:23:GLU:OE1   | 18:UO:23:GLU:N     | 2.24                     | 0.53              |
| 20:UQ:66:LEU:HD22  | 20:UQ:125:LEU:HD11 | 1.90                     | 0.53              |
| 20:UQ:372:LEU:HD23 | 20:UQ:384:SER:HA   | 1.92                     | 0.53              |
| 22:US:298:PHE:HA   | 22:US:301:ASP:OD1  | 2.09                     | 0.53              |
| 23:UT:41:TYR:CD2   | 23:UT:42:VAL:HG23  | 2.44                     | 0.53              |
| 23:UT:356:ASP:HB3  | 23:UT:747:TRP:CZ3  | 2.44                     | 0.53              |
| 23:UT:398:GLN:NE2  | 23:UT:746:ILE:HG21 | 2.23                     | 0.53              |
| 25:UV:376:SER:O    | 25:UV:388:PHE:N    | 2.42                     | 0.53              |
| 33:CJ:93:SER:OG    | 33:CJ:94:ARG:N     | 2.42                     | 0.53              |
| 34:CK:317:GLU:OE2  | 35:CL:1012:LYS:NZ  | 2.42                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:CK:507:ILE:HG13 | 34:CK:515:MET:HB2  | 1.90                     | 0.53              |
| 34:CK:530:ARG:NH1  | 66:D3:1643:U:OP2   | 2.42                     | 0.53              |
| 35:CL:56:VAL:HG23  | 61:DX:101:GLU:HG3  | 1.90                     | 0.53              |
| 37:CN:17:PRO:HB3   | 37:CN:34:LEU:HD12  | 1.91                     | 0.53              |
| 37:CN:180:LEU:O    | 37:CN:184:ILE:HG12 | 2.09                     | 0.53              |
| 39:JG:96:LEU:HG    | 39:JG:130:ILE:HD11 | 1.90                     | 0.53              |
| 47:JP:225:LEU:O    | 47:JP:226:LYS:HG3  | 2.09                     | 0.53              |
| 49:DE:64:ILE:HD13  | 62:DY:17:LEU:HD13  | 1.91                     | 0.53              |
| 54:DJ:7:THR:OG1    | 54:DJ:8:TYR:N      | 2.41                     | 0.53              |
| 65:D2:114:G:H2'    | 65:D2:115:G:H8     | 1.74                     | 0.53              |
| 65:D2:134:A:H2'    | 65:D2:135:G:C8     | 2.44                     | 0.53              |
| 4:UA:64:ASN:OD1    | 4:UA:65:LYS:N      | 2.42                     | 0.52              |
| 6:UC:538:ARG:HD2   | 35:CL:908:GLY:O    | 2.09                     | 0.52              |
| 6:UC:588:SER:O     | 30:CG:46:ARG:NH2   | 2.40                     | 0.52              |
| 8:UE:461:ASP:OD2   | 8:UE:464:VAL:N     | 2.36                     | 0.52              |
| 10:UG:531:HIS:CE1  | 65:D2:364:A:H2'    | 2.44                     | 0.52              |
| 11:UH:232:VAL:N    | 11:UH:237:GLN:O    | 2.42                     | 0.52              |
| 16:UM:522:ASN:OD1  | 16:UM:523:GLY:N    | 2.42                     | 0.52              |
| 16:UM:563:ASP:OD1  | 16:UM:564:THR:N    | 2.37                     | 0.52              |
| 16:UM:596:ASP:HB3  | 16:UM:598:LEU:HD22 | 1.90                     | 0.52              |
| 17:UN:832:ASN:HD21 | 17:UN:834:LYS:HZ3  | 1.57                     | 0.52              |
| 20:UQ:670:LEU:HB2  | 20:UQ:683:LEU:HD21 | 1.90                     | 0.52              |
| 23:UT:633:GLN:HA   | 51:DG:130:PRO:HB3  | 1.90                     | 0.52              |
| 23:UT:1897:PRO:HA  | 23:UT:1900:ARG:HE  | 1.74                     | 0.52              |
| 25:UV:132:TYR:O    | 25:UV:135:LEU:HG   | 2.09                     | 0.52              |
| 25:UV:422:PHE:O    | 25:UV:426:ILE:HG12 | 2.09                     | 0.52              |
| 25:UV:469:ASP:HB3  | 25:UV:474:VAL:HG22 | 1.91                     | 0.52              |
| 25:UV:941:PRO:HG2  | 25:UV:961:VAL:HG22 | 1.91                     | 0.52              |
| 27:UZ:73:LEU:HB2   | 27:UZ:122:PHE:CD2  | 2.44                     | 0.52              |
| 29:CE:310:ALA:HB1  | 29:CE:372:ARG:HG2  | 1.91                     | 0.52              |
| 31:CH:497:LYS:HG2  | 31:CH:513:GLU:OE1  | 2.08                     | 0.52              |
| 35:CL:548:ASN:O    | 35:CL:552:LEU:HG   | 2.09                     | 0.52              |
| 36:CM:52:PHE:CE1   | 36:CM:102:PRO:HG3  | 2.38                     | 0.52              |
| 36:CM:181:HIS:CE1  | 36:CM:309:GLY:HA2  | 2.43                     | 0.52              |
| 36:CM:220:GLN:NE2  | 36:CM:221:CYS:SG   | 2.82                     | 0.52              |
| 36:CM:245:LEU:HD12 | 36:CM:275:VAL:HG12 | 1.89                     | 0.52              |
| 36:CM:290:GLY:H    | 36:CM:293:GLN:NE2  | 2.07                     | 0.52              |
| 47:JP:205:ASP:HB2  | 47:JP:212:VAL:HG21 | 1.91                     | 0.52              |
| 47:JP:327:LYS:CE   | 47:JP:349:GLN:HA   | 2.39                     | 0.52              |
| 54:DJ:110:GLN:HG3  | 54:DJ:111:THR:N    | 2.24                     | 0.52              |
| 65:D2:145:A:H2'    | 65:D2:146:G:C8     | 2.44                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 66:D3:428:A:O2'    | 66:D3:439:U:O2'    | 2.27                     | 0.52              |
| 66:D3:1204:A:O2'   | 66:D3:1208:A:N3    | 2.34                     | 0.52              |
| 66:D3:1599:C:H2'   | 66:D3:1600:A:N7    | 2.23                     | 0.52              |
| 72:EE:139:ILE:HA   | 72:EE:157:SER:HA   | 1.90                     | 0.52              |
| 1:CA:236:MET:HE2   | 28:CD:132:ARG:HG2  | 1.91                     | 0.52              |
| 3:JA:34:ARG:HB3    | 3:JA:94:PHE:CG     | 2.44                     | 0.52              |
| 3:JA:52:ASN:OD1    | 3:JA:53:LYS:N      | 2.42                     | 0.52              |
| 3:JA:752:ASN:OD1   | 3:JA:755:THR:N     | 2.30                     | 0.52              |
| 4:UA:344:HIS:CE1   | 4:UA:370:LYS:HD2   | 2.44                     | 0.52              |
| 4:UA:515:TYR:CD1   | 58:DQ:118:ILE:HD11 | 2.44                     | 0.52              |
| 4:UA:576:ARG:HH12  | 32:CI:144:ASN:HB2  | 1.73                     | 0.52              |
| 7:UD:354:LYS:HB2   | 7:UD:374:THR:HG22  | 1.91                     | 0.52              |
| 7:UD:451:PHE:CE2   | 7:UD:464:LYS:HG2   | 2.45                     | 0.52              |
| 8:UE:162:GLN:HB2   | 8:UE:172:LEU:HD11  | 1.90                     | 0.52              |
| 11:UH:592:ARG:HH12 | 20:UQ:603:ASN:HB2  | 1.74                     | 0.52              |
| 21:UR:410:ASP:OD2  | 21:UR:411:TYR:N    | 2.43                     | 0.52              |
| 23:UT:431:LYS:NZ   | 23:UT:750:TYR:HB3  | 2.24                     | 0.52              |
| 23:UT:1803:ASN:OD1 | 23:UT:1804:SER:N   | 2.43                     | 0.52              |
| 24:UU:639:ASP:OD1  | 24:UU:640:LEU:N    | 2.42                     | 0.52              |
| 25:UV:486:GLN:HB3  | 25:UV:580:TYR:CE1  | 2.44                     | 0.52              |
| 25:UV:894:ARG:NH1  | 25:UV:894:ARG:HB2  | 2.24                     | 0.52              |
| 27:UZ:76:THR:OG1   | 27:UZ:77:LYS:O     | 2.28                     | 0.52              |
| 29:CE:5:LEU:HD11   | 29:CE:89:VAL:HG23  | 1.90                     | 0.52              |
| 31:CH:284:LEU:HD13 | 31:CH:300:ALA:HB2  | 1.91                     | 0.52              |
| 34:CK:493:GLN:HE22 | 66:D3:1633:A:H5'   | 1.73                     | 0.52              |
| 35:CL:1118:THR:HG1 | 65:D2:445:U:HO2'   | 1.57                     | 0.52              |
| 39:JF:77:LEU:HA    | 39:JF:80:MET:SD    | 2.49                     | 0.52              |
| 39:JF:90:ASP:O     | 39:JF:93:HIS:N     | 2.42                     | 0.52              |
| 39:JG:91:ILE:HG13  | 39:JG:92:THR:N     | 2.24                     | 0.52              |
| 46:JO:212:ARG:HB2  | 46:JO:214:GLU:OE1  | 2.09                     | 0.52              |
| 52:DH:31:SER:HB2   | 52:DH:34:LEU:HB3   | 1.89                     | 0.52              |
| 52:DH:141:ARG:HD3  | 52:DH:143:LEU:HD21 | 1.90                     | 0.52              |
| 55:DL:140:VAL:HG22 | 55:DL:141:LYS:HD3  | 1.90                     | 0.52              |
| 66:D3:1649:G:H2'   | 66:D3:1650:U:C6    | 2.45                     | 0.52              |
| 79:EN:87:GLN:N     | 79:EN:119:VAL:O    | 2.38                     | 0.52              |
| 2:DA:11:LYS:HG3    | 2:DA:12:GLY:H      | 1.73                     | 0.52              |
| 3:JA:727:TYR:O     | 3:JA:759:THR:OG1   | 2.17                     | 0.52              |
| 4:UA:7:PHE:HE2     | 4:UA:702:LEU:HD23  | 1.73                     | 0.52              |
| 4:UA:82:VAL:HG13   | 4:UA:88:ASN:O      | 2.08                     | 0.52              |
| 4:UA:518:VAL:HG23  | 4:UA:518:VAL:O     | 2.08                     | 0.52              |
| 1:CB:170:VAL:HA    | 1:CB:239:CYS:O     | 2.10                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CB:281:ASP:O     | 1:CB:284:THR:OG1   | 2.20                     | 0.52              |
| 5:UB:422:LEU:HD22  | 5:UB:466:TYR:HD2   | 1.72                     | 0.52              |
| 5:UB:651:TRP:O     | 5:UB:657:PHE:HB2   | 2.09                     | 0.52              |
| 7:UD:185:ARG:HH22  | 30:CF:126:ILE:HG22 | 1.74                     | 0.52              |
| 7:UD:427:ASN:HB2   | 7:UD:444:ARG:HD3   | 1.91                     | 0.52              |
| 7:UD:552:ILE:HG12  | 7:UD:563:LEU:HD11  | 1.91                     | 0.52              |
| 8:UE:435:GLY:HA2   | 22:US:298:PHE:HZ   | 1.73                     | 0.52              |
| 9:UF:318:ARG:HA    | 9:UF:321:LYS:NZ    | 2.24                     | 0.52              |
| 12:UI:498:GLY:HA3  | 18:UO:502:GLN:HE22 | 1.74                     | 0.52              |
| 13:UJ:753:ALA:HB1  | 13:UJ:791:VAL:HG11 | 1.91                     | 0.52              |
| 13:UJ:1418:ASN:OD1 | 13:UJ:1419:ILE:N   | 2.42                     | 0.52              |
| 13:UJ:1450:LEU:N   | 13:UJ:1452:GLU:OE2 | 2.43                     | 0.52              |
| 15:UL:232:ASP:OD1  | 15:UL:233:ILE:N    | 2.37                     | 0.52              |
| 20:UQ:714:ASP:N    | 20:UQ:718:GLY:O    | 2.41                     | 0.52              |
| 23:UT:340:ILE:HA   | 23:UT:343:ILE:HD12 | 1.91                     | 0.52              |
| 23:UT:374:LEU:HB3  | 23:UT:411:PHE:CZ   | 2.44                     | 0.52              |
| 23:UT:1148:GLY:O   | 23:UT:1151:ILE:N   | 2.42                     | 0.52              |
| 23:UT:1707:HIS:NE2 | 23:UT:1805:ASP:HB2 | 2.24                     | 0.52              |
| 29:CE:213:GLY:HA3  | 29:CE:252:LEU:HD21 | 1.90                     | 0.52              |
| 34:CK:297:LEU:HD23 | 34:CK:297:LEU:H    | 1.74                     | 0.52              |
| 35:CL:292:GLY:O    | 35:CL:1022:LEU:HG  | 2.09                     | 0.52              |
| 38:JC:14:TYR:HE2   | 38:JC:344:PRO:HG3  | 1.74                     | 0.52              |
| 38:JC:254:ILE:O    | 38:JC:263:SER:N    | 2.42                     | 0.52              |
| 39:JF:240:LYS:O    | 39:JG:243:HIS:HE1  | 1.93                     | 0.52              |
| 42:JJ:213:LYS:O    | 42:JJ:217:GLU:HG2  | 2.08                     | 0.52              |
| 47:JP:15:PRO:HB3   | 47:JP:20:GLN:NE2   | 2.24                     | 0.52              |
| 49:DE:38:LEU:CD1   | 49:DE:39:ARG:HG2   | 2.40                     | 0.52              |
| 50:DF:134:VAL:O    | 50:DF:138:THR:HG23 | 2.09                     | 0.52              |
| 66:D3:550:A:C6     | 66:D3:551:G:N7     | 2.78                     | 0.52              |
| 66:D3:1130:G:C6    | 66:D3:1131:A:C6    | 2.97                     | 0.52              |
| 67:D4:77:U:H2'     | 67:D4:78:G:C8      | 2.44                     | 0.52              |
| 73:EF:242:HIS:O    | 73:EF:246:GLN:N    | 2.41                     | 0.52              |
| 77:EJ:46:TYR:N     | 77:EJ:53:LEU:O     | 2.42                     | 0.52              |
| 78:EK:910:ASN:O    | 78:EK:911:GLU:CB   | 2.58                     | 0.52              |
| 2:DA:187:LYS:HE2   | 25:UV:752:SER:OG   | 2.10                     | 0.52              |
| 2:DA:216:LYS:NZ    | 66:D3:886:U:OP2    | 2.42                     | 0.52              |
| 3:JA:78:LYS:O      | 3:JA:82:LYS:HG2    | 2.10                     | 0.52              |
| 3:JA:476:TYR:HE2   | 3:JA:480:ASP:HB2   | 1.75                     | 0.52              |
| 4:UA:323:LYS:O     | 4:UA:324:LEU:HB2   | 2.08                     | 0.52              |
| 6:UC:557:ASP:O     | 6:UC:560:ASN:C     | 2.48                     | 0.52              |
| 13:UJ:106:SER:O    | 13:UJ:206:TYR:OH   | 2.22                     | 0.52              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 13:UJ:1361:VAL:HG22 | 13:UJ:1365:LYS:HE3 | 1.91                     | 0.52              |
| 18:UO:95:LEU:HA     | 18:UO:109:ASP:HA   | 1.90                     | 0.52              |
| 20:UQ:340:ILE:O     | 20:UQ:358:LEU:HA   | 2.08                     | 0.52              |
| 21:UR:269:ASP:O     | 21:UR:271:THR:HG23 | 2.08                     | 0.52              |
| 21:UR:288:LEU:HD21  | 21:UR:339:ILE:HG21 | 1.90                     | 0.52              |
| 23:UT:636:ARG:NH1   | 51:DG:129:VAL:O    | 2.33                     | 0.52              |
| 25:UV:516:SER:OG    | 25:UV:522:LYS:NZ   | 2.30                     | 0.52              |
| 27:UZ:229:ARG:HD3   | 27:UZ:233:GLY:HA3  | 1.91                     | 0.52              |
| 28:CD:171:ASP:OD2   | 28:CD:321:SER:OG   | 2.25                     | 0.52              |
| 38:JC:48:GLU:OE2    | 38:JC:50:ILE:N     | 2.42                     | 0.52              |
| 39:JG:90:ASP:HB3    | 39:JG:94:GLN:HE22  | 1.74                     | 0.52              |
| 47:JP:121:PRO:HD3   | 47:JP:135:PHE:CD1  | 2.45                     | 0.52              |
| 53:DI:36:THR:OG1    | 53:DI:57:ALA:O     | 2.27                     | 0.52              |
| 54:DJ:135:ALA:HB1   | 54:DJ:139:GLN:O    | 2.10                     | 0.52              |
| 66:D3:242:U:H2'     | 66:D3:243:G:C8     | 2.45                     | 0.52              |
| 66:D3:269:G:C6      | 66:D3:287:G:C6     | 2.98                     | 0.52              |
| 66:D3:491:C:H2'     | 66:D3:492:A:C8     | 2.44                     | 0.52              |
| 69:EB:40:PHE:HA     | 69:EB:47:VAL:HA    | 1.92                     | 0.52              |
| 1:CA:195:TYR:CD2    | 1:CA:234:ILE:HD12  | 2.45                     | 0.52              |
| 3:JA:494:VAL:HG23   | 3:JA:539:ALA:HB1   | 1.91                     | 0.52              |
| 5:UB:574:THR:HB     | 5:UB:593:LEU:HD12  | 1.92                     | 0.52              |
| 8:UE:544:ASP:OD2    | 18:UO:488:LYS:NZ   | 2.42                     | 0.52              |
| 9:UF:113:TYR:HD2    | 9:UF:132:ILE:HD12  | 1.72                     | 0.52              |
| 9:UF:159:ALA:HB1    | 9:UF:161:PHE:CE1   | 2.43                     | 0.52              |
| 12:UI:415:GLU:HA    | 12:UI:418:LYS:HZ2  | 1.74                     | 0.52              |
| 13:UJ:1599:GLU:HG2  | 13:UJ:1600:PRO:HD3 | 1.92                     | 0.52              |
| 14:UK:125:LEU:HD11  | 14:UK:198:PHE:CE1  | 2.45                     | 0.52              |
| 15:UL:275:GLN:HG3   | 15:UL:338:ILE:HD12 | 1.90                     | 0.52              |
| 15:UL:373:ASP:OD1   | 15:UL:373:ASP:N    | 2.40                     | 0.52              |
| 16:UM:495:ASN:OD1   | 16:UM:496:ALA:N    | 2.41                     | 0.52              |
| 20:UQ:246:SER:O     | 20:UQ:250:GLN:NE2  | 2.29                     | 0.52              |
| 20:UQ:443:ASN:HB3   | 20:UQ:448:ASN:H    | 1.73                     | 0.52              |
| 22:US:273:GLN:O     | 22:US:277:ILE:HD12 | 2.09                     | 0.52              |
| 23:UT:208:LEU:HD21  | 23:UT:254:ILE:HG23 | 1.91                     | 0.52              |
| 23:UT:468:ALA:O     | 23:UT:503:ARG:NH2  | 2.43                     | 0.52              |
| 23:UT:484:ILE:O     | 23:UT:487:LYS:HG2  | 2.10                     | 0.52              |
| 24:UU:66:LEU:HB3    | 24:UU:346:ARG:HD3  | 1.91                     | 0.52              |
| 24:UU:110:LEU:HD21  | 24:UU:140:TYR:CZ   | 2.45                     | 0.52              |
| 24:UU:670:GLU:N     | 24:UU:670:GLU:OE1  | 2.39                     | 0.52              |
| 25:UV:523:TYR:HA    | 25:UV:618:ILE:HD11 | 1.90                     | 0.52              |
| 25:UV:613:VAL:O     | 25:UV:614:ARG:NH2  | 2.42                     | 0.52              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 25:UV:641:GLU:H     | 25:UV:641:GLU:CD    | 2.13                     | 0.52              |
| 30:CG:8:ALA:HA      | 30:CG:80:PHE:HE2    | 1.73                     | 0.52              |
| 35:CL:250:THR:OG1   | 35:CL:270:ALA:HB3   | 2.09                     | 0.52              |
| 35:CL:874:TYR:OH    | 66:D3:578:U:OP2     | 2.21                     | 0.52              |
| 36:CM:7:LYS:N       | 36:CM:30:PRO:HB2    | 2.24                     | 0.52              |
| 36:CM:123:ALA:HB1   | 36:CM:261:ILE:HG21  | 1.91                     | 0.52              |
| 38:JC:57:GLU:OE1    | 38:JC:77:TYR:HB3    | 2.09                     | 0.52              |
| 39:JF:178:VAL:HA    | 39:JF:223:GLU:O     | 2.10                     | 0.52              |
| 39:JG:40:ARG:HD2    | 39:JG:42:ILE:HD11   | 1.91                     | 0.52              |
| 47:JP:393:LYS:NZ    | 67:D4:35:U:O2       | 2.43                     | 0.52              |
| 54:DJ:120:LYS:NZ    | 66:D3:480:G:OP1     | 2.41                     | 0.52              |
| 58:DQ:41:PRO:O      | 58:DQ:43:ILE:HD12   | 2.10                     | 0.52              |
| 60:DW:80:ASN:ND2    | 66:D3:747:C:O3'     | 2.43                     | 0.52              |
| 66:D3:389:G:C6      | 66:D3:390:G:C6      | 2.98                     | 0.52              |
| 66:D3:1435:G:H2'    | 66:D3:1437:U:H1'    | 1.92                     | 0.52              |
| 66:D3:1648:A:H2'    | 66:D3:1649:G:H8     | 1.73                     | 0.52              |
| 3:JA:748:ARG:HE     | 3:JA:759:THR:H      | 1.57                     | 0.52              |
| 4:UA:77:GLY:CA      | 4:UA:95:PHE:O       | 2.29                     | 0.52              |
| 4:UA:130:ASP:OD2    | 24:UU:25:SER:OG     | 2.16                     | 0.52              |
| 4:UA:450:LEU:HA     | 4:UA:475:PRO:HB3    | 1.92                     | 0.52              |
| 1:CB:167:GLY:HA2    | 1:CB:191:GLU:HG2    | 1.91                     | 0.52              |
| 8:UE:473:LYS:NZ     | 8:UE:475:ALA:HB3    | 2.25                     | 0.52              |
| 9:UF:143:ASN:O      | 9:UF:146:ILE:HG22   | 2.10                     | 0.52              |
| 13:UJ:25:ARG:NH1    | 47:JP:16:VAL:HA     | 2.25                     | 0.52              |
| 13:UJ:32:SER:OG     | 13:UJ:119:GLU:OE1   | 2.27                     | 0.52              |
| 13:UJ:257:ALA:O     | 13:UJ:261:LEU:HD23  | 2.10                     | 0.52              |
| 13:UJ:1545:ARG:HA   | 13:UJ:1593:TYR:HE1  | 1.73                     | 0.52              |
| 13:UJ:1670:ILE:HG22 | 13:UJ:1714:ILE:HD11 | 1.92                     | 0.52              |
| 15:UL:412:GLY:CA    | 15:UL:430:CYS:H     | 2.23                     | 0.52              |
| 16:UM:334:ALA:HB3   | 16:UM:381:VAL:HG21  | 1.91                     | 0.52              |
| 16:UM:509:ALA:HA    | 16:UM:515:CYS:HA    | 1.92                     | 0.52              |
| 20:UQ:534:LYS:HD3   | 20:UQ:541:TRP:CZ2   | 2.45                     | 0.52              |
| 23:UT:365:PHE:O     | 23:UT:369:SER:CB    | 2.57                     | 0.52              |
| 23:UT:558:TRP:CZ3   | 23:UT:603:LEU:HD21  | 2.45                     | 0.52              |
| 23:UT:621:SER:HA    | 23:UT:624:VAL:HG12  | 1.92                     | 0.52              |
| 23:UT:1055:ARG:O    | 23:UT:1059:LEU:HG   | 2.10                     | 0.52              |
| 23:UT:1087:VAL:HA   | 23:UT:1091:ILE:HD13 | 1.92                     | 0.52              |
| 25:UV:603:THR:OG1   | 25:UV:610:PHE:O     | 2.24                     | 0.52              |
| 29:CE:69:SER:OG     | 29:CE:72:LEU:HD23   | 2.09                     | 0.52              |
| 31:CH:341:ALA:HB1   | 31:CH:401:SER:OG    | 2.10                     | 0.52              |
| 31:CH:529:SER:OG    | 31:CH:530:GLY:N     | 2.43                     | 0.52              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 35:CL:274:TYR:O     | 35:CL:275:LEU:HD23  | 2.10                     | 0.52              |
| 37:CN:131:ALA:HA    | 37:CN:134:ILE:HG22  | 1.92                     | 0.52              |
| 42:JJ:153:GLN:NE2   | 42:JJ:157:ASP:OD2   | 2.36                     | 0.52              |
| 42:JJ:204:ARG:NH2   | 42:JJ:251:ILE:O     | 2.35                     | 0.52              |
| 42:JJ:220:THR:HG21  | 42:JJ:243:ALA:HB2   | 1.92                     | 0.52              |
| 46:JO:90:ASP:O      | 46:JO:93:ILE:HG22   | 2.09                     | 0.52              |
| 49:DE:238:LEU:HD23  | 49:DE:242:LYS:HD3   | 1.92                     | 0.52              |
| 51:DG:43:ASP:OD2    | 51:DG:44:GLU:N      | 2.42                     | 0.52              |
| 54:DJ:107:ARG:NH1   | 54:DJ:153:GLU:OE1   | 2.38                     | 0.52              |
| 65:D2:148:G:N2      | 65:D2:149:U:O2      | 2.42                     | 0.52              |
| 66:D3:195:G:H2'     | 66:D3:196:G:C8      | 2.45                     | 0.52              |
| 66:D3:387:A:H62     | 66:D3:402:C:P       | 2.31                     | 0.52              |
| 66:D3:1707:A:H2'    | 66:D3:1708:U:C6     | 2.45                     | 0.52              |
| 2:DA:121:ILE:HB     | 2:DA:141:ALA:O      | 2.08                     | 0.52              |
| 3:JA:26:PHE:CD1     | 3:JA:199:LEU:HB2    | 2.44                     | 0.52              |
| 3:JA:89:ASN:HD22    | 35:CL:95:LYS:NZ     | 2.08                     | 0.52              |
| 7:UD:112:LEU:HD23   | 7:UD:112:LEU:H      | 1.75                     | 0.52              |
| 8:UE:227:VAL:HG22   | 8:UE:228:ALA:O      | 2.08                     | 0.52              |
| 9:UF:89:GLN:OE1     | 9:UF:116:TYR:OH     | 2.26                     | 0.52              |
| 10:UG:183:GLU:O     | 10:UG:184:LEU:HD23  | 2.09                     | 0.52              |
| 10:UG:325:SER:HB2   | 10:UG:383:PHE:CZ    | 2.45                     | 0.52              |
| 13:UJ:1395:GLN:HA   | 13:UJ:1398:VAL:HG22 | 1.92                     | 0.52              |
| 14:UK:105:ASN:HB3   | 29:CE:330:LEU:HD22  | 1.91                     | 0.52              |
| 15:UL:222:THR:OG1   | 15:UL:223:ASP:OD1   | 2.26                     | 0.52              |
| 15:UL:248:PHE:HD2   | 15:UL:251:GLN:HE21  | 1.57                     | 0.52              |
| 17:UN:313:PHE:O     | 17:UN:315:LEU:N     | 2.43                     | 0.52              |
| 18:UO:34:GLN:OE1    | 18:UO:35:LEU:N      | 2.41                     | 0.52              |
| 18:UO:192:LEU:O     | 18:UO:194:ARG:HD2   | 2.10                     | 0.52              |
| 21:UR:145:LYS:HB2   | 65:D2:310:U:C5      | 2.44                     | 0.52              |
| 25:UV:313:ASN:ND2   | 25:UV:315:ILE:O     | 2.42                     | 0.52              |
| 25:UV:1115:LEU:HD23 | 25:UV:1115:LEU:H    | 1.74                     | 0.52              |
| 25:UV:1215:ASN:O    | 25:UV:1219:ILE:HG12 | 2.10                     | 0.52              |
| 29:CE:76:LEU:HA     | 29:CE:79:ILE:HG12   | 1.92                     | 0.52              |
| 32:CI:87:VAL:O      | 32:CI:105:ALA:HB1   | 2.10                     | 0.52              |
| 35:CL:776:GLN:HG3   | 35:CL:780:ILE:HD11  | 1.91                     | 0.52              |
| 37:CN:50:SER:O      | 37:CN:127:LYS:NZ    | 2.35                     | 0.52              |
| 38:JC:232:THR:OG1   | 38:JC:274:ILE:O     | 2.27                     | 0.52              |
| 39:JF:150:ILE:O     | 39:JF:159:LEU:N     | 2.32                     | 0.52              |
| 39:JF:177:LYS:HB3   | 39:JF:205:PHE:CE2   | 2.45                     | 0.52              |
| 42:JJ:124:LEU:HD21  | 42:JJ:151:ALA:HB1   | 1.91                     | 0.52              |
| 65:D2:215:U:H2'     | 65:D2:216:U:C6      | 2.45                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 75:EH:203:ASN:O    | 75:EH:207:CYS:N    | 2.40                     | 0.52              |
| 79:EN:351:GLU:O    | 79:EN:355:LYS:N    | 2.34                     | 0.52              |
| 7:UD:448:THR:OG1   | 7:UD:470:LEU:O     | 2.22                     | 0.52              |
| 8:UE:86:TRP:HE1    | 8:UE:98:LYS:HE3    | 1.74                     | 0.52              |
| 8:UE:525:SER:HB2   | 18:UO:17:PRO:HG2   | 1.92                     | 0.52              |
| 11:UH:529:HIS:CG   | 11:UH:530:PRO:HD2  | 2.45                     | 0.52              |
| 11:UH:639:SER:HB2  | 12:UI:499:ILE:HD11 | 1.91                     | 0.52              |
| 13:UJ:703:GLU:O    | 13:UJ:707:ILE:HG12 | 2.09                     | 0.52              |
| 13:UJ:1654:GLN:HA  | 13:UJ:1657:ASN:OD1 | 2.10                     | 0.52              |
| 15:UL:415:LYS:HB3  | 15:UL:417:TRP:HE1  | 1.75                     | 0.52              |
| 16:UM:542:CYS:HB2  | 16:UM:547:LEU:HB2  | 1.89                     | 0.52              |
| 16:UM:683:LEU:HD21 | 16:UM:727:ALA:HB1  | 1.91                     | 0.52              |
| 20:UQ:200:ASN:HD22 | 20:UQ:262:MET:HB3  | 1.75                     | 0.52              |
| 20:UQ:584:PHE:HD2  | 20:UQ:598:LYS:HB2  | 1.74                     | 0.52              |
| 23:UT:91:LEU:HD13  | 23:UT:110:LEU:HD13 | 1.91                     | 0.52              |
| 23:UT:399:PHE:O    | 23:UT:402:ARG:HG3  | 2.09                     | 0.52              |
| 25:UV:930:THR:OG1  | 25:UV:932:GLU:OE2  | 2.18                     | 0.52              |
| 25:UV:932:GLU:HA   | 25:UV:935:GLU:CD   | 2.30                     | 0.52              |
| 28:CD:188:ILE:HD11 | 28:CD:281:LEU:HG   | 1.91                     | 0.52              |
| 28:CD:310:VAL:O    | 28:CD:314:ARG:HG2  | 2.10                     | 0.52              |
| 29:CE:98:ILE:HD13  | 29:CE:101:LEU:HD21 | 1.91                     | 0.52              |
| 30:CG:54:MET:O     | 30:CG:80:PHE:HA    | 2.10                     | 0.52              |
| 31:CH:231:THR:HA   | 31:CH:273:VAL:HG11 | 1.91                     | 0.52              |
| 33:CJ:109:LEU:HD21 | 33:CJ:182:GLN:HG3  | 1.91                     | 0.52              |
| 33:CJ:139:LEU:HD23 | 33:CJ:266:LEU:HD21 | 1.92                     | 0.52              |
| 36:CM:70:THR:HG23  | 36:CM:72:THR:H     | 1.74                     | 0.52              |
| 39:JF:71:ASP:OD2   | 39:JG:136:ARG:NH1  | 2.43                     | 0.52              |
| 51:DG:48:TYR:HB3   | 51:DG:50:PHE:CE2   | 2.44                     | 0.52              |
| 53:DI:81:VAL:HG22  | 53:DI:91:VAL:HG13  | 1.91                     | 0.52              |
| 55:DL:46:LYS:HA    | 55:DL:49:ILE:HG12  | 1.91                     | 0.52              |
| 56:DN:46:THR:O     | 56:DN:50:ILE:HG12  | 2.10                     | 0.52              |
| 65:D2:409:C:H2'    | 65:D2:410:A:H8     | 1.75                     | 0.52              |
| 66:D3:151:G:H22    | 66:D3:163:G:H8     | 1.58                     | 0.52              |
| 66:D3:450:U:H2'    | 66:D3:451:A:H8     | 1.75                     | 0.52              |
| 66:D3:501:U:O2'    | 66:D3:502:U:OP2    | 2.26                     | 0.52              |
| 66:D3:1045:C:H2'   | 66:D3:1046:G:H8    | 1.75                     | 0.52              |
| 66:D3:1074:G:N2    | 66:D3:1075:C:N3    | 2.58                     | 0.52              |
| 67:D4:4:G:H2'      | 67:D4:5:A:C8       | 2.45                     | 0.52              |
| 67:D4:75:C:H2'     | 67:D4:76:U:C6      | 2.44                     | 0.52              |
| 79:EN:504:THR:O    | 79:EN:508:GLY:N    | 2.35                     | 0.52              |
| 2:DA:134:VAL:HG12  | 2:DA:219:LYS:HG2   | 1.92                     | 0.52              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:DA:168:ILE:HA     | 2:DA:171:ILE:HG22   | 1.92                     | 0.52              |
| 3:JA:25:ILE:O       | 3:JA:198:CYS:HA     | 2.10                     | 0.52              |
| 3:JA:162:TYR:HA     | 3:JA:165:THR:HG22   | 1.92                     | 0.52              |
| 3:JA:838:ASP:HA     | 3:JA:841:ARG:HH21   | 1.74                     | 0.52              |
| 4:UA:652:ASP:OD1    | 4:UA:653:LEU:N      | 2.42                     | 0.52              |
| 1:CB:91:HIS:ND1     | 14:UK:164:ASN:OD1   | 2.43                     | 0.52              |
| 5:UB:763:ALA:HA     | 34:CK:349:ARG:HE    | 1.75                     | 0.52              |
| 9:UF:107:LEU:HD21   | 9:UF:143:ASN:HD21   | 1.75                     | 0.52              |
| 11:UH:120:LEU:N     | 11:UH:168:LYS:O     | 2.42                     | 0.52              |
| 13:UJ:354:SER:O     | 13:UJ:358:TYR:HB2   | 2.10                     | 0.52              |
| 15:UL:362:ILE:O     | 15:UL:384:THR:HA    | 2.10                     | 0.52              |
| 18:UO:188:SER:OG    | 18:UO:190:ASP:OD1   | 2.19                     | 0.52              |
| 18:UO:383:ARG:HH22  | 18:UO:386:ARG:NH2   | 2.07                     | 0.52              |
| 21:UR:241:ALA:HB3   | 21:UR:586:VAL:HG21  | 1.92                     | 0.52              |
| 22:US:181:THR:HA    | 22:US:185:TYR:HB3   | 1.92                     | 0.52              |
| 23:UT:654:THR:HG21  | 23:UT:691:LYS:HD3   | 1.91                     | 0.52              |
| 23:UT:1017:LEU:HD22 | 23:UT:1022:VAL:HG21 | 1.92                     | 0.52              |
| 24:UU:166:GLU:O     | 24:UU:185:LYS:HG2   | 2.10                     | 0.52              |
| 24:UU:606:ASP:OD1   | 24:UU:608:THR:OG1   | 2.22                     | 0.52              |
| 27:UZ:42:THR:HG21   | 27:UZ:235:ILE:HD12  | 1.91                     | 0.52              |
| 31:CH:195:GLN:NE2   | 31:CH:196:LEU:O     | 2.42                     | 0.52              |
| 31:CH:371:ARG:HA    | 31:CH:374:LYS:HG2   | 1.90                     | 0.52              |
| 32:CI:61:LEU:HA     | 32:CI:64:LEU:HD12   | 1.91                     | 0.52              |
| 33:CJ:206:LEU:O     | 33:CJ:209:LEU:HB3   | 2.09                     | 0.52              |
| 34:CK:326:LEU:O     | 35:CL:930:LYS:NZ    | 2.43                     | 0.52              |
| 39:JF:130:ILE:HD12  | 39:JF:131:PRO:HD2   | 1.92                     | 0.52              |
| 44:JM:71:ALA:O      | 44:JM:75:LYS:HB2    | 2.10                     | 0.52              |
| 47:JP:289:TYR:HE1   | 47:JP:297:SER:HB3   | 1.74                     | 0.52              |
| 51:DG:28:PHE:HA     | 51:DG:102:VAL:HG13  | 1.91                     | 0.52              |
| 56:DN:121:ARG:HH22  | 66:D3:868:G:H5'     | 1.73                     | 0.52              |
| 60:DW:122:SER:OG    | 60:DW:123:GLY:N     | 2.43                     | 0.52              |
| 65:D2:208:A:H2'     | 65:D2:209:G:C8      | 2.44                     | 0.52              |
| 66:D3:192:U:O2'     | 66:D3:193:U:O5'     | 2.28                     | 0.52              |
| 66:D3:1050:G:C2     | 66:D3:1051:G:C4     | 2.98                     | 0.52              |
| 66:D3:1483:A:C6     | 66:D3:1524:A:C5     | 2.97                     | 0.52              |
| 79:EN:433:SER:O     | 79:EN:437:LYS:N     | 2.40                     | 0.52              |
| 1:CA:222:GLU:OE2    | 1:CA:229:LYS:HB3    | 2.10                     | 0.52              |
| 3:JA:128:GLU:N      | 3:JA:128:GLU:OE1    | 2.43                     | 0.52              |
| 1:CB:110:ASN:OD1    | 1:CB:142:ARG:HB2    | 2.09                     | 0.52              |
| 1:CB:110:ASN:HD21   | 1:CB:142:ARG:HD3    | 1.75                     | 0.52              |
| 3:JB:635:ILE:N      | 3:JB:724:GLY:O      | 2.42                     | 0.52              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 5:UB:546:LEU:HD12  | 5:UB:549:ILE:HD11   | 1.92                     | 0.52              |
| 7:UD:35:ARG:HA     | 7:UD:754:ILE:HG13   | 1.92                     | 0.52              |
| 7:UD:104:TRP:NE1   | 7:UD:114:LEU:HD13   | 2.25                     | 0.52              |
| 7:UD:298:ALA:HB1   | 7:UD:333:ILE:HG21   | 1.92                     | 0.52              |
| 8:UE:311:MET:HB3   | 8:UE:313:TYR:HE2    | 1.75                     | 0.52              |
| 10:UG:467:ALA:O    | 10:UG:471:MET:HG3   | 2.09                     | 0.52              |
| 11:UH:593:ASP:OD1  | 11:UH:594:SER:N     | 2.42                     | 0.52              |
| 15:UL:194:HIS:ND1  | 15:UL:194:HIS:O     | 2.43                     | 0.52              |
| 15:UL:273:TYR:HD1  | 15:UL:343:TRP:CZ2   | 2.27                     | 0.52              |
| 15:UL:287:ARG:NH2  | 15:UL:326:LEU:O     | 2.43                     | 0.52              |
| 16:UM:418:ASN:HD22 | 16:UM:423:LYS:HE3   | 1.75                     | 0.52              |
| 16:UM:461:LEU:O    | 16:UM:489:ALA:N     | 2.25                     | 0.52              |
| 16:UM:679:THR:HG21 | 16:UM:723:GLU:HG2   | 1.91                     | 0.52              |
| 18:UO:360:MET:HE3  | 65:D2:234:A:C4      | 2.45                     | 0.52              |
| 18:UO:420:GLU:OE1  | 18:UO:424:ARG:NE    | 2.42                     | 0.52              |
| 20:UQ:240:PRO:O    | 20:UQ:243:SER:OG    | 2.23                     | 0.52              |
| 23:UT:85:LYS:HA    | 23:UT:88:PHE:HD2    | 1.75                     | 0.52              |
| 23:UT:700:VAL:HG21 | 23:UT:782:MET:HG2   | 1.92                     | 0.52              |
| 23:UT:947:ILE:HA   | 23:UT:950:ILE:HG22  | 1.91                     | 0.52              |
| 23:UT:1112:TRP:HD1 | 23:UT:1118:LEU:HD13 | 1.75                     | 0.52              |
| 27:UZ:142:ARG:HE   | 66:D3:1515:A:N6     | 2.08                     | 0.52              |
| 29:CE:15:LEU:HD21  | 29:CE:42:PHE:HB3    | 1.91                     | 0.52              |
| 29:CE:65:GLU:O     | 29:CE:93:LYS:NZ     | 2.34                     | 0.52              |
| 32:CI:71:ARG:HE    | 33:CJ:61:SER:CB     | 2.22                     | 0.52              |
| 33:CJ:154:ILE:O    | 33:CJ:162:THR:HA    | 2.09                     | 0.52              |
| 33:CJ:259:PHE:O    | 33:CJ:260:GLU:HB3   | 2.10                     | 0.52              |
| 35:CL:772:MET:SD   | 35:CL:774:PRO:HD2   | 2.50                     | 0.52              |
| 36:CM:59:VAL:HG21  | 36:CM:103:MET:SD    | 2.50                     | 0.52              |
| 37:CN:58:LEU:HD12  | 37:CN:59:PRO:HD2    | 1.92                     | 0.52              |
| 38:JC:51:GLN:CD    | 51:DG:76:LEU:HD21   | 2.30                     | 0.52              |
| 38:JC:238:ASN:HB3  | 38:JC:279:TRP:CE3   | 2.45                     | 0.52              |
| 46:JO:146:VAL:HG23 | 46:JO:153:LEU:HD22  | 1.90                     | 0.52              |
| 55:DL:71:LEU:HD23  | 55:DL:72:THR:N      | 2.25                     | 0.52              |
| 61:DX:130:VAL:CG1  | 61:DX:135:LEU:HD11  | 2.40                     | 0.52              |
| 66:D3:420:A:H2'    | 66:D3:421:A:C8      | 2.45                     | 0.52              |
| 66:D3:542:A:H2'    | 66:D3:542:A:N3      | 2.23                     | 0.52              |
| 66:D3:1264:G:H2'   | 66:D3:1265:G:C8     | 2.45                     | 0.52              |
| 66:D3:1682:U:O2'   | 66:D3:1683:C:H5'    | 2.10                     | 0.52              |
| 67:D4:201:C:H2'    | 67:D4:202:G:H8      | 1.75                     | 0.52              |
| 1:CA:201:HIS:O     | 1:CA:204:GLY:N      | 2.44                     | 0.51              |
| 4:UA:221:THR:O     | 4:UA:249:ARG:NH1    | 2.41                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:UC:502:LYS:O     | 6:UC:506:LYS:HG2   | 2.10                     | 0.51              |
| 7:UD:645:ARG:HB3   | 7:UD:656:ARG:HD2   | 1.92                     | 0.51              |
| 8:UE:234:GLU:HG3   | 8:UE:293:ASN:OD1   | 2.10                     | 0.51              |
| 9:UF:319:TYR:O     | 9:UF:322:LEU:HB3   | 2.10                     | 0.51              |
| 13:UJ:32:SER:C     | 13:UJ:154:ILE:HD11 | 2.31                     | 0.51              |
| 13:UJ:493:LYS:O    | 13:UJ:496:SER:OG   | 2.24                     | 0.51              |
| 13:UJ:701:SER:HA   | 13:UJ:704:LYS:HD2  | 1.91                     | 0.51              |
| 13:UJ:1592:SER:O   | 13:UJ:1595:THR:OG1 | 2.21                     | 0.51              |
| 14:UK:59:ASN:O     | 14:UK:61:ASP:N     | 2.41                     | 0.51              |
| 15:UL:285:ARG:HB3  | 15:UL:327:HIS:ND1  | 2.25                     | 0.51              |
| 18:UO:486:ASP:O    | 18:UO:489:THR:OG1  | 2.24                     | 0.51              |
| 19:UP:155:ILE:O    | 19:UP:158:LYS:HG3  | 2.09                     | 0.51              |
| 20:UQ:450:TYR:CE2  | 20:UQ:500:PHE:HZ   | 2.28                     | 0.51              |
| 20:UQ:725:ASN:OD1  | 20:UQ:726:GLN:N    | 2.43                     | 0.51              |
| 22:US:339:MET:SD   | 22:US:453:PRO:HD3  | 2.50                     | 0.51              |
| 23:UT:114:CYS:O    | 23:UT:117:LEU:C    | 2.48                     | 0.51              |
| 23:UT:887:ASN:HA   | 23:UT:890:ASN:HD22 | 1.75                     | 0.51              |
| 24:UU:118:VAL:HA   | 24:UU:132:THR:HA   | 1.91                     | 0.51              |
| 25:UV:369:TRP:CZ2  | 25:UV:495:THR:HG21 | 2.45                     | 0.51              |
| 30:CG:22:ASP:OD1   | 31:CH:342:ARG:NH2  | 2.31                     | 0.51              |
| 31:CH:200:ASP:O    | 31:CH:208:PRO:HA   | 2.10                     | 0.51              |
| 36:CM:241:TRP:CZ2  | 36:CM:262:GLY:HA3  | 2.45                     | 0.51              |
| 36:CM:309:GLY:O    | 36:CM:353:THR:HA   | 2.10                     | 0.51              |
| 37:CN:99:ASP:OD1   | 37:CN:101:SER:OG   | 2.28                     | 0.51              |
| 38:JC:166:ASN:HB3  | 38:JC:169:LYS:HB2  | 1.92                     | 0.51              |
| 45:JN:157:GLN:HE21 | 45:JN:161:GLU:HG3  | 1.75                     | 0.51              |
| 52:DH:85:PHE:HD1   | 52:DH:88:ARG:HB2   | 1.75                     | 0.51              |
| 62:DY:40:LEU:HD13  | 62:DY:60:PHE:HE2   | 1.75                     | 0.51              |
| 66:D3:144:U:HO2'   | 66:D3:145:A:H8     | 1.58                     | 0.51              |
| 66:D3:208:U:H2'    | 66:D3:209:U:C6     | 2.44                     | 0.51              |
| 66:D3:462:G:H2'    | 66:D3:463:U:H6     | 1.75                     | 0.51              |
| 66:D3:1203:A:H2'   | 66:D3:1204:A:C8    | 2.45                     | 0.51              |
| 3:JA:500:PRO:HA    | 3:JA:504:THR:HG23  | 1.92                     | 0.51              |
| 4:UA:191:ARG:HH21  | 65:D2:323:A:H2     | 1.58                     | 0.51              |
| 5:UB:616:LEU:HD23  | 5:UB:619:LEU:HD13  | 1.92                     | 0.51              |
| 13:UJ:149:LYS:HZ1  | 13:UJ:173:PRO:HA   | 1.75                     | 0.51              |
| 13:UJ:491:TYR:HE2  | 13:UJ:528:ARG:HD3  | 1.75                     | 0.51              |
| 13:UJ:657:GLN:O    | 13:UJ:661:ILE:HG12 | 2.10                     | 0.51              |
| 13:UJ:658:ALA:O    | 13:UJ:667:LYS:NZ   | 2.28                     | 0.51              |
| 13:UJ:1708:ILE:O   | 13:UJ:1712:LYS:HG2 | 2.10                     | 0.51              |
| 15:UL:236:ASP:O    | 15:UL:241:LYS:NZ   | 2.31                     | 0.51              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 23:UT:1247:LEU:HD23 | 23:UT:1287:LEU:HD13 | 1.91                     | 0.51              |
| 23:UT:1433:ASP:O    | 23:UT:1437:MET:HG2  | 2.10                     | 0.51              |
| 29:CE:248:THR:OG1   | 29:CE:251:ASP:OD2   | 2.28                     | 0.51              |
| 29:CE:324:LYS:O     | 29:CE:328:ARG:HG3   | 2.11                     | 0.51              |
| 31:CH:443:LEU:HB3   | 31:CH:471:GLN:HG2   | 1.90                     | 0.51              |
| 37:CN:151:HIS:CE1   | 37:CN:154:GLU:HG3   | 2.44                     | 0.51              |
| 38:JC:237:ARG:HH22  | 38:JC:288:LYS:HG3   | 1.75                     | 0.51              |
| 39:JG:91:ILE:HD12   | 39:JG:208:ALA:O     | 2.10                     | 0.51              |
| 39:JG:99:LEU:HD21   | 39:JG:238:CYS:HB3   | 1.92                     | 0.51              |
| 47:JP:360:SER:O     | 47:JP:360:SER:OG    | 2.28                     | 0.51              |
| 47:JP:445:ARG:HB2   | 47:JP:445:ARG:CZ    | 2.40                     | 0.51              |
| 49:DE:223:ASN:OD1   | 49:DE:224:ASN:N     | 2.43                     | 0.51              |
| 52:DH:122:HIS:HA    | 52:DH:125:ILE:HD13  | 1.91                     | 0.51              |
| 52:DH:140:VAL:HA    | 52:DH:149:ILE:O     | 2.10                     | 0.51              |
| 55:DL:27:THR:OG1    | 55:DL:30:ARG:NH2    | 2.41                     | 0.51              |
| 60:DW:24:GLN:HB3    | 60:DW:64:GLN:HA     | 1.92                     | 0.51              |
| 61:DX:85:ALA:HB1    | 61:DX:122:PHE:HB2   | 1.91                     | 0.51              |
| 62:DY:38:ASP:OD1    | 62:DY:38:ASP:N      | 2.43                     | 0.51              |
| 66:D3:768:C:H5      | 66:D3:770:A:N1      | 2.09                     | 0.51              |
| 66:D3:1066:C:H2'    | 66:D3:1067:C:H6     | 1.76                     | 0.51              |
| 67:D4:52:U:H2'      | 67:D4:53:U:C6       | 2.44                     | 0.51              |
| 1:CA:107:VAL:CG1    | 1:CA:141:TYR:HB3    | 2.40                     | 0.51              |
| 3:JA:742:PHE:CD2    | 3:JA:764:ASN:HB2    | 2.45                     | 0.51              |
| 4:UA:420:ARG:O      | 4:UA:422:PHE:N      | 2.43                     | 0.51              |
| 4:UA:848:PHE:HA     | 15:UL:900:PHE:CE2   | 2.46                     | 0.51              |
| 1:CB:188:VAL:HB     | 1:CB:192:GLY:HA3    | 1.91                     | 0.51              |
| 1:CB:293:LEU:HD22   | 1:CB:298:ILE:HD12   | 1.92                     | 0.51              |
| 5:UB:485:TYR:CD2    | 5:UB:486:LYS:HD3    | 2.45                     | 0.51              |
| 5:UB:796:LYS:HA     | 61:DX:121:ARG:HH12  | 1.75                     | 0.51              |
| 8:UE:277:LYS:HG2    | 8:UE:324:ASN:HA     | 1.93                     | 0.51              |
| 9:UF:193:ILE:HD12   | 9:UF:266:ARG:HG2    | 1.92                     | 0.51              |
| 12:UI:424:ILE:HA    | 12:UI:427:VAL:HG12  | 1.93                     | 0.51              |
| 12:UI:450:ASN:O     | 12:UI:454:LEU:HG    | 2.10                     | 0.51              |
| 12:UI:495:VAL:O     | 12:UI:499:ILE:HG12  | 2.11                     | 0.51              |
| 13:UJ:753:ALA:O     | 13:UJ:757:ILE:HG12  | 2.10                     | 0.51              |
| 13:UJ:1682:GLU:O    | 13:UJ:1685:GLN:HG2  | 2.10                     | 0.51              |
| 14:UK:166:LEU:HD12  | 14:UK:170:GLN:HB3   | 1.92                     | 0.51              |
| 15:UL:330:GLN:NE2   | 15:UL:367:ILE:HG21  | 2.24                     | 0.51              |
| 16:UM:170:GLY:CA    | 16:UM:189:HIS:HB2   | 2.40                     | 0.51              |
| 20:UQ:73:LEU:O      | 20:UQ:77:ILE:HG12   | 2.11                     | 0.51              |
| 23:UT:1036:VAL:O    | 23:UT:1040:GLU:HG2  | 2.11                     | 0.51              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 23:UT:1147:ILE:HG22 | 23:UT:1151:ILE:HD11 | 1.92                     | 0.51              |
| 23:UT:1368:SER:O    | 23:UT:1372:MET:HG2  | 2.09                     | 0.51              |
| 23:UT:1658:LEU:HA   | 23:UT:1661:ILE:HG12 | 1.92                     | 0.51              |
| 24:UU:188:VAL:H     | 24:UU:202:SER:HG    | 1.58                     | 0.51              |
| 26:UX:84:ARG:CZ     | 60:DW:97:ARG:HH12   | 2.23                     | 0.51              |
| 27:UZ:110:PHE:CE2   | 27:UZ:118:LEU:HD11  | 2.46                     | 0.51              |
| 29:CE:300:ILE:HA    | 29:CE:309:LEU:HD22  | 1.92                     | 0.51              |
| 31:CH:301:ASP:O     | 31:CH:303:LYS:HG3   | 2.11                     | 0.51              |
| 35:CL:47:SER:OG     | 61:DX:46:SER:HB3    | 2.10                     | 0.51              |
| 38:JC:292:CYS:HB3   | 38:JC:296:ILE:HG22  | 1.92                     | 0.51              |
| 47:JP:310:ASP:OD1   | 47:JP:311:VAL:N     | 2.39                     | 0.51              |
| 51:DG:188:ARG:NH1   | 66:D3:284:G:O6      | 2.42                     | 0.51              |
| 52:DH:43:PHE:CB     | 52:DH:62:VAL:HG22   | 2.41                     | 0.51              |
| 65:D2:344:U:H2'     | 65:D2:345:U:C6      | 2.45                     | 0.51              |
| 65:D2:360:C:H2'     | 65:D2:361:G:C8      | 2.46                     | 0.51              |
| 66:D3:278:U:H4'     | 66:D3:279:G:O5'     | 2.09                     | 0.51              |
| 66:D3:420:A:H2'     | 66:D3:421:A:H8      | 1.76                     | 0.51              |
| 66:D3:485:A:N6      | 66:D3:486:G:O6      | 2.44                     | 0.51              |
| 66:D3:747:C:H2'     | 66:D3:748:U:C6      | 2.46                     | 0.51              |
| 66:D3:787:G:H3'     | 66:D3:788:A:C8      | 2.44                     | 0.51              |
| 67:D4:32:G:C2'      | 67:D4:33:A:H5''     | 2.41                     | 0.51              |
| 1:CA:142:ARG:NH1    | 1:CA:186:ASP:OD2    | 2.36                     | 0.51              |
| 3:JA:748:ARG:NH2    | 3:JA:752:ASN:HB3    | 2.25                     | 0.51              |
| 5:UB:796:LYS:CA     | 61:DX:121:ARG:HH12  | 2.23                     | 0.51              |
| 7:UD:151:ASP:OD2    | 7:UD:197:LYS:HE2    | 2.11                     | 0.51              |
| 8:UE:203:ILE:HD12   | 8:UE:213:ASN:O      | 2.11                     | 0.51              |
| 8:UE:546:ARG:NH1    | 11:UH:677:ASN:O     | 2.42                     | 0.51              |
| 9:UF:184:GLU:HA     | 9:UF:187:LYS:HG2    | 1.93                     | 0.51              |
| 9:UF:193:ILE:O      | 9:UF:197:ILE:HG12   | 2.11                     | 0.51              |
| 9:UF:342:TRP:CH2    | 9:UF:359:TYR:HA     | 2.45                     | 0.51              |
| 13:UJ:1541:ASP:HA   | 13:UJ:1544:PHE:CZ   | 2.45                     | 0.51              |
| 14:UK:100:LYS:NZ    | 14:UK:221:GLN:OE1   | 2.25                     | 0.51              |
| 15:UL:279:LYS:HD3   | 15:UL:336:TYR:HA    | 1.92                     | 0.51              |
| 15:UL:342:SER:O     | 15:UL:353:LEU:HD12  | 2.10                     | 0.51              |
| 15:UL:620:ASN:HB2   | 15:UL:633:CYS:SG    | 2.50                     | 0.51              |
| 16:UM:23:ALA:HA     | 16:UM:67:LEU:HD11   | 1.92                     | 0.51              |
| 16:UM:333:ILE:HD11  | 16:UM:379:LEU:HB3   | 1.93                     | 0.51              |
| 16:UM:345:TYR:HE2   | 16:UM:626:MET:N     | 2.09                     | 0.51              |
| 16:UM:414:VAL:HB    | 16:UM:428:ALA:CB    | 2.38                     | 0.51              |
| 16:UM:593:CYS:HB3   | 16:UM:620:LEU:HB3   | 1.92                     | 0.51              |
| 16:UM:690:HIS:CE1   | 34:CK:519:GLU:HB3   | 2.46                     | 0.51              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 16:UM:787:PRO:HB2  | 34:CK:492:PRO:HG3   | 1.92                     | 0.51              |
| 18:UO:227:VAL:HG12 | 18:UO:258:LEU:HD21  | 1.92                     | 0.51              |
| 20:UQ:295:TRP:CD1  | 65:D2:85:G:H5'      | 2.46                     | 0.51              |
| 21:UR:144:LYS:NZ   | 65:D2:312:U:C4      | 2.79                     | 0.51              |
| 21:UR:463:GLY:N    | 21:UR:479:ASN:OD1   | 2.37                     | 0.51              |
| 22:US:259:LYS:HE3  | 22:US:259:LYS:HA    | 1.92                     | 0.51              |
| 23:UT:50:SER:O     | 23:UT:54:TRP:HD1    | 1.93                     | 0.51              |
| 23:UT:643:LYS:NZ   | 23:UT:683:ASP:HB2   | 2.25                     | 0.51              |
| 25:UV:533:LEU:HB3  | 25:UV:606:ASN:HD22  | 1.75                     | 0.51              |
| 25:UV:698:ASN:H    | 25:UV:702:LYS:NZ    | 2.07                     | 0.51              |
| 25:UV:1057:PRO:HB2 | 25:UV:1060:ILE:HG12 | 1.92                     | 0.51              |
| 25:UV:1097:ASP:OD2 | 25:UV:1186:ILE:N    | 2.33                     | 0.51              |
| 26:UX:68:ASP:OD1   | 26:UX:69:THR:N      | 2.44                     | 0.51              |
| 28:CD:230:ASN:OD1  | 28:CD:233:SER:N     | 2.35                     | 0.51              |
| 28:CD:255:ALA:HA   | 28:CD:258:SER:HB2   | 1.91                     | 0.51              |
| 35:CL:830:ARG:HD2  | 35:CL:831:ARG:O     | 2.10                     | 0.51              |
| 38:JC:195:LEU:HB2  | 38:JC:207:TRP:HB2   | 1.92                     | 0.51              |
| 49:DE:87:MET:HE1   | 49:DE:123:LEU:N     | 2.20                     | 0.51              |
| 50:DF:76:ARG:HH22  | 58:DQ:122:ARG:HH21  | 1.59                     | 0.51              |
| 51:DG:35:GLU:OE2   | 51:DG:50:PHE:N      | 2.43                     | 0.51              |
| 65:D2:212:U:H2'    | 65:D2:213:G:H8      | 1.75                     | 0.51              |
| 65:D2:243:A:N3     | 65:D2:271:G:N2      | 2.58                     | 0.51              |
| 66:D3:196:G:O2'    | 66:D3:197:A:O5'     | 2.28                     | 0.51              |
| 67:D4:77:U:H2'     | 67:D4:78:G:H8       | 1.75                     | 0.51              |
| 2:DA:105:PHE:HD2   | 2:DA:213:ARG:HA     | 1.74                     | 0.51              |
| 4:UA:653:LEU:HD11  | 65:D2:331:U:H3      | 1.76                     | 0.51              |
| 1:CB:236:MET:H     | 29:CE:121:LYS:NZ    | 2.07                     | 0.51              |
| 3:JB:737:TRP:O     | 3:JB:740:ASN:C      | 2.49                     | 0.51              |
| 7:UD:309:GLN:NE2   | 7:UD:318:ASN:HA     | 2.25                     | 0.51              |
| 13:UJ:646:ASN:HB2  | 13:UJ:649:VAL:HB    | 1.92                     | 0.51              |
| 13:UJ:1586:LEU:O   | 13:UJ:1587:ARG:HD3  | 2.11                     | 0.51              |
| 13:UJ:1762:GLU:HG2 | 13:UJ:1763:PRO:HD2  | 1.91                     | 0.51              |
| 14:UK:70:ARG:HH21  | 14:UK:78:LEU:CD2    | 2.22                     | 0.51              |
| 14:UK:223:GLU:OE2  | 14:UK:226:LYS:HD2   | 2.11                     | 0.51              |
| 15:UL:634:SER:OG   | 15:UL:636:ASP:OD1   | 2.28                     | 0.51              |
| 15:UL:901:ASN:HD21 | 16:UM:761:ARG:N     | 2.08                     | 0.51              |
| 20:UQ:722:LEU:HD11 | 20:UQ:766:ILE:HD12  | 1.92                     | 0.51              |
| 23:UT:215:VAL:HA   | 23:UT:218:LYS:HD2   | 1.92                     | 0.51              |
| 23:UT:1755:GLU:HG3 | 23:UT:1795:ARG:HB3  | 1.92                     | 0.51              |
| 25:UV:439:HIS:N    | 25:UV:458:ILE:O     | 2.34                     | 0.51              |
| 25:UV:1010:GLU:OE1 | 25:UV:1010:GLU:N    | 2.43                     | 0.51              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 25:UV:1075:LEU:HD11 | 25:UV:1080:LEU:HD13 | 1.92                     | 0.51              |
| 29:CE:216:SER:O     | 29:CE:220:GLU:HG2   | 2.10                     | 0.51              |
| 31:CH:333:MET:SD    | 31:CH:335:ARG:NH1   | 2.83                     | 0.51              |
| 35:CL:51:GLU:O      | 61:DX:50:LYS:HE3    | 2.09                     | 0.51              |
| 35:CL:211:ILE:HG13  | 35:CL:212:ASN:N     | 2.25                     | 0.51              |
| 35:CL:871:MET:N     | 35:CL:929:VAL:O     | 2.42                     | 0.51              |
| 37:CN:262:VAL:HG13  | 37:CN:266:LYS:HZ3   | 1.76                     | 0.51              |
| 38:JC:4:LYS:HG3     | 38:JC:363:LEU:HD12  | 1.93                     | 0.51              |
| 38:JC:5:SER:O       | 38:JC:14:TYR:HA     | 2.11                     | 0.51              |
| 42:JJ:172:ILE:HB    | 42:JJ:176:ARG:HH12  | 1.75                     | 0.51              |
| 47:JP:15:PRO:HG3    | 47:JP:22:SER:HA     | 1.92                     | 0.51              |
| 54:DJ:133:HIS:ND1   | 54:DJ:162:SER:OG    | 2.22                     | 0.51              |
| 55:DL:99:ARG:HG2    | 55:DL:100:TYR:N     | 2.25                     | 0.51              |
| 65:D2:120:C:H2'     | 65:D2:121:G:O4'     | 2.10                     | 0.51              |
| 66:D3:480:G:C2      | 66:D3:509:G:N3      | 2.79                     | 0.51              |
| 66:D3:1155:G:N1     | 66:D3:1156:C:N3     | 2.59                     | 0.51              |
| 2:DA:46:THR:HG22    | 2:DA:47:LEU:H       | 1.74                     | 0.51              |
| 3:JA:81:ILE:HD11    | 3:JA:88:VAL:HA      | 1.91                     | 0.51              |
| 3:JA:505:ARG:HH12   | 3:JA:643:GLU:HB2    | 1.75                     | 0.51              |
| 3:JA:721:HIS:HB3    | 3:JA:769:ARG:HH11   | 1.75                     | 0.51              |
| 4:UA:549:GLN:HE21   | 4:UA:552:ASN:HB3    | 1.76                     | 0.51              |
| 7:UD:103:CYS:SG     | 7:UD:115:PHE:HB2    | 2.51                     | 0.51              |
| 7:UD:242:TRP:HD1    | 7:UD:282:ASP:HB2    | 1.76                     | 0.51              |
| 11:UH:80:ALA:HA     | 11:UH:88:ASP:HA     | 1.92                     | 0.51              |
| 13:UJ:77:SER:O      | 13:UJ:80:SER:N      | 2.44                     | 0.51              |
| 13:UJ:1683:HIS:HA   | 13:UJ:1686:ILE:HG12 | 1.93                     | 0.51              |
| 13:UJ:1701:SER:O    | 13:UJ:1705:LEU:HD23 | 2.10                     | 0.51              |
| 18:UO:435:ASP:OD1   | 18:UO:436:GLU:N     | 2.39                     | 0.51              |
| 20:UQ:33:ASN:ND2    | 20:UQ:345:GLN:HE22  | 2.08                     | 0.51              |
| 22:US:387:THR:HG22  | 22:US:398:VAL:HG11  | 1.93                     | 0.51              |
| 23:UT:1017:LEU:HD21 | 23:UT:1065:VAL:HG21 | 1.93                     | 0.51              |
| 23:UT:1296:PRO:O    | 23:UT:1297:GLU:HG3  | 2.11                     | 0.51              |
| 23:UT:1543:GLN:HA   | 23:UT:1546:GLN:NE2  | 2.26                     | 0.51              |
| 24:UU:234:ASN:OD1   | 24:UU:235:MET:N     | 2.43                     | 0.51              |
| 24:UU:829:ASP:OD1   | 24:UU:830:TYR:N     | 2.43                     | 0.51              |
| 30:CG:38:ASN:HA     | 30:CG:41:THR:HG22   | 1.92                     | 0.51              |
| 35:CL:219:GLU:HA    | 35:CL:222:ASN:OD1   | 2.11                     | 0.51              |
| 35:CL:243:TYR:O     | 35:CL:276:HIS:HB2   | 2.11                     | 0.51              |
| 35:CL:876:PRO:HB2   | 35:CL:879:THR:HG22  | 1.91                     | 0.51              |
| 39:JF:213:LYS:NZ    | 39:JF:215:ASN:HB3   | 2.25                     | 0.51              |
| 42:JJ:121:VAL:HG23  | 42:JJ:122:GLU:OE1   | 2.10                     | 0.51              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 56:DN:20:ARG:HH21  | 60:DW:56:HIS:CG     | 2.28                     | 0.51              |
| 66:D3:315:A:N3     | 66:D3:316:A:H1'     | 2.25                     | 0.51              |
| 66:D3:467:G:O2'    | 66:D3:469:C:OP2     | 2.29                     | 0.51              |
| 67:D4:318:U:H4'    | 67:D4:319:G:O5'     | 2.11                     | 0.51              |
| 2:DA:205:PHE:HE2   | 66:D3:1065:A:H4'    | 1.75                     | 0.51              |
| 3:JA:185:ASN:O     | 3:JA:189:ILE:HG12   | 2.11                     | 0.51              |
| 7:UD:41:PHE:CD1    | 7:UD:43:PRO:HD3     | 2.45                     | 0.51              |
| 12:UI:502:ARG:O    | 12:UI:506:LEU:HD23  | 2.10                     | 0.51              |
| 13:UJ:751:ILE:HA   | 13:UJ:754:GLU:HG3   | 1.93                     | 0.51              |
| 13:UJ:1742:GLU:CD  | 31:CH:58:ASN:HD21   | 2.14                     | 0.51              |
| 14:UK:151:PHE:HD2  | 14:UK:152:PHE:CE2   | 2.29                     | 0.51              |
| 15:UL:401:ASP:HB2  | 15:UL:403:ASN:HD22  | 1.75                     | 0.51              |
| 15:UL:580:ASP:OD1  | 15:UL:581:ILE:N     | 2.44                     | 0.51              |
| 15:UL:905:LEU:HD12 | 16:UM:760:ILE:HD11  | 1.93                     | 0.51              |
| 16:UM:126:ILE:HG12 | 16:UM:140:PHE:HB2   | 1.93                     | 0.51              |
| 16:UM:619:ARG:HB3  | 16:UM:637:ALA:H     | 1.76                     | 0.51              |
| 18:UO:128:HIS:CD2  | 18:UO:172:ARG:HE    | 2.29                     | 0.51              |
| 18:UO:259:ASP:O    | 18:UO:272:LEU:HD12  | 2.11                     | 0.51              |
| 18:UO:284:PHE:CD1  | 18:UO:292:VAL:HA    | 2.45                     | 0.51              |
| 19:UP:185:GLN:OE1  | 19:UP:185:GLN:N     | 2.39                     | 0.51              |
| 21:UR:511:LEU:HD13 | 21:UR:544:VAL:HG21  | 1.91                     | 0.51              |
| 22:US:350:MET:HE1  | 22:US:386:LEU:HB3   | 1.93                     | 0.51              |
| 23:UT:291:LEU:HB3  | 23:UT:295:TYR:CZ    | 2.45                     | 0.51              |
| 23:UT:363:ALA:HB1  | 23:UT:403:LEU:HD21  | 1.92                     | 0.51              |
| 23:UT:489:SER:O    | 23:UT:490:LYS:HG2   | 2.11                     | 0.51              |
| 23:UT:1001:VAL:O   | 23:UT:1005:ASN:ND2  | 2.44                     | 0.51              |
| 23:UT:1399:LEU:HA  | 23:UT:1402:ILE:HG22 | 1.91                     | 0.51              |
| 24:UU:738:ASP:HA   | 42:JJ:269:ARG:NH2   | 2.26                     | 0.51              |
| 25:UV:309:LEU:HB2  | 25:UV:312:ARG:HG2   | 1.91                     | 0.51              |
| 28:CD:44:PHE:CZ    | 28:CD:48:ILE:HD12   | 2.46                     | 0.51              |
| 28:CD:195:VAL:HG13 | 28:CD:216:PHE:HE2   | 1.76                     | 0.51              |
| 29:CE:188:TYR:HB3  | 29:CE:205:TYR:OH    | 2.11                     | 0.51              |
| 30:CG:50:GLU:N     | 30:CG:102:ILE:O     | 2.42                     | 0.51              |
| 31:CH:68:LYS:HE2   | 31:CH:71:LEU:HD12   | 1.91                     | 0.51              |
| 32:CI:142:LEU:HD23 | 32:CI:142:LEU:H     | 1.76                     | 0.51              |
| 33:CJ:139:LEU:HB2  | 33:CJ:157:PHE:CZ    | 2.46                     | 0.51              |
| 36:CM:48:TYR:CG    | 36:CM:94:LYS:HG3    | 2.46                     | 0.51              |
| 38:JC:162:LEU:N    | 38:JC:176:PHE:O     | 2.44                     | 0.51              |
| 39:JF:187:ILE:HD13 | 39:JF:225:VAL:HG11  | 1.92                     | 0.51              |
| 50:DF:200:ASN:HD21 | 50:DF:207:THR:C     | 2.13                     | 0.51              |
| 55:DL:104:HIS:NE2  | 66:D3:349:U:OP1     | 2.43                     | 0.51              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 56:DN:48:SER:OG     | 56:DN:86:GLU:OE2    | 2.25                     | 0.51              |
| 62:DY:15:ASN:HD22   | 62:DY:20:ARG:HE     | 1.59                     | 0.51              |
| 66:D3:647:G:N2      | 66:D3:687:G:H22     | 2.09                     | 0.51              |
| 1:CA:306:LEU:HD11   | 1:CA:313:HIS:HB2    | 1.92                     | 0.51              |
| 4:UA:772:ALA:HA     | 4:UA:775:LEU:HB2    | 1.92                     | 0.51              |
| 8:UE:232:ILE:HG13   | 8:UE:246:VAL:HG13   | 1.91                     | 0.51              |
| 9:UF:336:ASN:O      | 9:UF:339:LEU:HG     | 2.11                     | 0.51              |
| 10:UG:287:TYR:CD1   | 10:UG:304:ARG:HD2   | 2.46                     | 0.51              |
| 10:UG:379:GLU:N     | 10:UG:393:GLY:O     | 2.44                     | 0.51              |
| 13:UJ:81:LEU:HD11   | 13:UJ:125:PHE:HE1   | 1.75                     | 0.51              |
| 13:UJ:1472:VAL:O    | 13:UJ:1476:LEU:HG   | 2.11                     | 0.51              |
| 18:UO:84:VAL:HA     | 18:UO:100:ASP:HA    | 1.92                     | 0.51              |
| 18:UO:215:VAL:HA    | 18:UO:230:GLY:HA3   | 1.92                     | 0.51              |
| 18:UO:229:CYS:HB2   | 18:UO:258:LEU:HD22  | 1.93                     | 0.51              |
| 18:UO:245:LEU:HB3   | 18:UO:246:TYR:CD2   | 2.46                     | 0.51              |
| 18:UO:379:VAL:HG22  | 65:D2:90:G:H5"      | 1.92                     | 0.51              |
| 20:UQ:239:PHE:CD1   | 20:UQ:244:ILE:HD11  | 2.46                     | 0.51              |
| 23:UT:1079:MET:HE2  | 23:UT:1082:ILE:HG21 | 1.93                     | 0.51              |
| 23:UT:1357:ASN:HB2  | 23:UT:1363:LEU:HD11 | 1.92                     | 0.51              |
| 23:UT:1410:LEU:HD21 | 23:UT:1412:GLU:CD   | 2.30                     | 0.51              |
| 23:UT:1677:LEU:HD12 | 23:UT:1678:MET:HE2  | 1.93                     | 0.51              |
| 24:UU:51:VAL:HG12   | 24:UU:83:LEU:HD13   | 1.91                     | 0.51              |
| 24:UU:302:THR:O     | 24:UU:310:ILE:HA    | 2.10                     | 0.51              |
| 25:UV:1221:HIS:HE1  | 37:CN:26:LEU:HD22   | 1.76                     | 0.51              |
| 28:CD:187:ASP:OD2   | 29:CE:180:TYR:OH    | 2.27                     | 0.51              |
| 28:CD:388:ARG:HE    | 30:CG:66:HIS:CG     | 2.29                     | 0.51              |
| 29:CE:19:ASP:HB3    | 29:CE:23:TYR:OH     | 2.10                     | 0.51              |
| 30:CG:16:LEU:O      | 30:CG:20:ILE:HG12   | 2.10                     | 0.51              |
| 35:CL:212:ASN:HB3   | 35:CL:214:ARG:NH2   | 2.26                     | 0.51              |
| 36:CM:91:PRO:HD2    | 36:CM:99:PHE:HE2    | 1.76                     | 0.51              |
| 36:CM:241:TRP:CE2   | 36:CM:262:GLY:HA3   | 2.46                     | 0.51              |
| 36:CM:244:THR:HG22  | 36:CM:259:GLU:HB2   | 1.91                     | 0.51              |
| 47:JP:453:TYR:HE2   | 66:D3:-2:A:C5       | 2.29                     | 0.51              |
| 57:DO:84:ARG:HE     | 57:DO:120:PRO:CG    | 2.24                     | 0.51              |
| 65:D2:379:A:C2      | 65:D2:380:A:C4      | 2.98                     | 0.51              |
| 66:D3:1165:G:C2     | 66:D3:1166:A:C4     | 2.99                     | 0.51              |
| 75:EH:232:LYS:O     | 75:EH:236:THR:N     | 2.43                     | 0.51              |
| 79:EN:646:TYR:O     | 79:EN:650:GLU:N     | 2.40                     | 0.51              |
| 3:JA:6:ILE:HD13     | 3:JA:205:LEU:HB3    | 1.93                     | 0.51              |
| 4:UA:669:ASP:O      | 4:UA:672:THR:OG1    | 2.19                     | 0.51              |
| 1:CB:264:GLN:HB3    | 1:CB:319:ARG:HH21   | 1.75                     | 0.51              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 8:UE:305:TRP:NE1   | 8:UE:307:GLN:OE1    | 2.39                     | 0.51              |
| 8:UE:454:GLU:OE2   | 65:D2:136:U:H5''    | 2.11                     | 0.51              |
| 9:UF:63:VAL:HG22   | 21:UR:26:VAL:HG23   | 1.92                     | 0.51              |
| 13:UJ:247:ALA:HA   | 21:UR:205:ILE:HD11  | 1.91                     | 0.51              |
| 14:UK:196:LYS:HD2  | 65:D2:424:G:P       | 2.51                     | 0.51              |
| 15:UL:42:ILE:HG12  | 15:UL:51:ILE:HG22   | 1.91                     | 0.51              |
| 16:UM:268:GLN:NE2  | 16:UM:277:VAL:HG11  | 2.26                     | 0.51              |
| 16:UM:413:ILE:HB   | 16:UM:426:ILE:HD11  | 1.91                     | 0.51              |
| 16:UM:513:LYS:HE2  | 16:UM:513:LYS:HA    | 1.92                     | 0.51              |
| 16:UM:676:GLY:HA2  | 16:UM:678:TRP:CZ2   | 2.45                     | 0.51              |
| 20:UQ:53:LYS:HG2   | 20:UQ:65:THR:HG23   | 1.93                     | 0.51              |
| 20:UQ:875:MET:HB3  | 20:UQ:887:PHE:HE1   | 1.74                     | 0.51              |
| 22:US:289:PHE:HE2  | 22:US:292:PRO:HA    | 1.75                     | 0.51              |
| 23:UT:1104:SER:HA  | 23:UT:1107:ARG:HG2  | 1.93                     | 0.51              |
| 23:UT:1695:HIS:NE2 | 23:UT:1749:LYS:HD3  | 2.26                     | 0.51              |
| 24:UU:42:GLY:HA3   | 24:UU:49:TYR:CZ     | 2.46                     | 0.51              |
| 25:UV:532:PRO:HG2  | 25:UV:693:LYS:HB3   | 1.93                     | 0.51              |
| 28:CD:18:PHE:CD2   | 28:CD:50:LEU:HA     | 2.45                     | 0.51              |
| 36:CM:193:GLY:HA3  | 36:CM:245:LEU:HD23  | 1.92                     | 0.51              |
| 38:JC:253:TYR:CE1  | 38:JC:265:ILE:HG23  | 2.44                     | 0.51              |
| 45:JN:292:LYS:HG2  | 66:D3:9:U:OP2       | 2.11                     | 0.51              |
| 49:DE:161:LYS:O    | 49:DE:170:THR:OG1   | 2.22                     | 0.51              |
| 55:DL:116:ARG:HE   | 55:DL:117:VAL:H     | 1.59                     | 0.51              |
| 65:D2:426:G:N2     | 65:D2:428:A:H3'     | 2.26                     | 0.51              |
| 66:D3:175:G:C2     | 66:D3:266:A:C4      | 2.99                     | 0.51              |
| 66:D3:379:U:H2'    | 66:D3:380:U:C5      | 2.46                     | 0.51              |
| 66:D3:1130:G:H5''  | 66:D3:1131:A:H2'    | 1.93                     | 0.51              |
| 66:D3:1592:A:N3    | 66:D3:1605:G:C2     | 2.79                     | 0.51              |
| 1:CA:244:VAL:O     | 1:CA:249:GLN:NE2    | 2.43                     | 0.51              |
| 3:JA:658:ARG:HH12  | 3:JA:766:LEU:H      | 1.57                     | 0.51              |
| 3:JA:745:VAL:HG21  | 3:JA:763:LEU:HB3    | 1.93                     | 0.51              |
| 7:UD:533:HIS:HB2   | 7:UD:544:SER:OG     | 2.11                     | 0.51              |
| 8:UE:10:TYR:O      | 8:UE:65:TRP:NE1     | 2.43                     | 0.51              |
| 8:UE:46:TRP:HB3    | 8:UE:48:GLU:OE2     | 2.10                     | 0.51              |
| 9:UF:172:LEU:HD12  | 9:UF:182:TRP:CE2    | 2.45                     | 0.51              |
| 10:UG:284:ARG:HH22 | 47:JP:31:GLU:HG3    | 1.76                     | 0.51              |
| 13:UJ:272:LYS:HG2  | 13:UJ:306:LEU:HD11  | 1.93                     | 0.51              |
| 13:UJ:283:LEU:HD21 | 13:UJ:323:PHE:HA    | 1.92                     | 0.51              |
| 13:UJ:745:TYR:HD2  | 13:UJ:748:LEU:HB2   | 1.75                     | 0.51              |
| 13:UJ:1452:GLU:HA  | 13:UJ:1455:LYS:HD2  | 1.92                     | 0.51              |
| 13:UJ:1544:PHE:HA  | 13:UJ:1547:LEU:HD12 | 1.91                     | 0.51              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 13:UJ:1748:VAL:O    | 13:UJ:1752:LEU:HB2  | 2.11                     | 0.51              |
| 15:UL:22:ASN:ND2    | 15:UL:85:LEU:H      | 2.09                     | 0.51              |
| 15:UL:588:ILE:HB    | 15:UL:600:TRP:HB2   | 1.93                     | 0.51              |
| 17:UN:309:ASP:OD1   | 17:UN:310:HIS:N     | 2.44                     | 0.51              |
| 20:UQ:437:THR:HG22  | 20:UQ:709:ARG:HE    | 1.75                     | 0.51              |
| 21:UR:20:GLN:O      | 21:UR:24:LYS:HG2    | 2.11                     | 0.51              |
| 21:UR:365:ASN:HD21  | 21:UR:372:HIS:CE1   | 2.28                     | 0.51              |
| 23:UT:1352:LEU:O    | 23:UT:1355:ILE:HG22 | 2.11                     | 0.51              |
| 23:UT:1378:ILE:HG12 | 23:UT:1390:SER:OG   | 2.11                     | 0.51              |
| 23:UT:1492:TYR:O    | 23:UT:1495:SER:OG   | 2.29                     | 0.51              |
| 23:UT:1968:ARG:NH1  | 23:UT:2005:ALA:HB2  | 2.25                     | 0.51              |
| 25:UV:846:GLU:OE1   | 25:UV:846:GLU:N     | 2.42                     | 0.51              |
| 25:UV:900:GLU:OE2   | 25:UV:904:HIS:NE2   | 2.44                     | 0.51              |
| 25:UV:1136:LEU:HA   | 25:UV:1139:LEU:HD12 | 1.92                     | 0.51              |
| 29:CE:191:HIS:ND1   | 29:CE:247:ILE:HG12  | 2.27                     | 0.51              |
| 30:CG:81:VAL:HG11   | 30:CG:87:LEU:HD12   | 1.93                     | 0.51              |
| 31:CH:64:ARG:O      | 31:CH:68:LYS:HG2    | 2.11                     | 0.51              |
| 31:CH:449:ASN:OD1   | 31:CH:450:ASP:N     | 2.43                     | 0.51              |
| 35:CL:210:VAL:O     | 35:CL:210:VAL:HG22  | 2.10                     | 0.51              |
| 35:CL:854:PHE:CZ    | 35:CL:888:PRO:HD2   | 2.45                     | 0.51              |
| 38:JC:280:LEU:HB2   | 38:JC:287:ASN:HB2   | 1.92                     | 0.51              |
| 39:JG:104:ILE:HD11  | 39:JG:109:LYS:HB2   | 1.92                     | 0.51              |
| 46:JO:260:VAL:HA    | 46:JO:263:GLU:HG2   | 1.92                     | 0.51              |
| 51:DG:187:LYS:HZ2   | 66:D3:141:U:H5      | 1.58                     | 0.51              |
| 66:D3:487:G:N2      | 66:D3:488:G:C5      | 2.79                     | 0.51              |
| 66:D3:527:A:H2'     | 66:D3:528:U:C6      | 2.46                     | 0.51              |
| 67:D4:76:U:H2'      | 67:D4:77:U:C6       | 2.46                     | 0.51              |
| 69:EB:164:LYS:O     | 69:EB:185:VAL:N     | 2.35                     | 0.51              |
| 79:EN:93:VAL:O      | 79:EN:113:VAL:N     | 2.43                     | 0.51              |
| 79:EN:1022:GLY:O    | 79:EN:1026:ARG:N    | 2.42                     | 0.51              |
| 4:UA:254:HIS:HB3    | 4:UA:292:PHE:CD2    | 2.46                     | 0.50              |
| 4:UA:519:LEU:HD23   | 4:UA:519:LEU:H      | 1.75                     | 0.50              |
| 3:JB:751:ALA:HA     | 3:JB:758:HIS:HA     | 1.92                     | 0.50              |
| 5:UB:524:LEU:O      | 5:UB:527:GLN:HB3    | 2.11                     | 0.50              |
| 7:UD:213:TRP:NE1    | 7:UD:225:LEU:HB3    | 2.26                     | 0.50              |
| 7:UD:490:SER:O      | 7:UD:493:ASP:N      | 2.44                     | 0.50              |
| 10:UG:116:ILE:CG1   | 10:UG:398:ILE:HD12  | 2.41                     | 0.50              |
| 10:UG:482:ASP:OD2   | 10:UG:512:ARG:NE    | 2.43                     | 0.50              |
| 11:UH:606:ASP:OD2   | 11:UH:606:ASP:N     | 2.44                     | 0.50              |
| 13:UJ:187:ASP:OD2   | 29:CE:414:ARG:NH2   | 2.44                     | 0.50              |
| 13:UJ:771:ILE:O     | 13:UJ:775:ILE:HG12  | 2.11                     | 0.50              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 14:UK:221:GLN:O    | 14:UK:224:LEU:HB2   | 2.11                     | 0.50              |
| 15:UL:189:TRP:HD1  | 15:UL:196:CYS:HA    | 1.77                     | 0.50              |
| 15:UL:294:ARG:O    | 15:UL:297:LYS:HG3   | 2.12                     | 0.50              |
| 15:UL:789:GLN:OE1  | 15:UL:790:GLY:N     | 2.44                     | 0.50              |
| 16:UM:490:HIS:CE1  | 16:UM:514:THR:HG23  | 2.46                     | 0.50              |
| 21:UR:211:ILE:O    | 21:UR:214:THR:OG1   | 2.23                     | 0.50              |
| 21:UR:242:ASN:ND2  | 21:UR:247:SER:OG    | 2.44                     | 0.50              |
| 22:US:329:ARG:HA   | 22:US:329:ARG:NH1   | 2.25                     | 0.50              |
| 23:UT:1338:SER:HA  | 23:UT:1377:PHE:HE1  | 1.75                     | 0.50              |
| 23:UT:1441:LEU:O   | 23:UT:1468:ARG:NH2  | 2.45                     | 0.50              |
| 23:UT:1751:TYR:HB3 | 23:UT:1795:ARG:HG3  | 1.92                     | 0.50              |
| 25:UV:117:LYS:HB3  | 25:UV:119:LYS:HG2   | 1.92                     | 0.50              |
| 25:UV:960:LYS:HA   | 25:UV:963:LYS:HZ2   | 1.75                     | 0.50              |
| 25:UV:1048:SER:OG  | 25:UV:1050:ILE:HG22 | 2.11                     | 0.50              |
| 28:CD:400:PHE:CZ   | 30:CG:60:PRO:HD3    | 2.45                     | 0.50              |
| 29:CE:37:LYS:HA    | 29:CE:40:LYS:HE2    | 1.94                     | 0.50              |
| 30:CG:64:LEU:HD23  | 30:CG:64:LEU:H      | 1.75                     | 0.50              |
| 32:CI:62:SER:O     | 32:CI:71:ARG:NH1    | 2.44                     | 0.50              |
| 35:CL:40:ALA:O     | 35:CL:43:MET:HG3    | 2.11                     | 0.50              |
| 35:CL:310:THR:HG22 | 35:CL:312:PHE:H     | 1.75                     | 0.50              |
| 35:CL:551:LYS:O    | 35:CL:555:MET:HG2   | 2.11                     | 0.50              |
| 38:JC:210:ARG:NH1  | 43:JK:487:ASP:OD2   | 2.45                     | 0.50              |
| 38:JC:254:ILE:HB   | 38:JC:264:ILE:HB    | 1.93                     | 0.50              |
| 39:JG:204:VAL:HG21 | 39:JG:241:PHE:CE2   | 2.45                     | 0.50              |
| 50:DF:103:ASN:HA   | 50:DF:106:LYS:NZ    | 2.25                     | 0.50              |
| 51:DG:57:ASP:OD2   | 51:DG:61:PHE:HB2    | 2.11                     | 0.50              |
| 51:DG:139:ASN:HA   | 51:DG:142:ARG:HD2   | 1.93                     | 0.50              |
| 52:DH:60:ILE:HB    | 52:DH:92:PHE:HA     | 1.94                     | 0.50              |
| 61:DX:112:LYS:NZ   | 67:D4:10:C:OP1      | 2.45                     | 0.50              |
| 65:D2:288:G:N2     | 65:D2:289:U:C2      | 2.79                     | 0.50              |
| 66:D3:337:G:P      | 66:D3:339:C:H41     | 2.34                     | 0.50              |
| 66:D3:766:U:O2'    | 66:D3:767:U:OP2     | 2.29                     | 0.50              |
| 66:D3:1753:A:H2'   | 66:D3:1754:A:C8     | 2.45                     | 0.50              |
| 3:JA:106:VAL:HG23  | 3:JA:110:GLU:HG3    | 1.93                     | 0.50              |
| 3:JA:651:SER:O     | 3:JA:654:ILE:HG22   | 2.11                     | 0.50              |
| 4:UA:402:MET:CE    | 4:UA:416:LEU:HD21   | 2.42                     | 0.50              |
| 4:UA:441:SER:O     | 4:UA:443:GLU:N      | 2.45                     | 0.50              |
| 4:UA:467:ASP:OD1   | 4:UA:468:ALA:N      | 2.44                     | 0.50              |
| 4:UA:492:SER:C     | 4:UA:494:ASP:H      | 2.15                     | 0.50              |
| 5:UB:733:THR:O     | 5:UB:736:GLU:HG3    | 2.11                     | 0.50              |
| 7:UD:185:ARG:NH2   | 30:CF:126:ILE:HG22  | 2.25                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:UE:90:VAL:HG23   | 8:UE:91:LEU:H      | 1.76                     | 0.50              |
| 8:UE:94:GLU:OE1    | 8:UE:95:VAL:N      | 2.43                     | 0.50              |
| 10:UG:350:ASP:OD1  | 10:UG:351:SER:N    | 2.45                     | 0.50              |
| 13:UJ:763:LEU:HB3  | 13:UJ:768:LYS:HZ3  | 1.76                     | 0.50              |
| 13:UJ:1547:LEU:O   | 13:UJ:1551:LEU:HG  | 2.11                     | 0.50              |
| 14:UK:184:ILE:O    | 14:UK:184:ILE:HG13 | 2.11                     | 0.50              |
| 16:UM:18:GLY:HA3   | 16:UM:37:LEU:HA    | 1.92                     | 0.50              |
| 17:UN:298:TRP:CD1  | 47:JP:231:GLU:OE1  | 2.64                     | 0.50              |
| 18:UO:298:PHE:HE1  | 18:UO:330:ARG:HH21 | 1.58                     | 0.50              |
| 18:UO:374:ILE:HG12 | 21:UR:289:HIS:CD2  | 2.41                     | 0.50              |
| 18:UO:405:PHE:HE2  | 18:UO:442:LEU:HD13 | 1.76                     | 0.50              |
| 23:UT:332:ASP:O    | 23:UT:336:ILE:HG12 | 2.12                     | 0.50              |
| 23:UT:832:LEU:HB3  | 23:UT:868:LEU:HD22 | 1.93                     | 0.50              |
| 23:UT:1241:GLN:HA  | 23:UT:1244:LEU:HG  | 1.91                     | 0.50              |
| 24:UU:535:THR:OG1  | 24:UU:536:LEU:N    | 2.44                     | 0.50              |
| 28:CD:382:LYS:NZ   | 67:D4:256:G:OP1    | 2.37                     | 0.50              |
| 30:CG:35:LYS:NZ    | 67:D4:254:A:C5     | 2.80                     | 0.50              |
| 31:CH:545:LYS:HE2  | 31:CH:556:VAL:O    | 2.10                     | 0.50              |
| 35:CL:38:LYS:HA    | 35:CL:41:ARG:HG2   | 1.92                     | 0.50              |
| 35:CL:562:GLU:HA   | 35:CL:565:ARG:HG3  | 1.92                     | 0.50              |
| 35:CL:890:CYS:SG   | 35:CL:919:VAL:HG11 | 2.51                     | 0.50              |
| 36:CM:130:ILE:HG13 | 36:CM:131:GLU:N    | 2.27                     | 0.50              |
| 38:JC:329:PHE:O    | 38:JC:340:THR:HA   | 2.11                     | 0.50              |
| 39:JF:49:SER:H     | 39:JF:209:MET:HE3  | 1.75                     | 0.50              |
| 46:JO:166:VAL:HG12 | 46:JO:171:VAL:HG22 | 1.93                     | 0.50              |
| 47:JP:296:ARG:NH1  | 66:D3:-3:U:O2      | 2.45                     | 0.50              |
| 49:DE:100:ARG:HB3  | 49:DE:112:HIS:HB3  | 1.93                     | 0.50              |
| 52:DH:93:LEU:HA    | 52:DH:128:ASP:OD1  | 2.11                     | 0.50              |
| 52:DH:112:ARG:HH22 | 66:D3:638:U:H1'    | 1.75                     | 0.50              |
| 54:DJ:68:LYS:HG2   | 54:DJ:72:GLU:OE2   | 2.11                     | 0.50              |
| 65:D2:269:G:C2     | 65:D2:270:U:C2     | 2.99                     | 0.50              |
| 65:D2:307:C:O2'    | 65:D2:311:C:OP2    | 2.28                     | 0.50              |
| 65:D2:311:C:C2     | 65:D2:312:U:C5     | 2.99                     | 0.50              |
| 66:D3:1130:G:H3'   | 66:D3:1131:A:C8    | 2.46                     | 0.50              |
| 66:D3:1130:G:H3'   | 66:D3:1131:A:H8    | 1.76                     | 0.50              |
| 66:D3:1629:G:H1'   | 66:D3:1631:A:H62   | 1.76                     | 0.50              |
| 67:D4:12:U:H3      | 67:D4:13:C:N4      | 2.09                     | 0.50              |
| 78:EK:618:TYR:N    | 78:EK:648:SER:O    | 2.41                     | 0.50              |
| 4:UA:272:THR:O     | 4:UA:273:ARG:HD3   | 2.12                     | 0.50              |
| 4:UA:580:PHE:HZ    | 4:UA:602:CYS:HG    | 1.59                     | 0.50              |
| 4:UA:813:HIS:HB2   | 4:UA:817:PHE:HE2   | 1.76                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CB:214:ARG:HB2   | 1:CB:217:ILE:HD12  | 1.93                     | 0.50              |
| 7:UD:225:LEU:O     | 7:UD:225:LEU:HD12  | 2.12                     | 0.50              |
| 8:UE:234:GLU:HB3   | 8:UE:247:THR:HB    | 1.93                     | 0.50              |
| 9:UF:169:GLN:CD    | 17:UN:339:GLN:HE22 | 2.15                     | 0.50              |
| 9:UF:313:PHE:O     | 9:UF:316:SER:OG    | 2.25                     | 0.50              |
| 13:UJ:717:GLU:OE1  | 13:UJ:747:GLN:NE2  | 2.44                     | 0.50              |
| 13:UJ:1439:SER:O   | 13:UJ:1443:LEU:HG  | 2.12                     | 0.50              |
| 13:UJ:1567:THR:OG1 | 13:UJ:1570:GLU:OE1 | 2.26                     | 0.50              |
| 13:UJ:1614:GLU:HA  | 13:UJ:1619:ARG:NH2 | 2.27                     | 0.50              |
| 17:UN:337:GLU:CD   | 17:UN:337:GLU:H    | 2.14                     | 0.50              |
| 18:UO:90:ARG:HG3   | 18:UO:132:PHE:CD1  | 2.47                     | 0.50              |
| 18:UO:251:PHE:CD1  | 18:UO:255:VAL:HG12 | 2.46                     | 0.50              |
| 18:UO:405:PHE:CE2  | 18:UO:442:LEU:HD13 | 2.46                     | 0.50              |
| 20:UQ:663:LYS:O    | 20:UQ:670:LEU:HD12 | 2.11                     | 0.50              |
| 21:UR:41:ASN:ND2   | 21:UR:43:ASP:OD2   | 2.43                     | 0.50              |
| 22:US:447:ASP:OD1  | 22:US:448:VAL:N    | 2.44                     | 0.50              |
| 22:US:467:ALA:O    | 22:US:470:MET:HB3  | 2.10                     | 0.50              |
| 23:UT:197:SER:HA   | 23:UT:200:VAL:HG22 | 1.93                     | 0.50              |
| 23:UT:213:ARG:O    | 23:UT:217:GLU:HG2  | 2.11                     | 0.50              |
| 23:UT:216:PHE:CE1  | 23:UT:271:SER:HB2  | 2.46                     | 0.50              |
| 23:UT:366:ILE:HG22 | 23:UT:407:ARG:HD3  | 1.94                     | 0.50              |
| 23:UT:1531:ILE:O   | 23:UT:1535:LYS:HG2 | 2.11                     | 0.50              |
| 24:UU:484:ILE:HB   | 24:UU:498:TYR:HB2  | 1.94                     | 0.50              |
| 25:UV:141:TRP:NE1  | 25:UV:178:TYR:HB3  | 2.27                     | 0.50              |
| 25:UV:1166:ARG:NH2 | 25:UV:1179:LYS:O   | 2.45                     | 0.50              |
| 26:UX:155:THR:OG1  | 26:UX:156:ASN:N    | 2.43                     | 0.50              |
| 28:CD:159:SER:OG   | 28:CD:160:ARG:N    | 2.44                     | 0.50              |
| 29:CE:366:LYS:HE3  | 29:CE:393:LYS:NZ   | 2.27                     | 0.50              |
| 36:CM:200:VAL:HG11 | 36:CM:204:LEU:HD13 | 1.93                     | 0.50              |
| 47:JP:270:ASN:HB3  | 47:JP:313:PHE:CE2  | 2.46                     | 0.50              |
| 49:DE:15:PRO:HG2   | 49:DE:18:TRP:CD2   | 2.47                     | 0.50              |
| 49:DE:238:LEU:HD12 | 49:DE:239:PRO:HD2  | 1.93                     | 0.50              |
| 55:DL:59:PRO:HD2   | 55:DL:112:SER:HB2  | 1.93                     | 0.50              |
| 56:DN:31:GLU:H     | 56:DN:31:GLU:CD    | 2.14                     | 0.50              |
| 56:DN:61:THR:HG23  | 56:DN:62:GLN:H     | 1.75                     | 0.50              |
| 58:DQ:122:ARG:NH1  | 66:D3:1584:G:OP2   | 2.44                     | 0.50              |
| 65:D2:145:A:H2'    | 65:D2:146:G:H8     | 1.77                     | 0.50              |
| 66:D3:449:C:H2'    | 66:D3:450:U:C6     | 2.46                     | 0.50              |
| 66:D3:590:C:H2'    | 66:D3:591:A:H8     | 1.76                     | 0.50              |
| 66:D3:1590:G:N2    | 66:D3:1591:C:C2    | 2.79                     | 0.50              |
| 2:DA:127:VAL:HG21  | 2:DA:176:VAL:HG21  | 1.94                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:DA:214:LYS:HE2   | 2:DA:216:LYS:HG2   | 1.93                     | 0.50              |
| 3:JA:69:HIS:ND1    | 3:JA:71:LYS:HB3    | 2.27                     | 0.50              |
| 3:JA:752:ASN:ND2   | 3:JA:757:GLU:O     | 2.42                     | 0.50              |
| 4:UA:188:ASN:HD21  | 65:D2:321:G:H1'    | 1.75                     | 0.50              |
| 4:UA:793:GLU:HA    | 4:UA:796:LEU:HB2   | 1.93                     | 0.50              |
| 4:UA:836:VAL:O     | 4:UA:840:THR:HG23  | 2.11                     | 0.50              |
| 4:UA:845:THR:O     | 4:UA:849:LEU:HD23  | 2.12                     | 0.50              |
| 1:CB:286:PHE:O     | 1:CB:290:VAL:HG23  | 2.12                     | 0.50              |
| 5:UB:517:VAL:C     | 5:UB:520:PRO:HD2   | 2.32                     | 0.50              |
| 5:UB:769:GLU:O     | 5:UB:773:GLU:HG2   | 2.10                     | 0.50              |
| 8:UE:282:VAL:HG12  | 8:UE:283:SER:O     | 2.11                     | 0.50              |
| 8:UE:456:VAL:O     | 8:UE:459:ASN:HB2   | 2.11                     | 0.50              |
| 9:UF:50:ILE:HD11   | 9:UF:109:PHE:CG    | 2.46                     | 0.50              |
| 11:UH:673:THR:HG21 | 12:UI:493:LEU:HD13 | 1.93                     | 0.50              |
| 13:UJ:684:TYR:HE2  | 13:UJ:723:LEU:HD23 | 1.75                     | 0.50              |
| 13:UJ:1581:LYS:O   | 13:UJ:1584:GLU:HG3 | 2.11                     | 0.50              |
| 15:UL:19:SER:N     | 15:UL:44:SER:O     | 2.40                     | 0.50              |
| 15:UL:276:ASN:HD21 | 15:UL:282:GLU:HG2  | 1.76                     | 0.50              |
| 15:UL:279:LYS:HG2  | 15:UL:335:LEU:O    | 2.11                     | 0.50              |
| 15:UL:923:GLU:HG2  | 24:UU:745:LYS:HZ3  | 1.77                     | 0.50              |
| 16:UM:595:ALA:HA   | 16:UM:619:ARG:HD3  | 1.93                     | 0.50              |
| 18:UO:211:HIS:ND1  | 18:UO:235:LYS:HE2  | 2.27                     | 0.50              |
| 21:UR:241:ALA:HB3  | 21:UR:586:VAL:CG2  | 2.41                     | 0.50              |
| 21:UR:465:THR:HG23 | 21:UR:467:THR:H    | 1.76                     | 0.50              |
| 21:UR:560:THR:O    | 21:UR:562:LEU:N    | 2.43                     | 0.50              |
| 23:UT:95:ILE:O     | 23:UT:98:HIS:ND1   | 2.45                     | 0.50              |
| 23:UT:457:PHE:O    | 23:UT:461:ILE:HG12 | 2.11                     | 0.50              |
| 23:UT:472:ASP:O    | 23:UT:476:LEU:HG   | 2.11                     | 0.50              |
| 23:UT:1204:SER:O   | 23:UT:1208:MET:HG3 | 2.11                     | 0.50              |
| 24:UU:140:TYR:CD1  | 24:UU:153:PHE:HA   | 2.47                     | 0.50              |
| 24:UU:869:THR:O    | 24:UU:873:LYS:HG2  | 2.11                     | 0.50              |
| 25:UV:148:GLU:O    | 25:UV:151:SER:OG   | 2.20                     | 0.50              |
| 31:CH:162:CYS:SG   | 31:CH:525:GLN:HB3  | 2.51                     | 0.50              |
| 31:CH:296:TYR:HB3  | 31:CH:328:ILE:HD11 | 1.94                     | 0.50              |
| 33:CJ:201:ARG:O    | 33:CJ:205:ILE:HG13 | 2.11                     | 0.50              |
| 35:CL:126:ASN:HB3  | 35:CL:853:ARG:HE   | 1.76                     | 0.50              |
| 35:CL:1107:LYS:HZ2 | 65:D2:412:A:C5'    | 2.23                     | 0.50              |
| 36:CM:45:LEU:HG    | 36:CM:49:GLU:HB2   | 1.94                     | 0.50              |
| 38:JC:223:ASN:HB3  | 38:JC:229:PHE:CE1  | 2.46                     | 0.50              |
| 39:JF:130:ILE:HD11 | 39:JF:137:PHE:HD1  | 1.77                     | 0.50              |
| 44:JM:131:ASP:OD2  | 44:JM:132:PRO:HD2  | 2.12                     | 0.50              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 50:DF:30:PRO:O     | 50:DF:33:VAL:HB     | 2.12                     | 0.50              |
| 52:DH:50:ASP:HB3   | 52:DH:56:LYS:HE2    | 1.94                     | 0.50              |
| 54:DJ:110:GLN:OE1  | 54:DJ:126:ARG:HB2   | 2.11                     | 0.50              |
| 65:D2:187:A:H2'    | 65:D2:188:A:C8      | 2.47                     | 0.50              |
| 65:D2:306:G:C2     | 65:D2:307:C:C2      | 2.99                     | 0.50              |
| 65:D2:415:U:H2'    | 65:D2:416:A:H8      | 1.77                     | 0.50              |
| 66:D3:147:A:OP2    | 66:D3:166:C:N4      | 2.45                     | 0.50              |
| 66:D3:312:A:N3     | 66:D3:314:C:H3'     | 2.26                     | 0.50              |
| 66:D3:538:A:H5''   | 66:D3:543:C:H41     | 1.77                     | 0.50              |
| 66:D3:592:A:C5     | 66:D3:593:U:N3      | 2.80                     | 0.50              |
| 66:D3:949:C:H2'    | 66:D3:950:C:C6      | 2.46                     | 0.50              |
| 66:D3:1469:A:C5    | 66:D3:1470:C:C5     | 3.00                     | 0.50              |
| 5:UB:520:PRO:HG3   | 22:US:510:GLU:HG2   | 1.94                     | 0.50              |
| 5:UB:527:GLN:NE2   | 22:US:503:TYR:HD2   | 2.09                     | 0.50              |
| 7:UD:481:ILE:HB    | 7:UD:485:LYS:HB3    | 1.94                     | 0.50              |
| 8:UE:497:PRO:O     | 8:UE:500:VAL:HG22   | 2.11                     | 0.50              |
| 13:UJ:170:SER:OG   | 13:UJ:171:GLU:N     | 2.45                     | 0.50              |
| 13:UJ:572:ARG:CZ   | 13:UJ:669:VAL:HB    | 2.41                     | 0.50              |
| 15:UL:180:THR:HG23 | 15:UL:210:LEU:HD11  | 1.94                     | 0.50              |
| 15:UL:588:ILE:O    | 15:UL:599:ILE:HD12  | 2.11                     | 0.50              |
| 18:UO:186:THR:HG22 | 18:UO:194:ARG:HB2   | 1.93                     | 0.50              |
| 20:UQ:262:MET:SD   | 20:UQ:273:VAL:HG12  | 2.52                     | 0.50              |
| 22:US:228:HIS:HD2  | 22:US:288:HIS:HE1   | 1.58                     | 0.50              |
| 22:US:349:LEU:HD23 | 22:US:355:ARG:NH2   | 2.26                     | 0.50              |
| 23:UT:280:MET:HE1  | 23:UT:733:VAL:HG21  | 1.93                     | 0.50              |
| 23:UT:662:PHE:HE2  | 23:UT:688:VAL:HG21  | 1.76                     | 0.50              |
| 23:UT:801:TYR:HA   | 23:UT:853:HIS:NE2   | 2.27                     | 0.50              |
| 23:UT:1919:ILE:HA  | 23:UT:1922:ILE:HG22 | 1.93                     | 0.50              |
| 23:UT:2000:PHE:HB3 | 23:UT:2004:LYS:NZ   | 2.26                     | 0.50              |
| 24:UU:523:ASP:N    | 24:UU:523:ASP:OD1   | 2.44                     | 0.50              |
| 27:UZ:59:LEU:HD11  | 27:UZ:215:ASN:OD1   | 2.12                     | 0.50              |
| 28:CD:230:ASN:N    | 28:CD:233:SER:OG    | 2.44                     | 0.50              |
| 30:CG:66:HIS:CG    | 30:CG:67:LEU:N      | 2.79                     | 0.50              |
| 31:CH:174:GLU:HG3  | 31:CH:176:SER:H     | 1.77                     | 0.50              |
| 36:CM:15:GLN:O     | 36:CM:20:ARG:NH1    | 2.45                     | 0.50              |
| 38:JC:189:ASN:O    | 38:JC:193:GLY:CA    | 2.50                     | 0.50              |
| 38:JC:327:GLY:O    | 38:JC:342:TYR:HA    | 2.11                     | 0.50              |
| 39:JG:31:LEU:HD12  | 39:JG:40:ARG:NH2    | 2.27                     | 0.50              |
| 45:JN:262:ILE:HD13 | 46:JO:165:LEU:HD11  | 1.92                     | 0.50              |
| 47:JP:66:HIS:CE1   | 47:JP:93:LYS:HG3    | 2.47                     | 0.50              |
| 47:JP:121:PRO:HA   | 47:JP:192:SER:CB    | 2.42                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 52:DH:113:PRO:O    | 52:DH:117:THR:OG1  | 2.18                     | 0.50              |
| 53:DI:31:ARG:HB2   | 53:DI:56:ARG:HH22  | 1.77                     | 0.50              |
| 66:D3:332:U:H3     | 66:D3:334:G:H8     | 1.60                     | 0.50              |
| 66:D3:1054:U:H3    | 66:D3:1065:A:H61   | 1.58                     | 0.50              |
| 66:D3:1777:G:H2'   | 66:D3:1778:G:C8    | 2.47                     | 0.50              |
| 4:UA:426:THR:OG1   | 4:UA:427:GLY:N     | 2.43                     | 0.50              |
| 4:UA:580:PHE:HZ    | 4:UA:602:CYS:SG    | 2.34                     | 0.50              |
| 5:UB:314:MET:HA    | 5:UB:512:ASP:HA    | 1.92                     | 0.50              |
| 5:UB:571:ILE:HA    | 5:UB:574:THR:HG22  | 1.93                     | 0.50              |
| 7:UD:43:PRO:HD2    | 7:UD:757:ARG:NH1   | 2.26                     | 0.50              |
| 7:UD:375:VAL:HB    | 7:UD:757:ARG:HH21  | 1.76                     | 0.50              |
| 8:UE:344:ASP:N     | 8:UE:348:LYS:O     | 2.28                     | 0.50              |
| 8:UE:466:ARG:HD3   | 8:UE:504:TRP:CH2   | 2.47                     | 0.50              |
| 13:UJ:114:THR:O    | 13:UJ:118:THR:HG22 | 2.12                     | 0.50              |
| 13:UJ:1556:PHE:CZ  | 13:UJ:1600:PRO:HB2 | 2.47                     | 0.50              |
| 15:UL:361:THR:HG22 | 15:UL:386:GLU:HB3  | 1.92                     | 0.50              |
| 16:UM:585:ASN:ND2  | 16:UM:630:ASP:HA   | 2.27                     | 0.50              |
| 18:UO:85:TYR:CD2   | 18:UO:128:HIS:HA   | 2.46                     | 0.50              |
| 22:US:349:LEU:O    | 22:US:355:ARG:NH2  | 2.45                     | 0.50              |
| 23:UT:448:VAL:HA   | 23:UT:451:VAL:HG23 | 1.93                     | 0.50              |
| 23:UT:1846:PHE:CE2 | 26:UX:62:PRO:HD3   | 2.46                     | 0.50              |
| 25:UV:781:ASP:HA   | 25:UV:851:LYS:O    | 2.11                     | 0.50              |
| 27:UZ:243:PHE:HA   | 27:UZ:252:LEU:O    | 2.11                     | 0.50              |
| 30:CF:78:TYR:C     | 30:CF:121:ILE:HD11 | 2.32                     | 0.50              |
| 33:CJ:93:SER:HB3   | 33:CJ:142:LEU:O    | 2.12                     | 0.50              |
| 35:CL:257:LEU:O    | 35:CL:261:GLN:HG2  | 2.11                     | 0.50              |
| 38:JC:6:THR:HG23   | 38:JC:13:VAL:H     | 1.76                     | 0.50              |
| 39:JF:54:LYS:NZ    | 39:JF:63:ASP:OD2   | 2.44                     | 0.50              |
| 42:JJ:114:THR:HA   | 42:JJ:117:TYR:HE2  | 1.76                     | 0.50              |
| 51:DG:70:PRO:HB3   | 51:DG:101:ILE:HB   | 1.94                     | 0.50              |
| 58:DQ:58:ASP:HA    | 58:DQ:61:SER:HB3   | 1.92                     | 0.50              |
| 61:DX:121:ARG:HD2  | 61:DX:122:PHE:CZ   | 2.47                     | 0.50              |
| 66:D3:330:G:H2'    | 66:D3:331:A:C8     | 2.46                     | 0.50              |
| 66:D3:1671:A:H3'   | 66:D3:1672:G:C8    | 2.45                     | 0.50              |
| 1:CA:185:SER:OG    | 1:CA:216:ASN:HB2   | 2.12                     | 0.50              |
| 2:DA:145:LYS:HB2   | 2:DA:149:GLN:HG3   | 1.93                     | 0.50              |
| 3:JA:773:TRP:HA    | 3:JA:776:GLU:HB2   | 1.92                     | 0.50              |
| 1:CB:221:ILE:HD13  | 29:CE:148:GLY:HA3  | 1.93                     | 0.50              |
| 5:UB:537:LEU:HA    | 5:UB:540:ILE:HD12  | 1.92                     | 0.50              |
| 6:UC:548:LYS:HA    | 61:DX:139:LYS:NZ   | 2.26                     | 0.50              |
| 7:UD:389:ARG:CZ    | 7:UD:404:MET:HB3   | 2.42                     | 0.50              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 8:UE:150:LYS:HB2    | 8:UE:166:ALA:HB3   | 1.94                     | 0.50              |
| 8:UE:300:LEU:N      | 8:UE:319:TRP:HE1   | 2.10                     | 0.50              |
| 8:UE:434:THR:OG1    | 8:UE:467:ASP:OD2   | 2.18                     | 0.50              |
| 10:UG:527:ARG:HH12  | 65:D2:366:A:P      | 2.35                     | 0.50              |
| 13:UJ:109:TRP:CH2   | 13:UJ:118:THR:HG21 | 2.46                     | 0.50              |
| 13:UJ:585:ILE:HA    | 13:UJ:588:LEU:HD12 | 1.94                     | 0.50              |
| 13:UJ:728:GLU:HB2   | 13:UJ:732:PHE:HD1  | 1.76                     | 0.50              |
| 15:UL:359:SER:O     | 15:UL:361:THR:N    | 2.45                     | 0.50              |
| 16:UM:266:ILE:HB    | 16:UM:283:LYS:HZ3  | 1.75                     | 0.50              |
| 20:UQ:725:ASN:O     | 20:UQ:740:LYS:N    | 2.44                     | 0.50              |
| 22:US:208:TYR:O     | 22:US:212:LEU:HG   | 2.11                     | 0.50              |
| 23:UT:417:LEU:HD11  | 23:UT:451:VAL:HG11 | 1.94                     | 0.50              |
| 23:UT:535:ASN:HB3   | 23:UT:537:LEU:HD23 | 1.94                     | 0.50              |
| 23:UT:841:ILE:O     | 23:UT:844:VAL:HG12 | 2.12                     | 0.50              |
| 23:UT:1733:LYS:HD3  | 23:UT:1748:ASN:HB2 | 1.93                     | 0.50              |
| 24:UU:609:ILE:HD12  | 24:UU:625:VAL:HG21 | 1.93                     | 0.50              |
| 24:UU:846:ASP:OD2   | 24:UU:847:LEU:N    | 2.44                     | 0.50              |
| 25:UV:1100:VAL:HG22 | 25:UV:1234:PHE:CD1 | 2.47                     | 0.50              |
| 34:CK:311:ILE:O     | 34:CK:315:GLU:HG3  | 2.12                     | 0.50              |
| 35:CL:241:HIS:HB2   | 35:CL:851:TRP:HZ2  | 1.76                     | 0.50              |
| 35:CL:247:ASP:OD2   | 35:CL:273:GLY:HA2  | 2.12                     | 0.50              |
| 35:CL:560:PRO:HB2   | 36:CM:320:GLU:OE1  | 2.11                     | 0.50              |
| 36:CM:189:SER:N     | 36:CM:248:GLN:O    | 2.43                     | 0.50              |
| 42:JJ:105:ARG:HG3   | 42:JJ:163:THR:O    | 2.11                     | 0.50              |
| 49:DE:124:GLY:HA2   | 49:DE:142:HIS:CE1  | 2.46                     | 0.50              |
| 49:DE:209:HIS:CD2   | 49:DE:219:VAL:HG22 | 2.46                     | 0.50              |
| 55:DL:55:ASP:HB3    | 55:DL:58:CYS:HB2   | 1.94                     | 0.50              |
| 56:DN:20:ARG:HH12   | 66:D3:862:A:P      | 2.34                     | 0.50              |
| 66:D3:314:C:H42     | 66:D3:354:C:H42    | 1.59                     | 0.50              |
| 66:D3:491:C:H2'     | 66:D3:492:A:H8     | 1.75                     | 0.50              |
| 66:D3:528:U:H2'     | 66:D3:529:A:H8     | 1.77                     | 0.50              |
| 67:D4:98:U:H2'      | 67:D4:99:U:C6      | 2.47                     | 0.50              |
| 79:EN:123:VAL:HA    | 79:EN:315:HIS:HA   | 1.93                     | 0.50              |
| 1:CA:195:TYR:CD1    | 1:CA:218:ILE:HG12  | 2.46                     | 0.50              |
| 2:DA:209:ASN:OD1    | 2:DA:211:HIS:HE1   | 1.95                     | 0.50              |
| 3:JA:202:ASP:OD1    | 3:JA:203:ASP:N     | 2.42                     | 0.50              |
| 4:UA:259:ASN:OD1    | 4:UA:260:GLN:N     | 2.38                     | 0.50              |
| 4:UA:414:TRP:CE3    | 4:UA:421:ASN:HB3   | 2.46                     | 0.50              |
| 4:UA:785:PHE:O      | 4:UA:789:SER:HB2   | 2.12                     | 0.50              |
| 7:UD:32:ILE:HA      | 11:UH:720:TYR:HB2  | 1.94                     | 0.50              |
| 7:UD:744:VAL:HG22   | 7:UD:754:ILE:HG22  | 1.93                     | 0.50              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 11:UH:295:TYR:HA    | 11:UH:302:LEU:HA    | 1.93                     | 0.50              |
| 13:UJ:726:PRO:HB3   | 13:UJ:762:SER:HB2   | 1.94                     | 0.50              |
| 14:UK:14:ARG:HE     | 66:D3:583:C:HO2'    | 1.59                     | 0.50              |
| 15:UL:200:HIS:ND1   | 16:UM:664:GLU:OE2   | 2.44                     | 0.50              |
| 16:UM:556:THR:OG1   | 16:UM:557:VAL:N     | 2.45                     | 0.50              |
| 18:UO:173:THR:HG21  | 18:UO:217:ASN:HA    | 1.94                     | 0.50              |
| 20:UQ:573:CYS:SG    | 20:UQ:585:TRP:HB2   | 2.51                     | 0.50              |
| 21:UR:216:TYR:CZ    | 24:UU:247:PRO:HD2   | 2.46                     | 0.50              |
| 22:US:356:ALA:O     | 22:US:360:ARG:HD3   | 2.12                     | 0.50              |
| 22:US:406:ILE:HD13  | 22:US:412:CYS:HB2   | 1.93                     | 0.50              |
| 22:US:428:THR:HG22  | 22:US:431:GLN:HG2   | 1.93                     | 0.50              |
| 22:US:503:TYR:O     | 22:US:507:LEU:HG    | 2.11                     | 0.50              |
| 23:UT:75:GLN:HB2    | 31:CH:125:VAL:HG21  | 1.93                     | 0.50              |
| 23:UT:76:THR:O      | 23:UT:80:ILE:HG13   | 2.12                     | 0.50              |
| 23:UT:494:THR:OG1   | 23:UT:495:GLU:OE1   | 2.30                     | 0.50              |
| 23:UT:1670:LEU:HD21 | 23:UT:1701:MET:HE3  | 1.93                     | 0.50              |
| 23:UT:2004:LYS:HA   | 23:UT:2007:VAL:HG12 | 1.93                     | 0.50              |
| 24:UU:39:PHE:CD2    | 24:UU:313:SER:HB3   | 2.46                     | 0.50              |
| 24:UU:218:LEU:O     | 24:UU:220:ILE:HG12  | 2.12                     | 0.50              |
| 24:UU:328:LEU:HD21  | 29:CE:412:VAL:HG11  | 1.94                     | 0.50              |
| 25:UV:206:LEU:HD11  | 25:UV:297:GLY:HA3   | 1.94                     | 0.50              |
| 27:UZ:24:CYS:O      | 27:UZ:31:LYS:HG3    | 2.12                     | 0.50              |
| 28:CD:249:GLN:HA    | 28:CD:252:ILE:HG22  | 1.94                     | 0.50              |
| 29:CE:316:THR:O     | 29:CE:319:ILE:N     | 2.45                     | 0.50              |
| 30:CF:64:LEU:HD23   | 30:CF:98:ILE:HD12   | 1.94                     | 0.50              |
| 31:CH:69:GLN:HA     | 31:CH:72:GLU:OE2    | 2.11                     | 0.50              |
| 35:CL:89:LEU:HD21   | 35:CL:93:MET:HE1    | 1.93                     | 0.50              |
| 36:CM:205:VAL:O     | 36:CM:209:ILE:HG23  | 2.12                     | 0.50              |
| 39:JG:180:LEU:HD21  | 39:JG:237:ALA:HB1   | 1.94                     | 0.50              |
| 50:DF:149:VAL:HG22  | 50:DF:156:ARG:H     | 1.76                     | 0.50              |
| 55:DL:65:SER:HB3    | 66:D3:247:A:C2      | 2.46                     | 0.50              |
| 55:DL:132:SER:OG    | 66:D3:326:G:OP2     | 2.29                     | 0.50              |
| 65:D2:158:G:H2'     | 65:D2:159:A:H8      | 1.75                     | 0.50              |
| 66:D3:1270:G:H2'    | 66:D3:1271:G:H8     | 1.77                     | 0.50              |
| 66:D3:1450:U:H2'    | 66:D3:1451:C:C6     | 2.46                     | 0.50              |
| 67:D4:167:C:H2'     | 67:D4:168:C:C6      | 2.47                     | 0.50              |
| 2:DA:22:ASP:O       | 2:DA:25:THR:N       | 2.45                     | 0.50              |
| 3:JA:71:LYS:NZ      | 66:D3:158:U:O3'     | 2.45                     | 0.50              |
| 3:JA:591:GLU:OE2    | 3:JA:613:LEU:N      | 2.45                     | 0.50              |
| 3:JA:748:ARG:HH12   | 3:JA:752:ASN:N      | 2.10                     | 0.50              |
| 1:CB:88:ILE:HD11    | 1:CB:97:TYR:HB3     | 1.94                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:UB:534:PHE:N     | 5:UB:594:ASP:OD2   | 2.44                     | 0.50              |
| 7:UD:76:ILE:CG1    | 7:UD:91:ILE:HB     | 2.42                     | 0.50              |
| 7:UD:249:ARG:NE    | 7:UD:291:ASP:O     | 2.37                     | 0.50              |
| 7:UD:326:ARG:HH11  | 7:UD:365:SER:HA    | 1.77                     | 0.50              |
| 7:UD:347:LEU:HD21  | 7:UD:359:ASN:HB2   | 1.94                     | 0.50              |
| 8:UE:8:SER:HG      | 8:UE:293:ASN:HD22  | 1.57                     | 0.50              |
| 8:UE:484:LEU:O     | 8:UE:488:ILE:HG13  | 2.12                     | 0.50              |
| 8:UE:504:TRP:HZ3   | 12:UI:512:LEU:HD21 | 1.76                     | 0.50              |
| 11:UH:675:LEU:HD12 | 12:UI:456:LEU:HD22 | 1.94                     | 0.50              |
| 15:UL:147:VAL:HG12 | 15:UL:156:LEU:HB3  | 1.93                     | 0.50              |
| 15:UL:171:CYS:SG   | 15:UL:172:GLN:N    | 2.85                     | 0.50              |
| 16:UM:224:ASP:HB3  | 16:UM:234:LEU:HD11 | 1.93                     | 0.50              |
| 18:UO:427:VAL:HG12 | 18:UO:462:TRP:CH2  | 2.46                     | 0.50              |
| 20:UQ:473:LEU:HD23 | 20:UQ:532:TRP:CE2  | 2.47                     | 0.50              |
| 20:UQ:778:ASP:OD1  | 20:UQ:779:ILE:N    | 2.45                     | 0.50              |
| 24:UU:95:GLU:HA    | 24:UU:117:ASN:OD1  | 2.12                     | 0.50              |
| 24:UU:176:TYR:HB3  | 24:UU:179:LYS:HB2  | 1.94                     | 0.50              |
| 25:UV:124:VAL:HG11 | 25:UV:290:PHE:HD2  | 1.75                     | 0.50              |
| 25:UV:527:TYR:HB2  | 25:UV:615:VAL:HB   | 1.94                     | 0.50              |
| 25:UV:933:LEU:HB2  | 25:UV:1052:TYR:HB3 | 1.94                     | 0.50              |
| 25:UV:1022:MET:O   | 25:UV:1026:ASN:ND2 | 2.45                     | 0.50              |
| 27:UZ:97:PHE:HB3   | 27:UZ:100:ILE:HD11 | 1.93                     | 0.50              |
| 29:CE:15:LEU:HD11  | 29:CE:42:PHE:HB3   | 1.92                     | 0.50              |
| 29:CE:267:ALA:HA   | 29:CE:270:GLU:OE2  | 2.12                     | 0.50              |
| 30:CF:9:PHE:HB3    | 30:CF:10:PRO:HD3   | 1.94                     | 0.50              |
| 30:CG:95:ARG:CZ    | 31:CH:551:ARG:HB2  | 2.42                     | 0.50              |
| 31:CH:474:TRP:HB2  | 31:CH:492:TRP:HZ3  | 1.76                     | 0.50              |
| 35:CL:78:PRO:HD3   | 35:CL:122:ALA:HB3  | 1.91                     | 0.50              |
| 36:CM:131:GLU:CD   | 36:CM:194:VAL:HG11 | 2.32                     | 0.50              |
| 38:JC:192:ASN:ND2  | 38:JC:257:LEU:HD21 | 2.26                     | 0.50              |
| 38:JC:207:TRP:CE2  | 38:JC:214:ARG:HB2  | 2.47                     | 0.50              |
| 39:JG:89:PRO:HG2   | 39:JG:134:PHE:CZ   | 2.40                     | 0.50              |
| 47:JP:246:LEU:O    | 47:JP:255:THR:HG22 | 2.12                     | 0.50              |
| 55:DL:116:ARG:HG3  | 55:DL:118:GLN:HE22 | 1.77                     | 0.50              |
| 66:D3:37:U:C4      | 66:D3:38:C:C4      | 3.00                     | 0.50              |
| 66:D3:887:A:H2'    | 66:D3:888:U:H6     | 1.76                     | 0.50              |
| 66:D3:1638:G:HO2'  | 66:D3:1639:C:P     | 2.32                     | 0.50              |
| 67:D4:143:G:O2'    | 67:D4:144:G:OP1    | 2.24                     | 0.50              |
| 67:D4:160:G:H2'    | 67:D4:161:G:C8     | 2.47                     | 0.50              |
| 72:EE:168:VAL:O    | 72:EE:172:LYS:N    | 2.45                     | 0.50              |
| 1:CA:85:LYS:HG2    | 44:JM:151:THR:HG22 | 1.94                     | 0.49              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 3:JA:108:TYR:CE2   | 3:JA:126:ASP:HB2    | 2.47                     | 0.49              |
| 3:JA:615:PRO:HA    | 3:JA:618:ILE:HG22   | 1.92                     | 0.49              |
| 4:UA:215:VAL:HG11  | 4:UA:289:LEU:HD11   | 1.94                     | 0.49              |
| 4:UA:597:ASN:HA    | 4:UA:680:ARG:HB2    | 1.94                     | 0.49              |
| 5:UB:481:MET:CE    | 5:UB:484:ARG:HH21   | 2.25                     | 0.49              |
| 7:UD:289:ASP:OD2   | 7:UD:294:TYR:HB2    | 2.11                     | 0.49              |
| 9:UF:276:VAL:HG21  | 17:UN:338:LEU:HD21  | 1.94                     | 0.49              |
| 10:UG:319:GLY:HA2  | 10:UG:334:ARG:HB3   | 1.93                     | 0.49              |
| 10:UG:453:ASP:OD1  | 10:UG:453:ASP:N     | 2.44                     | 0.49              |
| 12:UI:437:ILE:HG12 | 12:UI:452:LEU:HD11  | 1.94                     | 0.49              |
| 16:UM:26:SER:HB2   | 16:UM:71:PRO:O      | 2.11                     | 0.49              |
| 16:UM:174:VAL:O    | 16:UM:183:LEU:N     | 2.45                     | 0.49              |
| 16:UM:663:VAL:HA   | 16:UM:666:GLU:OE2   | 2.12                     | 0.49              |
| 18:UO:312:ALA:O    | 18:UO:313:GLN:HG2   | 2.12                     | 0.49              |
| 18:UO:368:GLY:HA3  | 21:UR:289:HIS:CD2   | 2.47                     | 0.49              |
| 18:UO:418:LEU:HD12 | 18:UO:462:TRP:NE1   | 2.27                     | 0.49              |
| 20:UQ:511:GLU:OE1  | 20:UQ:511:GLU:N     | 2.45                     | 0.49              |
| 21:UR:241:ALA:HA   | 21:UR:282:ASN:ND2   | 2.27                     | 0.49              |
| 23:UT:77:LEU:HD22  | 31:CH:67:ALA:CB     | 2.42                     | 0.49              |
| 23:UT:582:LEU:O    | 23:UT:586:THR:HG23  | 2.12                     | 0.49              |
| 23:UT:969:SER:O    | 23:UT:972:LEU:O     | 2.30                     | 0.49              |
| 23:UT:1018:HIS:O   | 23:UT:1022:VAL:HG22 | 2.11                     | 0.49              |
| 23:UT:1079:MET:HA  | 23:UT:1082:ILE:HG22 | 1.93                     | 0.49              |
| 24:UU:120:HIS:NE2  | 24:UU:168:VAL:O     | 2.45                     | 0.49              |
| 25:UV:139:PRO:HG2  | 25:UV:238:HIS:CE1   | 2.47                     | 0.49              |
| 25:UV:178:TYR:HD1  | 25:UV:231:TYR:CZ    | 2.29                     | 0.49              |
| 30:CG:116:ALA:O    | 30:CG:120:LYS:HG2   | 2.12                     | 0.49              |
| 35:CL:364:VAL:HA   | 35:CL:372:TYR:O     | 2.12                     | 0.49              |
| 35:CL:1104:GLY:O   | 35:CL:1107:LYS:HB3  | 2.12                     | 0.49              |
| 36:CM:191:ILE:O    | 36:CM:223:VAL:HA    | 2.12                     | 0.49              |
| 45:JN:277:SER:O    | 45:JN:281:LYS:HG3   | 2.11                     | 0.49              |
| 46:JO:90:ASP:OD2   | 46:JO:93:ILE:N      | 2.44                     | 0.49              |
| 47:JP:178:GLY:HA3  | 47:JP:182:PHE:HZ    | 1.77                     | 0.49              |
| 47:JP:324:SER:OG   | 47:JP:326:ASP:O     | 2.30                     | 0.49              |
| 53:DI:98:LYS:HG2   | 66:D3:329:G:O3'     | 2.12                     | 0.49              |
| 54:DJ:2:PRO:HB3    | 66:D3:380:U:H4'     | 1.93                     | 0.49              |
| 55:DL:140:VAL:C    | 55:DL:141:LYS:HD3   | 2.33                     | 0.49              |
| 61:DX:51:GLY:HA2   | 61:DX:77:ILE:HG13   | 1.94                     | 0.49              |
| 65:D2:20:C:H2'     | 65:D2:21:A:H8       | 1.75                     | 0.49              |
| 65:D2:277:C:H5     | 65:D2:278:G:C4      | 2.30                     | 0.49              |
| 66:D3:27:U:O4      | 66:D3:599:A:N6      | 2.42                     | 0.49              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 67:D4:50:U:N3      | 67:D4:51:C:N3       | 2.60                     | 0.49              |
| 70:EC:164:GLY:HA2  | 70:EC:184:THR:HA    | 1.93                     | 0.49              |
| 74:EG:193:ALA:HA   | 74:EG:202:SER:HA    | 1.94                     | 0.49              |
| 3:JA:86:ARG:HG2    | 3:JA:87:GLU:H       | 1.77                     | 0.49              |
| 3:JA:517:VAL:HG11  | 3:JA:715:GLN:HG3    | 1.94                     | 0.49              |
| 4:UA:334:SER:HB3   | 42:JJ:271:LYS:HB3   | 1.93                     | 0.49              |
| 1:CB:268:VAL:HA    | 1:CB:316:VAL:O      | 2.13                     | 0.49              |
| 5:UB:209:GLU:HA    | 66:D3:1206:U:O2'    | 2.12                     | 0.49              |
| 7:UD:81:PRO:HB3    | 7:UD:85:TRP:CE3     | 2.47                     | 0.49              |
| 7:UD:427:ASN:OD1   | 19:UP:190:LEU:HD11  | 2.12                     | 0.49              |
| 7:UD:536:VAL:HG22  | 7:UD:537:ASP:O      | 2.12                     | 0.49              |
| 10:UG:115:HIS:CE1  | 10:UG:380:ASN:ND2   | 2.79                     | 0.49              |
| 11:UH:564:ASN:ND2  | 11:UH:598:GLU:OE2   | 2.45                     | 0.49              |
| 13:UJ:1656:SER:HB3 | 13:UJ:1694:HIS:NE2  | 2.26                     | 0.49              |
| 14:UK:107:VAL:HG13 | 14:UK:211:LEU:HD12  | 1.94                     | 0.49              |
| 14:UK:147:THR:HG22 | 14:UK:149:GLU:H     | 1.76                     | 0.49              |
| 15:UL:299:ARG:O    | 15:UL:303:LEU:HG    | 2.12                     | 0.49              |
| 16:UM:248:PHE:HB3  | 16:UM:256:ARG:NH2   | 2.27                     | 0.49              |
| 16:UM:538:ASP:O    | 16:UM:550:THR:HA    | 2.12                     | 0.49              |
| 23:UT:1544:ALA:O   | 23:UT:1548:ILE:HG12 | 2.13                     | 0.49              |
| 24:UU:87:PHE:HD1   | 65:D2:308:A:C2      | 2.29                     | 0.49              |
| 24:UU:321:GLU:O    | 24:UU:343:LEU:HB3   | 2.11                     | 0.49              |
| 24:UU:860:GLU:OE1  | 24:UU:860:GLU:N     | 2.24                     | 0.49              |
| 25:UV:654:SER:HG   | 25:UV:666:CYS:HG    | 1.54                     | 0.49              |
| 27:UZ:226:LYS:HA   | 27:UZ:229:ARG:NH2   | 2.27                     | 0.49              |
| 35:CL:102:GLN:O    | 35:CL:359:SER:HB2   | 2.12                     | 0.49              |
| 35:CL:211:ILE:HG13 | 35:CL:212:ASN:H     | 1.77                     | 0.49              |
| 35:CL:254:HIS:HB3  | 35:CL:256:GLU:CD    | 2.31                     | 0.49              |
| 36:CM:285:LYS:HA   | 36:CM:316:GLU:OE2   | 2.12                     | 0.49              |
| 39:JG:43:VAL:O     | 39:JG:112:VAL:HA    | 2.12                     | 0.49              |
| 39:JG:181:SER:HB2  | 39:JG:214:ASP:OD2   | 2.12                     | 0.49              |
| 47:JP:405:ARG:HB3  | 47:JP:405:ARG:CZ    | 2.40                     | 0.49              |
| 49:DE:188:ASN:HB3  | 49:DE:191:ARG:CZ    | 2.42                     | 0.49              |
| 54:DJ:49:LEU:HD22  | 54:DJ:101:VAL:HG22  | 1.93                     | 0.49              |
| 56:DN:18:TYR:CE2   | 60:DW:56:HIS:CD2    | 2.99                     | 0.49              |
| 58:DQ:58:ASP:OD1   | 58:DQ:59:LYS:N      | 2.45                     | 0.49              |
| 67:D4:11:U:H2'     | 67:D4:12:U:C6       | 2.47                     | 0.49              |
| 79:EN:399:LYS:O    | 79:EN:403:LYS:N     | 2.38                     | 0.49              |
| 3:JA:16:ASN:HA     | 3:JA:19:GLN:HG2     | 1.94                     | 0.49              |
| 3:JA:76:LYS:HA     | 3:JA:79:LYS:NZ      | 2.27                     | 0.49              |
| 3:JA:789:LEU:HA    | 3:JA:793:PHE:CE1    | 2.47                     | 0.49              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 4:UA:360:VAL:HG21  | 4:UA:374:ILE:HD11   | 1.95                     | 0.49              |
| 7:UD:199:ASP:CA    | 7:UD:215:ALA:O      | 2.59                     | 0.49              |
| 7:UD:310:ASN:OD1   | 7:UD:311:THR:N      | 2.44                     | 0.49              |
| 7:UD:614:TRP:O     | 7:UD:618:ASN:HB2    | 2.11                     | 0.49              |
| 9:UF:317:LEU:HD23  | 9:UF:321:LYS:NZ     | 2.28                     | 0.49              |
| 10:UG:533:ILE:HG12 | 10:UG:539:SER:HA    | 1.94                     | 0.49              |
| 13:UJ:248:SER:O    | 13:UJ:254:GLN:NE2   | 2.45                     | 0.49              |
| 13:UJ:345:ASP:HA   | 13:UJ:348:ILE:HD12  | 1.94                     | 0.49              |
| 13:UJ:561:PHE:CE2  | 13:UJ:619:SER:HB2   | 2.47                     | 0.49              |
| 13:UJ:1600:PRO:O   | 13:UJ:1604:LEU:HG   | 2.12                     | 0.49              |
| 13:UJ:1644:PHE:CD2 | 13:UJ:1683:HIS:HD2  | 2.30                     | 0.49              |
| 16:UM:490:HIS:HE1  | 16:UM:514:THR:HG23  | 1.78                     | 0.49              |
| 17:UN:864:PRO:HG3  | 47:JP:36:GLU:OE1    | 2.12                     | 0.49              |
| 20:UQ:435:ASP:HB3  | 20:UQ:701:VAL:O     | 2.11                     | 0.49              |
| 23:UT:78:PRO:HB3   | 31:CH:71:LEU:HD21   | 1.94                     | 0.49              |
| 23:UT:1199:LEU:O   | 23:UT:1203:VAL:HG23 | 2.12                     | 0.49              |
| 23:UT:1397:ILE:O   | 23:UT:1400:PRO:HD2  | 2.12                     | 0.49              |
| 24:UU:90:VAL:HG23  | 24:UU:101:TYR:HB2   | 1.93                     | 0.49              |
| 24:UU:865:ILE:HD13 | 24:UU:909:LEU:HD22  | 1.94                     | 0.49              |
| 25:UV:106:GLN:HB3  | 25:UV:507:PHE:CE2   | 2.47                     | 0.49              |
| 25:UV:824:PHE:O    | 25:UV:840:LEU:HD12  | 2.13                     | 0.49              |
| 26:UX:90:LEU:HD22  | 26:UX:94:CYS:SG     | 2.52                     | 0.49              |
| 26:UX:152:ILE:HB   | 26:UX:171:PRO:HG2   | 1.94                     | 0.49              |
| 27:UZ:93:THR:HA    | 27:UZ:96:LEU:HB3    | 1.94                     | 0.49              |
| 29:CE:420:GLU:OE1  | 29:CE:420:GLU:N     | 2.45                     | 0.49              |
| 30:CF:28:ALA:HB2   | 30:CF:33:LEU:HD23   | 1.94                     | 0.49              |
| 30:CF:39:GLU:OE1   | 30:CF:42:LYS:NZ     | 2.40                     | 0.49              |
| 30:CG:54:MET:HE1   | 30:CG:67:LEU:HD22   | 1.94                     | 0.49              |
| 31:CH:433:ILE:HD11 | 31:CH:506:ARG:HG3   | 1.93                     | 0.49              |
| 33:CJ:92:THR:CG2   | 33:CJ:96:PRO:HB3    | 2.41                     | 0.49              |
| 35:CL:198:VAL:HG12 | 35:CL:199:TYR:N     | 2.27                     | 0.49              |
| 40:JH:260:TYR:HA   | 40:JH:306:ALA:HB2   | 1.93                     | 0.49              |
| 42:JJ:205:ILE:O    | 42:JJ:212:THR:OG1   | 2.29                     | 0.49              |
| 46:JO:80:MET:SD    | 46:JO:101:ILE:HB    | 2.52                     | 0.49              |
| 47:JP:16:VAL:HG23  | 47:JP:17:LYS:H      | 1.77                     | 0.49              |
| 47:JP:303:ASP:O    | 47:JP:330:ARG:NH2   | 2.45                     | 0.49              |
| 47:JP:361:LYS:O    | 47:JP:377:SER:OG    | 2.21                     | 0.49              |
| 49:DE:126:VAL:HG13 | 49:DE:139:VAL:CG2   | 2.42                     | 0.49              |
| 53:DI:23:LYS:H     | 53:DI:25:ARG:HH21   | 1.61                     | 0.49              |
| 56:DN:126:ALA:O    | 56:DN:130:ARG:HG3   | 2.13                     | 0.49              |
| 58:DQ:69:VAL:HG11  | 58:DQ:81:ILE:HG12   | 1.94                     | 0.49              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 66:D3:282:C:H2'     | 66:D3:283:U:H6     | 1.78                     | 0.49              |
| 66:D3:828:U:O4      | 66:D3:829:A:N6     | 2.46                     | 0.49              |
| 79:EN:93:VAL:N      | 79:EN:113:VAL:O    | 2.42                     | 0.49              |
| 1:CA:221:ILE:HB     | 28:CD:162:LYS:HE2  | 1.93                     | 0.49              |
| 2:DA:112:SER:O      | 46:JO:44:LEU:HD13  | 2.13                     | 0.49              |
| 2:DA:189:ILE:CB     | 2:DA:190:PRO:HD3   | 2.36                     | 0.49              |
| 4:UA:126:ASP:HB3    | 4:UA:129:LYS:NZ    | 2.28                     | 0.49              |
| 4:UA:162:LEU:CB     | 4:UA:172:ILE:HG22  | 2.42                     | 0.49              |
| 3:JB:202:ASP:N      | 3:JB:206:ASN:O     | 2.41                     | 0.49              |
| 5:UB:552:GLN:HA     | 5:UB:555:ARG:NE    | 2.28                     | 0.49              |
| 7:UD:511:VAL:HG23   | 7:UD:558:ARG:HB3   | 1.94                     | 0.49              |
| 13:UJ:88:LYS:O      | 13:UJ:92:LYS:HG3   | 2.12                     | 0.49              |
| 13:UJ:1535:TYR:O    | 13:UJ:1539:MET:HG2 | 2.12                     | 0.49              |
| 14:UK:190:LEU:O     | 14:UK:194:LYS:HG2  | 2.12                     | 0.49              |
| 18:UO:11:SER:O      | 18:UO:12:LYS:HD3   | 2.11                     | 0.49              |
| 18:UO:322:LEU:HD12  | 18:UO:326:LEU:HB2  | 1.94                     | 0.49              |
| 19:UP:204:ARG:NH2   | 65:D2:170:U:H4'    | 2.23                     | 0.49              |
| 20:UQ:265:ASP:HB2   | 20:UQ:270:GLN:O    | 2.12                     | 0.49              |
| 20:UQ:693:ASP:OD1   | 20:UQ:693:ASP:N    | 2.43                     | 0.49              |
| 21:UR:458:ILE:O     | 21:UR:459:GLN:NE2  | 2.46                     | 0.49              |
| 22:US:251:SER:OG    | 65:D2:111:C:OP1    | 2.30                     | 0.49              |
| 23:UT:47:PHE:CD1    | 23:UT:113:PHE:HB2  | 2.47                     | 0.49              |
| 23:UT:54:TRP:HA     | 23:UT:57:ILE:CG2   | 2.40                     | 0.49              |
| 23:UT:1083:TYR:CE1  | 23:UT:1121:PHE:HB3 | 2.47                     | 0.49              |
| 23:UT:1211:ILE:HD12 | 23:UT:1216:VAL:CG2 | 2.41                     | 0.49              |
| 24:UU:631:ASN:HB2   | 24:UU:644:THR:CG2  | 2.42                     | 0.49              |
| 25:UV:145:SER:OG    | 25:UV:148:GLU:HB2  | 2.11                     | 0.49              |
| 28:CD:4:ILE:HG23    | 28:CD:20:VAL:HG11  | 1.95                     | 0.49              |
| 29:CE:159:VAL:O     | 29:CE:162:MET:HG3  | 2.12                     | 0.49              |
| 31:CH:140:LEU:HD12  | 31:CH:568:ILE:CG2  | 2.42                     | 0.49              |
| 31:CH:314:GLN:N     | 62:DY:2:SER:O      | 2.24                     | 0.49              |
| 32:CI:5:LEU:HD22    | 32:CI:13:LEU:HD12  | 1.94                     | 0.49              |
| 32:CI:59:ASN:ND2    | 65:D2:335:G:H4'    | 2.27                     | 0.49              |
| 32:CI:94:ILE:HG12   | 33:CJ:58:TYR:HB3   | 1.93                     | 0.49              |
| 35:CL:145:ASN:HA    | 35:CL:177:PHE:CE1  | 2.43                     | 0.49              |
| 36:CM:96:VAL:HG21   | 36:CM:122:THR:HG22 | 1.94                     | 0.49              |
| 45:JN:313:ARG:O     | 45:JN:319:LEU:HD12 | 2.12                     | 0.49              |
| 47:JP:453:TYR:HE2   | 66:D3:-2:A:C6      | 2.31                     | 0.49              |
| 51:DG:92:ARG:HH12   | 66:D3:406:U:H4'    | 1.77                     | 0.49              |
| 54:DJ:11:THR:OG1    | 66:D3:472:U:OP1    | 2.28                     | 0.49              |
| 55:DL:131:ILE:O     | 66:D3:336:G:O2'    | 2.19                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 56:DN:96:VAL:HG21  | 56:DN:150:VAL:HG21 | 1.93                     | 0.49              |
| 65:D2:2:U:H2'      | 65:D2:3:G:H8       | 1.75                     | 0.49              |
| 65:D2:306:G:C6     | 65:D2:307:C:C4     | 3.01                     | 0.49              |
| 66:D3:882:U:H2'    | 66:D3:883:C:H6     | 1.77                     | 0.49              |
| 66:D3:1575:G:H2'   | 66:D3:1576:A:C8    | 2.46                     | 0.49              |
| 66:D3:1786:G:H2'   | 66:D3:1787:C:C6    | 2.47                     | 0.49              |
| 79:EN:398:VAL:O    | 79:EN:402:TRP:N    | 2.34                     | 0.49              |
| 3:JA:794:HIS:HB3   | 3:JA:795:LYS:HD2   | 1.93                     | 0.49              |
| 4:UA:315:GLU:O     | 4:UA:331:GLU:HG2   | 2.11                     | 0.49              |
| 4:UA:429:GLU:C     | 4:UA:430:ARG:HD3   | 2.33                     | 0.49              |
| 1:CB:107:VAL:HG21  | 1:CB:141:TYR:HB3   | 1.93                     | 0.49              |
| 1:CB:195:TYR:HA    | 1:CB:218:ILE:HG23  | 1.93                     | 0.49              |
| 6:UC:433:ARG:O     | 6:UC:435:LYS:HG3   | 2.13                     | 0.49              |
| 7:UD:270:ALA:HB3   | 21:UR:446:ARG:HH22 | 1.78                     | 0.49              |
| 7:UD:768:ALA:HA    | 19:UP:213:LYS:NZ   | 2.28                     | 0.49              |
| 8:UE:523:LEU:HB2   | 8:UE:527:HIS:NE2   | 2.27                     | 0.49              |
| 10:UG:79:GLU:OE2   | 65:D2:313:A:N6     | 2.45                     | 0.49              |
| 13:UJ:290:GLU:H    | 13:UJ:290:GLU:CD   | 2.16                     | 0.49              |
| 13:UJ:390:LEU:O    | 13:UJ:394:LEU:HB3  | 2.11                     | 0.49              |
| 13:UJ:760:PHE:CD2  | 13:UJ:795:LEU:HD22 | 2.47                     | 0.49              |
| 13:UJ:1443:LEU:O   | 13:UJ:1446:GLU:HG3 | 2.12                     | 0.49              |
| 16:UM:753:HIS:O    | 16:UM:757:GLN:HG2  | 2.11                     | 0.49              |
| 18:UO:391:ASN:ND2  | 18:UO:399:GLU:HG3  | 2.26                     | 0.49              |
| 20:UQ:105:HIS:CE1  | 20:UQ:122:LYS:HB3  | 2.47                     | 0.49              |
| 20:UQ:201:ILE:C    | 20:UQ:264:ILE:HD13 | 2.32                     | 0.49              |
| 21:UR:317:ARG:NE   | 21:UR:356:GLU:OE1  | 2.40                     | 0.49              |
| 21:UR:386:ILE:HB   | 21:UR:396:MET:O    | 2.12                     | 0.49              |
| 23:UT:228:LEU:O    | 23:UT:232:LEU:HG   | 2.12                     | 0.49              |
| 23:UT:498:ILE:HA   | 23:UT:501:LEU:HD12 | 1.94                     | 0.49              |
| 23:UT:841:ILE:HG13 | 23:UT:844:VAL:HB   | 1.95                     | 0.49              |
| 23:UT:1584:ASN:HB2 | 23:UT:1587:LYS:NZ  | 2.26                     | 0.49              |
| 25:UV:344:ASN:OD1  | 25:UV:347:LYS:HE3  | 2.12                     | 0.49              |
| 25:UV:801:LYS:HD3  | 37:CN:184:ILE:HD13 | 1.94                     | 0.49              |
| 28:CD:326:SER:OG   | 28:CD:388:ARG:HA   | 2.13                     | 0.49              |
| 34:CK:315:GLU:O    | 34:CK:319:VAL:HG13 | 2.13                     | 0.49              |
| 34:CK:358:THR:HG22 | 34:CK:361:VAL:HG23 | 1.94                     | 0.49              |
| 35:CL:86:ILE:HD11  | 35:CL:117:PHE:HD2  | 1.77                     | 0.49              |
| 35:CL:125:LEU:O    | 35:CL:129:ILE:HG13 | 2.13                     | 0.49              |
| 35:CL:833:ARG:NH1  | 61:DX:139:LYS:O    | 2.45                     | 0.49              |
| 36:CM:209:ILE:HB   | 36:CM:225:ILE:HD11 | 1.95                     | 0.49              |
| 37:CN:37:MET:SD    | 37:CN:59:PRO:HD3   | 2.52                     | 0.49              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 47:JP:146:LYS:HB3  | 47:JP:148:TRP:HE1   | 1.76                     | 0.49              |
| 47:JP:147:LEU:C    | 47:JP:148:TRP:HD1   | 2.14                     | 0.49              |
| 49:DE:32:SER:N     | 49:DE:81:THR:O      | 2.30                     | 0.49              |
| 50:DF:84:LYS:HZ1   | 66:D3:1613:U:P      | 2.34                     | 0.49              |
| 51:DG:137:ARG:HD2  | 51:DG:177:ARG:HD3   | 1.95                     | 0.49              |
| 51:DG:199:GLN:O    | 51:DG:203:GLU:HG2   | 2.13                     | 0.49              |
| 53:DI:65:PHE:HA    | 53:DI:181:GLY:O     | 2.12                     | 0.49              |
| 65:D2:242:C:H2'    | 65:D2:243:A:C8      | 2.28                     | 0.49              |
| 65:D2:349:G:C2     | 65:D2:376:U:O2      | 2.65                     | 0.49              |
| 66:D3:108:A:H2'    | 66:D3:109:G:H8      | 1.78                     | 0.49              |
| 66:D3:252:U:H2'    | 66:D3:253:A:H8      | 1.77                     | 0.49              |
| 66:D3:353:A:OP2    | 66:D3:354:C:N4      | 2.42                     | 0.49              |
| 66:D3:477:A:C2     | 66:D3:512:A:N1      | 2.80                     | 0.49              |
| 66:D3:940:A:H2'    | 66:D3:941:A:H8      | 1.77                     | 0.49              |
| 67:D4:91:C:H5''    | 67:D4:92:A:OP2      | 2.11                     | 0.49              |
| 73:EF:9:SER:O      | 73:EF:13:ASP:N      | 2.45                     | 0.49              |
| 79:EN:1050:LEU:O   | 79:EN:1054:MET:N    | 2.45                     | 0.49              |
| 1:CA:222:GLU:HB2   | 28:CD:162:LYS:HZ2   | 1.77                     | 0.49              |
| 1:CA:302:GLU:HG2   | 1:CA:317:VAL:HB     | 1.93                     | 0.49              |
| 2:DA:99:ASN:OD1    | 2:DA:100:PHE:N      | 2.46                     | 0.49              |
| 3:JA:632:GLY:HA2   | 3:JA:720:LEU:HB2    | 1.94                     | 0.49              |
| 4:UA:386:HIS:CE1   | 4:UA:412:ARG:HG3    | 2.47                     | 0.49              |
| 4:UA:518:VAL:HB    | 4:UA:532:VAL:CG2    | 2.41                     | 0.49              |
| 5:UB:547:VAL:O     | 5:UB:550:VAL:HG22   | 2.12                     | 0.49              |
| 5:UB:678:PHE:HD2   | 5:UB:680:LYS:HE3    | 1.76                     | 0.49              |
| 7:UD:561:LYS:HZ2   | 7:UD:563:LEU:HD23   | 1.78                     | 0.49              |
| 11:UH:671:ARG:O    | 11:UH:675:LEU:HD23  | 2.13                     | 0.49              |
| 13:UJ:98:ILE:HD13  | 13:UJ:131:ASN:ND2   | 2.28                     | 0.49              |
| 13:UJ:407:PHE:O    | 13:UJ:410:ILE:C     | 2.51                     | 0.49              |
| 15:UL:438:PHE:HE1  | 15:UL:443:LEU:HA    | 1.77                     | 0.49              |
| 16:UM:406:ALA:HB2  | 16:UM:440:VAL:HG13  | 1.94                     | 0.49              |
| 16:UM:491:GLU:OE2  | 16:UM:492:LYS:HG3   | 2.13                     | 0.49              |
| 16:UM:572:GLU:CG   | 16:UM:573:GLY:H     | 2.24                     | 0.49              |
| 17:UN:881:PRO:HG2  | 17:UN:884:MET:HG2   | 1.94                     | 0.49              |
| 23:UT:899:ASP:OD1  | 53:DI:41:LYS:NZ     | 2.43                     | 0.49              |
| 23:UT:1644:ARG:NH2 | 23:UT:1645:SER:HA   | 2.27                     | 0.49              |
| 23:UT:1693:THR:O   | 23:UT:1697:ILE:HG12 | 2.13                     | 0.49              |
| 24:UU:274:ILE:HG12 | 24:UU:286:VAL:HG23  | 1.94                     | 0.49              |
| 25:UV:178:TYR:CE1  | 25:UV:235:LEU:HD21  | 2.47                     | 0.49              |
| 25:UV:218:ASP:O    | 25:UV:224:CYS:N     | 2.45                     | 0.49              |
| 29:CE:17:ALA:HA    | 29:CE:42:PHE:CE2    | 2.48                     | 0.49              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 30:CG:63:ILE:HG23   | 30:CG:64:LEU:N     | 2.27                     | 0.49              |
| 31:CH:295:LEU:HD12  | 31:CH:296:TYR:H    | 1.78                     | 0.49              |
| 35:CL:154:GLU:OE1   | 35:CL:912:ARG:HD2  | 2.12                     | 0.49              |
| 35:CL:798:MET:N     | 35:CL:798:MET:SD   | 2.84                     | 0.49              |
| 35:CL:969:VAL:HG23  | 66:D3:556:A:O4'    | 2.12                     | 0.49              |
| 36:CM:306:GLU:HA    | 36:CM:356:GLY:O    | 2.12                     | 0.49              |
| 38:JC:189:ASN:ND2   | 38:JC:240:GLY:O    | 2.46                     | 0.49              |
| 39:JF:137:PHE:O     | 39:JF:141:MET:HG2  | 2.13                     | 0.49              |
| 42:JJ:182:ILE:HA    | 42:JJ:233:ILE:O    | 2.13                     | 0.49              |
| 46:JO:259:LYS:HA    | 46:JO:262:LEU:HD12 | 1.93                     | 0.49              |
| 49:DE:45:ILE:HB     | 49:DE:80:THR:HG1   | 1.77                     | 0.49              |
| 55:DL:17:PRO:O      | 55:DL:19:ILE:HD12  | 2.12                     | 0.49              |
| 61:DX:60:GLU:OE1    | 61:DX:60:GLU:N     | 2.43                     | 0.49              |
| 65:D2:355:C:H2'     | 65:D2:356:C:C6     | 2.47                     | 0.49              |
| 66:D3:951:A:H2'     | 66:D3:952:A:C8     | 2.46                     | 0.49              |
| 66:D3:1125:A:H2'    | 66:D3:1126:G:C4    | 2.48                     | 0.49              |
| 66:D3:1130:G:N2     | 66:D3:1138:A:H62   | 2.11                     | 0.49              |
| 66:D3:1213:G:O6     | 66:D3:1451:C:N4    | 2.45                     | 0.49              |
| 66:D3:1643:U:H2'    | 66:D3:1644:C:H6    | 1.77                     | 0.49              |
| 67:D4:57:A:N6       | 67:D4:58:A:N1      | 2.60                     | 0.49              |
| 76:EI:176:LEU:HA    | 76:EI:182:ALA:HA   | 1.94                     | 0.49              |
| 79:EN:205:SER:O     | 79:EN:209:TYR:N    | 2.33                     | 0.49              |
| 79:EN:793:SER:O     | 79:EN:797:VAL:N    | 2.43                     | 0.49              |
| 1:CA:176:ALA:O      | 1:CA:203:PRO:HB3   | 2.12                     | 0.49              |
| 3:JA:60:LYS:HD2     | 3:JA:61:LYS:HB2    | 1.95                     | 0.49              |
| 3:JA:87:GLU:HG3     | 3:JA:88:VAL:H      | 1.78                     | 0.49              |
| 3:JA:509:HIS:CG     | 3:JA:510:PRO:HD2   | 2.47                     | 0.49              |
| 4:UA:432:GLN:O      | 4:UA:449:SER:HB2   | 2.13                     | 0.49              |
| 5:UB:784:ILE:O      | 5:UB:788:ILE:HD12  | 2.13                     | 0.49              |
| 6:UC:554:ARG:NE     | 66:D3:546:U:OP2    | 2.39                     | 0.49              |
| 7:UD:63:SER:OG      | 7:UD:687:PHE:O     | 2.30                     | 0.49              |
| 7:UD:191:LEU:N      | 7:UD:204:GLY:O     | 2.29                     | 0.49              |
| 7:UD:435:PRO:HD3    | 7:UD:480:PHE:CZ    | 2.48                     | 0.49              |
| 7:UD:638:SER:HB3    | 7:UD:646:LEU:HD13  | 1.95                     | 0.49              |
| 8:UE:473:LYS:HE3    | 8:UE:476:LEU:HD23  | 1.94                     | 0.49              |
| 11:UH:57:ILE:O      | 11:UH:70:PRO:HA    | 2.12                     | 0.49              |
| 13:UJ:1572:LEU:HD12 | 13:UJ:1576:PHE:HE2 | 1.77                     | 0.49              |
| 13:UJ:1593:TYR:O    | 13:UJ:1597:LEU:HG  | 2.13                     | 0.49              |
| 15:UL:92:ASP:OD1    | 15:UL:108:LEU:HB2  | 2.13                     | 0.49              |
| 15:UL:656:HIS:NE2   | 15:UL:660:VAL:HG22 | 2.28                     | 0.49              |
| 15:UL:760:ILE:O     | 15:UL:763:ILE:N    | 2.44                     | 0.49              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 16:UM:463:ILE:HG23  | 16:UM:489:ALA:HB2   | 1.93                     | 0.49              |
| 18:UO:42:VAL:HG23   | 18:UO:58:THR:O      | 2.12                     | 0.49              |
| 18:UO:85:TYR:HD2    | 18:UO:128:HIS:HA    | 1.77                     | 0.49              |
| 22:US:227:LYS:NZ    | 22:US:235:ASP:O     | 2.46                     | 0.49              |
| 23:UT:858:LEU:HD11  | 23:UT:928:ILE:HD13  | 1.93                     | 0.49              |
| 23:UT:1034:TYR:OH   | 23:UT:1090:ARG:NH2  | 2.46                     | 0.49              |
| 23:UT:1278:ARG:HA   | 23:UT:1315:ARG:HE   | 1.77                     | 0.49              |
| 23:UT:1725:ILE:HG23 | 23:UT:1726:PHE:CD1  | 2.48                     | 0.49              |
| 23:UT:1966:PHE:CD1  | 23:UT:1970:THR:HG21 | 2.48                     | 0.49              |
| 24:UU:539:LYS:HG3   | 24:UU:539:LYS:O     | 2.13                     | 0.49              |
| 24:UU:606:ASP:O     | 24:UU:607:SER:OG    | 2.26                     | 0.49              |
| 24:UU:613:ASP:OD1   | 24:UU:615:PRO:HD2   | 2.12                     | 0.49              |
| 24:UU:630:THR:HG23  | 24:UU:644:THR:HG23  | 1.94                     | 0.49              |
| 25:UV:304:GLU:OE1   | 25:UV:306:LYS:HG2   | 2.13                     | 0.49              |
| 27:UZ:11:GLY:HA2    | 27:UZ:14:GLU:OE2    | 2.12                     | 0.49              |
| 29:CE:113:THR:OG1   | 29:CE:116:ILE:HB    | 2.13                     | 0.49              |
| 34:CK:466:GLU:OE2   | 34:CK:468:ARG:NH2   | 2.46                     | 0.49              |
| 35:CL:126:ASN:HB3   | 35:CL:853:ARG:NE    | 2.28                     | 0.49              |
| 35:CL:248:ARG:HB3   | 35:CL:272:TYR:CD1   | 2.48                     | 0.49              |
| 37:CN:256:ASP:N     | 37:CN:256:ASP:OD1   | 2.46                     | 0.49              |
| 38:JC:124:GLN:HG2   | 38:JC:134:THR:HG23  | 1.95                     | 0.49              |
| 39:JF:44:VAL:HA     | 39:JF:113:TYR:O     | 2.12                     | 0.49              |
| 42:JJ:148:ASP:OD2   | 42:JJ:151:ALA:N     | 2.45                     | 0.49              |
| 46:JO:165:LEU:HB3   | 46:JO:172:SER:OG    | 2.13                     | 0.49              |
| 47:JP:300:VAL:O     | 47:JP:300:VAL:HG13  | 2.13                     | 0.49              |
| 49:DE:98:ASN:HB2    | 49:DE:114:ILE:O     | 2.12                     | 0.49              |
| 54:DJ:133:HIS:NE2   | 66:D3:512:A:O2'     | 2.44                     | 0.49              |
| 66:D3:0:U:H1'       | 66:D3:1:U:OP2       | 2.12                     | 0.49              |
| 66:D3:230:C:H2'     | 66:D3:231:U:H4'     | 1.93                     | 0.49              |
| 66:D3:296:U:H2'     | 66:D3:297:U:C6      | 2.48                     | 0.49              |
| 66:D3:1708:U:H2'    | 66:D3:1709:C:C2     | 2.47                     | 0.49              |
| 67:D4:44:U:H2'      | 67:D4:45:U:C6       | 2.47                     | 0.49              |
| 72:EE:138:ILE:O     | 72:EE:158:LEU:N     | 2.36                     | 0.49              |
| 77:EJ:270:THR:N     | 77:EJ:274:MET:O     | 2.45                     | 0.49              |
| 1:CA:306:LEU:HD11   | 1:CA:313:HIS:CB     | 2.42                     | 0.49              |
| 3:JA:912:MET:HA     | 3:JA:915:LYS:HD2    | 1.94                     | 0.49              |
| 4:UA:114:ALA:CB     | 4:UA:152:LEU:HD11   | 2.42                     | 0.49              |
| 4:UA:475:PRO:O      | 4:UA:492:SER:HB2    | 2.13                     | 0.49              |
| 4:UA:531:ALA:HB2    | 4:UA:585:TYR:CZ     | 2.48                     | 0.49              |
| 7:UD:426:GLN:HE21   | 19:UP:190:LEU:HD12  | 1.78                     | 0.49              |
| 10:UG:546:ILE:HG12  | 25:UV:808:LEU:HD22  | 1.94                     | 0.49              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 11:UH:595:ILE:O    | 11:UH:599:MET:HG2   | 2.13                     | 0.49              |
| 13:UJ:22:ARG:NH1   | 47:JP:15:PRO:HG2    | 2.28                     | 0.49              |
| 14:UK:32:LYS:HA    | 14:UK:35:VAL:HG12   | 1.94                     | 0.49              |
| 14:UK:187:LYS:HD2  | 14:UK:188:GLU:HB3   | 1.95                     | 0.49              |
| 15:UL:876:LEU:HA   | 15:UL:879:GLN:HG2   | 1.95                     | 0.49              |
| 16:UM:583:PHE:HA   | 16:UM:590:LEU:HD23  | 1.95                     | 0.49              |
| 17:UN:292:ARG:HG2  | 47:JP:292:ARG:HG3   | 1.94                     | 0.49              |
| 18:UO:16:LEU:HG    | 18:UO:17:PRO:HD2    | 1.95                     | 0.49              |
| 18:UO:90:ARG:HH21  | 18:UO:137:ASN:HB3   | 1.77                     | 0.49              |
| 18:UO:499:LYS:O    | 18:UO:503:ARG:HG2   | 2.13                     | 0.49              |
| 20:UQ:155:THR:O    | 20:UQ:171:TYR:HA    | 2.13                     | 0.49              |
| 20:UQ:200:ASN:ND2  | 20:UQ:262:MET:O     | 2.46                     | 0.49              |
| 20:UQ:378:ASP:HB2  | 20:UQ:380:THR:HG22  | 1.93                     | 0.49              |
| 21:UR:490:PHE:CE2  | 30:CF:89:ARG:HG3    | 2.48                     | 0.49              |
| 23:UT:100:GLU:OE1  | 23:UT:100:GLU:N     | 2.29                     | 0.49              |
| 23:UT:243:THR:HB   | 23:UT:246:THR:O     | 2.13                     | 0.49              |
| 23:UT:260:HIS:O    | 23:UT:263:LEU:HG    | 2.13                     | 0.49              |
| 23:UT:593:ASP:HB2  | 23:UT:596:ILE:HG22  | 1.94                     | 0.49              |
| 23:UT:668:GLY:O    | 23:UT:672:VAL:HG23  | 2.12                     | 0.49              |
| 23:UT:1069:VAL:O   | 23:UT:1072:THR:HG23 | 2.13                     | 0.49              |
| 23:UT:1477:LYS:NZ  | 23:UT:1479:ASN:HB3  | 2.28                     | 0.49              |
| 23:UT:1543:GLN:O   | 23:UT:1547:LEU:HD23 | 2.13                     | 0.49              |
| 27:UZ:17:LEU:HD23  | 27:UZ:20:LEU:HD21   | 1.95                     | 0.49              |
| 28:CD:17:VAL:HG12  | 28:CD:52:SER:HB2    | 1.94                     | 0.49              |
| 33:CJ:188:HIS:C    | 33:CJ:189:LEU:HD12  | 2.33                     | 0.49              |
| 36:CM:175:ALA:HA   | 36:CM:361:ASN:HB2   | 1.94                     | 0.49              |
| 37:CN:91:ASP:OD2   | 37:CN:96:HIS:N      | 2.36                     | 0.49              |
| 38:JC:108:SER:OG   | 38:JC:109:ASP:N     | 2.46                     | 0.49              |
| 39:JF:156:GLU:OE1  | 39:JF:156:GLU:N     | 2.43                     | 0.49              |
| 39:JF:243:HIS:HB2  | 39:JG:243:HIS:ND1   | 2.28                     | 0.49              |
| 44:JM:135:HIS:CE1  | 66:D3:487:G:N1      | 2.81                     | 0.49              |
| 46:JO:182:GLU:HG2  | 46:JO:203:LEU:HD11  | 1.95                     | 0.49              |
| 47:JP:50:LEU:HD23  | 47:JP:53:MET:SD     | 2.53                     | 0.49              |
| 47:JP:276:ASN:OD1  | 66:D3:-7:A:N6       | 2.44                     | 0.49              |
| 49:DE:147:ILE:HD13 | 49:DE:169:ILE:HD11  | 1.95                     | 0.49              |
| 53:DI:7:SER:OG     | 53:DI:10:LYS:HD3    | 2.13                     | 0.49              |
| 58:DQ:51:PRO:O     | 58:DQ:55:VAL:HG22   | 2.13                     | 0.49              |
| 58:DQ:98:ASP:OD1   | 58:DQ:101:SER:OG    | 2.26                     | 0.49              |
| 65:D2:413:C:H2'    | 65:D2:414:G:H8      | 1.77                     | 0.49              |
| 65:D2:428:A:H2'    | 65:D2:429:A:C8      | 2.47                     | 0.49              |
| 66:D3:254:A:H2'    | 66:D3:255:U:C6      | 2.48                     | 0.49              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 66:D3:538:A:O4'     | 66:D3:543:C:N4      | 2.46                     | 0.49              |
| 66:D3:555:A:O3'     | 66:D3:574:G:N2      | 2.45                     | 0.49              |
| 66:D3:752:A:H2'     | 66:D3:753:A:H8      | 1.78                     | 0.49              |
| 66:D3:862:A:C2      | 66:D3:963:A:C4      | 3.01                     | 0.49              |
| 66:D3:1138:A:H2'    | 66:D3:1139:A:O4'    | 2.13                     | 0.49              |
| 71:ED:377:SER:O     | 71:ED:381:SER:N     | 2.45                     | 0.49              |
| 78:EK:778:ILE:HA    | 78:EK:789:SER:CB    | 2.43                     | 0.49              |
| 3:JA:70:ARG:NH2     | 66:D3:415:C:OP1     | 2.44                     | 0.49              |
| 3:JA:520:ARG:HH12   | 3:JA:562:HIS:HB2    | 1.78                     | 0.49              |
| 3:JA:541:TYR:CE1    | 3:JA:637:ARG:HG2    | 2.48                     | 0.49              |
| 1:CB:264:GLN:HA     | 1:CB:320:TYR:O      | 2.13                     | 0.49              |
| 7:UD:268:GLN:O      | 7:UD:269:PHE:HB2    | 2.13                     | 0.49              |
| 9:UF:300:MET:HA     | 9:UF:303:GLU:HG3    | 1.95                     | 0.49              |
| 10:UG:63:THR:HG21   | 47:JP:28:LEU:HD23   | 1.94                     | 0.49              |
| 15:UL:159:LEU:HD13  | 15:UL:189:TRP:CD2   | 2.48                     | 0.49              |
| 15:UL:177:LEU:HD22  | 15:UL:189:TRP:HE3   | 1.78                     | 0.49              |
| 15:UL:808:THR:O     | 15:UL:812:ILE:HG12  | 2.13                     | 0.49              |
| 16:UM:340:ILE:HA    | 16:UM:357:THR:HA    | 1.95                     | 0.49              |
| 16:UM:756:ALA:O     | 16:UM:759:THR:HG22  | 2.12                     | 0.49              |
| 19:UP:200:ARG:HG3   | 19:UP:204:ARG:HD3   | 1.94                     | 0.49              |
| 20:UQ:535:ASN:N     | 20:UQ:538:GLU:OE2   | 2.45                     | 0.49              |
| 21:UR:295:ILE:HD11  | 21:UR:298:CYS:CB    | 2.34                     | 0.49              |
| 21:UR:324:TRP:HE1   | 21:UR:337:ALA:HB1   | 1.78                     | 0.49              |
| 21:UR:414:ILE:HD11  | 21:UR:420:ARG:HD2   | 1.95                     | 0.49              |
| 21:UR:436:ASP:O     | 21:UR:437:LEU:HD23  | 2.13                     | 0.49              |
| 23:UT:508:PHE:O     | 23:UT:548:TYR:OH    | 2.21                     | 0.49              |
| 23:UT:1284:LEU:HD13 | 23:UT:1287:LEU:HD12 | 1.94                     | 0.49              |
| 23:UT:1592:PRO:HA   | 23:UT:1595:SER:HB2  | 1.95                     | 0.49              |
| 23:UT:1688:HIS:CE1  | 23:UT:1745:ILE:HG23 | 2.48                     | 0.49              |
| 23:UT:1927:SER:OG   | 23:UT:1928:ASP:N    | 2.45                     | 0.49              |
| 24:UU:66:LEU:HD13   | 24:UU:346:ARG:HG2   | 1.94                     | 0.49              |
| 24:UU:132:THR:OG1   | 24:UU:133:ASP:N     | 2.45                     | 0.49              |
| 24:UU:586:ASN:OD1   | 24:UU:587:ARG:N     | 2.41                     | 0.49              |
| 25:UV:699:GLU:O     | 25:UV:703:LYS:HE2   | 2.11                     | 0.49              |
| 25:UV:947:PRO:HD2   | 25:UV:948:TYR:CD2   | 2.48                     | 0.49              |
| 25:UV:1046:ASP:HB2  | 25:UV:1051:LEU:HD13 | 1.94                     | 0.49              |
| 31:CH:364:GLU:HG2   | 31:CH:367:LYS:HB3   | 1.94                     | 0.49              |
| 31:CH:425:TRP:CZ2   | 31:CH:432:PRO:HG3   | 2.48                     | 0.49              |
| 35:CL:921:GLU:OE2   | 36:CM:366:ILE:N     | 2.46                     | 0.49              |
| 37:CN:225:SER:HB2   | 66:D3:1059:U:O2     | 2.13                     | 0.49              |
| 45:JN:280:LYS:HE3   | 65:D2:382:U:H5      | 1.77                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:JO:218:GLU:O    | 66:D3:904:G:N1     | 2.33                     | 0.49              |
| 47:JP:389:ARG:NH1  | 67:D4:38:U:OP1     | 2.45                     | 0.49              |
| 49:DE:117:GLU:OE1  | 49:DE:117:GLU:N    | 2.43                     | 0.49              |
| 54:DJ:30:LEU:HD12  | 54:DJ:105:LEU:HD13 | 1.95                     | 0.49              |
| 54:DJ:48:GLN:O     | 54:DJ:52:ILE:HG12  | 2.13                     | 0.49              |
| 58:DQ:97:VAL:CG1   | 58:DQ:98:ASP:H     | 2.24                     | 0.49              |
| 61:DX:74:VAL:HG21  | 61:DX:104:LEU:HD11 | 1.95                     | 0.49              |
| 65:D2:198:A:H3'    | 65:D2:199:A:C8     | 2.48                     | 0.49              |
| 65:D2:255:U:O2'    | 65:D2:256:U:OP1    | 2.26                     | 0.49              |
| 66:D3:30:G:N2      | 66:D3:31:C:C2      | 2.81                     | 0.49              |
| 66:D3:1616:G:C6    | 66:D3:1617:U:N3    | 2.81                     | 0.49              |
| 66:D3:1753:A:H2'   | 66:D3:1754:A:H8    | 1.78                     | 0.49              |
| 3:JA:24:SER:OG     | 3:JA:25:ILE:N      | 2.45                     | 0.49              |
| 3:JA:760:CYS:SG    | 3:JA:762:MET:HB2   | 2.52                     | 0.49              |
| 3:JA:798:ALA:O     | 3:JA:802:LEU:HG    | 2.12                     | 0.49              |
| 3:JA:805:ILE:HB    | 3:JA:809:LYS:HZ3   | 1.78                     | 0.49              |
| 4:UA:852:THR:HB    | 24:UU:897:HIS:CE1  | 2.48                     | 0.49              |
| 3:JB:44:MET:O      | 3:JB:47:ALA:C      | 2.51                     | 0.49              |
| 5:UB:747:GLU:O     | 5:UB:751:THR:HG22  | 2.13                     | 0.49              |
| 7:UD:78:ILE:HD12   | 7:UD:104:TRP:HZ2   | 1.78                     | 0.49              |
| 7:UD:262:ILE:HD11  | 7:UD:283:VAL:HG21  | 1.95                     | 0.49              |
| 7:UD:326:ARG:NH1   | 7:UD:364:PHE:O     | 2.46                     | 0.49              |
| 7:UD:551:ASP:OD1   | 7:UD:552:ILE:N     | 2.46                     | 0.49              |
| 9:UF:14:GLU:CD     | 9:UF:15:MET:HG3    | 2.33                     | 0.49              |
| 9:UF:28:GLU:HG2    | 21:UR:27:PHE:CZ    | 2.48                     | 0.49              |
| 10:UG:194:ARG:H    | 10:UG:209:GLY:HA2  | 1.77                     | 0.49              |
| 11:UH:582:ILE:O    | 11:UH:586:ILE:HG12 | 2.12                     | 0.49              |
| 11:UH:635:PHE:HD1  | 11:UH:638:LEU:HD12 | 1.78                     | 0.49              |
| 15:UL:545:TYR:HE1  | 15:UL:559:PHE:CZ   | 2.31                     | 0.49              |
| 16:UM:211:LEU:HD11 | 16:UM:225:PHE:CD1  | 2.48                     | 0.49              |
| 16:UM:454:LEU:HD23 | 16:UM:466:TRP:O    | 2.12                     | 0.49              |
| 16:UM:542:CYS:HB2  | 16:UM:547:LEU:H    | 1.77                     | 0.49              |
| 20:UQ:396:ILE:HG22 | 20:UQ:397:LYS:HG2  | 1.94                     | 0.49              |
| 23:UT:394:LEU:HD11 | 23:UT:435:PHE:CG   | 2.48                     | 0.49              |
| 23:UT:514:PHE:O    | 23:UT:518:MET:HG3  | 2.12                     | 0.49              |
| 23:UT:1090:ARG:O   | 23:UT:1094:PHE:N   | 2.46                     | 0.49              |
| 23:UT:1344:TRP:O   | 23:UT:1348:LEU:HG  | 2.13                     | 0.49              |
| 24:UU:552:HIS:CD2  | 24:UU:555:SER:H    | 2.26                     | 0.49              |
| 28:CD:46:LYS:NZ    | 65:D2:485:G:OP2    | 2.46                     | 0.49              |
| 29:CE:194:GLU:OE2  | 29:CE:242:SER:HA   | 2.12                     | 0.49              |
| 30:CG:95:ARG:NE    | 31:CH:551:ARG:HB2  | 2.28                     | 0.49              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 31:CH:233:GLU:OE1  | 31:CH:233:GLU:N     | 2.46                     | 0.49              |
| 32:CI:137:ARG:HA   | 32:CI:142:LEU:HA    | 1.95                     | 0.49              |
| 35:CL:111:LYS:HD2  | 35:CL:312:PHE:CE1   | 2.48                     | 0.49              |
| 35:CL:143:ASP:OD1  | 35:CL:144:GLY:N     | 2.46                     | 0.49              |
| 37:CN:223:LEU:CG   | 37:CN:227:ARG:HH12  | 2.25                     | 0.49              |
| 38:JC:33:ARG:HE    | 38:JC:34:LYS:HE3    | 1.78                     | 0.49              |
| 38:JC:100:GLU:O    | 38:JC:100:GLU:HG2   | 2.13                     | 0.49              |
| 38:JC:277:ILE:HD12 | 38:JC:288:LYS:HZ3   | 1.78                     | 0.49              |
| 39:JG:189:VAL:HG23 | 39:JG:244:GLY:HA3   | 1.95                     | 0.49              |
| 39:JG:218:ASP:HA   | 39:JG:221:VAL:HG22  | 1.94                     | 0.49              |
| 49:DE:11:ARG:NH2   | 49:DE:20:LEU:HD12   | 2.27                     | 0.49              |
| 49:DE:130:GLN:HB3  | 49:DE:138:TYR:CZ    | 2.48                     | 0.49              |
| 50:DF:34:GLN:O     | 50:DF:38:THR:HG23   | 2.13                     | 0.49              |
| 50:DF:205:SER:O    | 50:DF:205:SER:OG    | 2.26                     | 0.49              |
| 51:DG:122:GLU:HG2  | 51:DG:123:GLY:N     | 2.28                     | 0.49              |
| 51:DG:185:GLN:O    | 51:DG:188:ARG:HG2   | 2.13                     | 0.49              |
| 52:DH:62:VAL:HG11  | 52:DH:70:PHE:CE2    | 2.47                     | 0.49              |
| 53:DI:79:ALA:HB2   | 53:DI:164:ARG:NH1   | 2.25                     | 0.49              |
| 53:DI:166:TYR:CE2  | 53:DI:193:LEU:HD21  | 2.47                     | 0.49              |
| 56:DN:91:LEU:HB3   | 56:DN:122:ILE:HD12  | 1.93                     | 0.49              |
| 65:D2:287:G:C5     | 67:D4:67:G:C2       | 3.01                     | 0.49              |
| 66:D3:325:G:H2'    | 66:D3:326:G:H8      | 1.77                     | 0.49              |
| 66:D3:1057:U:O2'   | 66:D3:1058:U:O5'    | 2.27                     | 0.49              |
| 77:EJ:67:GLU:O     | 77:EJ:107:LEU:N     | 2.45                     | 0.49              |
| 2:DA:243:LYS:HA    | 25:UV:656:ARG:HG2   | 1.95                     | 0.48              |
| 4:UA:15:TYR:CD1    | 4:UA:20:ILE:HD11    | 2.48                     | 0.48              |
| 4:UA:155:SER:OG    | 4:UA:157:ASP:OD1    | 2.13                     | 0.48              |
| 4:UA:846:TYR:O     | 4:UA:850:VAL:HG22   | 2.13                     | 0.48              |
| 7:UD:285:CYS:SG    | 7:UD:335:ALA:HA     | 2.53                     | 0.48              |
| 7:UD:547:CYS:O     | 7:UD:566:LEU:O      | 2.31                     | 0.48              |
| 7:UD:769:PHE:HE1   | 19:UP:211:LEU:HB2   | 1.78                     | 0.48              |
| 10:UG:527:ARG:HH22 | 65:D2:366:A:P       | 2.35                     | 0.48              |
| 11:UH:650:LEU:HD12 | 11:UH:655:LEU:HG    | 1.94                     | 0.48              |
| 13:UJ:1418:ASN:O   | 13:UJ:1422:VAL:HG23 | 2.13                     | 0.48              |
| 14:UK:237:SER:OG   | 14:UK:239:LYS:HD3   | 2.13                     | 0.48              |
| 15:UL:594:ASP:OD1  | 15:UL:594:ASP:N     | 2.33                     | 0.48              |
| 17:UN:848:PRO:HG3  | 47:JP:406:HIS:CE1   | 2.48                     | 0.48              |
| 20:UQ:153:ILE:CG1  | 20:UQ:174:TYR:HB2   | 2.43                     | 0.48              |
| 20:UQ:698:VAL:HG13 | 20:UQ:702:TYR:HD2   | 1.77                     | 0.48              |
| 23:UT:356:ASP:OD1  | 23:UT:357:LYS:N     | 2.46                     | 0.48              |
| 23:UT:1140:GLN:HG2 | 23:UT:1188:LYS:HD2  | 1.94                     | 0.48              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 23:UT:1189:LEU:HD23 | 23:UT:1198:PHE:CE2  | 2.48                     | 0.48              |
| 23:UT:1520:TRP:HE1  | 23:UT:1587:LYS:HE3  | 1.77                     | 0.48              |
| 23:UT:1696:TYR:HA   | 23:UT:1699:LYS:NZ   | 2.28                     | 0.48              |
| 23:UT:1924:LEU:HD23 | 23:UT:1925:ASP:N    | 2.28                     | 0.48              |
| 25:UV:249:ASP:N     | 25:UV:249:ASP:OD1   | 2.44                     | 0.48              |
| 25:UV:369:TRP:HZ2   | 25:UV:495:THR:HG21  | 1.77                     | 0.48              |
| 27:UZ:55:ARG:HH21   | 48:JQ:189:PRO:HA    | 1.78                     | 0.48              |
| 28:CD:44:PHE:CD1    | 28:CD:47:LEU:HD23   | 2.47                     | 0.48              |
| 29:CE:93:LYS:HD2    | 29:CE:94:LEU:HD22   | 1.94                     | 0.48              |
| 29:CE:411:LYS:NZ    | 67:D4:69:A:OP1      | 2.42                     | 0.48              |
| 30:CG:11:LEU:HG     | 30:CG:80:PHE:O      | 2.12                     | 0.48              |
| 31:CH:443:LEU:HB3   | 31:CH:471:GLN:NE2   | 2.28                     | 0.48              |
| 33:CJ:189:LEU:HD23  | 33:CJ:191:PHE:CZ    | 2.47                     | 0.48              |
| 36:CM:18:ARG:HD3    | 36:CM:98:TYR:CE1    | 2.47                     | 0.48              |
| 39:JF:45:LEU:HD13   | 39:JF:206:VAL:HG23  | 1.94                     | 0.48              |
| 39:JF:52:THR:HG21   | 39:JF:146:HIS:CE1   | 2.42                     | 0.48              |
| 39:JG:167:ILE:O     | 39:JG:171:LEU:HG    | 2.13                     | 0.48              |
| 39:JG:192:TYR:HA    | 39:JG:195:LYS:HZ1   | 1.78                     | 0.48              |
| 51:DG:3:LEU:O       | 51:DG:15:THR:HA     | 2.12                     | 0.48              |
| 56:DN:14:SER:HB3    | 66:D3:958:U:H2'     | 1.95                     | 0.48              |
| 66:D3:554:C:H5      | 66:D3:571:G:N1      | 2.10                     | 0.48              |
| 3:JA:23:ARG:HH11    | 3:JA:475:ARG:NH2    | 2.10                     | 0.48              |
| 1:CB:194:VAL:HG23   | 1:CB:217:ILE:HA     | 1.95                     | 0.48              |
| 1:CB:195:TYR:CD1    | 1:CB:234:ILE:HG23   | 2.48                     | 0.48              |
| 1:CB:236:MET:HE1    | 29:CE:118:ARG:HG3   | 1.95                     | 0.48              |
| 1:CB:255:LEU:O      | 1:CB:259:MET:HG3    | 2.14                     | 0.48              |
| 7:UD:52:SER:OG      | 7:UD:53:HIS:N       | 2.46                     | 0.48              |
| 10:UG:81:GLU:O      | 10:UG:82:LYS:HD3    | 2.13                     | 0.48              |
| 10:UG:304:ARG:HG3   | 10:UG:304:ARG:HH21  | 1.77                     | 0.48              |
| 12:UI:511:LYS:O     | 12:UI:514:GLU:HG2   | 2.12                     | 0.48              |
| 13:UJ:248:SER:OG    | 13:UJ:249:LYS:N     | 2.47                     | 0.48              |
| 13:UJ:684:TYR:O     | 13:UJ:688:PHE:HB2   | 2.13                     | 0.48              |
| 13:UJ:1394:GLU:O    | 13:UJ:1397:GLN:HG3  | 2.13                     | 0.48              |
| 13:UJ:1534:SER:HA   | 13:UJ:1537:LEU:HD12 | 1.94                     | 0.48              |
| 13:UJ:1607:ARG:HB3  | 13:UJ:1612:ASP:HB2  | 1.96                     | 0.48              |
| 15:UL:420:LYS:H     | 15:UL:420:LYS:HD2   | 1.79                     | 0.48              |
| 18:UO:480:LEU:HD23  | 18:UO:483:LEU:HD12  | 1.95                     | 0.48              |
| 20:UQ:37:LEU:HD12   | 20:UQ:43:ASN:O      | 2.13                     | 0.48              |
| 20:UQ:510:TYR:HB2   | 20:UQ:557:ILE:HD11  | 1.95                     | 0.48              |
| 21:UR:235:ILE:HD12  | 21:UR:590:LYS:O     | 2.14                     | 0.48              |
| 21:UR:319:ARG:HD3   | 21:UR:353:ARG:HH11  | 1.78                     | 0.48              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 22:US:254:LYS:O    | 22:US:258:GLU:HG2   | 2.12                     | 0.48              |
| 22:US:474:HIS:CD2  | 22:US:477:VAL:HG23  | 2.48                     | 0.48              |
| 22:US:499:LEU:O    | 22:US:501:TRP:N     | 2.42                     | 0.48              |
| 23:UT:77:LEU:HD21  | 23:UT:81:LEU:HD22   | 1.94                     | 0.48              |
| 23:UT:773:LEU:O    | 23:UT:777:GLN:HG2   | 2.13                     | 0.48              |
| 23:UT:940:GLY:HA2  | 23:UT:943:ARG:HE    | 1.79                     | 0.48              |
| 23:UT:1888:THR:HB  | 23:UT:1891:HIS:ND1  | 2.28                     | 0.48              |
| 24:UU:253:SER:OG   | 24:UU:254:LEU:N     | 2.46                     | 0.48              |
| 25:UV:1157:TYR:HD2 | 25:UV:1161:LEU:HD23 | 1.78                     | 0.48              |
| 33:CJ:43:PRO:HD2   | 33:CJ:46:LEU:HD12   | 1.94                     | 0.48              |
| 33:CJ:92:THR:HG21  | 33:CJ:96:PRO:CB     | 2.41                     | 0.48              |
| 33:CJ:97:SER:HG    | 33:CJ:144:GLU:CD    | 2.16                     | 0.48              |
| 33:CJ:121:ASN:HB2  | 66:D3:1585:U:OP1    | 2.12                     | 0.48              |
| 34:CK:452:SER:O    | 34:CK:453:SER:OG    | 2.28                     | 0.48              |
| 35:CL:75:VAL:HG22  | 35:CL:120:CYS:SG    | 2.53                     | 0.48              |
| 35:CL:805:ASN:HD21 | 35:CL:807:LYS:HB2   | 1.79                     | 0.48              |
| 35:CL:847:LEU:HA   | 35:CL:898:GLY:HA2   | 1.95                     | 0.48              |
| 36:CM:80:ILE:HG22  | 36:CM:81:ILE:H      | 1.77                     | 0.48              |
| 36:CM:139:PRO:O    | 36:CM:142:GLU:HG2   | 2.13                     | 0.48              |
| 36:CM:231:ARG:NH1  | 66:D3:1133:A:O5'    | 2.31                     | 0.48              |
| 39:JG:137:PHE:O    | 39:JG:141:MET:HG2   | 2.13                     | 0.48              |
| 45:JN:170:ASN:HB2  | 65:D2:382:U:O4      | 2.13                     | 0.48              |
| 47:JP:209:LEU:O    | 47:JP:210:LYS:HE2   | 2.12                     | 0.48              |
| 50:DF:112:ARG:HD2  | 66:D3:1528:U:H5''   | 1.95                     | 0.48              |
| 51:DG:69:LEU:O     | 51:DG:100:ALA:N     | 2.46                     | 0.48              |
| 51:DG:79:LYS:HD3   | 51:DG:89:ASP:HA     | 1.94                     | 0.48              |
| 52:DH:43:PHE:HB2   | 52:DH:62:VAL:HG22   | 1.93                     | 0.48              |
| 65:D2:109:C:H5'    | 65:D2:110:G:OP1     | 2.12                     | 0.48              |
| 66:D3:282:C:H2'    | 66:D3:283:U:C6      | 2.48                     | 0.48              |
| 66:D3:305:C:H2'    | 66:D3:306:U:C6      | 2.48                     | 0.48              |
| 66:D3:462:G:H2'    | 66:D3:463:U:C6      | 2.48                     | 0.48              |
| 66:D3:539:G:O2'    | 66:D3:540:G:O5'     | 2.29                     | 0.48              |
| 72:EE:190:GLN:O    | 72:EE:194:LEU:N     | 2.46                     | 0.48              |
| 1:CA:127:GLU:OE1   | 44:JM:107:PRO:HG3   | 2.13                     | 0.48              |
| 2:DA:27:LYS:HA     | 2:DA:49:ASN:O       | 2.13                     | 0.48              |
| 3:JA:57:TRP:NE1    | 3:JA:125:GLN:HB2    | 2.28                     | 0.48              |
| 3:JA:384:VAL:O     | 3:JA:406:VAL:HA     | 2.13                     | 0.48              |
| 4:UA:319:PHE:HB2   | 4:UA:328:LEU:HB3    | 1.95                     | 0.48              |
| 4:UA:549:GLN:NE2   | 4:UA:552:ASN:HB3    | 2.28                     | 0.48              |
| 1:CB:185:SER:HB2   | 1:CB:194:VAL:HG21   | 1.95                     | 0.48              |
| 11:UH:524:THR:HA   | 11:UH:527:LEU:HD12  | 1.94                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:UJ:525:PHE:O    | 13:UJ:529:VAL:HG23 | 2.13                     | 0.48              |
| 13:UJ:547:ILE:O    | 13:UJ:551:ILE:HG12 | 2.14                     | 0.48              |
| 13:UJ:551:ILE:HG21 | 13:UJ:588:LEU:HB3  | 1.95                     | 0.48              |
| 13:UJ:585:ILE:O    | 13:UJ:589:ILE:HG12 | 2.13                     | 0.48              |
| 15:UL:216:LEU:HD23 | 15:UL:216:LEU:H    | 1.77                     | 0.48              |
| 16:UM:7:TYR:HE1    | 16:UM:648:THR:HG23 | 1.78                     | 0.48              |
| 16:UM:389:ASP:HB3  | 16:UM:409:ASP:HB2  | 1.95                     | 0.48              |
| 16:UM:592:SER:OG   | 16:UM:600:LYS:HB2  | 2.12                     | 0.48              |
| 20:UQ:36:ARG:HH12  | 20:UQ:90:LYS:HD2   | 1.77                     | 0.48              |
| 20:UQ:36:ARG:HH12  | 20:UQ:90:LYS:CD    | 2.27                     | 0.48              |
| 20:UQ:714:ASP:HB3  | 20:UQ:718:GLY:H    | 1.79                     | 0.48              |
| 22:US:286:ILE:HA   | 22:US:289:PHE:CB   | 2.42                     | 0.48              |
| 23:UT:37:ARG:HG3   | 23:UT:40:ASP:HB2   | 1.95                     | 0.48              |
| 23:UT:140:ILE:HD11 | 23:UT:188:LEU:HD21 | 1.95                     | 0.48              |
| 23:UT:178:ILE:HA   | 23:UT:181:LEU:HG   | 1.95                     | 0.48              |
| 23:UT:315:LEU:HD11 | 23:UT:358:VAL:HG22 | 1.93                     | 0.48              |
| 23:UT:465:PHE:HA   | 23:UT:468:ALA:HB2  | 1.94                     | 0.48              |
| 23:UT:708:ASP:OD1  | 23:UT:775:ARG:NH1  | 2.45                     | 0.48              |
| 23:UT:1763:LEU:HA  | 23:UT:1766:PHE:CE2 | 2.45                     | 0.48              |
| 25:UV:528:ASP:CA   | 25:UV:614:ARG:HH21 | 2.19                     | 0.48              |
| 26:UX:128:LEU:HD11 | 26:UX:144:ARG:HH12 | 1.77                     | 0.48              |
| 27:UZ:109:ARG:HH12 | 66:D3:1478:G:P     | 2.37                     | 0.48              |
| 28:CD:261:GLN:HG3  | 29:CE:154:PHE:HZ   | 1.78                     | 0.48              |
| 29:CE:179:THR:HG23 | 29:CE:180:TYR:HD1  | 1.78                     | 0.48              |
| 35:CL:75:VAL:O     | 35:CL:141:LEU:HD23 | 2.13                     | 0.48              |
| 36:CM:319:ASP:O    | 36:CM:323:ILE:HG12 | 2.13                     | 0.48              |
| 38:JC:161:GLU:OE2  | 38:JC:177:LYS:NZ   | 2.46                     | 0.48              |
| 39:JG:167:ILE:O    | 39:JG:170:HIS:N    | 2.44                     | 0.48              |
| 42:JJ:106:MET:HE1  | 42:JJ:135:LYS:HD2  | 1.95                     | 0.48              |
| 42:JJ:106:MET:HE2  | 42:JJ:135:LYS:HB3  | 1.95                     | 0.48              |
| 43:JK:460:LYS:NZ   | 66:D3:342:C:H41    | 2.10                     | 0.48              |
| 45:JN:291:ILE:HG22 | 45:JN:294:ARG:H    | 1.77                     | 0.48              |
| 47:JP:301:PHE:HD1  | 47:JP:337:GLY:HA2  | 1.79                     | 0.48              |
| 47:JP:314:SER:O    | 47:JP:316:THR:N    | 2.46                     | 0.48              |
| 49:DE:161:LYS:HB3  | 49:DE:171:ASP:OD1  | 2.12                     | 0.48              |
| 50:DF:186:ASN:HD21 | 50:DF:188:LYS:HB2  | 1.78                     | 0.48              |
| 52:DH:21:ALA:O     | 52:DH:25:VAL:HG23  | 2.14                     | 0.48              |
| 52:DH:78:THR:OG1   | 52:DH:79:ARG:NH1   | 2.46                     | 0.48              |
| 53:DI:5:ARG:NH2    | 66:D3:331:A:O2'    | 2.46                     | 0.48              |
| 56:DN:61:THR:HG23  | 56:DN:62:GLN:N     | 2.29                     | 0.48              |
| 66:D3:327:U:O4     | 66:D3:328:A:N6     | 2.47                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 66:D3:477:A:H2     | 66:D3:512:A:N1     | 2.12                     | 0.48              |
| 66:D3:689:G:H2'    | 66:D3:690:G:C8     | 2.48                     | 0.48              |
| 66:D3:846:G:H2'    | 66:D3:847:A:N7     | 2.27                     | 0.48              |
| 66:D3:1682:U:O2'   | 66:D3:1683:C:H6    | 1.96                     | 0.48              |
| 66:D3:1729:C:H2'   | 66:D3:1730:A:O4'   | 2.13                     | 0.48              |
| 66:D3:1783:C:H2'   | 66:D3:1784:C:C6    | 2.48                     | 0.48              |
| 67:D4:148:G:O6     | 67:D4:150:A:N6     | 2.46                     | 0.48              |
| 67:D4:149:C:H1'    | 67:D4:150:A:N7     | 2.28                     | 0.48              |
| 67:D4:156:U:H5''   | 67:D4:157:A:C8     | 2.49                     | 0.48              |
| 4:UA:88:ASN:ND2    | 24:UU:659:GLN:HE21 | 2.07                     | 0.48              |
| 4:UA:385:GLU:HB2   | 4:UA:414:TRP:CH2   | 2.45                     | 0.48              |
| 1:CB:169:LYS:HG2   | 1:CB:193:VAL:CG1   | 2.43                     | 0.48              |
| 1:CB:302:GLU:OE1   | 14:UK:135:ILE:HA   | 2.14                     | 0.48              |
| 7:UD:299:GLY:O     | 7:UD:333:ILE:HB    | 2.13                     | 0.48              |
| 7:UD:647:TRP:CD2   | 7:UD:656:ARG:HB2   | 2.47                     | 0.48              |
| 9:UF:311:TYR:HD2   | 9:UF:312:LEU:HD22  | 1.78                     | 0.48              |
| 10:UG:157:ALA:CB   | 10:UG:168:VAL:HG12 | 2.42                     | 0.48              |
| 12:UI:439:LYS:HA   | 12:UI:442:THR:HG22 | 1.95                     | 0.48              |
| 15:UL:170:TRP:HB3  | 15:UL:178:ILE:HG22 | 1.94                     | 0.48              |
| 15:UL:861:ILE:O    | 15:UL:865:HIS:HB2  | 2.13                     | 0.48              |
| 16:UM:592:SER:HB3  | 16:UM:602:TRP:CH2  | 2.48                     | 0.48              |
| 18:UO:123:SER:HB3  | 18:UO:150:ARG:NH1  | 2.27                     | 0.48              |
| 20:UQ:578:ASN:ND2  | 65:D2:7:A:H62      | 2.11                     | 0.48              |
| 21:UR:137:ILE:HG22 | 21:UR:138:LEU:HD23 | 1.95                     | 0.48              |
| 24:UU:279:ASP:OD1  | 24:UU:280:ARG:N    | 2.46                     | 0.48              |
| 25:UV:626:LYS:NZ   | 25:UV:628:VAL:H    | 2.08                     | 0.48              |
| 25:UV:688:LYS:HE2  | 25:UV:689:HIS:HD2  | 1.77                     | 0.48              |
| 30:CF:33:LEU:HD12  | 30:CF:101:SER:O    | 2.14                     | 0.48              |
| 30:CF:42:LYS:O     | 30:CF:46:ARG:HG2   | 2.13                     | 0.48              |
| 30:CG:51:PHE:CE2   | 30:CG:53:ILE:HD11  | 2.49                     | 0.48              |
| 31:CH:132:VAL:HG13 | 31:CH:409:ASP:HB3  | 1.95                     | 0.48              |
| 31:CH:437:ARG:C    | 31:CH:439:ALA:H    | 2.15                     | 0.48              |
| 35:CL:931:LYS:HB2  | 35:CL:1006:TRP:HZ3 | 1.78                     | 0.48              |
| 38:JC:242:THR:OG1  | 38:JC:255:TYR:O    | 2.21                     | 0.48              |
| 38:JC:281:ASP:OD1  | 38:JC:281:ASP:N    | 2.43                     | 0.48              |
| 50:DF:117:THR:O    | 50:DF:121:ILE:HG12 | 2.14                     | 0.48              |
| 62:DY:109:LYS:HZ2  | 66:D3:55:A:P       | 2.36                     | 0.48              |
| 66:D3:387:A:N6     | 66:D3:402:C:O5'    | 2.35                     | 0.48              |
| 66:D3:647:G:H22    | 66:D3:687:G:N2     | 2.11                     | 0.48              |
| 66:D3:1662:G:H2'   | 66:D3:1663:G:C8    | 2.49                     | 0.48              |
| 79:EN:960:ALA:O    | 79:EN:964:LYS:N    | 2.38                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:JA:16:ASN:O      | 3:JA:20:THR:HG22   | 2.13                     | 0.48              |
| 3:JA:138:THR:HA    | 3:JA:141:THR:HG22  | 1.96                     | 0.48              |
| 4:UA:14:VAL:HG21   | 4:UA:341:GLN:HB3   | 1.94                     | 0.48              |
| 4:UA:284:PHE:CZ    | 4:UA:298:LEU:HB2   | 2.49                     | 0.48              |
| 4:UA:369:ILE:HD11  | 4:UA:390:VAL:HG21  | 1.94                     | 0.48              |
| 4:UA:728:GLU:HA    | 4:UA:731:ARG:HG2   | 1.95                     | 0.48              |
| 7:UD:374:THR:OG1   | 7:UD:375:VAL:N     | 2.45                     | 0.48              |
| 7:UD:535:GLU:HG3   | 7:UD:573:VAL:HG13  | 1.96                     | 0.48              |
| 9:UF:89:GLN:HB3    | 9:UF:120:ARG:CZ    | 2.43                     | 0.48              |
| 9:UF:271:LEU:HG    | 9:UF:337:HIS:HB3   | 1.96                     | 0.48              |
| 10:UG:121:ASN:HB2  | 10:UG:123:THR:HG22 | 1.94                     | 0.48              |
| 15:UL:49:VAL:CG1   | 15:UL:63:LEU:HB2   | 2.43                     | 0.48              |
| 15:UL:261:PHE:N    | 15:UL:343:TRP:HE1  | 2.11                     | 0.48              |
| 15:UL:791:ASN:OD1  | 15:UL:792:ALA:N    | 2.46                     | 0.48              |
| 16:UM:155:GLN:HB2  | 16:UM:158:SER:HB3  | 1.94                     | 0.48              |
| 16:UM:760:ILE:HA   | 16:UM:763:ILE:HG22 | 1.96                     | 0.48              |
| 18:UO:251:PHE:HD1  | 18:UO:255:VAL:HG12 | 1.78                     | 0.48              |
| 20:UQ:313:LEU:HD23 | 20:UQ:323:LEU:HG   | 1.94                     | 0.48              |
| 20:UQ:420:SER:HA   | 20:UQ:423:LYS:HG2  | 1.95                     | 0.48              |
| 20:UQ:728:LEU:HD23 | 20:UQ:728:LEU:H    | 1.78                     | 0.48              |
| 22:US:376:VAL:O    | 22:US:380:ILE:HG13 | 2.13                     | 0.48              |
| 23:UT:853:HIS:HA   | 23:UT:856:VAL:HG22 | 1.94                     | 0.48              |
| 24:UU:37:VAL:HB    | 24:UU:53:CYS:HB3   | 1.96                     | 0.48              |
| 25:UV:931:ASP:OD1  | 25:UV:932:GLU:N    | 2.46                     | 0.48              |
| 26:UX:80:VAL:HG11  | 26:UX:178:HIS:O    | 2.13                     | 0.48              |
| 29:CE:58:GLU:OE2   | 29:CE:150:HIS:HB3  | 2.12                     | 0.48              |
| 34:CK:358:THR:OG1  | 34:CK:359:SER:N    | 2.46                     | 0.48              |
| 35:CL:56:VAL:CG2   | 61:DX:101:GLU:HG3  | 2.43                     | 0.48              |
| 35:CL:623:LYS:HA   | 35:CL:626:LYS:HG2  | 1.95                     | 0.48              |
| 35:CL:750:TRP:HE3  | 61:DX:77:ILE:HG23  | 1.77                     | 0.48              |
| 36:CM:181:HIS:HE1  | 36:CM:309:GLY:HA2  | 1.78                     | 0.48              |
| 38:JC:53:PHE:CE1   | 38:JC:338:MET:HG2  | 2.47                     | 0.48              |
| 39:JG:55:ILE:O     | 39:JG:63:ASP:N     | 2.47                     | 0.48              |
| 42:JJ:106:MET:CE   | 42:JJ:135:LYS:HB3  | 2.43                     | 0.48              |
| 42:JJ:213:LYS:NZ   | 66:D3:1770:U:H1'   | 2.28                     | 0.48              |
| 47:JP:188:HIS:CD2  | 47:JP:190:GLU:H    | 2.31                     | 0.48              |
| 47:JP:391:LYS:HG2  | 47:JP:395:GLU:OE1  | 2.13                     | 0.48              |
| 52:DH:29:ASN:HA    | 52:DH:35:LYS:HZ1   | 1.77                     | 0.48              |
| 57:DO:28:VAL:HG23  | 57:DO:67:VAL:HG21  | 1.95                     | 0.48              |
| 66:D3:955:A:C5     | 66:D3:956:C:N3     | 2.82                     | 0.48              |
| 69:EB:256:MET:O    | 70:EC:196:LEU:N    | 2.45                     | 0.48              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 76:EI:348:ILE:O     | 76:EI:352:GLU:N     | 2.46                     | 0.48              |
| 3:JA:568:LEU:HD12   | 3:JA:569:PRO:HD2    | 1.94                     | 0.48              |
| 4:UA:116:GLY:O      | 4:UA:148:ASP:HA     | 2.14                     | 0.48              |
| 4:UA:341:GLN:NE2    | 4:UA:378:PHE:HB3    | 2.28                     | 0.48              |
| 4:UA:432:GLN:O      | 4:UA:432:GLN:HG3    | 2.14                     | 0.48              |
| 7:UD:312:ASN:HA     | 7:UD:315:GLN:NE2    | 2.28                     | 0.48              |
| 7:UD:485:LYS:HA     | 7:UD:498:VAL:O      | 2.13                     | 0.48              |
| 9:UF:28:GLU:HG2     | 21:UR:27:PHE:CE2    | 2.48                     | 0.48              |
| 9:UF:96:TYR:O       | 9:UF:100:THR:HG23   | 2.13                     | 0.48              |
| 12:UI:414:PRO:O     | 12:UI:418:LYS:HG3   | 2.12                     | 0.48              |
| 13:UJ:271:LYS:NZ    | 21:UR:217:ASN:O     | 2.36                     | 0.48              |
| 13:UJ:531:ILE:HD11  | 13:UJ:566:CYS:HB3   | 1.96                     | 0.48              |
| 13:UJ:666:ALA:HA    | 13:UJ:669:VAL:HG12  | 1.94                     | 0.48              |
| 13:UJ:1392:LEU:O    | 13:UJ:1396:LEU:HG   | 2.14                     | 0.48              |
| 14:UK:117:LYS:NZ    | 14:UK:204:HIS:CE1   | 2.81                     | 0.48              |
| 16:UM:296:ILE:C     | 16:UM:298:SER:H     | 2.16                     | 0.48              |
| 20:UQ:146:HIS:HB3   | 20:UQ:151:TYR:CD2   | 2.49                     | 0.48              |
| 21:UR:233:LEU:HD11  | 21:UR:552:PHE:CG    | 2.48                     | 0.48              |
| 22:US:155:LEU:O     | 22:US:158:SER:OG    | 2.31                     | 0.48              |
| 23:UT:100:GLU:HG2   | 23:UT:101:PHE:N     | 2.29                     | 0.48              |
| 23:UT:220:GLU:HG3   | 23:UT:268:PRO:HG3   | 1.95                     | 0.48              |
| 23:UT:903:THR:O     | 53:DI:77:ARG:NH2    | 2.42                     | 0.48              |
| 23:UT:1588:GLN:O    | 23:UT:1592:PRO:HD3  | 2.12                     | 0.48              |
| 23:UT:1670:LEU:HD11 | 23:UT:1701:MET:HE3  | 1.94                     | 0.48              |
| 23:UT:1674:ILE:HA   | 23:UT:1677:LEU:HG   | 1.96                     | 0.48              |
| 23:UT:1777:LEU:HD12 | 23:UT:1863:LEU:HD22 | 1.96                     | 0.48              |
| 24:UU:220:ILE:HD13  | 24:UU:234:ASN:HA    | 1.95                     | 0.48              |
| 28:CD:172:ASN:OD1   | 28:CD:173:HIS:N     | 2.46                     | 0.48              |
| 28:CD:194:ARG:HG2   | 29:CE:169:LEU:HD13  | 1.95                     | 0.48              |
| 29:CE:5:LEU:HD21    | 29:CE:89:VAL:HG23   | 1.95                     | 0.48              |
| 31:CH:551:ARG:O     | 31:CH:553:ILE:N     | 2.47                     | 0.48              |
| 33:CJ:80:THR:HA     | 33:CJ:83:ILE:HD13   | 1.96                     | 0.48              |
| 35:CL:65:ASP:N      | 35:CL:65:ASP:OD1    | 2.46                     | 0.48              |
| 35:CL:177:PHE:CD2   | 35:CL:183:LEU:HA    | 2.46                     | 0.48              |
| 35:CL:635:PHE:HZ    | 36:CM:221:CYS:HB2   | 1.77                     | 0.48              |
| 36:CM:274:LYS:CD    | 36:CM:278:GLN:HE22  | 2.24                     | 0.48              |
| 37:CN:62:SER:HA     | 37:CN:66:HIS:CD2    | 2.49                     | 0.48              |
| 37:CN:66:HIS:CE1    | 37:CN:161:THR:H     | 2.32                     | 0.48              |
| 38:JC:144:LEU:HD21  | 38:JC:153:LEU:HD12  | 1.94                     | 0.48              |
| 38:JC:230:GLN:N     | 38:JC:247:THR:OG1   | 2.41                     | 0.48              |
| 38:JC:262:PRO:HB2   | 38:JC:265:ILE:HG13  | 1.95                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 43:JK:460:LYS:NZ   | 66:D3:341:A:N7     | 2.56                     | 0.48              |
| 47:JP:235:LEU:HD23 | 47:JP:236:ALA:N    | 2.29                     | 0.48              |
| 49:DE:212:ASP:O    | 49:DE:215:ASP:CA   | 2.62                     | 0.48              |
| 50:DF:100:ASN:O    | 50:DF:104:ASN:ND2  | 2.47                     | 0.48              |
| 50:DF:127:GLN:HG3  | 50:DF:128:ASN:N    | 2.25                     | 0.48              |
| 53:DI:36:THR:HB    | 53:DI:96:LEU:HB2   | 1.94                     | 0.48              |
| 60:DW:111:MET:HE3  | 60:DW:115:GLU:OE1  | 2.13                     | 0.48              |
| 66:D3:29:U:H2'     | 66:D3:30:G:C8      | 2.44                     | 0.48              |
| 66:D3:104:A:O5'    | 66:D3:308:C:N4     | 2.37                     | 0.48              |
| 66:D3:1049:U:C2    | 66:D3:1050:G:C8    | 3.02                     | 0.48              |
| 1:CA:142:ARG:HH21  | 1:CA:183:HIS:CG    | 2.31                     | 0.48              |
| 2:DA:105:PHE:CE2   | 2:DA:211:HIS:HB3   | 2.49                     | 0.48              |
| 2:DA:121:ILE:HD13  | 2:DA:164:ILE:CD1   | 2.42                     | 0.48              |
| 3:JA:747:LEU:HD13  | 3:JA:760:CYS:HB2   | 1.94                     | 0.48              |
| 3:JA:771:SER:HB3   | 3:JA:774:LEU:HG    | 1.95                     | 0.48              |
| 4:UA:29:LEU:HD21   | 4:UA:327:LEU:HD21  | 1.95                     | 0.48              |
| 4:UA:162:LEU:HD22  | 4:UA:199:PHE:CE2   | 2.49                     | 0.48              |
| 5:UB:616:LEU:HB3   | 5:UB:619:LEU:HB3   | 1.95                     | 0.48              |
| 7:UD:32:ILE:HA     | 11:UH:720:TYR:CB   | 2.44                     | 0.48              |
| 7:UD:370:ARG:HH11  | 7:UD:371:LYS:H     | 1.62                     | 0.48              |
| 7:UD:426:GLN:OE1   | 7:UD:426:GLN:N     | 2.46                     | 0.48              |
| 10:UG:69:GLU:HG2   | 10:UG:409:ALA:HB1  | 1.96                     | 0.48              |
| 10:UG:74:LEU:HG    | 47:JP:3:ILE:HD12   | 1.95                     | 0.48              |
| 11:UH:676:TRP:CB   | 12:UI:486:LEU:HD13 | 2.42                     | 0.48              |
| 13:UJ:251:LYS:O    | 13:UJ:255:ILE:HG12 | 2.14                     | 0.48              |
| 13:UJ:309:GLN:NE2  | 21:UR:225:SER:HA   | 2.29                     | 0.48              |
| 13:UJ:663:SER:O    | 13:UJ:667:LYS:HG2  | 2.14                     | 0.48              |
| 14:UK:200:GLN:NE2  | 14:UK:204:HIS:NE2  | 2.62                     | 0.48              |
| 15:UL:878:LEU:HG   | 15:UL:882:ARG:HH21 | 1.79                     | 0.48              |
| 16:UM:16:TYR:O     | 16:UM:336:ASN:HB2  | 2.14                     | 0.48              |
| 16:UM:519:ASN:OD1  | 16:UM:520:LEU:N    | 2.46                     | 0.48              |
| 20:UQ:15:VAL:HA    | 20:UQ:67:LYS:NZ    | 2.28                     | 0.48              |
| 20:UQ:720:ILE:HG22 | 20:UQ:745:ILE:HA   | 1.95                     | 0.48              |
| 23:UT:636:ARG:NH2  | 66:D3:165:G:O2'    | 2.44                     | 0.48              |
| 24:UU:885:MET:HE3  | 24:UU:889:PHE:CZ   | 2.48                     | 0.48              |
| 25:UV:339:SER:HA   | 25:UV:342:HIS:CD2  | 2.48                     | 0.48              |
| 25:UV:433:ASP:HB3  | 25:UV:437:ASP:HB3  | 1.96                     | 0.48              |
| 25:UV:525:LEU:O    | 25:UV:616:LYS:HA   | 2.14                     | 0.48              |
| 25:UV:652:LYS:HD3  | 25:UV:684:PHE:CZ   | 2.49                     | 0.48              |
| 29:CE:234:ARG:O    | 29:CE:237:THR:HG22 | 2.14                     | 0.48              |
| 33:CJ:189:LEU:HD21 | 33:CJ:210:PHE:CG   | 2.49                     | 0.48              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 35:CL:777:ARG:NH2   | 35:CL:781:GLU:OE1  | 2.46                     | 0.48              |
| 36:CM:231:ARG:HH12  | 66:D3:1133:A:P     | 2.36                     | 0.48              |
| 38:JC:145:VAL:HB    | 38:JC:154:TYR:CZ   | 2.48                     | 0.48              |
| 38:JC:255:TYR:CD1   | 38:JC:262:PRO:HA   | 2.48                     | 0.48              |
| 47:JP:137:LEU:HD21  | 47:JP:147:LEU:HD12 | 1.95                     | 0.48              |
| 49:DE:183:VAL:HG13  | 49:DE:189:LEU:HA   | 1.96                     | 0.48              |
| 50:DF:133:VAL:HG22  | 50:DF:198:LEU:HD13 | 1.95                     | 0.48              |
| 56:DN:72:MET:HE1    | 66:D3:962:C:H5'    | 1.96                     | 0.48              |
| 57:DO:18:ARG:HH12   | 66:D3:919:A:P      | 2.37                     | 0.48              |
| 65:D2:359:U:H2'     | 65:D2:360:C:C6     | 2.48                     | 0.48              |
| 66:D3:330:G:C6      | 66:D3:331:A:C6     | 3.01                     | 0.48              |
| 66:D3:363:G:H2'     | 66:D3:364:G:H8     | 1.79                     | 0.48              |
| 66:D3:1531:G:H2'    | 66:D3:1532:U:H6    | 1.79                     | 0.48              |
| 1:CA:107:VAL:HG22   | 1:CA:143:VAL:HA    | 1.94                     | 0.48              |
| 4:UA:762:GLU:OE1    | 4:UA:762:GLU:N     | 2.47                     | 0.48              |
| 5:UB:598:LEU:HD12   | 5:UB:598:LEU:O     | 2.14                     | 0.48              |
| 6:UC:566:ARG:HH12   | 66:D3:479:C:P      | 2.36                     | 0.48              |
| 7:UD:52:SER:OG      | 7:UD:65:LEU:HD12   | 2.13                     | 0.48              |
| 7:UD:297:SER:OG     | 7:UD:305:PHE:HB2   | 2.14                     | 0.48              |
| 8:UE:546:ARG:NH1    | 11:UH:677:ASN:OD1  | 2.47                     | 0.48              |
| 10:UG:414:LEU:HD22  | 67:D4:37:G:C6      | 2.49                     | 0.48              |
| 12:UI:458:TRP:HA    | 12:UI:461:THR:HG22 | 1.96                     | 0.48              |
| 13:UJ:364:ASN:OD1   | 13:UJ:365:ILE:N    | 2.47                     | 0.48              |
| 13:UJ:1712:LYS:HZ2  | 13:UJ:1751:GLY:HA3 | 1.78                     | 0.48              |
| 14:UK:11:LYS:O      | 14:UK:12:GLN:HB3   | 2.14                     | 0.48              |
| 15:UL:170:TRP:CZ3   | 15:UL:172:GLN:HB2  | 2.49                     | 0.48              |
| 16:UM:401:LEU:HD23  | 16:UM:417:TYR:CD1  | 2.49                     | 0.48              |
| 16:UM:580:ARG:HB3   | 16:UM:593:CYS:SG   | 2.54                     | 0.48              |
| 19:UP:185:GLN:HA    | 19:UP:188:LYS:HZ2  | 1.78                     | 0.48              |
| 21:UR:241:ALA:HA    | 21:UR:282:ASN:HD22 | 1.77                     | 0.48              |
| 21:UR:541:LEU:HD23  | 21:UR:542:ARG:N    | 2.29                     | 0.48              |
| 23:UT:123:LYS:H     | 23:UT:123:LYS:HD3  | 1.77                     | 0.48              |
| 23:UT:362:PHE:O     | 23:UT:366:ILE:HG12 | 2.14                     | 0.48              |
| 23:UT:367:ARG:O     | 23:UT:407:ARG:NH2  | 2.45                     | 0.48              |
| 23:UT:674:PHE:CD2   | 23:UT:676:PRO:HD2  | 2.49                     | 0.48              |
| 23:UT:1689:VAL:HG23 | 23:UT:1744:GLU:OE1 | 2.13                     | 0.48              |
| 24:UU:859:ASP:N     | 24:UU:859:ASP:OD1  | 2.47                     | 0.48              |
| 25:UV:565:LYS:HZ2   | 25:UV:690:VAL:HG22 | 1.79                     | 0.48              |
| 27:UZ:222:PHE:HD2   | 27:UZ:223:LEU:HD22 | 1.79                     | 0.48              |
| 30:CF:42:LYS:NZ     | 67:D4:327:G:O6     | 2.37                     | 0.48              |
| 30:CG:79:VAL:CG2    | 30:CG:121:ILE:HD12 | 2.40                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:CH:142:ILE:H    | 31:CH:142:ILE:HD12 | 1.77                     | 0.48              |
| 31:CH:155:ASN:OD1  | 31:CH:561:ASN:ND2  | 2.47                     | 0.48              |
| 35:CL:805:ASN:ND2  | 35:CL:807:LYS:HB2  | 2.29                     | 0.48              |
| 37:CN:62:SER:HA    | 37:CN:66:HIS:CG    | 2.49                     | 0.48              |
| 37:CN:262:VAL:HG13 | 37:CN:266:LYS:NZ   | 2.28                     | 0.48              |
| 38:JC:285:THR:OG1  | 38:JC:286:GLU:N    | 2.46                     | 0.48              |
| 47:JP:201:ILE:CG2  | 47:JP:215:LEU:HB2  | 2.44                     | 0.48              |
| 49:DE:68:ARG:HE    | 49:DE:76:VAL:HG11  | 1.78                     | 0.48              |
| 51:DG:56:ASN:HD21  | 66:D3:153:G:H21    | 1.62                     | 0.48              |
| 51:DG:60:GLY:HA2   | 66:D3:154:G:O2'    | 2.14                     | 0.48              |
| 52:DH:119:THR:OG1  | 52:DH:120:ALA:N    | 2.47                     | 0.48              |
| 52:DH:138:LYS:HB3  | 60:DW:54:ASP:OD1   | 2.13                     | 0.48              |
| 54:DJ:108:ARG:NH1  | 54:DJ:110:GLN:HE21 | 2.12                     | 0.48              |
| 58:DQ:40:GLU:OE2   | 66:D3:1481:C:H5'   | 2.14                     | 0.48              |
| 60:DW:15:ASN:ND2   | 60:DW:71:LYS:HG3   | 2.24                     | 0.48              |
| 65:D2:212:U:H2'    | 65:D2:213:G:C8     | 2.48                     | 0.48              |
| 66:D3:575:C:O2'    | 66:D3:576:G:H8     | 1.96                     | 0.48              |
| 66:D3:972:G:C2     | 66:D3:973:A:C4     | 3.02                     | 0.48              |
| 66:D3:1587:A:C2    | 66:D3:1588:G:C8    | 3.02                     | 0.48              |
| 66:D3:1617:U:H5''  | 66:D3:1618:C:OP2   | 2.13                     | 0.48              |
| 70:EC:105:VAL:O    | 70:EC:109:GLU:N    | 2.47                     | 0.48              |
| 72:EE:217:ILE:O    | 72:EE:221:LEU:N    | 2.45                     | 0.48              |
| 79:EN:92:GLU:HA    | 79:EN:114:ARG:HA   | 1.95                     | 0.48              |
| 3:JA:69:HIS:CE1    | 3:JA:71:LYS:HB3    | 2.48                     | 0.48              |
| 3:JA:309:PHE:O     | 3:JA:384:VAL:HA    | 2.14                     | 0.48              |
| 4:UA:492:SER:O     | 4:UA:494:ASP:N     | 2.47                     | 0.48              |
| 5:UB:511:SER:HA    | 5:UB:557:SER:HA    | 1.96                     | 0.48              |
| 8:UE:247:THR:HG21  | 8:UE:292:TYR:HA    | 1.95                     | 0.48              |
| 8:UE:453:LEU:O     | 8:UE:457:LEU:HD23  | 2.14                     | 0.48              |
| 11:UH:596:LYS:NZ   | 11:UH:600:LYS:HD3  | 2.29                     | 0.48              |
| 13:UJ:216:CYS:O    | 13:UJ:220:VAL:HG23 | 2.14                     | 0.48              |
| 13:UJ:1517:ASP:OD1 | 13:UJ:1520:THR:OG1 | 2.23                     | 0.48              |
| 14:UK:16:ARG:CZ    | 66:D3:575:C:C4     | 2.97                     | 0.48              |
| 15:UL:88:HIS:HD2   | 15:UL:91:THR:HG23  | 1.79                     | 0.48              |
| 16:UM:292:GLY:HA3  | 16:UM:305:VAL:HB   | 1.96                     | 0.48              |
| 16:UM:446:VAL:HG12 | 16:UM:450:TYR:O    | 2.14                     | 0.48              |
| 16:UM:486:THR:OG1  | 16:UM:487:ARG:NH2  | 2.47                     | 0.48              |
| 17:UN:880:LYS:NZ   | 65:D2:486:U:H2'    | 2.28                     | 0.48              |
| 18:UO:31:THR:OG1   | 18:UO:32:SER:N     | 2.46                     | 0.48              |
| 20:UQ:320:VAL:HA   | 20:UQ:334:LEU:O    | 2.14                     | 0.48              |
| 20:UQ:554:SER:O    | 20:UQ:554:SER:OG   | 2.32                     | 0.48              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 21:UR:480:ARG:HD3   | 21:UR:481:TRP:NE1  | 2.29                     | 0.48              |
| 22:US:199:PHE:HD2   | 22:US:260:ASN:ND2  | 2.12                     | 0.48              |
| 23:UT:187:TYR:HB2   | 23:UT:191:PHE:CZ   | 2.49                     | 0.48              |
| 23:UT:1020:ASN:OD1  | 23:UT:1024:GLN:NE2 | 2.47                     | 0.48              |
| 23:UT:1130:ALA:O    | 23:UT:1134:MET:HG2 | 2.13                     | 0.48              |
| 23:UT:1410:LEU:HD23 | 23:UT:1413:VAL:H   | 1.79                     | 0.48              |
| 24:UU:476:PHE:CD1   | 24:UU:486:ILE:HG12 | 2.49                     | 0.48              |
| 24:UU:910:GLN:O     | 24:UU:913:GLU:HG3  | 2.14                     | 0.48              |
| 25:UV:674:SER:HA    | 25:UV:705:HIS:HB3  | 1.95                     | 0.48              |
| 25:UV:808:LEU:HD23  | 25:UV:812:GLU:OE1  | 2.13                     | 0.48              |
| 27:UZ:220:ILE:HG13  | 27:UZ:221:ASN:N    | 2.29                     | 0.48              |
| 29:CE:256:ASN:O     | 29:CE:260:GLU:HG3  | 2.13                     | 0.48              |
| 31:CH:367:LYS:HD2   | 31:CH:370:ARG:HD2  | 1.96                     | 0.48              |
| 35:CL:138:VAL:HG23  | 35:CL:167:VAL:HG23 | 1.95                     | 0.48              |
| 38:JC:289:ILE:HD12  | 38:JC:299:ILE:HG13 | 1.96                     | 0.48              |
| 51:DG:21:GLU:OE1    | 51:DG:24:ILE:HD11  | 2.14                     | 0.48              |
| 51:DG:45:PHE:HA     | 51:DG:48:TYR:CD1   | 2.48                     | 0.48              |
| 51:DG:106:LEU:HD21  | 51:DG:109:LEU:HG   | 1.95                     | 0.48              |
| 52:DH:97:ARG:HH22   | 66:D3:641:G:N2     | 2.11                     | 0.48              |
| 53:DI:11:ARG:HB2    | 66:D3:323:A:H5''   | 1.94                     | 0.48              |
| 55:DL:136:ARG:HD3   | 66:D3:304:U:H5''   | 1.94                     | 0.48              |
| 65:D2:339:A:N7      | 65:D2:340:U:C4     | 2.82                     | 0.48              |
| 66:D3:89:G:C6       | 66:D3:452:A:C6     | 3.02                     | 0.48              |
| 66:D3:117:U:H2'     | 66:D3:118:U:O4'    | 2.13                     | 0.48              |
| 66:D3:209:U:H2'     | 66:D3:210:A:H8     | 1.78                     | 0.48              |
| 66:D3:481:A:C6      | 66:D3:482:U:C4     | 3.01                     | 0.48              |
| 66:D3:561:G:C2      | 66:D3:567:A:C2     | 3.02                     | 0.48              |
| 66:D3:902:G:H1'     | 66:D3:907:A:H61    | 1.78                     | 0.48              |
| 66:D3:968:U:H2'     | 66:D3:969:C:O4'    | 2.14                     | 0.48              |
| 66:D3:1202:A:H3'    | 66:D3:1203:A:H8    | 1.79                     | 0.48              |
| 66:D3:1599:C:H2'    | 66:D3:1600:A:C8    | 2.49                     | 0.48              |
| 67:D4:111:G:C2      | 67:D4:260:U:C4     | 3.01                     | 0.48              |
| 79:EN:400:MET:O     | 79:EN:404:LYS:N    | 2.44                     | 0.48              |
| 3:JA:25:ILE:HG13    | 3:JA:148:VAL:O     | 2.14                     | 0.48              |
| 3:JA:805:ILE:HB     | 3:JA:809:LYS:NZ    | 2.28                     | 0.48              |
| 3:JA:818:GLU:HB2    | 3:JA:819:LYS:NZ    | 2.29                     | 0.48              |
| 1:CB:172:TYR:HD2    | 1:CB:175:ALA:HB2   | 1.79                     | 0.48              |
| 5:UB:444:ASN:H      | 5:UB:446:GLN:NE2   | 2.04                     | 0.48              |
| 5:UB:573:LEU:HD21   | 5:UB:667:LEU:HD21  | 1.95                     | 0.48              |
| 5:UB:781:MET:HE1    | 61:DX:68:ILE:HD11  | 1.95                     | 0.48              |
| 6:UC:569:TYR:CG     | 54:DJ:32:GLY:HA3   | 2.49                     | 0.48              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 7:UD:237:GLU:OE1   | 19:UP:208:ARG:NE    | 2.47                     | 0.48              |
| 7:UD:246:TYR:HD1   | 7:UD:253:ILE:HG22   | 1.77                     | 0.48              |
| 7:UD:767:LYS:NZ    | 19:UP:214:GLY:H     | 2.08                     | 0.48              |
| 8:UE:288:LYS:HE2   | 8:UE:289:VAL:O      | 2.14                     | 0.48              |
| 10:UG:136:SER:OG   | 10:UG:159:TYR:OH    | 1.99                     | 0.48              |
| 11:UH:651:GLU:O    | 11:UH:655:LEU:HD23  | 2.14                     | 0.48              |
| 11:UH:676:TRP:NE1  | 11:UH:680:ASP:OD2   | 2.47                     | 0.48              |
| 13:UJ:316:PRO:HB2  | 13:UJ:319:ILE:HD12  | 1.96                     | 0.48              |
| 13:UJ:1362:LEU:HA  | 13:UJ:1365:LYS:HB2  | 1.95                     | 0.48              |
| 14:UK:199:LYS:O    | 14:UK:202:LYS:N     | 2.47                     | 0.48              |
| 15:UL:75:ARG:NE    | 15:UL:76:GLY:H      | 2.11                     | 0.48              |
| 15:UL:432:TYR:HD2  | 66:D3:1657:U:C5     | 2.32                     | 0.48              |
| 15:UL:635:LYS:O    | 15:UL:659:GLU:HG3   | 2.14                     | 0.48              |
| 15:UL:866:LYS:HA   | 15:UL:866:LYS:HD2   | 1.75                     | 0.48              |
| 18:UO:495:ILE:O    | 18:UO:498:SER:OG    | 2.30                     | 0.48              |
| 20:UQ:491:GLN:NE2  | 20:UQ:514:TYR:HB2   | 2.28                     | 0.48              |
| 21:UR:141:ASN:HD22 | 65:D2:307:C:C5'     | 2.26                     | 0.48              |
| 21:UR:500:MET:HG3  | 21:UR:501:THR:HG23  | 1.95                     | 0.48              |
| 23:UT:498:ILE:HG23 | 23:UT:499:PRO:HD3   | 1.96                     | 0.48              |
| 23:UT:648:GLU:HA   | 23:UT:651:LYS:HG2   | 1.95                     | 0.48              |
| 23:UT:1013:THR:N   | 53:DI:115:ALA:O     | 2.39                     | 0.48              |
| 23:UT:1144:GLU:HB2 | 23:UT:1189:LEU:HG   | 1.96                     | 0.48              |
| 23:UT:1363:LEU:HA  | 23:UT:1366:ASN:HD21 | 1.78                     | 0.48              |
| 25:UV:572:TYR:HE2  | 25:UV:648:PHE:CG    | 2.32                     | 0.48              |
| 29:CE:328:ARG:O    | 29:CE:332:THR:HG22  | 2.12                     | 0.48              |
| 30:CF:34:LYS:HE3   | 30:CF:39:GLU:CG     | 2.44                     | 0.48              |
| 30:CF:34:LYS:HE3   | 30:CF:39:GLU:HG2    | 1.96                     | 0.48              |
| 30:CF:111:LYS:O    | 30:CF:114:ILE:HG22  | 2.14                     | 0.48              |
| 32:CI:109:ARG:HD2  | 32:CI:109:ARG:HA    | 1.65                     | 0.48              |
| 33:CJ:188:HIS:ND1  | 34:CK:378:PHE:CE1   | 2.82                     | 0.48              |
| 35:CL:237:TRP:CZ2  | 35:CL:850:GLY:HA2   | 2.49                     | 0.48              |
| 38:JC:17:SER:OG    | 38:JC:340:THR:N     | 2.28                     | 0.48              |
| 38:JC:60:ASN:HB3   | 38:JC:74:THR:HB     | 1.96                     | 0.48              |
| 47:JP:196:THR:HB   | 47:JP:204:TRP:HE1   | 1.79                     | 0.48              |
| 66:D3:551:G:N2     | 66:D3:588:U:O2      | 2.47                     | 0.48              |
| 66:D3:1068:C:H2'   | 66:D3:1069:A:C8     | 2.48                     | 0.48              |
| 66:D3:1148:C:H2'   | 66:D3:1149:G:C8     | 2.49                     | 0.48              |
| 66:D3:1508:U:H2'   | 66:D3:1509:C:H6     | 1.79                     | 0.48              |
| 4:UA:482:SER:HB3   | 4:UA:487:VAL:HG22   | 1.96                     | 0.47              |
| 5:UB:490:PHE:CD1   | 5:UB:493:LEU:HD21   | 2.48                     | 0.47              |
| 6:UC:511:GLU:HA    | 6:UC:514:LYS:HG2    | 1.96                     | 0.47              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 7:UD:116:SER:CB    | 7:UD:126:TRP:HE1    | 2.27                     | 0.47              |
| 7:UD:519:THR:H     | 7:UD:522:SER:HB2    | 1.79                     | 0.47              |
| 15:UL:284:PHE:CD1  | 15:UL:328:PRO:HA    | 2.49                     | 0.47              |
| 16:UM:542:CYS:O    | 16:UM:546:LYS:CA    | 2.62                     | 0.47              |
| 17:UN:298:TRP:CZ2  | 17:UN:896:ALA:HB2   | 2.49                     | 0.47              |
| 18:UO:253:LYS:HG2  | 18:UO:278:ASP:OD1   | 2.14                     | 0.47              |
| 20:UQ:554:SER:OG   | 65:D2:7:A:N3        | 2.47                     | 0.47              |
| 21:UR:232:LYS:HA   | 21:UR:554:ASN:ND2   | 2.28                     | 0.47              |
| 22:US:208:TYR:O    | 22:US:211:LEU:HG    | 2.13                     | 0.47              |
| 22:US:295:LEU:HD13 | 22:US:298:PHE:CD1   | 2.48                     | 0.47              |
| 22:US:419:PRO:HG3  | 39:JG:19:LEU:HD21   | 1.95                     | 0.47              |
| 23:UT:790:GLU:OE2  | 23:UT:839:LYS:NZ    | 2.41                     | 0.47              |
| 23:UT:850:LEU:O    | 23:UT:854:LEU:HG    | 2.14                     | 0.47              |
| 23:UT:885:ARG:HA   | 23:UT:888:LEU:HD12  | 1.95                     | 0.47              |
| 23:UT:954:PRO:HG3  | 23:UT:1010:VAL:HG22 | 1.95                     | 0.47              |
| 23:UT:1706:LYS:HB2 | 23:UT:1709:ASP:OD2  | 2.14                     | 0.47              |
| 23:UT:1929:GLU:OE1 | 23:UT:1929:GLU:N    | 2.43                     | 0.47              |
| 23:UT:1948:SER:HB2 | 47:JP:208:ARG:HH12  | 1.79                     | 0.47              |
| 24:UU:69:LEU:HB3   | 24:UU:70:PHE:CD2    | 2.49                     | 0.47              |
| 24:UU:125:GLY:HA3  | 29:CE:433:THR:OG1   | 2.14                     | 0.47              |
| 24:UU:323:VAL:HG11 | 29:CE:419:VAL:HG11  | 1.96                     | 0.47              |
| 24:UU:760:LEU:HA   | 24:UU:763:SER:OG    | 2.14                     | 0.47              |
| 25:UV:724:LEU:HB2  | 25:UV:728:PHE:CZ    | 2.49                     | 0.47              |
| 25:UV:958:PHE:CE1  | 25:UV:962:LEU:HD11  | 2.49                     | 0.47              |
| 27:UZ:53:ILE:HG21  | 48:JQ:189:PRO:HG2   | 1.96                     | 0.47              |
| 27:UZ:141:SER:HA   | 27:UZ:144:TYR:HB2   | 1.96                     | 0.47              |
| 34:CK:538:LYS:HG2  | 66:D3:1628:U:N3     | 2.29                     | 0.47              |
| 39:JF:38:THR:OG1   | 39:JF:40:ARG:NH2    | 2.47                     | 0.47              |
| 39:JG:44:VAL:HA    | 39:JG:113:TYR:O     | 2.14                     | 0.47              |
| 49:DE:63:ALA:O     | 49:DE:67:GLN:HG3    | 2.14                     | 0.47              |
| 50:DF:184:PHE:CD2  | 50:DF:185:ARG:HG2   | 2.49                     | 0.47              |
| 50:DF:222:LYS:HD2  | 50:DF:225:ARG:CZ    | 2.44                     | 0.47              |
| 56:DN:31:GLU:O     | 56:DN:35:GLU:OE1    | 2.32                     | 0.47              |
| 62:DY:18:LEU:HB2   | 62:DY:20:ARG:HG2    | 1.96                     | 0.47              |
| 65:D2:235:A:O2'    | 65:D2:236:C:OP2     | 2.30                     | 0.47              |
| 66:D3:473:A:N6     | 66:D3:474:A:H62     | 2.12                     | 0.47              |
| 66:D3:478:A:C2     | 66:D3:479:C:C2      | 3.02                     | 0.47              |
| 66:D3:575:C:O2'    | 66:D3:576:G:P       | 2.72                     | 0.47              |
| 66:D3:1586:A:C2    | 66:D3:1611:A:C4     | 3.02                     | 0.47              |
| 1:CB:181:VAL:HA    | 1:CB:184:VAL:HG22   | 1.96                     | 0.47              |
| 1:CB:294:ARG:HH22  | 19:UP:187:SER:HG    | 1.56                     | 0.47              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 5:UB:715:PRO:C      | 5:UB:716:LYS:HD2    | 2.34                     | 0.47              |
| 7:UD:767:LYS:HZ2    | 19:UP:213:LYS:HA    | 1.80                     | 0.47              |
| 9:UF:183:TYR:HE2    | 9:UF:318:ARG:HG2    | 1.79                     | 0.47              |
| 11:UH:587:LEU:HD23  | 20:UQ:605:ASN:ND2   | 2.28                     | 0.47              |
| 13:UJ:631:VAL:HG13  | 13:UJ:633:GLU:H     | 1.78                     | 0.47              |
| 13:UJ:1732:VAL:O    | 13:UJ:1736:LEU:HG   | 2.14                     | 0.47              |
| 14:UK:66:ALA:HB3    | 35:CL:1079:PHE:CZ   | 2.49                     | 0.47              |
| 15:UL:42:ILE:HA     | 15:UL:51:ILE:HG22   | 1.96                     | 0.47              |
| 15:UL:148:TRP:HA    | 15:UL:155:GLY:HA2   | 1.96                     | 0.47              |
| 16:UM:738:LEU:O     | 16:UM:742:ARG:HG2   | 2.14                     | 0.47              |
| 19:UP:196:SER:HA    | 19:UP:199:ILE:HG12  | 1.95                     | 0.47              |
| 23:UT:219:LEU:O     | 23:UT:223:ASP:HB3   | 2.14                     | 0.47              |
| 23:UT:526:TYR:CE2   | 23:UT:561:LEU:HD23  | 2.49                     | 0.47              |
| 23:UT:758:ILE:O     | 23:UT:762:ILE:HG12  | 2.13                     | 0.47              |
| 23:UT:1199:LEU:HD11 | 23:UT:1243:ILE:HG12 | 1.97                     | 0.47              |
| 23:UT:1584:ASN:HB2  | 23:UT:1587:LYS:HZ2  | 1.79                     | 0.47              |
| 23:UT:1794:ARG:HH11 | 23:UT:1795:ARG:HE   | 1.62                     | 0.47              |
| 24:UU:610:ARG:HH21  | 24:UU:673:PHE:HD2   | 1.62                     | 0.47              |
| 25:UV:99:LYS:HZ2    | 25:UV:419:TYR:HE2   | 1.61                     | 0.47              |
| 25:UV:146:LEU:HD13  | 25:UV:176:PHE:HZ    | 1.79                     | 0.47              |
| 25:UV:306:LYS:O     | 25:UV:312:ARG:HG3   | 2.13                     | 0.47              |
| 25:UV:867:ILE:HD11  | 25:UV:879:GLU:CD    | 2.34                     | 0.47              |
| 25:UV:1051:LEU:H    | 25:UV:1051:LEU:HD12 | 1.79                     | 0.47              |
| 25:UV:1145:PRO:O    | 25:UV:1149:LEU:HG   | 2.14                     | 0.47              |
| 26:UX:64:GLN:OE1    | 26:UX:97:LEU:HD11   | 2.13                     | 0.47              |
| 26:UX:79:LYS:NZ     | 45:JN:310:SER:H     | 2.12                     | 0.47              |
| 27:UZ:90:ASP:O      | 27:UZ:92:HIS:N      | 2.47                     | 0.47              |
| 31:CH:327:ASP:HB3   | 31:CH:339:VAL:HG22  | 1.95                     | 0.47              |
| 35:CL:549:ILE:HB    | 35:CL:567:TRP:NE1   | 2.29                     | 0.47              |
| 38:JC:147:ASN:HB3   | 38:JC:152:ASP:HB3   | 1.96                     | 0.47              |
| 45:JN:231:LEU:H     | 45:JN:231:LEU:HD12  | 1.80                     | 0.47              |
| 45:JN:268:LYS:HB2   | 45:JN:271:GLN:OE1   | 2.14                     | 0.47              |
| 47:JP:173:ILE:HG22  | 47:JP:174:ARG:HG3   | 1.96                     | 0.47              |
| 47:JP:284:HIS:NE2   | 47:JP:306:SER:HA    | 2.29                     | 0.47              |
| 47:JP:453:TYR:CE2   | 66:D3:-2:A:C5       | 3.01                     | 0.47              |
| 57:DO:18:ARG:NH1    | 66:D3:919:A:OP1     | 2.47                     | 0.47              |
| 58:DQ:26:LYS:N      | 58:DQ:64:ASP:OD1    | 2.47                     | 0.47              |
| 60:DW:82:LYS:NZ     | 66:D3:748:U:H5''    | 2.24                     | 0.47              |
| 62:DY:25:VAL:HG12   | 62:DY:71:GLY:O      | 2.15                     | 0.47              |
| 65:D2:13:U:H1'      | 65:D2:70:A:N7       | 2.29                     | 0.47              |
| 65:D2:219:U:H2'     | 65:D2:220:U:C6      | 2.49                     | 0.47              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 65:D2:453:A:N7     | 65:D2:454:C:C4      | 2.82                     | 0.47              |
| 66:D3:233:C:H4'    | 66:D3:234:G:H5''    | 1.95                     | 0.47              |
| 66:D3:568:G:N2     | 66:D3:569:C:C2      | 2.82                     | 0.47              |
| 3:JA:70:ARG:HA     | 3:JA:73:ARG:HD3     | 1.97                     | 0.47              |
| 4:UA:328:LEU:HD11  | 4:UA:337:TYR:CE2    | 2.49                     | 0.47              |
| 6:UC:595:LYS:N     | 6:UC:595:LYS:HD2    | 2.29                     | 0.47              |
| 7:UD:512:GLU:OE2   | 7:UD:560:SER:N      | 2.47                     | 0.47              |
| 8:UE:357:VAL:HG13  | 8:UE:357:VAL:O      | 2.14                     | 0.47              |
| 10:UG:431:ARG:NH2  | 67:D4:37:G:C4       | 2.83                     | 0.47              |
| 10:UG:546:ILE:H    | 10:UG:546:ILE:HD12  | 1.79                     | 0.47              |
| 12:UI:425:ASN:HD21 | 12:UI:463:LYS:HG3   | 1.77                     | 0.47              |
| 15:UL:438:PHE:CZ   | 15:UL:440:PRO:HA    | 2.48                     | 0.47              |
| 16:UM:631:MET:CE   | 16:UM:643:PHE:HB3   | 2.44                     | 0.47              |
| 18:UO:40:ASN:OD1   | 18:UO:41:SER:N      | 2.41                     | 0.47              |
| 18:UO:502:GLN:HA   | 18:UO:505:GLU:OE2   | 2.14                     | 0.47              |
| 20:UQ:184:GLN:N    | 20:UQ:184:GLN:OE1   | 2.47                     | 0.47              |
| 20:UQ:376:ALA:HA   | 20:UQ:379:LEU:HD23  | 1.96                     | 0.47              |
| 22:US:350:MET:HG2  | 22:US:355:ARG:NH1   | 2.29                     | 0.47              |
| 23:UT:977:PHE:CZ   | 23:UT:982:HIS:HA    | 2.49                     | 0.47              |
| 23:UT:1269:SER:O   | 23:UT:1273:LYS:HG2  | 2.14                     | 0.47              |
| 23:UT:1643:LEU:HA  | 23:UT:1654:VAL:HG11 | 1.95                     | 0.47              |
| 25:UV:523:TYR:HE2  | 25:UV:582:GLN:HG2   | 1.80                     | 0.47              |
| 25:UV:606:ASN:HD21 | 25:UV:610:PHE:HE1   | 1.61                     | 0.47              |
| 25:UV:827:ARG:HG2  | 37:CN:175:LEU:HD11  | 1.96                     | 0.47              |
| 27:UZ:172:ASP:OD1  | 27:UZ:175:TYR:HB3   | 2.15                     | 0.47              |
| 28:CD:103:LYS:HG3  | 47:JP:156:SER:HB2   | 1.95                     | 0.47              |
| 31:CH:266:GLU:OE2  | 67:D4:167:C:H5''    | 2.15                     | 0.47              |
| 32:CI:135:HIS:O    | 32:CI:160:TRP:HE3   | 1.97                     | 0.47              |
| 32:CI:172:ARG:HB2  | 32:CI:177:ILE:HD11  | 1.96                     | 0.47              |
| 35:CL:86:ILE:HD11  | 35:CL:117:PHE:CD2   | 2.50                     | 0.47              |
| 53:DI:42:ARG:NH1   | 53:DI:42:ARG:HA     | 2.30                     | 0.47              |
| 56:DN:16:ILE:HB    | 60:DW:57:ARG:NH2    | 2.28                     | 0.47              |
| 61:DX:87:VAL:HA    | 61:DX:124:VAL:HG22  | 1.96                     | 0.47              |
| 66:D3:1620:C:HO2'  | 66:D3:1621:U:P      | 2.37                     | 0.47              |
| 67:D4:75:C:H2'     | 67:D4:76:U:H6       | 1.77                     | 0.47              |
| 67:D4:174:U:O4     | 67:D4:175:A:N6      | 2.47                     | 0.47              |
| 73:EF:37:PHE:O     | 73:EF:49:ARG:N      | 2.45                     | 0.47              |
| 79:EN:622:GLU:O    | 79:EN:626:ALA:N     | 2.40                     | 0.47              |
| 2:DA:121:ILE:HD13  | 2:DA:164:ILE:HD11   | 1.95                     | 0.47              |
| 3:JA:91:MET:HB2    | 3:JA:95:GLU:OE2     | 2.15                     | 0.47              |
| 3:JA:499:ASN:O     | 3:JA:503:ALA:N      | 2.47                     | 0.47              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 3:JA:541:TYR:HE1   | 3:JA:637:ARG:HG2    | 1.79                     | 0.47              |
| 1:CB:288:ARG:HE    | 7:UD:121:THR:HG21   | 1.79                     | 0.47              |
| 5:UB:656:ALA:O     | 5:UB:660:ILE:HG13   | 2.14                     | 0.47              |
| 6:UC:498:VAL:O     | 6:UC:502:LYS:HG2    | 2.12                     | 0.47              |
| 8:UE:490:ARG:HD3   | 18:UO:16:LEU:HD23   | 1.96                     | 0.47              |
| 9:UF:138:LYS:HZ1   | 28:CD:84:LEU:HG     | 1.79                     | 0.47              |
| 13:UJ:348:ILE:O    | 13:UJ:352:THR:HG23  | 2.15                     | 0.47              |
| 13:UJ:364:ASN:HA   | 13:UJ:367:LEU:HG    | 1.96                     | 0.47              |
| 13:UJ:1567:THR:N   | 13:UJ:1570:GLU:OE2  | 2.48                     | 0.47              |
| 13:UJ:1688:ASN:OD1 | 13:UJ:1725:LEU:HD13 | 2.13                     | 0.47              |
| 15:UL:631:PHE:HB3  | 15:UL:663:LEU:HD21  | 1.97                     | 0.47              |
| 19:UP:199:ILE:HG13 | 19:UP:200:ARG:N     | 2.29                     | 0.47              |
| 20:UQ:152:ARG:NE   | 20:UQ:231:PHE:HA    | 2.29                     | 0.47              |
| 20:UQ:255:ASN:O    | 20:UQ:276:ALA:HB3   | 2.15                     | 0.47              |
| 20:UQ:708:ASP:N    | 20:UQ:708:ASP:OD1   | 2.47                     | 0.47              |
| 20:UQ:821:ILE:O    | 20:UQ:825:GLN:HG3   | 2.14                     | 0.47              |
| 21:UR:324:TRP:NE1  | 21:UR:337:ALA:HB1   | 2.29                     | 0.47              |
| 21:UR:360:VAL:HG22 | 21:UR:375:VAL:HG22  | 1.96                     | 0.47              |
| 21:UR:496:ARG:O    | 21:UR:500:MET:HG2   | 2.15                     | 0.47              |
| 22:US:502:ASN:OD1  | 22:US:503:TYR:N     | 2.41                     | 0.47              |
| 22:US:508:ASN:O    | 22:US:511:SER:OG    | 2.22                     | 0.47              |
| 23:UT:1341:GLU:HG3 | 23:UT:1342:LEU:H    | 1.79                     | 0.47              |
| 23:UT:1852:SER:HB2 | 26:UX:123:PRO:HG2   | 1.96                     | 0.47              |
| 23:UT:1877:ARG:HB2 | 23:UT:1917:ILE:HD11 | 1.97                     | 0.47              |
| 24:UU:419:ILE:HG13 | 24:UU:430:ILE:HG12  | 1.95                     | 0.47              |
| 24:UU:536:LEU:HD22 | 50:DF:14:PHE:HB2    | 1.96                     | 0.47              |
| 25:UV:237:HIS:CE1  | 25:UV:241:ILE:HD11  | 2.49                     | 0.47              |
| 25:UV:401:LEU:HD11 | 25:UV:414:HIS:CE1   | 2.48                     | 0.47              |
| 25:UV:522:LYS:HG2  | 25:UV:523:TYR:CD1   | 2.49                     | 0.47              |
| 25:UV:1137:ASN:O   | 25:UV:1141:GLU:OE1  | 2.33                     | 0.47              |
| 25:UV:1147:TYR:HA  | 25:UV:1150:VAL:HG12 | 1.96                     | 0.47              |
| 25:UV:1214:LEU:HG  | 25:UV:1216:LYS:HD3  | 1.96                     | 0.47              |
| 25:UV:1221:HIS:HB2 | 37:CN:20:LEU:HD22   | 1.96                     | 0.47              |
| 28:CD:158:TYR:CE1  | 28:CD:162:LYS:HD3   | 2.50                     | 0.47              |
| 28:CD:223:ILE:HD11 | 28:CD:226:LYS:HA    | 1.96                     | 0.47              |
| 31:CH:314:GLN:N    | 62:DY:2:SER:OG      | 2.47                     | 0.47              |
| 31:CH:516:GLY:HA3  | 31:CH:564:TYR:CE1   | 2.50                     | 0.47              |
| 36:CM:205:VAL:O    | 36:CM:208:MET:HG2   | 2.14                     | 0.47              |
| 36:CM:339:LEU:HD12 | 36:CM:350:MET:CG    | 2.44                     | 0.47              |
| 38:JC:55:PHE:HD1   | 38:JC:82:HIS:NE2    | 2.11                     | 0.47              |
| 38:JC:199:THR:HG22 | 38:JC:201:THR:H     | 1.79                     | 0.47              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 42:JJ:138:GLU:OE1   | 42:JJ:138:GLU:N     | 2.48                     | 0.47              |
| 58:DQ:39:VAL:HG23   | 58:DQ:45:ARG:HG3    | 1.96                     | 0.47              |
| 62:DY:52:LYS:O      | 62:DY:55:VAL:HG12   | 2.14                     | 0.47              |
| 62:DY:60:PHE:HD1    | 62:DY:71:GLY:HA3    | 1.79                     | 0.47              |
| 65:D2:243:A:H1'     | 65:D2:271:G:H22     | 1.79                     | 0.47              |
| 1:CA:171:LEU:HB2    | 1:CA:237:VAL:HG21   | 1.95                     | 0.47              |
| 3:JA:160:GLN:HG3    | 3:JA:164:MET:HE1    | 1.95                     | 0.47              |
| 3:JA:200:VAL:HG13   | 3:JA:208:LEU:HB2    | 1.96                     | 0.47              |
| 3:JA:393:PRO:O      | 3:JA:397:VAL:N      | 2.44                     | 0.47              |
| 4:UA:792:ILE:O      | 4:UA:796:LEU:HD23   | 2.14                     | 0.47              |
| 5:UB:430:LEU:O      | 5:UB:434:ILE:HG12   | 2.14                     | 0.47              |
| 7:UD:52:SER:HA      | 7:UD:104:TRP:CE3    | 2.45                     | 0.47              |
| 8:UE:115:ASN:OD1    | 8:UE:131:LEU:HB2    | 2.15                     | 0.47              |
| 9:UF:138:LYS:HA     | 9:UF:138:LYS:HE3    | 1.94                     | 0.47              |
| 9:UF:155:TYR:HD2    | 9:UF:156:GLU:CD     | 2.18                     | 0.47              |
| 9:UF:183:TYR:CE1    | 9:UF:322:LEU:HD12   | 2.48                     | 0.47              |
| 10:UG:246:VAL:HG13  | 10:UG:248:HIS:CE1   | 2.49                     | 0.47              |
| 13:UJ:491:TYR:CE2   | 13:UJ:528:ARG:HD3   | 2.49                     | 0.47              |
| 13:UJ:647:GLU:HG2   | 13:UJ:648:LYS:HD3   | 1.96                     | 0.47              |
| 14:UK:250:ARG:HG3   | 14:UK:250:ARG:NH2   | 2.28                     | 0.47              |
| 15:UL:336:TYR:OH    | 15:UL:391:ARG:NH1   | 2.47                     | 0.47              |
| 15:UL:621:VAL:HA    | 15:UL:631:PHE:O     | 2.15                     | 0.47              |
| 16:UM:63:GLU:O      | 16:UM:81:GLN:N      | 2.48                     | 0.47              |
| 16:UM:241:GLN:OE1   | 16:UM:266:ILE:HG23  | 2.13                     | 0.47              |
| 16:UM:544:TYR:HD2   | 16:UM:587:GLN:HB3   | 1.79                     | 0.47              |
| 18:UO:173:THR:HG21  | 18:UO:218:VAL:N     | 2.29                     | 0.47              |
| 18:UO:431:LEU:HA    | 18:UO:434:ARG:HG3   | 1.96                     | 0.47              |
| 20:UQ:29:THR:HG23   | 20:UQ:32:LYS:HG2    | 1.96                     | 0.47              |
| 20:UQ:213:LYS:HG2   | 20:UQ:216:SER:HB2   | 1.96                     | 0.47              |
| 20:UQ:579:ASN:HD21  | 65:D2:7:A:H61       | 1.62                     | 0.47              |
| 22:US:188:PHE:O     | 22:US:191:ILE:HG22  | 2.14                     | 0.47              |
| 23:UT:395:GLU:O     | 23:UT:398:GLN:HG3   | 2.14                     | 0.47              |
| 23:UT:942:LYS:HG2   | 23:UT:945:ARG:NH1   | 2.30                     | 0.47              |
| 23:UT:1102:PRO:HD3  | 23:UT:1143:LYS:HZ1  | 1.78                     | 0.47              |
| 23:UT:1268:ILE:HG23 | 23:UT:1288:PHE:HE1  | 1.80                     | 0.47              |
| 23:UT:1463:GLN:HG3  | 23:UT:1467:LYS:HZ1  | 1.79                     | 0.47              |
| 23:UT:1684:GLY:O    | 23:UT:1687:ILE:HG12 | 2.15                     | 0.47              |
| 24:UU:349:HIS:CE1   | 24:UU:370:SER:HB3   | 2.49                     | 0.47              |
| 25:UV:126:LYS:HZ1   | 25:UV:283:TYR:HA    | 1.80                     | 0.47              |
| 25:UV:771:PHE:HA    | 25:UV:1132:PHE:CE1  | 2.50                     | 0.47              |
| 25:UV:909:TYR:CD1   | 25:UV:939:ILE:HD13  | 2.50                     | 0.47              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 25:UV:1069:LYS:HA  | 25:UV:1072:VAL:HG12 | 1.95                     | 0.47              |
| 26:UX:115:ILE:HG23 | 26:UX:116:ALA:H     | 1.78                     | 0.47              |
| 26:UX:155:THR:HB   | 26:UX:160:LEU:HD23  | 1.95                     | 0.47              |
| 27:UZ:67:PRO:HB2   | 27:UZ:96:LEU:HD11   | 1.96                     | 0.47              |
| 29:CE:85:SER:N     | 29:CE:106:ASN:OD1   | 2.48                     | 0.47              |
| 31:CH:221:ILE:HG12 | 31:CH:236:TYR:CD2   | 2.49                     | 0.47              |
| 35:CL:549:ILE:HD13 | 35:CL:567:TRP:CG    | 2.49                     | 0.47              |
| 36:CM:9:THR:HB     | 36:CM:31:ILE:HG22   | 1.96                     | 0.47              |
| 38:JC:98:ASP:CG    | 38:JC:124:GLN:HE22  | 2.18                     | 0.47              |
| 38:JC:250:GLY:HA3  | 38:JC:268:GLN:O     | 2.15                     | 0.47              |
| 39:JF:192:TYR:O    | 39:JF:195:LYS:HG2   | 2.15                     | 0.47              |
| 47:JP:280:ALA:HB2  | 47:JP:311:VAL:HB    | 1.96                     | 0.47              |
| 47:JP:327:LYS:HG2  | 47:JP:350:HIS:N     | 2.15                     | 0.47              |
| 47:JP:415:ARG:HH22 | 66:D3:4:C:N4        | 2.11                     | 0.47              |
| 50:DF:172:ILE:O    | 50:DF:176:THR:HG23  | 2.14                     | 0.47              |
| 52:DH:74:GLN:HG3   | 52:DH:92:PHE:CE2    | 2.49                     | 0.47              |
| 52:DH:141:ARG:O    | 52:DH:148:LYS:HA    | 2.15                     | 0.47              |
| 53:DI:11:ARG:HG2   | 53:DI:17:LYS:HD2    | 1.96                     | 0.47              |
| 53:DI:29:LEU:HD13  | 53:DI:31:ARG:NE     | 2.30                     | 0.47              |
| 53:DI:168:CYS:HB2  | 53:DI:184:LEU:HD21  | 1.96                     | 0.47              |
| 60:DW:115:GLU:OE2  | 60:DW:118:ARG:NH2   | 2.48                     | 0.47              |
| 65:D2:83:U:H1'     | 65:D2:84:G:C2       | 2.50                     | 0.47              |
| 65:D2:470:U:H2'    | 65:D2:471:C:H6      | 1.80                     | 0.47              |
| 65:D2:472:A:C2     | 67:D4:47:G:C2       | 3.02                     | 0.47              |
| 66:D3:395:U:H2'    | 66:D3:396:G:O4'     | 2.14                     | 0.47              |
| 66:D3:1124:A:H1'   | 67:D4:1:G:N1        | 2.29                     | 0.47              |
| 66:D3:1221:A:H2'   | 66:D3:1222:C:C6     | 2.49                     | 0.47              |
| 66:D3:1725:U:H2'   | 66:D3:1726:G:C8     | 2.50                     | 0.47              |
| 67:D4:78:G:N1      | 67:D4:330:A:C6      | 2.82                     | 0.47              |
| 67:D4:150:A:H2'    | 67:D4:150:A:N3      | 2.30                     | 0.47              |
| 3:JA:91:MET:SD     | 35:CL:96:SER:HA     | 2.55                     | 0.47              |
| 3:JA:737:TRP:HA    | 3:JA:740:ASN:HB2    | 1.97                     | 0.47              |
| 3:JA:823:LYS:O     | 3:JA:870:LYS:HG2    | 2.15                     | 0.47              |
| 4:UA:12:GLY:HA2    | 4:UA:372:TRP:CH2    | 2.49                     | 0.47              |
| 4:UA:85:LYS:HB2    | 4:UA:85:LYS:HE3     | 1.68                     | 0.47              |
| 1:CB:228:GLN:HA    | 1:CB:231:ARG:HD2    | 1.95                     | 0.47              |
| 5:UB:478:ILE:HA    | 5:UB:481:MET:HG2    | 1.97                     | 0.47              |
| 5:UB:490:PHE:CE1   | 5:UB:539:ARG:HG2    | 2.49                     | 0.47              |
| 5:UB:576:ILE:O     | 5:UB:576:ILE:HG22   | 2.14                     | 0.47              |
| 6:UC:576:LEU:HD11  | 6:UC:580:ARG:HD3    | 1.96                     | 0.47              |
| 7:UD:105:SER:O     | 7:UD:112:LEU:HA     | 2.15                     | 0.47              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 8:UE:118:TRP:HA     | 8:UE:127:TYR:O      | 2.14                     | 0.47              |
| 9:UF:83:LEU:HD23    | 9:UF:87:SER:HB3     | 1.97                     | 0.47              |
| 13:UJ:108:LYS:O     | 13:UJ:114:THR:HG21  | 2.15                     | 0.47              |
| 13:UJ:141:ASN:HD22  | 13:UJ:209:GLN:HG3   | 1.79                     | 0.47              |
| 13:UJ:523:ILE:O     | 13:UJ:526:LEU:HG    | 2.15                     | 0.47              |
| 13:UJ:1544:PHE:O    | 13:UJ:1548:PHE:N    | 2.36                     | 0.47              |
| 13:UJ:1683:HIS:O    | 13:UJ:1687:LEU:HG   | 2.14                     | 0.47              |
| 15:UL:446:ILE:HG13  | 15:UL:456:LEU:HD13  | 1.95                     | 0.47              |
| 16:UM:211:LEU:HG    | 16:UM:225:PHE:HB2   | 1.96                     | 0.47              |
| 20:UQ:19:LYS:O      | 20:UQ:49:ASN:N      | 2.35                     | 0.47              |
| 20:UQ:42:ARG:HH21   | 20:UQ:42:ARG:HG2    | 1.79                     | 0.47              |
| 20:UQ:335:PRO:HB3   | 65:D2:86:C:O2       | 2.14                     | 0.47              |
| 20:UQ:598:LYS:HB3   | 20:UQ:638:PHE:CE2   | 2.49                     | 0.47              |
| 20:UQ:768:TRP:HA    | 20:UQ:774:PHE:HA    | 1.96                     | 0.47              |
| 21:UR:240:ASP:OD2   | 21:UR:587:ARG:HG2   | 2.14                     | 0.47              |
| 21:UR:353:ARG:HG3   | 21:UR:353:ARG:O     | 2.14                     | 0.47              |
| 23:UT:619:LEU:O     | 23:UT:623:MET:HE2   | 2.15                     | 0.47              |
| 23:UT:655:ASP:OD1   | 23:UT:658:VAL:HG22  | 2.14                     | 0.47              |
| 23:UT:736:LEU:O     | 23:UT:740:ILE:HG12  | 2.15                     | 0.47              |
| 23:UT:1004:VAL:O    | 23:UT:1008:LEU:HD23 | 2.15                     | 0.47              |
| 23:UT:1119:TYR:CE2  | 23:UT:1157:ILE:HG13 | 2.48                     | 0.47              |
| 23:UT:1600:THR:O    | 23:UT:1609:ARG:NH2  | 2.48                     | 0.47              |
| 23:UT:1601:ARG:NH1  | 23:UT:1603:ASP:HA   | 2.29                     | 0.47              |
| 25:UV:1081:ASN:O    | 25:UV:1084:THR:OG1  | 2.25                     | 0.47              |
| 25:UV:1108:LEU:HD12 | 25:UV:1169:ILE:HG21 | 1.97                     | 0.47              |
| 25:UV:1166:ARG:NH2  | 25:UV:1172:ASN:O    | 2.48                     | 0.47              |
| 26:UX:130:CYS:SG    | 26:UX:132:HIS:CD2   | 3.07                     | 0.47              |
| 27:UZ:38:ILE:HD13   | 27:UZ:216:ILE:HD12  | 1.95                     | 0.47              |
| 31:CH:306:THR:OG1   | 31:CH:316:GLU:O     | 2.24                     | 0.47              |
| 31:CH:456:ASP:HB2   | 31:CH:459:LEU:HD12  | 1.96                     | 0.47              |
| 32:CI:128:VAL:O     | 32:CI:132:GLU:HG3   | 2.15                     | 0.47              |
| 34:CK:324:TRP:HE3   | 34:CK:330:VAL:HG21  | 1.79                     | 0.47              |
| 34:CK:534:ARG:HH22  | 66:D3:1628:U:P      | 2.38                     | 0.47              |
| 35:CL:932:LEU:O     | 35:CL:1005:SER:OG   | 2.20                     | 0.47              |
| 36:CM:281:GLU:O     | 36:CM:284:SER:OG    | 2.22                     | 0.47              |
| 37:CN:218:LYS:NZ    | 66:D3:1064:G:N7     | 2.63                     | 0.47              |
| 38:JC:54:GLU:H      | 38:JC:84:TYR:HH     | 1.60                     | 0.47              |
| 38:JC:63:LYS:HE2    | 38:JC:106:ILE:HB    | 1.95                     | 0.47              |
| 38:JC:185:HIS:HB3   | 38:JC:234:THR:HG23  | 1.97                     | 0.47              |
| 39:JF:181:SER:HB3   | 39:JF:184:ALA:HB2   | 1.96                     | 0.47              |
| 39:JF:230:TYR:O     | 39:JF:232:LEU:HD12  | 2.14                     | 0.47              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 45:JN:316:ARG:CD   | 66:D3:1036:A:H1'    | 2.45                     | 0.47              |
| 49:DE:153:ASN:O    | 49:DE:174:LYS:NZ    | 2.28                     | 0.47              |
| 50:DF:208:SER:OG   | 50:DF:211:ILE:HG22  | 2.15                     | 0.47              |
| 54:DJ:65:LYS:H     | 54:DJ:70:LEU:HD21   | 1.80                     | 0.47              |
| 65:D2:338:A:H5''   | 65:D2:339:A:OP1     | 2.14                     | 0.47              |
| 65:D2:437:G:H2'    | 65:D2:438:U:C6      | 2.49                     | 0.47              |
| 66:D3:1134:C:O2'   | 66:D3:1135:U:H5'    | 2.15                     | 0.47              |
| 67:D4:45:U:H2'     | 67:D4:46:U:O4'      | 2.15                     | 0.47              |
| 1:CA:212:LYS:HE2   | 1:CA:212:LYS:HB2    | 1.80                     | 0.47              |
| 2:DA:81:PHE:HE2    | 2:DA:105:PHE:HE1    | 1.63                     | 0.47              |
| 2:DA:243:LYS:N     | 25:UV:656:ARG:HE    | 2.12                     | 0.47              |
| 3:JA:3:LYS:HG3     | 35:CL:372:TYR:HB3   | 1.96                     | 0.47              |
| 3:JA:59:TYR:O      | 3:JA:108:TYR:N      | 2.47                     | 0.47              |
| 3:JA:75:ASN:O      | 3:JA:79:LYS:HG2     | 2.14                     | 0.47              |
| 3:JA:842:LEU:HD21  | 3:JA:921:SER:HA     | 1.97                     | 0.47              |
| 5:UB:440:ASN:ND2   | 5:UB:442:LEU:HD23   | 2.28                     | 0.47              |
| 7:UD:79:TRP:HE1    | 7:UD:85:TRP:C       | 2.17                     | 0.47              |
| 7:UD:79:TRP:CH2    | 7:UD:87:GLN:HB2     | 2.50                     | 0.47              |
| 7:UD:331:ASN:O     | 7:UD:768:ALA:HB1    | 2.14                     | 0.47              |
| 7:UD:347:LEU:HD23  | 7:UD:347:LEU:H      | 1.80                     | 0.47              |
| 7:UD:645:ARG:HH21  | 7:UD:656:ARG:NH1    | 2.11                     | 0.47              |
| 8:UE:51:LEU:HD22   | 8:UE:88:TYR:CE1     | 2.50                     | 0.47              |
| 8:UE:536:LEU:HB3   | 8:UE:540:LEU:HD11   | 1.97                     | 0.47              |
| 9:UF:8:LEU:HB3     | 10:UG:66:LEU:HD13   | 1.96                     | 0.47              |
| 9:UF:93:GLY:O      | 9:UF:97:GLN:HG2     | 2.14                     | 0.47              |
| 9:UF:360:LEU:HA    | 9:UF:363:VAL:HG12   | 1.97                     | 0.47              |
| 10:UG:464:LYS:HA   | 66:D3:-2:A:C2       | 2.50                     | 0.47              |
| 11:UH:655:LEU:HA   | 11:UH:658:LEU:HD12  | 1.97                     | 0.47              |
| 13:UJ:304:GLN:HE22 | 13:UJ:346:LYS:N     | 2.13                     | 0.47              |
| 13:UJ:529:VAL:O    | 13:UJ:532:SER:OG    | 2.21                     | 0.47              |
| 13:UJ:1437:ARG:HA  | 13:UJ:1440:VAL:HG22 | 1.96                     | 0.47              |
| 13:UJ:1615:ASN:O   | 13:UJ:1619:ARG:HD2  | 2.14                     | 0.47              |
| 14:UK:246:LYS:NZ   | 65:D2:233:G:OP1     | 2.46                     | 0.47              |
| 15:UL:38:PRO:HG2   | 15:UL:54:ILE:HB     | 1.96                     | 0.47              |
| 15:UL:444:LEU:HD22 | 15:UL:458:ASP:HA    | 1.96                     | 0.47              |
| 15:UL:580:ASP:HB3  | 15:UL:589:ILE:HD11  | 1.96                     | 0.47              |
| 15:UL:814:MET:O    | 15:UL:816:GLN:N     | 2.47                     | 0.47              |
| 16:UM:89:HIS:ND1   | 16:UM:92:THR:HG23   | 2.30                     | 0.47              |
| 16:UM:253:ASP:OD1  | 16:UM:253:ASP:N     | 2.47                     | 0.47              |
| 16:UM:436:ALA:O    | 16:UM:459:ASN:N     | 2.48                     | 0.47              |
| 16:UM:590:LEU:HB2  | 16:UM:602:TRP:NE1   | 2.29                     | 0.47              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 16:UM:802:GLN:O    | 16:UM:805:ILE:HG22  | 2.15                     | 0.47              |
| 16:UM:804:TYR:O    | 16:UM:807:ASP:HB2   | 2.15                     | 0.47              |
| 18:UO:182:HIS:CE1  | 18:UO:183:LEU:HG    | 2.50                     | 0.47              |
| 22:US:210:ASP:O    | 22:US:214:LYS:HG2   | 2.15                     | 0.47              |
| 22:US:386:LEU:O    | 22:US:389:GLU:O     | 2.33                     | 0.47              |
| 22:US:387:THR:HB   | 22:US:469:LEU:HD11  | 1.97                     | 0.47              |
| 23:UT:288:ILE:HA   | 23:UT:291:LEU:HB2   | 1.96                     | 0.47              |
| 23:UT:692:ASP:O    | 23:UT:696:VAL:HG22  | 2.15                     | 0.47              |
| 23:UT:1154:ALA:HA  | 23:UT:1157:ILE:HG22 | 1.96                     | 0.47              |
| 23:UT:1273:LYS:HB3 | 23:UT:1349:PHE:CG   | 2.50                     | 0.47              |
| 23:UT:1367:ALA:O   | 23:UT:1371:ILE:HG12 | 2.15                     | 0.47              |
| 23:UT:1398:LEU:HA  | 23:UT:1401:ASN:HD21 | 1.79                     | 0.47              |
| 23:UT:1595:SER:C   | 23:UT:1597:ILE:H    | 2.18                     | 0.47              |
| 23:UT:1676:GLU:O   | 23:UT:1680:THR:HG22 | 2.14                     | 0.47              |
| 23:UT:1987:LEU:HA  | 23:UT:1990:LEU:HB2  | 1.97                     | 0.47              |
| 24:UU:24:PHE:O     | 24:UU:657:ARG:NH1   | 2.46                     | 0.47              |
| 24:UU:125:GLY:HA2  | 29:CE:430:ASP:HA    | 1.97                     | 0.47              |
| 24:UU:242:ARG:NH2  | 24:UU:281:ARG:HG3   | 2.26                     | 0.47              |
| 24:UU:263:HIS:CD2  | 24:UU:284:ILE:HD11  | 2.49                     | 0.47              |
| 24:UU:509:SER:O    | 24:UU:517:MET:HG2   | 2.14                     | 0.47              |
| 24:UU:544:ALA:HB3  | 24:UU:562:LEU:HD23  | 1.97                     | 0.47              |
| 25:UV:130:LYS:HD2  | 25:UV:283:TYR:CZ    | 2.49                     | 0.47              |
| 25:UV:167:PRO:HB3  | 25:UV:226:HIS:CD2   | 2.49                     | 0.47              |
| 25:UV:549:SER:O    | 25:UV:553:VAL:HG23  | 2.15                     | 0.47              |
| 25:UV:723:ASN:OD1  | 25:UV:725:SER:N     | 2.47                     | 0.47              |
| 25:UV:738:TYR:HA   | 25:UV:741:ILE:HG22  | 1.96                     | 0.47              |
| 25:UV:1166:ARG:NE  | 25:UV:1172:ASN:HB3  | 2.29                     | 0.47              |
| 27:UZ:155:ARG:HD3  | 27:UZ:175:TYR:OH    | 2.14                     | 0.47              |
| 27:UZ:226:LYS:HD2  | 27:UZ:229:ARG:HE    | 1.79                     | 0.47              |
| 28:CD:9:PHE:CE2    | 28:CD:11:GLU:HG3    | 2.49                     | 0.47              |
| 28:CD:176:GLN:HB3  | 29:CE:187:TRP:NE1   | 2.30                     | 0.47              |
| 30:CG:16:LEU:HA    | 30:CG:19:GLN:OE1    | 2.15                     | 0.47              |
| 31:CH:68:LYS:HE2   | 31:CH:68:LYS:HA     | 1.96                     | 0.47              |
| 31:CH:160:ILE:HG22 | 31:CH:189:THR:HG22  | 1.95                     | 0.47              |
| 31:CH:316:GLU:OE1  | 62:DY:8:ARG:NH2     | 2.31                     | 0.47              |
| 32:CI:22:LYS:NZ    | 65:D2:388:C:OP2     | 2.36                     | 0.47              |
| 33:CJ:141:VAL:HB   | 33:CJ:153:THR:OG1   | 2.15                     | 0.47              |
| 34:CK:527:ARG:NH1  | 66:D3:1639:C:O2     | 2.40                     | 0.47              |
| 37:CN:135:ASN:O    | 37:CN:139:ASN:ND2   | 2.48                     | 0.47              |
| 37:CN:176:ASP:O    | 37:CN:180:LEU:HB2   | 2.15                     | 0.47              |
| 38:JC:62:ILE:HG13  | 38:JC:332:ALA:HB2   | 1.97                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 43:JK:487:ASP:HA   | 43:JK:490:ILE:HD12 | 1.96                     | 0.47              |
| 46:JO:52:TYR:CZ    | 46:JO:56:ILE:HG21  | 2.49                     | 0.47              |
| 47:JP:58:PHE:CE2   | 67:D4:31:G:C4      | 3.03                     | 0.47              |
| 50:DF:130:ILE:H    | 50:DF:130:ILE:HD12 | 1.79                     | 0.47              |
| 51:DG:116:LYS:HZ2  | 51:DG:117:GLY:C    | 2.18                     | 0.47              |
| 52:DH:166:LEU:HD12 | 52:DH:183:PHE:HB2  | 1.96                     | 0.47              |
| 56:DN:30:SER:O     | 56:DN:33:VAL:HG12  | 2.15                     | 0.47              |
| 58:DQ:60:PHE:HE1   | 58:DQ:89:LEU:HD13  | 1.80                     | 0.47              |
| 61:DX:92:CYS:HB3   | 61:DX:132:LEU:HD23 | 1.96                     | 0.47              |
| 62:DY:2:SER:O      | 62:DY:2:SER:OG     | 2.32                     | 0.47              |
| 62:DY:110:GLN:HA   | 62:DY:110:GLN:OE1  | 2.13                     | 0.47              |
| 65:D2:8:A:N6       | 65:D2:9:G:N3       | 2.63                     | 0.47              |
| 65:D2:281:G:C6     | 67:D4:73:A:C2      | 3.03                     | 0.47              |
| 65:D2:329:A:C5     | 65:D2:385:A:C6     | 3.02                     | 0.47              |
| 65:D2:341:G:C5     | 65:D2:342:C:C4     | 3.03                     | 0.47              |
| 65:D2:424:G:H2'    | 65:D2:425:U:C6     | 2.50                     | 0.47              |
| 65:D2:437:G:C2     | 65:D2:438:U:C2     | 3.02                     | 0.47              |
| 65:D2:464:G:N2     | 67:D4:53:U:O2      | 2.47                     | 0.47              |
| 65:D2:465:G:H2'    | 65:D2:466:A:C8     | 2.49                     | 0.47              |
| 66:D3:160:C:H2'    | 66:D3:161:U:O4'    | 2.14                     | 0.47              |
| 66:D3:170:U:N3     | 66:D3:289:U:O2'    | 2.25                     | 0.47              |
| 66:D3:188:A:N6     | 66:D3:197:A:H1'    | 2.29                     | 0.47              |
| 66:D3:590:C:H2'    | 66:D3:591:A:C8     | 2.50                     | 0.47              |
| 66:D3:878:G:H2'    | 66:D3:879:G:H8     | 1.80                     | 0.47              |
| 66:D3:890:C:H2'    | 66:D3:891:A:C8     | 2.49                     | 0.47              |
| 66:D3:1440:C:H2'   | 66:D3:1441:C:C6    | 2.49                     | 0.47              |
| 66:D3:1590:G:C2    | 66:D3:1591:C:C4    | 3.02                     | 0.47              |
| 66:D3:1688:U:H3    | 66:D3:1713:G:H22   | 1.62                     | 0.47              |
| 78:EK:723:THR:O    | 78:EK:726:LEU:CB   | 2.62                     | 0.47              |
| 79:EN:242:LEU:O    | 79:EN:246:LEU:N    | 2.47                     | 0.47              |
| 2:DA:85:LYS:C      | 2:DA:86:LEU:HD12   | 2.35                     | 0.47              |
| 2:DA:158:SER:HA    | 2:DA:161:ILE:HD12  | 1.97                     | 0.47              |
| 2:DA:243:LYS:HG3   | 25:UV:656:ARG:NE   | 2.29                     | 0.47              |
| 3:JA:38:PRO:HG2    | 3:JA:94:PHE:HA     | 1.96                     | 0.47              |
| 4:UA:328:LEU:HD11  | 4:UA:337:TYR:CD2   | 2.50                     | 0.47              |
| 5:UB:637:LEU:O     | 5:UB:641:GLU:HG2   | 2.15                     | 0.47              |
| 7:UD:565:ARG:HH11  | 7:UD:567:ASN:H     | 1.61                     | 0.47              |
| 8:UE:255:ILE:HB    | 8:UE:277:LYS:HB2   | 1.97                     | 0.47              |
| 8:UE:463:ARG:HA    | 8:UE:466:ARG:NH1   | 2.29                     | 0.47              |
| 11:UH:647:LEU:HB3  | 12:UI:509:GLN:HE22 | 1.80                     | 0.47              |
| 12:UI:421:LEU:HD22 | 12:UI:462:LEU:HD22 | 1.96                     | 0.47              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 13:UJ:57:GLU:O     | 13:UJ:61:GLN:HG2    | 2.15                     | 0.47              |
| 13:UJ:109:TRP:HB2  | 13:UJ:142:TYR:CE2   | 2.50                     | 0.47              |
| 13:UJ:1579:PHE:HA  | 13:UJ:1582:LEU:HG   | 1.96                     | 0.47              |
| 13:UJ:1643:ARG:O   | 13:UJ:1647:ILE:HG12 | 2.14                     | 0.47              |
| 20:UQ:343:ASP:HB3  | 20:UQ:357:ILE:HG12  | 1.96                     | 0.47              |
| 23:UT:220:GLU:CG   | 23:UT:268:PRO:HG3   | 2.45                     | 0.47              |
| 23:UT:1774:LYS:O   | 23:UT:1778:MET:HG2  | 2.14                     | 0.47              |
| 25:UV:522:LYS:HG2  | 25:UV:523:TYR:CE1   | 2.50                     | 0.47              |
| 25:UV:864:LEU:O    | 25:UV:867:ILE:HG22  | 2.14                     | 0.47              |
| 27:UZ:204:ILE:HD12 | 27:UZ:205:GLN:HE22  | 1.79                     | 0.47              |
| 28:CD:178:ILE:HD12 | 28:CD:313:ALA:HB3   | 1.97                     | 0.47              |
| 29:CE:308:SER:O    | 29:CE:311:LYS:HB3   | 2.15                     | 0.47              |
| 30:CF:62:GLU:HA    | 30:CF:65:LEU:CB     | 2.41                     | 0.47              |
| 31:CH:219:LYS:HE3  | 31:CH:220:TYR:CZ    | 2.50                     | 0.47              |
| 32:CI:53:ASP:OD2   | 34:CK:444:LEU:HD13  | 2.14                     | 0.47              |
| 35:CL:245:LEU:HD23 | 35:CL:245:LEU:H     | 1.79                     | 0.47              |
| 35:CL:616:ASP:OD1  | 35:CL:620:LYS:HE3   | 2.15                     | 0.47              |
| 36:CM:105:TYR:CE2  | 36:CM:296:LEU:HA    | 2.49                     | 0.47              |
| 36:CM:155:LYS:O    | 36:CM:165:GLU:N     | 2.34                     | 0.47              |
| 55:DL:99:ARG:HG2   | 55:DL:100:TYR:H     | 1.80                     | 0.47              |
| 65:D2:104:A:H61    | 65:D2:140:U:H3      | 1.62                     | 0.47              |
| 65:D2:290:G:C2     | 67:D4:64:A:C2       | 3.03                     | 0.47              |
| 66:D3:8:U:C4       | 66:D3:9:U:C2        | 3.03                     | 0.47              |
| 66:D3:525:A:C6     | 66:D3:526:A:C5      | 3.03                     | 0.47              |
| 67:D4:96:C:H2'     | 67:D4:97:C:C6       | 2.50                     | 0.47              |
| 77:EJ:259:ALA:O    | 77:EJ:264:GLY:N     | 2.44                     | 0.47              |
| 3:JA:527:HIS:O     | 3:JA:530:SER:OG     | 2.18                     | 0.47              |
| 4:UA:515:TYR:CE1   | 58:DQ:118:ILE:HD11  | 2.50                     | 0.47              |
| 1:CB:258:HIS:HE1   | 1:CB:297:ARG:HD3    | 1.80                     | 0.47              |
| 7:UD:31:MET:HE1    | 7:UD:752:LEU:HG     | 1.97                     | 0.47              |
| 7:UD:100:GLU:HG3   | 7:UD:118:GLY:C      | 2.35                     | 0.47              |
| 8:UE:479:ILE:HD11  | 8:UE:483:ARG:NH2    | 2.29                     | 0.47              |
| 13:UJ:255:ILE:HD11 | 20:UQ:884:MET:CG    | 2.45                     | 0.47              |
| 14:UK:48:LEU:HD23  | 14:UK:48:LEU:HA     | 1.67                     | 0.47              |
| 15:UL:390:GLN:HG2  | 15:UL:394:VAL:HG22  | 1.97                     | 0.47              |
| 16:UM:128:VAL:O    | 16:UM:137:THR:N     | 2.48                     | 0.47              |
| 16:UM:416:ARG:O    | 16:UM:424:PHE:HA    | 2.15                     | 0.47              |
| 18:UO:224:THR:C    | 18:UO:239:LEU:HD23  | 2.35                     | 0.47              |
| 18:UO:428:ARG:HB3  | 18:UO:432:TYR:CE1   | 2.50                     | 0.47              |
| 18:UO:496:HIS:HB3  | 18:UO:497:LYS:NZ    | 2.28                     | 0.47              |
| 23:UT:201:ARG:O    | 23:UT:250:LYS:NZ    | 2.39                     | 0.47              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 23:UT:422:LYS:NZ    | 23:UT:456:GLU:HG2   | 2.30                     | 0.47              |
| 23:UT:636:ARG:NH1   | 51:DG:129:VAL:HG13  | 2.29                     | 0.47              |
| 23:UT:673:ARG:HA    | 23:UT:678:TRP:NE1   | 2.29                     | 0.47              |
| 23:UT:886:ASP:O     | 23:UT:890:ASN:ND2   | 2.48                     | 0.47              |
| 23:UT:1003:ILE:O    | 23:UT:1007:THR:HG23 | 2.15                     | 0.47              |
| 23:UT:1247:LEU:HA   | 23:UT:1250:ILE:HG22 | 1.96                     | 0.47              |
| 23:UT:1268:ILE:HG23 | 23:UT:1288:PHE:CE1  | 2.50                     | 0.47              |
| 23:UT:1681:LEU:HD23 | 23:UT:1686:GLN:O    | 2.15                     | 0.47              |
| 23:UT:1771:SER:N    | 23:UT:1772:PRO:HD2  | 2.30                     | 0.47              |
| 25:UV:120:HIS:CE1   | 25:UV:287:LYS:HD2   | 2.49                     | 0.47              |
| 25:UV:184:SER:OG    | 25:UV:206:LEU:HB3   | 2.15                     | 0.47              |
| 25:UV:232:LEU:HB3   | 25:UV:296:ILE:HG13  | 1.96                     | 0.47              |
| 25:UV:377:SER:O     | 25:UV:479:LYS:NZ    | 2.30                     | 0.47              |
| 25:UV:565:LYS:NZ    | 25:UV:689:HIS:O     | 2.38                     | 0.47              |
| 25:UV:1140:SER:HA   | 25:UV:1143:MET:HE3  | 1.95                     | 0.47              |
| 27:UZ:201:VAL:HG13  | 27:UZ:215:ASN:ND2   | 2.30                     | 0.47              |
| 28:CD:226:LYS:HD2   | 28:CD:258:SER:OG    | 2.15                     | 0.47              |
| 28:CD:226:LYS:NZ    | 28:CD:262:ASP:HB2   | 2.30                     | 0.47              |
| 29:CE:359:ILE:HA    | 29:CE:362:VAL:HG22  | 1.96                     | 0.47              |
| 35:CL:86:ILE:O      | 35:CL:90:VAL:HG12   | 2.15                     | 0.47              |
| 35:CL:243:TYR:CZ    | 35:CL:276:HIS:HB3   | 2.50                     | 0.47              |
| 35:CL:1119:ILE:HG22 | 44:JM:129:ALA:HB1   | 1.97                     | 0.47              |
| 37:CN:17:PRO:HG2    | 37:CN:148:HIS:ND1   | 2.30                     | 0.47              |
| 37:CN:88:LEU:HB2    | 37:CN:125:LEU:HB2   | 1.97                     | 0.47              |
| 37:CN:259:ARG:HG2   | 56:DN:83:GLU:HG3    | 1.97                     | 0.47              |
| 39:JG:227:LEU:HD11  | 39:JG:232:LEU:HD21  | 1.97                     | 0.47              |
| 46:JO:92:ALA:HB1    | 57:DO:99:GLN:HG3    | 1.96                     | 0.47              |
| 47:JP:2:LYS:O       | 47:JP:3:ILE:HD13    | 2.15                     | 0.47              |
| 53:DI:25:ARG:HH22   | 66:D3:386:G:P       | 2.38                     | 0.47              |
| 65:D2:123:C:OP2     | 65:D2:124:A:N6      | 2.48                     | 0.47              |
| 65:D2:210:U:H2'     | 65:D2:211:G:C8      | 2.49                     | 0.47              |
| 66:D3:56:U:H4'      | 66:D3:57:G:OP1      | 2.15                     | 0.47              |
| 66:D3:96:G:C2       | 66:D3:97:C:C2       | 3.03                     | 0.47              |
| 66:D3:168:A:H2'     | 66:D3:169:A:C8      | 2.49                     | 0.47              |
| 66:D3:524:U:N3      | 66:D3:527:A:OP2     | 2.43                     | 0.47              |
| 66:D3:591:A:C2      | 66:D3:592:A:C6      | 3.02                     | 0.47              |
| 66:D3:929:A:N6      | 66:D3:930:A:N1      | 2.62                     | 0.47              |
| 66:D3:1049:U:H3     | 66:D3:1069:A:H61    | 1.62                     | 0.47              |
| 66:D3:1613:U:C2     | 66:D3:1614:A:H2     | 2.33                     | 0.47              |
| 69:EB:164:LYS:N     | 69:EB:185:VAL:O     | 2.35                     | 0.47              |
| 1:CA:261:LEU:HG     | 1:CA:262:LYS:O      | 2.15                     | 0.47              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 3:JA:117:ASN:O     | 3:JA:141:THR:OG1    | 2.33                     | 0.47              |
| 3:JA:495:THR:HA    | 3:JA:498:LYS:HE2    | 1.96                     | 0.47              |
| 3:JA:779:LYS:HG3   | 3:JA:783:LYS:HZ3    | 1.79                     | 0.47              |
| 3:JA:898:ILE:HA    | 3:JA:901:GLU:HG3    | 1.97                     | 0.47              |
| 1:CB:235:GLY:HA2   | 29:CE:121:LYS:HD2   | 1.97                     | 0.47              |
| 1:CB:283:GLU:OE2   | 1:CB:283:GLU:N      | 2.46                     | 0.47              |
| 8:UE:527:HIS:ND1   | 18:UO:508:LEU:HD23  | 2.30                     | 0.47              |
| 9:UF:42:ARG:HD2    | 9:UF:52:ASP:OD1     | 2.15                     | 0.47              |
| 10:UG:184:LEU:HD23 | 10:UG:184:LEU:HA    | 1.67                     | 0.47              |
| 10:UG:244:ASN:HB3  | 10:UG:246:VAL:HG12  | 1.97                     | 0.47              |
| 10:UG:388:ASP:HB2  | 10:UG:403:VAL:O     | 2.14                     | 0.47              |
| 13:UJ:229:GLU:O    | 13:UJ:232:ASN:N     | 2.48                     | 0.47              |
| 13:UJ:1425:VAL:O   | 13:UJ:1429:SER:HB3  | 2.15                     | 0.47              |
| 14:UK:40:ASP:HA    | 14:UK:43:ARG:HH11   | 1.79                     | 0.47              |
| 15:UL:55:LYS:HA    | 15:UL:383:HIS:CE1   | 2.50                     | 0.47              |
| 15:UL:253:LYS:HZ2  | 66:D3:1741:U:P      | 2.35                     | 0.47              |
| 16:UM:352:LYS:HD3  | 16:UM:366:PRO:HA    | 1.96                     | 0.47              |
| 16:UM:649:GLU:OE1  | 16:UM:649:GLU:N     | 2.29                     | 0.47              |
| 18:UO:424:ARG:HB3  | 18:UO:426:LYS:NZ    | 2.30                     | 0.47              |
| 20:UQ:293:LEU:HD12 | 20:UQ:324:TRP:CE3   | 2.50                     | 0.47              |
| 21:UR:296:GLN:O    | 21:UR:297:THR:OG1   | 2.24                     | 0.47              |
| 21:UR:433:TRP:HB3  | 21:UR:435:PHE:CE1   | 2.50                     | 0.47              |
| 22:US:225:HIS:HB2  | 22:US:228:HIS:CE1   | 2.50                     | 0.47              |
| 23:UT:247:LEU:HG   | 23:UT:248:HIS:H     | 1.81                     | 0.47              |
| 23:UT:481:TRP:CE2  | 23:UT:485:ILE:HD11  | 2.50                     | 0.47              |
| 23:UT:851:HIS:CE1  | 23:UT:924:TYR:HH    | 2.33                     | 0.47              |
| 23:UT:947:ILE:HG12 | 66:D3:257:A:H5'     | 1.97                     | 0.47              |
| 23:UT:1463:GLN:HG3 | 23:UT:1467:LYS:NZ   | 2.30                     | 0.47              |
| 24:UU:62:ASP:O     | 24:UU:66:LEU:HD23   | 2.15                     | 0.47              |
| 24:UU:222:ALA:HB1  | 24:UU:254:LEU:HD13  | 1.98                     | 0.47              |
| 24:UU:766:LYS:HB2  | 24:UU:766:LYS:HE3   | 1.70                     | 0.47              |
| 25:UV:127:PHE:O    | 25:UV:131:LEU:HG    | 2.14                     | 0.47              |
| 25:UV:529:VAL:CG2  | 25:UV:613:VAL:HB    | 2.45                     | 0.47              |
| 27:UZ:28:PRO:HA    | 27:UZ:31:LYS:HE3    | 1.97                     | 0.47              |
| 28:CD:222:PHE:CE2  | 28:CD:240:LEU:HD22  | 2.50                     | 0.47              |
| 29:CE:90:SER:HB3   | 29:CE:117:TYR:CE2   | 2.50                     | 0.47              |
| 31:CH:438:ILE:HD12 | 31:CH:442:ILE:HG13  | 1.97                     | 0.47              |
| 34:CK:335:ARG:HH21 | 34:CK:340:LEU:HD11  | 1.79                     | 0.47              |
| 35:CL:555:MET:HB2  | 35:CL:558:ILE:HD12  | 1.97                     | 0.47              |
| 35:CL:800:PHE:HB2  | 35:CL:1022:LEU:HD23 | 1.97                     | 0.47              |
| 36:CM:197:SER:OG   | 36:CM:229:VAL:HG12  | 2.15                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:JC:54:GLU:N     | 38:JC:84:TYR:OH    | 2.40                     | 0.47              |
| 38:JC:356:LEU:HA   | 38:JC:359:ILE:HG12 | 1.97                     | 0.47              |
| 39:JF:214:ASP:HA   | 39:JF:216:PHE:CE2  | 2.50                     | 0.47              |
| 39:JG:193:ILE:HD13 | 39:JG:196:LEU:HD12 | 1.96                     | 0.47              |
| 49:DE:45:ILE:HB    | 49:DE:80:THR:OG1   | 2.15                     | 0.47              |
| 58:DQ:98:ASP:O     | 58:DQ:101:SER:OG   | 2.32                     | 0.47              |
| 66:D3:386:G:C2     | 66:D3:387:A:H2     | 2.33                     | 0.47              |
| 66:D3:876:G:C2     | 66:D3:944:A:C6     | 3.04                     | 0.47              |
| 66:D3:1115:U:C2    | 66:D3:1116:A:C8    | 3.03                     | 0.47              |
| 66:D3:1584:G:O2'   | 66:D3:1610:G:O6    | 2.33                     | 0.47              |
| 3:JA:202:ASP:HB3   | 3:JA:206:ASN:OD1   | 2.15                     | 0.46              |
| 4:UA:843:LYS:O     | 4:UA:847:ARG:HG2   | 2.15                     | 0.46              |
| 1:CB:293:LEU:HB3   | 1:CB:298:ILE:HD12  | 1.96                     | 0.46              |
| 5:UB:552:GLN:O     | 5:UB:555:ARG:HG2   | 2.15                     | 0.46              |
| 7:UD:151:ASP:O     | 7:UD:152:SER:OG    | 2.30                     | 0.46              |
| 7:UD:394:TRP:HA    | 7:UD:398:THR:O     | 2.15                     | 0.46              |
| 8:UE:181:VAL:HG23  | 8:UE:182:MET:N     | 2.30                     | 0.46              |
| 9:UF:3:LYS:HG3     | 65:D2:487:A:H62    | 1.80                     | 0.46              |
| 9:UF:186:VAL:HG21  | 9:UF:319:TYR:CE2   | 2.49                     | 0.46              |
| 13:UJ:272:LYS:HE3  | 13:UJ:309:GLN:O    | 2.14                     | 0.46              |
| 15:UL:225:GLN:OE1  | 15:UL:247:ILE:HG23 | 2.15                     | 0.46              |
| 15:UL:487:ARG:HA   | 15:UL:500:TRP:O    | 2.15                     | 0.46              |
| 15:UL:631:PHE:HE2  | 15:UL:641:TYR:CD1  | 2.34                     | 0.46              |
| 16:UM:50:ARG:O     | 16:UM:51:LYS:HD2   | 2.15                     | 0.46              |
| 16:UM:223:TRP:CZ3  | 16:UM:233:LEU:HG   | 2.50                     | 0.46              |
| 16:UM:584:ILE:HG22 | 16:UM:589:GLN:H    | 1.80                     | 0.46              |
| 18:UO:79:ARG:NH1   | 66:D3:1534:G:N7    | 2.62                     | 0.46              |
| 18:UO:219:ILE:HG22 | 18:UO:227:VAL:HB   | 1.95                     | 0.46              |
| 20:UQ:255:ASN:OD1  | 20:UQ:256:THR:N    | 2.48                     | 0.46              |
| 20:UQ:503:ASP:HB3  | 20:UQ:570:SER:OG   | 2.14                     | 0.46              |
| 20:UQ:682:ASN:HB2  | 20:UQ:689:ILE:HD11 | 1.98                     | 0.46              |
| 21:UR:175:PRO:HG2  | 21:UR:177:TRP:CD1  | 2.50                     | 0.46              |
| 23:UT:386:LEU:HD22 | 23:UT:393:PHE:CE2  | 2.50                     | 0.46              |
| 23:UT:480:TYR:HE1  | 23:UT:518:MET:HA   | 1.80                     | 0.46              |
| 23:UT:1349:PHE:O   | 23:UT:1352:LEU:HG  | 2.15                     | 0.46              |
| 27:UZ:23:GLN:O     | 27:UZ:26:GLU:HG3   | 2.15                     | 0.46              |
| 27:UZ:169:GLU:OE1  | 27:UZ:169:GLU:N    | 2.48                     | 0.46              |
| 28:CD:5:GLU:O      | 28:CD:20:VAL:HG12  | 2.15                     | 0.46              |
| 30:CF:34:LYS:HA    | 30:CF:34:LYS:HD2   | 1.73                     | 0.46              |
| 31:CH:118:ALA:C    | 31:CH:122:LYS:HZ3  | 2.18                     | 0.46              |
| 31:CH:160:ILE:HG23 | 31:CH:542:SER:HB2  | 1.97                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:CI:98:GLU:HG3   | 33:CJ:58:TYR:OH    | 2.15                     | 0.46              |
| 32:CI:151:THR:OG1  | 34:CK:455:HIS:CD2  | 2.68                     | 0.46              |
| 33:CJ:131:CYS:HB3  | 33:CJ:136:THR:OG1  | 2.15                     | 0.46              |
| 36:CM:47:ASP:N     | 36:CM:47:ASP:OD1   | 2.47                     | 0.46              |
| 37:CN:138:TRP:O    | 37:CN:141:LEU:HG   | 2.16                     | 0.46              |
| 38:JC:171:ARG:NE   | 43:JK:468:VAL:HA   | 2.30                     | 0.46              |
| 38:JC:207:TRP:HA   | 38:JC:214:ARG:HA   | 1.97                     | 0.46              |
| 39:JF:168:THR:HA   | 39:JF:171:LEU:HD13 | 1.96                     | 0.46              |
| 39:JG:104:ILE:HG13 | 39:JG:110:LEU:HD22 | 1.97                     | 0.46              |
| 42:JJ:200:ARG:CZ   | 42:JJ:204:ARG:HD3  | 2.45                     | 0.46              |
| 46:JO:189:ASP:O    | 46:JO:192:LYS:C    | 2.54                     | 0.46              |
| 47:JP:58:PHE:HE1   | 47:JP:60:GLY:O     | 1.97                     | 0.46              |
| 47:JP:121:PRO:HA   | 47:JP:192:SER:HB2  | 1.95                     | 0.46              |
| 49:DE:172:PHE:CE2  | 49:DE:174:LYS:HE3  | 2.50                     | 0.46              |
| 51:DG:58:LYS:HA    | 51:DG:107:ALA:HB2  | 1.97                     | 0.46              |
| 52:DH:91:ILE:HG21  | 52:DH:129:LEU:HD12 | 1.96                     | 0.46              |
| 55:DL:57:LYS:NZ    | 66:D3:327:U:OP1    | 2.47                     | 0.46              |
| 62:DY:18:LEU:HD12  | 62:DY:20:ARG:CZ    | 2.45                     | 0.46              |
| 62:DY:127:LYS:NZ   | 66:D3:151:G:OP2    | 2.35                     | 0.46              |
| 65:D2:217:C:H2'    | 65:D2:218:U:H6     | 1.79                     | 0.46              |
| 66:D3:326:G:H2'    | 66:D3:327:U:C6     | 2.50                     | 0.46              |
| 66:D3:473:A:H62    | 66:D3:474:A:N6     | 2.13                     | 0.46              |
| 72:EE:15:GLY:O     | 72:EE:30:VAL:N     | 2.41                     | 0.46              |
| 1:CA:173:LEU:HD21  | 1:CA:256:ASN:ND2   | 2.30                     | 0.46              |
| 2:DA:48:VAL:HG21   | 2:DA:61:LEU:HD11   | 1.97                     | 0.46              |
| 3:JA:112:GLU:O     | 3:JA:115:LEU:HD23  | 2.16                     | 0.46              |
| 3:JA:484:LYS:HA    | 3:JA:487:ASN:HD21  | 1.81                     | 0.46              |
| 3:JA:855:ILE:HG21  | 3:JA:913:PHE:CZ    | 2.51                     | 0.46              |
| 4:UA:119:LEU:HD21  | 4:UA:161:ILE:HD13  | 1.98                     | 0.46              |
| 4:UA:555:CYS:HG    | 4:UA:580:PHE:HD2   | 1.60                     | 0.46              |
| 4:UA:794:PHE:HB2   | 24:UU:720:LEU:HD21 | 1.96                     | 0.46              |
| 1:CB:91:HIS:CE1    | 14:UK:164:ASN:HA   | 2.47                     | 0.46              |
| 5:UB:646:THR:HA    | 5:UB:649:THR:HG22  | 1.97                     | 0.46              |
| 5:UB:716:LYS:H     | 39:JG:150:ILE:CG2  | 2.28                     | 0.46              |
| 7:UD:271:THR:CG2   | 7:UD:272:LEU:H     | 2.21                     | 0.46              |
| 8:UE:364:THR:HG22  | 8:UE:365:SER:N     | 2.30                     | 0.46              |
| 10:UG:447:ASN:O    | 47:JP:37:ARG:NH1   | 2.48                     | 0.46              |
| 11:UH:597:GLN:HA   | 11:UH:600:LYS:NZ   | 2.31                     | 0.46              |
| 13:UJ:197:ASP:OD1  | 13:UJ:244:LYS:HD3  | 2.15                     | 0.46              |
| 13:UJ:576:ILE:HG13 | 13:UJ:579:ARG:HH12 | 1.79                     | 0.46              |
| 13:UJ:1483:SER:HA  | 13:UJ:1486:GLU:CD  | 2.35                     | 0.46              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 13:UJ:1593:TYR:HA   | 13:UJ:1596:TYR:CD2 | 2.50                     | 0.46              |
| 15:UL:633:CYS:HB3   | 15:UL:663:LEU:HD22 | 1.97                     | 0.46              |
| 15:UL:761:ALA:HA    | 15:UL:764:GLU:OE2  | 2.15                     | 0.46              |
| 15:UL:925:ASP:O     | 15:UL:928:GLU:HG3  | 2.15                     | 0.46              |
| 16:UM:245:SER:OG    | 16:UM:246:CYS:N    | 2.48                     | 0.46              |
| 16:UM:354:ALA:HA    | 16:UM:364:ILE:HD13 | 1.96                     | 0.46              |
| 19:UP:165:ASN:HA    | 19:UP:168:LYS:HE2  | 1.97                     | 0.46              |
| 21:UR:304:LEU:HD23  | 21:UR:371:VAL:HG21 | 1.97                     | 0.46              |
| 21:UR:484:VAL:CG1   | 21:UR:492:ASN:HB2  | 2.45                     | 0.46              |
| 22:US:277:ILE:HA    | 22:US:280:ILE:HG22 | 1.98                     | 0.46              |
| 22:US:342:TYR:CE1   | 22:US:382:LYS:HD2  | 2.50                     | 0.46              |
| 23:UT:60:SER:O      | 23:UT:64:THR:OG1   | 2.24                     | 0.46              |
| 23:UT:74:VAL:HG21   | 23:UT:80:ILE:HG12  | 1.96                     | 0.46              |
| 23:UT:146:ASN:HB3   | 23:UT:150:TRP:CZ2  | 2.50                     | 0.46              |
| 23:UT:1185:LEU:HA   | 23:UT:1189:LEU:HB2 | 1.97                     | 0.46              |
| 23:UT:1851:GLU:HG2  | 23:UT:1853:LYS:HB3 | 1.96                     | 0.46              |
| 24:UU:264:LEU:HB2   | 24:UU:278:LEU:HD21 | 1.97                     | 0.46              |
| 24:UU:437:GLU:HA    | 24:UU:437:GLU:OE2  | 2.14                     | 0.46              |
| 25:UV:434:LEU:HD12  | 25:UV:439:HIS:HA   | 1.97                     | 0.46              |
| 31:CH:363:ASP:OD2   | 31:CH:437:ARG:NH1  | 2.29                     | 0.46              |
| 35:CL:161:HIS:NE2   | 35:CL:916:THR:HG21 | 2.30                     | 0.46              |
| 35:CL:619:GLU:C     | 35:CL:623:LYS:HZ2  | 2.18                     | 0.46              |
| 35:CL:1004:ARG:HH21 | 35:CL:1006:TRP:HZ2 | 1.60                     | 0.46              |
| 36:CM:159:PRO:HA    | 36:CM:160:PRO:HA   | 1.68                     | 0.46              |
| 38:JC:101:ASN:HD21  | 38:JC:104:PHE:HB3  | 1.80                     | 0.46              |
| 39:JF:164:LYS:NZ    | 39:JF:165:ASN:O    | 2.39                     | 0.46              |
| 42:JJ:115:LYS:HE2   | 42:JJ:115:LYS:HA   | 1.96                     | 0.46              |
| 47:JP:354:VAL:O     | 47:JP:355:LYS:HG2  | 2.15                     | 0.46              |
| 49:DE:32:SER:O      | 49:DE:83:PRO:HG3   | 2.15                     | 0.46              |
| 49:DE:123:LEU:HA    | 49:DE:160:VAL:O    | 2.15                     | 0.46              |
| 49:DE:128:LYS:HB3   | 49:DE:140:VAL:HB   | 1.98                     | 0.46              |
| 49:DE:130:GLN:HG3   | 49:DE:131:LEU:H    | 1.80                     | 0.46              |
| 58:DQ:46:PHE:O      | 58:DQ:50:GLU:HG2   | 2.15                     | 0.46              |
| 58:DQ:58:ASP:O      | 58:DQ:61:SER:N     | 2.49                     | 0.46              |
| 60:DW:105:THR:HG23  | 60:DW:126:LEU:HD11 | 1.96                     | 0.46              |
| 65:D2:90:G:C4       | 65:D2:162:U:C4     | 3.03                     | 0.46              |
| 65:D2:101:G:C2      | 65:D2:103:G:C4     | 3.03                     | 0.46              |
| 65:D2:223:C:H2'     | 65:D2:224:G:C8     | 2.50                     | 0.46              |
| 65:D2:286:U:H3      | 67:D4:67:G:H1      | 1.62                     | 0.46              |
| 66:D3:42:G:OP2      | 66:D3:438:A:N6     | 2.45                     | 0.46              |
| 66:D3:52:U:H2'      | 66:D3:53:G:C8      | 2.45                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 66:D3:292:U:H2'    | 66:D3:293:U:C6     | 2.49                     | 0.46              |
| 66:D3:521:A:H2'    | 66:D3:522:U:O4'    | 2.15                     | 0.46              |
| 66:D3:541:A:H4'    | 66:D3:544:A:C2     | 2.50                     | 0.46              |
| 66:D3:549:G:N2     | 66:D3:550:A:C4     | 2.83                     | 0.46              |
| 66:D3:904:G:C6     | 66:D3:905:A:C5     | 3.03                     | 0.46              |
| 66:D3:929:A:N6     | 66:D3:930:A:C6     | 2.84                     | 0.46              |
| 1:CA:226:HIS:HB3   | 1:CA:229:LYS:HB2   | 1.96                     | 0.46              |
| 3:JA:825:LEU:HD21  | 3:JA:923:TYR:CE2   | 2.49                     | 0.46              |
| 4:UA:370:LYS:NZ    | 4:UA:379:CYS:SG    | 2.67                     | 0.46              |
| 4:UA:516:SER:HB2   | 4:UA:534:THR:HB    | 1.97                     | 0.46              |
| 1:CB:297:ARG:CZ    | 1:CB:323:SER:HA    | 2.45                     | 0.46              |
| 5:UB:659:GLU:HA    | 5:UB:662:LEU:HG    | 1.97                     | 0.46              |
| 7:UD:46:ILE:HD12   | 7:UD:46:ILE:H      | 1.80                     | 0.46              |
| 7:UD:220:GLU:OE1   | 7:UD:220:GLU:N     | 2.32                     | 0.46              |
| 7:UD:326:ARG:CD    | 7:UD:328:LEU:HD11  | 2.45                     | 0.46              |
| 7:UD:571:THR:CG2   | 7:UD:632:ASN:HB3   | 2.45                     | 0.46              |
| 7:UD:626:TRP:CH2   | 7:UD:657:ILE:HD11  | 2.48                     | 0.46              |
| 9:UF:146:ILE:HA    | 9:UF:146:ILE:HD12  | 1.81                     | 0.46              |
| 9:UF:155:TYR:HA    | 9:UF:159:ALA:HA    | 1.96                     | 0.46              |
| 10:UG:74:LEU:HD12  | 10:UG:404:PRO:HG2  | 1.96                     | 0.46              |
| 10:UG:122:GLY:HA2  | 10:UG:385:PRO:HG2  | 1.97                     | 0.46              |
| 13:UJ:238:LEU:HA   | 13:UJ:241:ILE:HG22 | 1.96                     | 0.46              |
| 13:UJ:257:ALA:HA   | 13:UJ:260:ILE:HG22 | 1.98                     | 0.46              |
| 13:UJ:611:ILE:HD12 | 13:UJ:612:PRO:HD2  | 1.97                     | 0.46              |
| 15:UL:183:ASP:OD1  | 15:UL:183:ASP:N    | 2.48                     | 0.46              |
| 15:UL:845:LEU:HD12 | 15:UL:848:SER:OG   | 2.15                     | 0.46              |
| 17:UN:890:VAL:HG23 | 47:JP:358:MET:HB3  | 1.96                     | 0.46              |
| 18:UO:373:ILE:HG23 | 21:UR:288:LEU:CD1  | 2.45                     | 0.46              |
| 21:UR:401:GLU:HG3  | 21:UR:402:GLY:N    | 2.30                     | 0.46              |
| 22:US:488:PHE:O    | 39:JG:24:VAL:HG11  | 2.16                     | 0.46              |
| 22:US:504:ASP:HA   | 22:US:507:LEU:HD12 | 1.98                     | 0.46              |
| 23:UT:173:THR:O    | 23:UT:176:LEU:HG   | 2.15                     | 0.46              |
| 23:UT:1208:MET:SD  | 23:UT:1210:PHE:HB3 | 2.55                     | 0.46              |
| 23:UT:1949:PRO:HB2 | 47:JP:252:ASN:ND2  | 2.31                     | 0.46              |
| 24:UU:58:PHE:CE2   | 24:UU:60:ILE:HD11  | 2.51                     | 0.46              |
| 24:UU:367:LEU:HD11 | 24:UU:419:ILE:HD12 | 1.97                     | 0.46              |
| 24:UU:412:PRO:HG2  | 24:UU:437:GLU:HG3  | 1.97                     | 0.46              |
| 24:UU:414:ILE:HG12 | 24:UU:434:HIS:CE1  | 2.50                     | 0.46              |
| 25:UV:376:SER:O    | 25:UV:387:GLY:N    | 2.49                     | 0.46              |
| 25:UV:391:PHE:O    | 25:UV:395:ILE:HG12 | 2.15                     | 0.46              |
| 25:UV:529:VAL:O    | 25:UV:612:PHE:HB2  | 2.16                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:UV:1098:PHE:CZ  | 25:UV:1184:GLY:HA3 | 2.51                     | 0.46              |
| 25:UV:1165:SER:OG  | 25:UV:1166:ARG:N   | 2.48                     | 0.46              |
| 29:CE:361:ARG:NH1  | 67:D4:83:A:OP2     | 2.48                     | 0.46              |
| 31:CH:334:GLU:OE1  | 31:CH:352:PRO:HG3  | 2.14                     | 0.46              |
| 31:CH:492:TRP:HD1  | 31:CH:556:VAL:HG21 | 1.80                     | 0.46              |
| 33:CJ:162:THR:HG21 | 33:CJ:266:LEU:N    | 2.30                     | 0.46              |
| 35:CL:874:TYR:OH   | 66:D3:577:G:H3'    | 2.15                     | 0.46              |
| 35:CL:980:LEU:HD23 | 35:CL:987:TYR:HA   | 1.96                     | 0.46              |
| 37:CN:42:HIS:CD2   | 37:CN:125:LEU:HD11 | 2.50                     | 0.46              |
| 38:JC:55:PHE:HA    | 38:JC:82:HIS:HE1   | 1.80                     | 0.46              |
| 38:JC:254:ILE:HD13 | 38:JC:264:ILE:HB   | 1.97                     | 0.46              |
| 42:JJ:139:LEU:HD23 | 42:JJ:139:LEU:H    | 1.80                     | 0.46              |
| 42:JJ:190:VAL:HG21 | 42:JJ:251:ILE:CD1  | 2.45                     | 0.46              |
| 47:JP:405:ARG:HG2  | 47:JP:405:ARG:O    | 2.16                     | 0.46              |
| 50:DF:49:GLU:OE1   | 50:DF:50:GLU:HG2   | 2.15                     | 0.46              |
| 52:DH:47:ARG:NH1   | 66:D3:642:G:O3'    | 2.49                     | 0.46              |
| 55:DL:78:THR:HG22  | 55:DL:84:ILE:HD12  | 1.96                     | 0.46              |
| 65:D2:263:C:H2'    | 65:D2:264:C:H6     | 1.81                     | 0.46              |
| 66:D3:84:A:H2'     | 66:D3:85:A:O4'     | 2.15                     | 0.46              |
| 66:D3:417:A:H4'    | 66:D3:418:G:O5'    | 2.14                     | 0.46              |
| 66:D3:1502:G:C2    | 66:D3:1506:G:C6    | 3.04                     | 0.46              |
| 66:D3:1648:A:H2'   | 66:D3:1649:G:C8    | 2.50                     | 0.46              |
| 77:EJ:34:ASN:N     | 77:EJ:104:LYS:O    | 2.48                     | 0.46              |
| 1:CA:253:ILE:HA    | 1:CA:253:ILE:HD13  | 1.77                     | 0.46              |
| 2:DA:23:PRO:O      | 2:DA:27:LYS:HG2    | 2.15                     | 0.46              |
| 2:DA:133:TYR:CZ    | 2:DA:221:PRO:HD2   | 2.51                     | 0.46              |
| 3:JA:195:ASN:HB3   | 3:JA:198:CYS:SG    | 2.56                     | 0.46              |
| 3:JA:755:THR:OG1   | 3:JA:757:GLU:HG2   | 2.15                     | 0.46              |
| 4:UA:792:ILE:HG23  | 4:UA:793:GLU:N     | 2.31                     | 0.46              |
| 1:CB:236:MET:H     | 29:CE:121:LYS:HZ2  | 1.64                     | 0.46              |
| 1:CB:271:ILE:O     | 1:CB:313:HIS:HA    | 2.16                     | 0.46              |
| 7:UD:68:ALA:HB2    | 7:UD:104:TRP:CZ2   | 2.50                     | 0.46              |
| 7:UD:145:TRP:CD1   | 7:UD:161:ASP:HB2   | 2.50                     | 0.46              |
| 7:UD:595:ASN:N     | 7:UD:610:VAL:O     | 2.49                     | 0.46              |
| 7:UD:769:PHE:HD1   | 19:UP:211:LEU:HD12 | 1.79                     | 0.46              |
| 8:UE:120:ILE:HG21  | 8:UE:148:LEU:HD22  | 1.97                     | 0.46              |
| 8:UE:356:TYR:CZ    | 20:UQ:475:SER:HB3  | 2.50                     | 0.46              |
| 9:UF:59:TYR:O      | 9:UF:63:VAL:HG23   | 2.16                     | 0.46              |
| 10:UG:111:PHE:HZ   | 10:UG:149:PHE:CE1  | 2.33                     | 0.46              |
| 10:UG:321:ASN:ND2  | 10:UG:379:GLU:O    | 2.49                     | 0.46              |
| 13:UJ:683:SER:OG   | 13:UJ:684:TYR:N    | 2.49                     | 0.46              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 13:UJ:689:GLU:HA   | 13:UJ:692:ILE:HD12  | 1.96                     | 0.46              |
| 16:UM:14:PRO:HD3   | 16:UM:639:GLY:C     | 2.36                     | 0.46              |
| 16:UM:194:ARG:NE   | 16:UM:216:ARG:HH11  | 2.13                     | 0.46              |
| 16:UM:535:GLY:C    | 16:UM:553:GLY:H     | 2.19                     | 0.46              |
| 18:UO:30:TYR:HD2   | 18:UO:332:LYS:HB2   | 1.79                     | 0.46              |
| 18:UO:493:HIS:CE1  | 18:UO:497:LYS:HE2   | 2.50                     | 0.46              |
| 21:UR:150:TYR:CD2  | 65:D2:313:A:C5      | 3.03                     | 0.46              |
| 23:UT:122:LEU:H    | 23:UT:122:LEU:HD12  | 1.80                     | 0.46              |
| 23:UT:394:LEU:HD11 | 23:UT:435:PHE:CB    | 2.46                     | 0.46              |
| 23:UT:403:LEU:HD12 | 23:UT:404:SER:HB3   | 1.97                     | 0.46              |
| 23:UT:777:GLN:O    | 23:UT:781:VAL:HG13  | 2.15                     | 0.46              |
| 23:UT:1386:GLU:HA  | 23:UT:1389:LYS:HG2  | 1.97                     | 0.46              |
| 23:UT:1654:VAL:O   | 23:UT:1658:LEU:HD23 | 2.15                     | 0.46              |
| 24:UU:86:HIS:N     | 24:UU:89:TYR:O      | 2.48                     | 0.46              |
| 24:UU:378:PHE:HD1  | 24:UU:386:SER:HB2   | 1.80                     | 0.46              |
| 28:CD:321:SER:OG   | 28:CD:322:LEU:N     | 2.49                     | 0.46              |
| 28:CD:392:TYR:CE2  | 30:CG:66:HIS:HB2    | 2.50                     | 0.46              |
| 29:CE:70:SER:HA    | 29:CE:73:GLU:OE2    | 2.15                     | 0.46              |
| 29:CE:295:VAL:O    | 29:CE:299:LEU:HD23  | 2.16                     | 0.46              |
| 30:CG:57:ASP:OD2   | 30:CG:83:SER:HA     | 2.16                     | 0.46              |
| 31:CH:457:GLU:OE1  | 31:CH:460:ARG:NH1   | 2.48                     | 0.46              |
| 35:CL:125:LEU:HD22 | 35:CL:912:ARG:HD3   | 1.98                     | 0.46              |
| 35:CL:833:ARG:CZ   | 35:CL:834:TRP:NE1   | 2.79                     | 0.46              |
| 36:CM:289:VAL:O    | 36:CM:317:GLN:NE2   | 2.44                     | 0.46              |
| 38:JC:4:LYS:HD2    | 38:JC:4:LYS:HA      | 1.75                     | 0.46              |
| 38:JC:53:PHE:HD1   | 38:JC:84:TYR:HE2    | 1.63                     | 0.46              |
| 39:JF:106:LYS:NZ   | 39:JG:230:TYR:HD1   | 2.13                     | 0.46              |
| 47:JP:270:ASN:HD21 | 47:JP:273:GLU:HB2   | 1.80                     | 0.46              |
| 49:DE:10:LYS:HZ3   | 66:D3:381:C:P       | 2.38                     | 0.46              |
| 51:DG:28:PHE:CE1   | 51:DG:102:VAL:HG22  | 2.51                     | 0.46              |
| 51:DG:98:ARG:HH21  | 51:DG:99:GLY:H      | 1.63                     | 0.46              |
| 52:DH:114:ARG:NH1  | 66:D3:860:U:O2      | 2.49                     | 0.46              |
| 62:DY:59:GLY:HA2   | 66:D3:523:G:H5''    | 1.96                     | 0.46              |
| 65:D2:349:G:N2     | 65:D2:350:A:H1'     | 2.30                     | 0.46              |
| 66:D3:1069:A:H2'   | 66:D3:1070:C:C6     | 2.50                     | 0.46              |
| 79:EN:699:ALA:N    | 79:EN:718:ILE:O     | 2.48                     | 0.46              |
| 1:CA:249:GLN:O     | 1:CA:252:ILE:HG22   | 2.15                     | 0.46              |
| 2:DA:161:ILE:HG22  | 2:DA:165:ARG:NH1    | 2.31                     | 0.46              |
| 3:JA:612:ASP:O     | 3:JA:616:TRP:CB     | 2.58                     | 0.46              |
| 1:CB:303:GLN:HA    | 1:CB:315:ILE:O      | 2.16                     | 0.46              |
| 7:UD:757:ARG:HG2   | 7:UD:759:PRO:CD     | 2.44                     | 0.46              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 8:UE:11:ASP:HB3     | 8:UE:65:TRP:CE3    | 2.51                     | 0.46              |
| 9:UF:14:GLU:OE1     | 9:UF:15:MET:HG3    | 2.15                     | 0.46              |
| 11:UH:315:SER:N     | 11:UH:320:LEU:O    | 2.39                     | 0.46              |
| 13:UJ:418:CYS:O     | 13:UJ:421:SER:OG   | 2.23                     | 0.46              |
| 13:UJ:585:ILE:HD13  | 13:UJ:588:LEU:HD12 | 1.97                     | 0.46              |
| 13:UJ:1662:ILE:HA   | 13:UJ:1665:TYR:CD2 | 2.49                     | 0.46              |
| 14:UK:100:LYS:HE3   | 35:CL:1094:TYR:CE1 | 2.50                     | 0.46              |
| 14:UK:249:LYS:HE3   | 30:CF:31:ARG:HH11  | 1.81                     | 0.46              |
| 15:UL:17:ILE:HD11   | 15:UL:388:GLN:HG2  | 1.96                     | 0.46              |
| 15:UL:98:TYR:HB2    | 15:UL:102:VAL:CG2  | 2.45                     | 0.46              |
| 15:UL:189:TRP:CD1   | 15:UL:196:CYS:HA   | 2.51                     | 0.46              |
| 15:UL:212:VAL:HG22  | 15:UL:217:LEU:HD13 | 1.97                     | 0.46              |
| 15:UL:532:ASP:HB3   | 15:UL:550:LEU:HD11 | 1.96                     | 0.46              |
| 16:UM:154:GLY:HA3   | 16:UM:161:TRP:HD1  | 1.81                     | 0.46              |
| 16:UM:456:THR:HG22  | 16:UM:464:LYS:HG2  | 1.97                     | 0.46              |
| 16:UM:585:ASN:ND2   | 16:UM:630:ASP:OD1  | 2.48                     | 0.46              |
| 17:UN:849:PHE:CZ    | 66:D3:-4:A:C5      | 3.03                     | 0.46              |
| 18:UO:65:ILE:O      | 18:UO:74:ILE:HG22  | 2.15                     | 0.46              |
| 18:UO:329:ILE:HG13  | 18:UO:329:ILE:O    | 2.16                     | 0.46              |
| 20:UQ:122:LYS:O     | 20:UQ:122:LYS:HD3  | 2.16                     | 0.46              |
| 21:UR:298:CYS:HA    | 21:UR:313:PHE:O    | 2.16                     | 0.46              |
| 22:US:385:ARG:O     | 22:US:388:LEU:HB3  | 2.15                     | 0.46              |
| 23:UT:125:TYR:O     | 23:UT:129:ILE:HG12 | 2.15                     | 0.46              |
| 23:UT:618:LEU:HD21  | 23:UT:649:PHE:N    | 2.30                     | 0.46              |
| 23:UT:972:LEU:HD22  | 23:UT:997:MET:CE   | 2.46                     | 0.46              |
| 23:UT:977:PHE:O     | 23:UT:980:ASN:C    | 2.54                     | 0.46              |
| 24:UU:499:LYS:NZ    | 50:DF:15:GLU:HB2   | 2.31                     | 0.46              |
| 25:UV:124:VAL:HG11  | 25:UV:290:PHE:CD2  | 2.50                     | 0.46              |
| 25:UV:126:LYS:HG2   | 25:UV:283:TYR:CE1  | 2.50                     | 0.46              |
| 25:UV:162:PHE:HD2   | 25:UV:166:LYS:HZ2  | 1.63                     | 0.46              |
| 25:UV:1169:ILE:HD11 | 25:UV:1178:ASP:HA  | 1.98                     | 0.46              |
| 33:CJ:226:ASN:O     | 33:CJ:227:ARG:HD3  | 2.16                     | 0.46              |
| 33:CJ:229:ASP:HB2   | 33:CJ:288:ASP:OD1  | 2.15                     | 0.46              |
| 35:CL:88:SER:OG     | 35:CL:214:ARG:HA   | 2.16                     | 0.46              |
| 35:CL:124:ASP:CG    | 35:CL:127:ALA:H    | 2.19                     | 0.46              |
| 35:CL:231:LYS:C     | 35:CL:232:PHE:HD2  | 2.19                     | 0.46              |
| 35:CL:800:PHE:HB2   | 35:CL:1022:LEU:CD2 | 2.46                     | 0.46              |
| 38:JC:72:MET:SD     | 38:JC:83:VAL:HG22  | 2.56                     | 0.46              |
| 39:JF:33:SER:HB3    | 39:JF:113:TYR:OH   | 2.16                     | 0.46              |
| 39:JF:91:ILE:HD13   | 39:JF:94:GLN:NE2   | 2.26                     | 0.46              |
| 39:JG:54:LYS:O      | 39:JG:55:ILE:HD13  | 2.16                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 42:JJ:216:ILE:O    | 42:JJ:220:THR:HG22 | 2.15                     | 0.46              |
| 47:JP:270:ASN:HA   | 47:JP:313:PHE:CD2  | 2.49                     | 0.46              |
| 47:JP:276:ASN:HB3  | 47:JP:288:TYR:HE1  | 1.79                     | 0.46              |
| 49:DE:180:LEU:HD13 | 49:DE:231:GLN:HA   | 1.97                     | 0.46              |
| 50:DF:206:SER:O    | 50:DF:212:LYS:NZ   | 2.48                     | 0.46              |
| 51:DG:74:LYS:HD2   | 51:DG:96:SER:HB3   | 1.98                     | 0.46              |
| 52:DH:47:ARG:HD2   | 52:DH:61:PHE:HE2   | 1.80                     | 0.46              |
| 56:DN:14:SER:HB2   | 66:D3:959:U:H5''   | 1.96                     | 0.46              |
| 57:DO:37:GLU:OE1   | 66:D3:895:G:H4'    | 2.16                     | 0.46              |
| 65:D2:292:A:C5     | 65:D2:293:U:N3     | 2.82                     | 0.46              |
| 65:D2:471:C:H2'    | 65:D2:472:A:C8     | 2.51                     | 0.46              |
| 66:D3:647:G:H1     | 66:D3:687:G:N2     | 2.12                     | 0.46              |
| 66:D3:1155:G:C2    | 66:D3:1156:C:C2    | 3.03                     | 0.46              |
| 66:D3:1509:C:H2'   | 66:D3:1510:U:O4'   | 2.16                     | 0.46              |
| 66:D3:1541:G:H22   | 66:D3:1569:A:N6    | 2.14                     | 0.46              |
| 1:CA:228:GLN:HA    | 1:CA:231:ARG:HH11  | 1.80                     | 0.46              |
| 2:DA:212:VAL:HG13  | 2:DA:212:VAL:O     | 2.16                     | 0.46              |
| 3:JA:16:ASN:ND2    | 3:JA:218:PRO:HA    | 2.27                     | 0.46              |
| 3:JA:763:LEU:HD12  | 3:JA:764:ASN:H     | 1.81                     | 0.46              |
| 3:JA:893:LYS:HD2   | 3:JA:898:ILE:HG22  | 1.98                     | 0.46              |
| 1:CB:225:ARG:O     | 1:CB:227:PRO:HD3   | 2.16                     | 0.46              |
| 3:JB:515:LEU:HA    | 3:JB:567:LEU:HA    | 1.96                     | 0.46              |
| 5:UB:519:THR:OG1   | 5:UB:520:PRO:HD3   | 2.15                     | 0.46              |
| 5:UB:604:VAL:HG22  | 5:UB:606:PHE:H     | 1.81                     | 0.46              |
| 5:UB:658:ASN:O     | 5:UB:662:LEU:HG    | 2.15                     | 0.46              |
| 10:UG:150:LEU:HD22 | 10:UG:154:CYS:SG   | 2.56                     | 0.46              |
| 10:UG:318:PRO:O    | 10:UG:334:ARG:HB2  | 2.16                     | 0.46              |
| 11:UH:71:SER:HA    | 11:UH:77:ALA:HA    | 1.97                     | 0.46              |
| 11:UH:185:SER:HA   | 11:UH:201:PHE:HA   | 1.98                     | 0.46              |
| 13:UJ:301:LYS:O    | 13:UJ:301:LYS:HD2  | 2.15                     | 0.46              |
| 16:UM:619:ARG:HD3  | 16:UM:620:LEU:H    | 1.80                     | 0.46              |
| 18:UO:5:ARG:NH2    | 18:UO:393:ASN:HD21 | 2.14                     | 0.46              |
| 18:UO:5:ARG:CA     | 20:UQ:336:ARG:HH22 | 2.20                     | 0.46              |
| 18:UO:368:GLY:HA3  | 21:UR:289:HIS:NE2  | 2.31                     | 0.46              |
| 20:UQ:318:GLU:O    | 20:UQ:320:VAL:HG12 | 2.15                     | 0.46              |
| 20:UQ:875:MET:SD   | 20:UQ:875:MET:N    | 2.88                     | 0.46              |
| 21:UR:216:TYR:OH   | 24:UU:247:PRO:HD2  | 2.15                     | 0.46              |
| 21:UR:237:ARG:HG3  | 21:UR:589:TRP:NE1  | 2.31                     | 0.46              |
| 23:UT:99:ASP:O     | 23:UT:102:SER:OG   | 2.23                     | 0.46              |
| 23:UT:445:LEU:O    | 23:UT:449:ARG:NE   | 2.45                     | 0.46              |
| 23:UT:559:ASN:HA   | 23:UT:562:VAL:HG12 | 1.98                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:UT:1899:LEU:O   | 23:UT:1902:SER:OG  | 2.28                     | 0.46              |
| 24:UU:187:ASN:HA   | 24:UU:205:PHE:HE1  | 1.81                     | 0.46              |
| 25:UV:273:SER:OG   | 25:UV:274:LYS:N    | 2.49                     | 0.46              |
| 25:UV:484:SER:HA   | 25:UV:487:ILE:HG22 | 1.98                     | 0.46              |
| 25:UV:936:LEU:HA   | 25:UV:939:ILE:HG22 | 1.98                     | 0.46              |
| 28:CD:262:ASP:OD1  | 28:CD:263:ILE:N    | 2.48                     | 0.46              |
| 29:CE:48:SER:HB2   | 29:CE:75:LEU:HD11  | 1.96                     | 0.46              |
| 29:CE:313:PRO:O    | 29:CE:316:THR:OG1  | 2.30                     | 0.46              |
| 31:CH:190:VAL:HG12 | 31:CH:196:LEU:HD13 | 1.98                     | 0.46              |
| 35:CL:619:GLU:HG2  | 35:CL:620:LYS:N    | 2.31                     | 0.46              |
| 35:CL:996:LEU:HD11 | 66:D3:1490:C:H4'   | 1.97                     | 0.46              |
| 35:CL:1034:LEU:H   | 35:CL:1037:GLN:NE2 | 2.13                     | 0.46              |
| 37:CN:41:ARG:NH2   | 37:CN:135:ASN:HA   | 2.31                     | 0.46              |
| 38:JC:192:ASN:O    | 38:JC:194:LEU:N    | 2.48                     | 0.46              |
| 46:JO:112:GLN:HB3  | 46:JO:174:MET:HE3  | 1.98                     | 0.46              |
| 47:JP:296:ARG:HH11 | 47:JP:458:LYS:HE2  | 1.80                     | 0.46              |
| 51:DG:27:PHE:CE1   | 51:DG:36:VAL:HG11  | 2.51                     | 0.46              |
| 52:DH:85:PHE:CD1   | 52:DH:88:ARG:HB2   | 2.51                     | 0.46              |
| 52:DH:158:ASP:O    | 52:DH:162:ILE:HG12 | 2.16                     | 0.46              |
| 55:DL:99:ARG:HB3   | 55:DL:99:ARG:NH1   | 2.31                     | 0.46              |
| 62:DY:110:GLN:HB3  | 62:DY:114:ARG:HH12 | 1.81                     | 0.46              |
| 65:D2:101:G:C4     | 65:D2:103:G:C2     | 3.03                     | 0.46              |
| 65:D2:246:G:N2     | 65:D2:268:G:C4     | 2.84                     | 0.46              |
| 65:D2:324:U:H2'    | 65:D2:327:A:H8     | 1.77                     | 0.46              |
| 65:D2:381:G:H5'    | 65:D2:382:U:OP2    | 2.15                     | 0.46              |
| 66:D3:160:C:C4     | 66:D3:161:U:C4     | 3.04                     | 0.46              |
| 66:D3:264:G:H5''   | 66:D3:265:A:H5''   | 1.97                     | 0.46              |
| 66:D3:1689:A:H2'   | 66:D3:1690:G:C8    | 2.51                     | 0.46              |
| 71:ED:298:GLY:N    | 71:ED:331:ILE:O    | 2.39                     | 0.46              |
| 79:EN:153:PHE:O    | 79:EN:157:ALA:N    | 2.49                     | 0.46              |
| 79:EN:864:LYS:O    | 79:EN:868:ARG:N    | 2.38                     | 0.46              |
| 2:DA:149:GLN:CD    | 66:D3:1066:C:H4'   | 2.36                     | 0.46              |
| 3:JA:12:SER:HB2    | 3:JA:218:PRO:HB3   | 1.96                     | 0.46              |
| 3:JA:73:ARG:O      | 3:JA:77:ILE:HG22   | 2.16                     | 0.46              |
| 3:JA:113:LYS:NZ    | 66:D3:417:A:OP2    | 2.41                     | 0.46              |
| 3:JA:114:ILE:O     | 3:JA:114:ILE:HG22  | 2.15                     | 0.46              |
| 4:UA:593:VAL:HG12  | 4:UA:603:LEU:HD13  | 1.97                     | 0.46              |
| 1:CB:230:TYR:CD1   | 1:CB:234:ILE:HD12  | 2.47                     | 0.46              |
| 5:UB:396:LEU:O     | 5:UB:399:HIS:N     | 2.48                     | 0.46              |
| 5:UB:548:ARG:CZ    | 5:UB:642:SER:HB3   | 2.45                     | 0.46              |
| 5:UB:717:TYR:OH    | 39:JG:136:ARG:HD3  | 2.15                     | 0.46              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 7:UD:119:GLY:HA3   | 19:UP:194:LYS:HB2   | 1.96                     | 0.46              |
| 7:UD:242:TRP:CD1   | 7:UD:282:ASP:HB2    | 2.51                     | 0.46              |
| 7:UD:423:LYS:HE2   | 19:UP:167:ARG:HD3   | 1.98                     | 0.46              |
| 7:UD:545:ARG:HB3   | 7:UD:549:VAL:CG1    | 2.46                     | 0.46              |
| 8:UE:514:VAL:CG1   | 18:UO:511:LEU:HD12  | 2.45                     | 0.46              |
| 9:UF:92:ILE:HG21   | 9:UF:116:TYR:CE1    | 2.51                     | 0.46              |
| 10:UG:143:GLN:NE2  | 65:D2:472:A:OP1     | 2.49                     | 0.46              |
| 10:UG:217:HIS:ND1  | 10:UG:218:ASP:O     | 2.47                     | 0.46              |
| 13:UJ:308:GLY:N    | 13:UJ:311:ASN:OD1   | 2.48                     | 0.46              |
| 14:UK:12:GLN:HG3   | 14:UK:12:GLN:O      | 2.16                     | 0.46              |
| 15:UL:901:ASN:HD21 | 16:UM:761:ARG:CA    | 2.29                     | 0.46              |
| 16:UM:532:HIS:CE1  | 16:UM:558:LYS:HE2   | 2.51                     | 0.46              |
| 17:UN:298:TRP:O    | 17:UN:301:ILE:HG22  | 2.15                     | 0.46              |
| 17:UN:306:ARG:HH12 | 66:D3:-5:G:P        | 2.33                     | 0.46              |
| 17:UN:306:ARG:HH22 | 66:D3:-5:G:P        | 2.38                     | 0.46              |
| 17:UN:835:VAL:HG12 | 65:D2:376:U:OP1     | 2.16                     | 0.46              |
| 17:UN:842:TYR:O    | 47:JP:407:MET:HE1   | 2.15                     | 0.46              |
| 18:UO:63:VAL:HG23  | 18:UO:80:PHE:HE2    | 1.81                     | 0.46              |
| 18:UO:227:VAL:CG1  | 18:UO:258:LEU:HD21  | 2.46                     | 0.46              |
| 18:UO:454:ARG:NH1  | 65:D2:102:A:C6      | 2.82                     | 0.46              |
| 20:UQ:433:ARG:HE   | 65:D2:4:C:P         | 2.39                     | 0.46              |
| 20:UQ:769:ASN:OD1  | 20:UQ:770:TYR:N     | 2.48                     | 0.46              |
| 21:UR:15:PRO:HB2   | 21:UR:20:GLN:NE2    | 2.31                     | 0.46              |
| 21:UR:181:GLU:HG2  | 21:UR:182:SER:N     | 2.30                     | 0.46              |
| 21:UR:520:ASN:ND2  | 21:UR:567:SER:HA    | 2.30                     | 0.46              |
| 22:US:274:TYR:O    | 22:US:278:LEU:HD23  | 2.15                     | 0.46              |
| 22:US:426:PHE:CZ   | 39:JG:250:ASN:HB3   | 2.50                     | 0.46              |
| 23:UT:145:SER:HA   | 23:UT:148:PHE:HD1   | 1.78                     | 0.46              |
| 23:UT:414:LEU:HD21 | 23:UT:447:LYS:HB3   | 1.98                     | 0.46              |
| 23:UT:1143:LYS:NZ  | 23:UT:1146:VAL:HG23 | 2.30                     | 0.46              |
| 25:UV:808:LEU:HA   | 25:UV:825:PHE:HZ    | 1.81                     | 0.46              |
| 29:CE:339:TYR:CE1  | 29:CE:357:GLY:HA2   | 2.49                     | 0.46              |
| 29:CE:427:TYR:CG   | 29:CE:428:ASN:N     | 2.84                     | 0.46              |
| 30:CG:94:SER:O     | 30:CG:95:ARG:NE     | 2.49                     | 0.46              |
| 31:CH:245:SER:OG   | 31:CH:247:ASP:OD1   | 2.22                     | 0.46              |
| 31:CH:419:ASN:HD21 | 31:CH:421:ASN:ND2   | 2.13                     | 0.46              |
| 34:CK:474:ILE:HG23 | 34:CK:485:SER:O     | 2.14                     | 0.46              |
| 35:CL:1024:LYS:HG3 | 35:CL:1025:GLU:N    | 2.30                     | 0.46              |
| 36:CM:271:LEU:O    | 36:CM:274:LYS:HB3   | 2.15                     | 0.46              |
| 36:CM:291:ARG:HA   | 36:CM:294:LEU:HG    | 1.97                     | 0.46              |
| 39:JF:64:LYS:HD2   | 39:JF:64:LYS:HA     | 1.78                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:JG:179:THR:OG1  | 39:JG:221:VAL:HG11 | 2.15                     | 0.46              |
| 42:JJ:256:PRO:O    | 42:JJ:260:TYR:HD1  | 1.99                     | 0.46              |
| 47:JP:311:VAL:HG23 | 47:JP:322:THR:HG22 | 1.97                     | 0.46              |
| 49:DE:59:ARG:HH11  | 49:DE:59:ARG:HG3   | 1.81                     | 0.46              |
| 50:DF:46:TRP:CE2   | 50:DF:129:PRO:HG3  | 2.51                     | 0.46              |
| 52:DH:5:GLN:NE2    | 52:DH:21:ALA:HB3   | 2.30                     | 0.46              |
| 52:DH:166:LEU:HD12 | 52:DH:183:PHE:CB   | 2.45                     | 0.46              |
| 53:DI:52:ASN:OD1   | 53:DI:53:LYS:N     | 2.49                     | 0.46              |
| 56:DN:121:ARG:HH22 | 66:D3:868:G:P      | 2.39                     | 0.46              |
| 58:DQ:66:ARG:NH1   | 58:DQ:68:ARG:HH21  | 2.14                     | 0.46              |
| 60:DW:76:SER:HB3   | 60:DW:77:PRO:HD3   | 1.98                     | 0.46              |
| 61:DX:104:LEU:HD23 | 61:DX:124:VAL:HA   | 1.97                     | 0.46              |
| 62:DY:93:ARG:HH21  | 66:D3:526:A:P      | 2.34                     | 0.46              |
| 65:D2:360:C:H2'    | 65:D2:361:G:H8     | 1.80                     | 0.46              |
| 66:D3:550:A:C6     | 66:D3:551:G:C8     | 3.04                     | 0.46              |
| 66:D3:885:G:O5'    | 66:D3:885:G:H8     | 1.99                     | 0.46              |
| 66:D3:1038:U:O2'   | 66:D3:1039:A:O4'   | 2.34                     | 0.46              |
| 66:D3:1150:G:H2'   | 66:D3:1151:A:C8    | 2.51                     | 0.46              |
| 67:D4:67:G:H2'     | 67:D4:68:A:C8      | 2.49                     | 0.46              |
| 67:D4:256:G:H2'    | 67:D4:256:G:OP2    | 2.16                     | 0.46              |
| 71:ED:387:ASP:O    | 71:ED:391:ARG:N    | 2.49                     | 0.46              |
| 75:EH:231:PHE:O    | 75:EH:235:LEU:N    | 2.35                     | 0.46              |
| 1:CA:228:GLN:HB3   | 28:CD:102:ASP:OD1  | 2.16                     | 0.46              |
| 4:UA:331:GLU:OE2   | 4:UA:333:GLN:HB2   | 2.16                     | 0.46              |
| 4:UA:520:ALA:HB3   | 4:UA:533:SER:HB3   | 1.97                     | 0.46              |
| 1:CB:145:ASN:ND2   | 1:CB:148:ARG:HG2   | 2.30                     | 0.46              |
| 1:CB:202:ARG:HA    | 1:CB:205:ARG:HE    | 1.79                     | 0.46              |
| 1:CB:294:ARG:HE    | 19:UP:181:LEU:CD2  | 2.29                     | 0.46              |
| 5:UB:512:ASP:OD1   | 5:UB:512:ASP:N     | 2.48                     | 0.46              |
| 5:UB:548:ARG:O     | 5:UB:551:SER:OG    | 2.26                     | 0.46              |
| 7:UD:625:GLU:O     | 7:UD:629:LEU:HG    | 2.16                     | 0.46              |
| 8:UE:10:TYR:HB3    | 8:UE:14:GLY:HA2    | 1.98                     | 0.46              |
| 8:UE:79:GLY:HA2    | 8:UE:85:ILE:HD13   | 1.98                     | 0.46              |
| 10:UG:227:GLU:C    | 10:UG:228:LEU:HD12 | 2.35                     | 0.46              |
| 10:UG:274:ARG:HG2  | 65:D2:322:A:C2     | 2.51                     | 0.46              |
| 12:UI:454:LEU:HA   | 12:UI:457:LYS:HG2  | 1.97                     | 0.46              |
| 13:UJ:25:ARG:HH11  | 47:JP:16:VAL:HA    | 1.81                     | 0.46              |
| 13:UJ:68:ILE:O     | 13:UJ:71:ARG:HB3   | 2.16                     | 0.46              |
| 13:UJ:87:THR:O     | 13:UJ:91:ILE:HG12  | 2.15                     | 0.46              |
| 13:UJ:98:ILE:HD13  | 13:UJ:131:ASN:HD22 | 1.81                     | 0.46              |
| 13:UJ:729:LYS:O    | 13:UJ:732:PHE:N    | 2.47                     | 0.46              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 13:UJ:801:ILE:O    | 13:UJ:805:ILE:HG12  | 2.15                     | 0.46              |
| 13:UJ:1352:LEU:HA  | 13:UJ:1355:ILE:HG12 | 1.96                     | 0.46              |
| 13:UJ:1501:PHE:HA  | 13:UJ:1504:LEU:HG   | 1.98                     | 0.46              |
| 14:UK:11:LYS:HD3   | 14:UK:13:HIS:HD2    | 1.81                     | 0.46              |
| 15:UL:339:LYS:HD2  | 15:UL:339:LYS:HA    | 1.72                     | 0.46              |
| 15:UL:874:GLU:OE1  | 15:UL:874:GLU:N     | 2.48                     | 0.46              |
| 16:UM:111:ASP:HB2  | 16:UM:116:LEU:HG    | 1.97                     | 0.46              |
| 16:UM:403:ILE:CG1  | 16:UM:415:TRP:HB2   | 2.45                     | 0.46              |
| 18:UO:438:THR:O    | 18:UO:441:PRO:HD2   | 2.16                     | 0.46              |
| 21:UR:237:ARG:O    | 21:UR:238:LEU:HD12  | 2.16                     | 0.46              |
| 23:UT:431:LYS:HZ1  | 23:UT:750:TYR:HB3   | 1.81                     | 0.46              |
| 23:UT:1653:ALA:O   | 23:UT:1657:THR:HG23 | 2.16                     | 0.46              |
| 24:UU:53:CYS:SG    | 24:UU:80:ILE:HB     | 2.56                     | 0.46              |
| 24:UU:125:GLY:HA3  | 29:CE:433:THR:CB    | 2.46                     | 0.46              |
| 24:UU:373:ARG:HB3  | 24:UU:411:PHE:O     | 2.15                     | 0.46              |
| 25:UV:1102:LEU:N   | 25:UV:1103:ARG:HH21 | 2.13                     | 0.46              |
| 29:CE:431:ALA:HB3  | 65:D2:309:A:N6      | 2.31                     | 0.46              |
| 33:CJ:55:ASP:O     | 33:CJ:57:ARG:N      | 2.42                     | 0.46              |
| 33:CJ:87:ARG:N     | 33:CJ:137:THR:OG1   | 2.49                     | 0.46              |
| 33:CJ:187:PRO:HB3  | 33:CJ:220:ARG:HE    | 1.81                     | 0.46              |
| 33:CJ:189:LEU:HD23 | 33:CJ:191:PHE:HZ    | 1.79                     | 0.46              |
| 35:CL:304:LEU:O    | 35:CL:788:TYR:CB    | 2.63                     | 0.46              |
| 35:CL:565:ARG:HD2  | 35:CL:566:ARG:N     | 2.31                     | 0.46              |
| 36:CM:155:LYS:HG2  | 36:CM:165:GLU:HG2   | 1.98                     | 0.46              |
| 37:CN:87:LEU:HD11  | 37:CN:124:ALA:HB1   | 1.98                     | 0.46              |
| 42:JJ:187:VAL:HG22 | 42:JJ:229:SER:OG    | 2.16                     | 0.46              |
| 46:JO:74:ASP:HB3   | 46:JO:79:SER:OG     | 2.15                     | 0.46              |
| 47:JP:147:LEU:C    | 47:JP:148:TRP:CD1   | 2.88                     | 0.46              |
| 49:DE:240:LYS:HD2  | 49:DE:240:LYS:HA    | 1.75                     | 0.46              |
| 62:DY:112:LYS:HD2  | 66:D3:57:G:OP1      | 2.16                     | 0.46              |
| 65:D2:107:G:H2'    | 65:D2:108:U:O4'     | 2.15                     | 0.46              |
| 65:D2:243:A:C4     | 65:D2:271:G:N2      | 2.84                     | 0.46              |
| 66:D3:188:A:H3'    | 66:D3:189:C:C6      | 2.51                     | 0.46              |
| 66:D3:326:G:O6     | 66:D3:341:A:N6      | 2.49                     | 0.46              |
| 66:D3:339:C:H2'    | 66:D3:340:U:O4'     | 2.16                     | 0.46              |
| 66:D3:849:C:H2'    | 66:D3:850:A:H8      | 1.80                     | 0.46              |
| 78:EK:368:LYS:O    | 78:EK:372:LEU:N     | 2.37                     | 0.46              |
| 1:CB:121:LYS:H     | 14:UK:123:LYS:NZ    | 2.14                     | 0.46              |
| 9:UF:96:TYR:CD1    | 9:UF:113:TYR:HB2    | 2.51                     | 0.46              |
| 9:UF:172:LEU:HD22  | 9:UF:181:LEU:HD21   | 1.98                     | 0.46              |
| 11:UH:522:THR:O    | 11:UH:526:LEU:HD23  | 2.15                     | 0.46              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 13:UJ:716:PHE:O    | 13:UJ:720:LEU:HG    | 2.15                     | 0.46              |
| 15:UL:14:PHE:CE2   | 15:UL:422:HIS:HB3   | 2.51                     | 0.46              |
| 15:UL:88:HIS:CD2   | 15:UL:90:ASP:HB2    | 2.51                     | 0.46              |
| 15:UL:105:VAL:O    | 15:UL:113:VAL:HA    | 2.16                     | 0.46              |
| 15:UL:252:SER:OG   | 15:UL:276:ASN:OD1   | 2.31                     | 0.46              |
| 15:UL:365:TYR:HD2  | 15:UL:379:PRO:HB2   | 1.81                     | 0.46              |
| 15:UL:678:ASP:N    | 15:UL:678:ASP:OD1   | 2.48                     | 0.46              |
| 15:UL:920:PHE:H    | 15:UL:926:GLN:CD    | 2.19                     | 0.46              |
| 16:UM:38:ASP:HB2   | 16:UM:62:GLN:NE2    | 2.31                     | 0.46              |
| 16:UM:78:TYR:CE1   | 16:UM:86:LYS:HB2    | 2.51                     | 0.46              |
| 18:UO:379:VAL:HG11 | 65:D2:89:C:C4       | 2.50                     | 0.46              |
| 20:UQ:515:PRO:HB2  | 20:UQ:522:SER:HA    | 1.97                     | 0.46              |
| 20:UQ:586:SER:OG   | 20:UQ:587:PHE:N     | 2.49                     | 0.46              |
| 22:US:470:MET:CE   | 22:US:485:ALA:HB2   | 2.43                     | 0.46              |
| 23:UT:37:ARG:O     | 23:UT:41:TYR:HB2    | 2.15                     | 0.46              |
| 23:UT:464:PHE:CD2  | 23:UT:482:ARG:HG2   | 2.51                     | 0.46              |
| 23:UT:1288:PHE:HB3 | 23:UT:1301:ILE:HG23 | 1.98                     | 0.46              |
| 24:UU:841:SER:O    | 24:UU:845:VAL:HG23  | 2.16                     | 0.46              |
| 25:UV:125:GLU:HA   | 25:UV:128:LEU:HG    | 1.97                     | 0.46              |
| 25:UV:909:TYR:OH   | 25:UV:935:GLU:HB2   | 2.16                     | 0.46              |
| 25:UV:1138:ASP:HA  | 25:UV:1141:GLU:CD   | 2.36                     | 0.46              |
| 27:UZ:75:ILE:HB    | 27:UZ:127:ALA:HB2   | 1.97                     | 0.46              |
| 27:UZ:194:ASP:OD1  | 27:UZ:195:ASN:N     | 2.47                     | 0.46              |
| 28:CD:176:GLN:HB3  | 29:CE:187:TRP:HE1   | 1.81                     | 0.46              |
| 29:CE:7:GLU:OE1    | 29:CE:12:TYR:HD1    | 1.98                     | 0.46              |
| 29:CE:229:GLU:O    | 29:CE:232:GLU:HG3   | 2.16                     | 0.46              |
| 31:CH:288:PHE:HE1  | 31:CH:309:ILE:HG13  | 1.79                     | 0.46              |
| 32:CI:42:GLU:HG3   | 32:CI:46:LYS:HE3    | 1.98                     | 0.46              |
| 35:CL:866:ARG:N    | 35:CL:866:ARG:HD2   | 2.31                     | 0.46              |
| 37:CN:14:ILE:HG23  | 37:CN:145:SER:HB3   | 1.96                     | 0.46              |
| 39:JF:115:GLN:NE2  | 39:JF:119:GLY:HA2   | 2.30                     | 0.46              |
| 39:JF:193:ILE:O    | 39:JF:196:LEU:HB2   | 2.16                     | 0.46              |
| 46:JO:288:GLN:HG3  | 66:D3:316:A:H62     | 1.79                     | 0.46              |
| 50:DF:66:GLN:OE1   | 50:DF:67:PRO:HD2    | 2.16                     | 0.46              |
| 52:DH:129:LEU:HG   | 52:DH:169:PHE:CE1   | 2.51                     | 0.46              |
| 56:DN:102:LEU:O    | 56:DN:105:ASN:C     | 2.54                     | 0.46              |
| 61:DX:42:PRO:HD2   | 61:DX:44:GLY:O      | 2.15                     | 0.46              |
| 62:DY:105:ARG:NH2  | 62:DY:109:LYS:HD2   | 2.31                     | 0.46              |
| 65:D2:411:A:H2'    | 65:D2:412:A:C8      | 2.51                     | 0.46              |
| 66:D3:395:U:C4     | 66:D3:396:G:C6      | 3.04                     | 0.46              |
| 66:D3:514:G:C2     | 66:D3:515:A:C5      | 3.04                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 66:D3:1167:G:H2'   | 66:D3:1167:G:N3    | 2.30                     | 0.46              |
| 66:D3:1213:G:N1    | 66:D3:1451:C:N3    | 2.63                     | 0.46              |
| 78:EK:771:ASN:O    | 78:EK:775:ASN:HA   | 2.16                     | 0.46              |
| 1:CA:224:ALA:O     | 1:CA:252:ILE:HD11  | 2.16                     | 0.46              |
| 2:DA:77:GLU:HA     | 2:DA:80:SER:HB3    | 1.98                     | 0.46              |
| 3:JA:536:LYS:HD2   | 3:JA:536:LYS:HA    | 1.72                     | 0.46              |
| 4:UA:32:PRO:HB3    | 4:UA:61:ILE:HD11   | 1.97                     | 0.46              |
| 4:UA:358:SER:O     | 4:UA:374:ILE:HG12  | 2.16                     | 0.46              |
| 5:UB:482:GLN:HB2   | 5:UB:486:LYS:HZ1   | 1.80                     | 0.46              |
| 5:UB:521:ALA:O     | 5:UB:525:MET:HG2   | 2.16                     | 0.46              |
| 5:UB:799:TYR:O     | 5:UB:802:GLU:HB2   | 2.16                     | 0.46              |
| 6:UC:609:LYS:HD3   | 6:UC:609:LYS:HA    | 1.53                     | 0.46              |
| 7:UD:52:SER:OG     | 7:UD:65:LEU:HA     | 2.16                     | 0.46              |
| 8:UE:343:ARG:HA    | 8:UE:349:ASP:HA    | 1.98                     | 0.46              |
| 12:UI:442:THR:HB   | 12:UI:482:LEU:HB3  | 1.98                     | 0.46              |
| 13:UJ:126:GLN:HB3  | 13:UJ:129:VAL:HG22 | 1.98                     | 0.46              |
| 13:UJ:339:GLU:OE1  | 13:UJ:339:GLU:N    | 2.49                     | 0.46              |
| 13:UJ:605:TYR:CZ   | 13:UJ:660:LEU:HG   | 2.51                     | 0.46              |
| 13:UJ:768:LYS:HB2  | 13:UJ:768:LYS:HE2  | 1.72                     | 0.46              |
| 16:UM:351:ASN:O    | 16:UM:367:VAL:HG12 | 2.16                     | 0.46              |
| 16:UM:584:ILE:HG23 | 16:UM:586:LYS:N    | 2.31                     | 0.46              |
| 18:UO:479:VAL:O    | 18:UO:482:GLU:HG3  | 2.15                     | 0.46              |
| 20:UQ:139:GLU:HB2  | 20:UQ:157:PHE:HB2  | 1.97                     | 0.46              |
| 20:UQ:200:ASN:ND2  | 20:UQ:262:MET:HB3  | 2.31                     | 0.46              |
| 20:UQ:510:TYR:CE1  | 20:UQ:527:HIS:HB3  | 2.49                     | 0.46              |
| 22:US:175:LEU:O    | 22:US:179:GLU:HG3  | 2.16                     | 0.46              |
| 22:US:198:GLU:HA   | 22:US:201:GLN:OE1  | 2.16                     | 0.46              |
| 22:US:227:LYS:O    | 22:US:227:LYS:HG2  | 2.16                     | 0.46              |
| 22:US:347:PRO:O    | 22:US:351:HIS:ND1  | 2.28                     | 0.46              |
| 22:US:414:ILE:CD1  | 39:JG:19:LEU:HD23  | 2.46                     | 0.46              |
| 23:UT:536:ASN:OD1  | 23:UT:537:LEU:N    | 2.49                     | 0.46              |
| 23:UT:689:TYR:CE1  | 23:UT:696:VAL:HG21 | 2.51                     | 0.46              |
| 23:UT:944:SER:O    | 23:UT:947:ILE:HG22 | 2.16                     | 0.46              |
| 23:UT:1067:GLU:HA  | 23:UT:1111:TYR:CE2 | 2.51                     | 0.46              |
| 23:UT:1930:SER:O   | 23:UT:1934:PHE:HD2 | 1.99                     | 0.46              |
| 24:UU:546:ILE:HG21 | 24:UU:560:LEU:HD22 | 1.97                     | 0.46              |
| 25:UV:648:PHE:O    | 25:UV:689:HIS:NE2  | 2.44                     | 0.46              |
| 25:UV:781:ASP:HA   | 25:UV:851:LYS:HG3  | 1.98                     | 0.46              |
| 25:UV:939:ILE:O    | 25:UV:943:VAL:HG23 | 2.16                     | 0.46              |
| 26:UX:152:ILE:HD11 | 26:UX:182:ILE:HD12 | 1.97                     | 0.46              |
| 27:UZ:129:TYR:CE1  | 27:UZ:155:ARG:HG3  | 2.50                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:CD:138:LEU:HD23 | 28:CD:138:LEU:HA   | 1.83                     | 0.46              |
| 28:CD:284:TYR:HE1  | 29:CE:257:ALA:HB1  | 1.80                     | 0.46              |
| 29:CE:144:ALA:HA   | 29:CE:147:ILE:HG22 | 1.97                     | 0.46              |
| 31:CH:443:LEU:HB3  | 31:CH:471:GLN:HE21 | 1.80                     | 0.46              |
| 33:CJ:223:THR:O    | 33:CJ:233:VAL:HA   | 2.15                     | 0.46              |
| 35:CL:69:PRO:HB2   | 35:CL:116:THR:HG23 | 1.98                     | 0.46              |
| 35:CL:150:MET:O    | 35:CL:154:GLU:HG3  | 2.16                     | 0.46              |
| 37:CN:77:LYS:HE2   | 37:CN:147:LEU:HD22 | 1.97                     | 0.46              |
| 38:JC:49:LEU:HD12  | 38:JC:356:LEU:HD11 | 1.98                     | 0.46              |
| 38:JC:143:SER:O    | 38:JC:155:VAL:HA   | 2.16                     | 0.46              |
| 38:JC:165:LEU:HD21 | 38:JC:170:GLY:HA2  | 1.97                     | 0.46              |
| 43:JK:460:LYS:O    | 66:D3:321:C:H3'    | 2.16                     | 0.46              |
| 43:JK:486:SER:H    | 43:JK:489:GLN:HE22 | 1.63                     | 0.46              |
| 46:JO:192:LYS:HE2  | 46:JO:192:LYS:HA   | 1.97                     | 0.46              |
| 47:JP:218:GLY:O    | 47:JP:220:ASP:N    | 2.45                     | 0.46              |
| 47:JP:296:ARG:HH22 | 66:D3:-3:U:C1'     | 2.28                     | 0.46              |
| 50:DF:200:ASN:HA   | 50:DF:203:LYS:HZ3  | 1.81                     | 0.46              |
| 56:DN:46:THR:HG23  | 56:DN:49:GLN:H     | 1.80                     | 0.46              |
| 61:DX:64:PRO:HA    | 61:DX:69:ARG:NH2   | 2.31                     | 0.46              |
| 61:DX:74:VAL:HG21  | 61:DX:104:LEU:CD1  | 2.45                     | 0.46              |
| 62:DY:19:ALA:HB1   | 62:DY:77:ASN:ND2   | 2.31                     | 0.46              |
| 62:DY:56:SER:N     | 62:DY:74:LEU:O     | 2.32                     | 0.46              |
| 65:D2:132:C:H2'    | 65:D2:133:U:H6     | 1.80                     | 0.46              |
| 66:D3:527:A:H2'    | 66:D3:528:U:H6     | 1.80                     | 0.46              |
| 66:D3:883:C:C2     | 66:D3:946:U:N3     | 2.85                     | 0.46              |
| 66:D3:1158:C:N4    | 66:D3:1581:C:N3    | 2.64                     | 0.46              |
| 66:D3:1168:U:C5    | 66:D3:1169:G:C5    | 3.04                     | 0.46              |
| 66:D3:1728:A:H2'   | 66:D3:1729:C:C6    | 2.51                     | 0.46              |
| 78:EK:328:ALA:N    | 78:EK:386:ILE:HA   | 2.31                     | 0.46              |
| 3:JA:57:TRP:HB2    | 3:JA:103:ILE:HD11  | 1.98                     | 0.45              |
| 3:JA:88:VAL:O      | 3:JA:89:ASN:ND2    | 2.49                     | 0.45              |
| 3:JA:585:VAL:HG13  | 3:JA:639:ALA:HB3   | 1.98                     | 0.45              |
| 3:JA:748:ARG:NE    | 3:JA:759:THR:HG22  | 2.30                     | 0.45              |
| 3:JA:753:ASP:OD1   | 3:JA:754:LEU:N     | 2.49                     | 0.45              |
| 3:JA:906:SER:HB3   | 3:JA:908:GLN:NE2   | 2.31                     | 0.45              |
| 4:UA:426:THR:O     | 4:UA:458:TRP:NE1   | 2.49                     | 0.45              |
| 4:UA:810:ILE:CD1   | 24:UU:936:VAL:HG11 | 2.46                     | 0.45              |
| 4:UA:842:ASN:ND2   | 24:UU:882:GLU:O    | 2.41                     | 0.45              |
| 5:UB:460:LYS:O     | 5:UB:464:GLU:OE1   | 2.34                     | 0.45              |
| 5:UB:502:SER:O     | 5:UB:506:ILE:HG12  | 2.16                     | 0.45              |
| 5:UB:520:PRO:HA    | 5:UB:523:ILE:HG12  | 1.98                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:UD:30:ARG:HD2    | 11:UH:720:TYR:CE1  | 2.51                     | 0.45              |
| 7:UD:241:VAL:HG23  | 7:UD:241:VAL:O     | 2.16                     | 0.45              |
| 7:UD:654:ILE:HB    | 7:UD:735:THR:HG22  | 1.97                     | 0.45              |
| 8:UE:4:PRO:HB3     | 21:UR:278:ASP:OD2  | 2.16                     | 0.45              |
| 8:UE:441:LEU:HD12  | 8:UE:442:SER:N     | 2.30                     | 0.45              |
| 9:UF:23:LEU:HG     | 9:UF:24:PHE:CD1    | 2.50                     | 0.45              |
| 10:UG:179:HIS:CD2  | 10:UG:180:GLU:HB2  | 2.51                     | 0.45              |
| 10:UG:334:ARG:HH22 | 10:UG:337:HIS:CD2  | 2.34                     | 0.45              |
| 10:UG:493:LYS:HE3  | 65:D2:357:G:N7     | 2.32                     | 0.45              |
| 10:UG:543:LYS:HZ1  | 10:UG:544:ASP:H    | 1.62                     | 0.45              |
| 13:UJ:59:LEU:HB3   | 13:UJ:66:PHE:CE2   | 2.51                     | 0.45              |
| 13:UJ:317:SER:OG   | 13:UJ:321:LYS:NZ   | 2.24                     | 0.45              |
| 14:UK:11:LYS:HD3   | 14:UK:13:HIS:CD2   | 2.50                     | 0.45              |
| 15:UL:260:GLU:OE2  | 15:UL:342:SER:HA   | 2.15                     | 0.45              |
| 17:UN:876:GLN:HE22 | 65:D2:487:A:H2     | 1.63                     | 0.45              |
| 18:UO:364:SER:O    | 21:UR:270:LYS:NZ   | 2.49                     | 0.45              |
| 18:UO:493:HIS:O    | 18:UO:497:LYS:HG2  | 2.17                     | 0.45              |
| 20:UQ:252:LEU:O    | 20:UQ:257:ARG:NH1  | 2.34                     | 0.45              |
| 20:UQ:443:ASN:HA   | 20:UQ:500:PHE:CD2  | 2.51                     | 0.45              |
| 20:UQ:658:GLU:OE1  | 20:UQ:658:GLU:N    | 2.42                     | 0.45              |
| 21:UR:396:MET:HE3  | 21:UR:440:ASN:OD1  | 2.16                     | 0.45              |
| 22:US:179:GLU:HA   | 22:US:182:GLU:HG3  | 1.98                     | 0.45              |
| 22:US:260:ASN:O    | 22:US:263:SER:OG   | 2.29                     | 0.45              |
| 23:UT:625:ILE:HD11 | 23:UT:641:ARG:CB   | 2.46                     | 0.45              |
| 23:UT:905:LEU:HG   | 23:UT:956:PHE:CE1  | 2.50                     | 0.45              |
| 23:UT:1668:GLU:HG2 | 23:UT:1669:TYR:N   | 2.31                     | 0.45              |
| 24:UU:583:GLY:HA3  | 24:UU:610:ARG:NH1  | 2.28                     | 0.45              |
| 25:UV:813:GLU:OE1  | 25:UV:814:LEU:HD22 | 2.16                     | 0.45              |
| 25:UV:945:PRO:HB3  | 25:UV:950:ILE:HA   | 1.96                     | 0.45              |
| 26:UX:159:GLY:O    | 26:UX:163:ARG:HG3  | 2.17                     | 0.45              |
| 27:UZ:174:ILE:HD12 | 27:UZ:174:ILE:H    | 1.81                     | 0.45              |
| 29:CE:192:PHE:CD2  | 29:CE:195:LEU:HB2  | 2.51                     | 0.45              |
| 31:CH:131:ARG:N    | 31:CH:131:ARG:HD2  | 2.31                     | 0.45              |
| 31:CH:363:ASP:N    | 31:CH:363:ASP:OD1  | 2.46                     | 0.45              |
| 35:CL:85:LEU:HD12  | 35:CL:215:TYR:HE2  | 1.79                     | 0.45              |
| 35:CL:199:TYR:CE2  | 66:D3:436:A:C8     | 3.05                     | 0.45              |
| 35:CL:272:TYR:CE2  | 35:CL:790:ARG:HD3  | 2.52                     | 0.45              |
| 38:JC:102:VAL:CG2  | 38:JC:119:ASN:HB3  | 2.46                     | 0.45              |
| 38:JC:257:LEU:HG   | 43:JK:493:PHE:HE2  | 1.82                     | 0.45              |
| 46:JO:274:ARG:O    | 46:JO:277:GLN:HG3  | 2.16                     | 0.45              |
| 49:DE:42:LEU:CD2   | 49:DE:47:PHE:HB2   | 2.46                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 49:DE:60:GLU:OE1   | 62:DY:18:LEU:HD11  | 2.15                     | 0.45              |
| 51:DG:64:LYS:HB3   | 51:DG:67:VAL:HG12  | 1.98                     | 0.45              |
| 53:DI:172:ARG:HH21 | 53:DI:175:GLN:NE2  | 2.14                     | 0.45              |
| 62:DY:125:LEU:O    | 62:DY:128:LYS:HG3  | 2.15                     | 0.45              |
| 65:D2:243:A:C2     | 65:D2:244:U:C2     | 3.04                     | 0.45              |
| 66:D3:70:C:H2'     | 66:D3:71:A:C8      | 2.51                     | 0.45              |
| 66:D3:448:C:H2'    | 66:D3:449:C:C6     | 2.50                     | 0.45              |
| 66:D3:502:U:H2'    | 66:D3:503:G:C8     | 2.37                     | 0.45              |
| 66:D3:648:G:C2     | 66:D3:687:G:C2     | 3.04                     | 0.45              |
| 66:D3:762:A:N1     | 66:D3:787:G:N2     | 2.64                     | 0.45              |
| 66:D3:870:C:H2'    | 66:D3:871:G:C8     | 2.48                     | 0.45              |
| 66:D3:1613:U:C6    | 66:D3:1614:A:H2    | 2.34                     | 0.45              |
| 66:D3:1787:C:N4    | 66:D3:1788:G:O6    | 2.49                     | 0.45              |
| 67:D4:64:A:C2      | 67:D4:65:C:C2      | 3.04                     | 0.45              |
| 67:D4:266:C:N3     | 67:D4:306:G:N1     | 2.63                     | 0.45              |
| 71:ED:297:TYR:N    | 71:ED:347:ILE:O    | 2.49                     | 0.45              |
| 79:EN:445:ASN:O    | 79:EN:449:ALA:N    | 2.50                     | 0.45              |
| 1:CA:107:VAL:HG11  | 1:CA:141:TYR:HB3   | 1.97                     | 0.45              |
| 1:CA:171:LEU:HB3   | 1:CA:240:VAL:HG12  | 1.99                     | 0.45              |
| 2:DA:66:VAL:HG12   | 2:DA:67:GLU:O      | 2.15                     | 0.45              |
| 2:DA:139:ALA:HA    | 2:DA:211:HIS:O     | 2.16                     | 0.45              |
| 3:JA:769:ARG:NH2   | 3:JA:771:SER:HB2   | 2.31                     | 0.45              |
| 4:UA:152:LEU:O     | 4:UA:153:THR:OG1   | 2.30                     | 0.45              |
| 4:UA:524:ARG:HA    | 4:UA:585:TYR:HD2   | 1.82                     | 0.45              |
| 4:UA:675:MET:HE3   | 4:UA:675:MET:HB3   | 1.86                     | 0.45              |
| 1:CB:98:ILE:HA     | 1:CB:105:LEU:O     | 2.16                     | 0.45              |
| 3:JB:858:MET:O     | 3:JB:862:LEU:N     | 2.42                     | 0.45              |
| 5:UB:612:THR:OG1   | 5:UB:613:ILE:N     | 2.49                     | 0.45              |
| 7:UD:66:ARG:HE     | 7:UD:88:GLU:CD     | 2.20                     | 0.45              |
| 7:UD:95:LYS:HG3    | 19:UP:193:LYS:HE2  | 1.98                     | 0.45              |
| 7:UD:644:SER:OG    | 7:UD:660:ASP:OD2   | 2.32                     | 0.45              |
| 7:UD:733:PHE:HE2   | 7:UD:735:THR:HB    | 1.81                     | 0.45              |
| 8:UE:281:ILE:HD13  | 8:UE:328:VAL:HB    | 1.98                     | 0.45              |
| 8:UE:361:ALA:HB2   | 20:UQ:543:LEU:O    | 2.16                     | 0.45              |
| 9:UF:50:ILE:HD11   | 9:UF:109:PHE:HB2   | 1.99                     | 0.45              |
| 11:UH:596:LYS:O    | 11:UH:600:LYS:HG3  | 2.15                     | 0.45              |
| 13:UJ:539:LEU:HA   | 13:UJ:542:ILE:HG22 | 1.97                     | 0.45              |
| 13:UJ:554:ILE:HD11 | 13:UJ:592:ARG:HD2  | 1.98                     | 0.45              |
| 13:UJ:643:PRO:HD2  | 13:UJ:647:GLU:HA   | 1.97                     | 0.45              |
| 13:UJ:1439:SER:O   | 13:UJ:1442:SER:OG  | 2.20                     | 0.45              |
| 13:UJ:1524:ILE:O   | 13:UJ:1527:SER:OG  | 2.28                     | 0.45              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 15:UL:51:ILE:HD11  | 15:UL:61:SER:HB2    | 1.98                     | 0.45              |
| 15:UL:451:ASN:OD1  | 15:UL:452:GLY:N     | 2.49                     | 0.45              |
| 16:UM:560:TRP:HD1  | 16:UM:566:SER:O     | 1.99                     | 0.45              |
| 17:UN:848:PRO:HB3  | 47:JP:406:HIS:CD2   | 2.51                     | 0.45              |
| 18:UO:411:LYS:HE2  | 65:D2:102:A:C6      | 2.51                     | 0.45              |
| 18:UO:462:TRP:O    | 18:UO:466:VAL:HG23  | 2.16                     | 0.45              |
| 20:UQ:508:ILE:HD13 | 20:UQ:531:PHE:CE1   | 2.51                     | 0.45              |
| 23:UT:248:HIS:CE1  | 23:UT:251:ALA:HB2   | 2.52                     | 0.45              |
| 23:UT:1614:GLU:HA  | 23:UT:1617:VAL:HG22 | 1.98                     | 0.45              |
| 23:UT:1906:GLU:OE1 | 23:UT:1906:GLU:N    | 2.49                     | 0.45              |
| 29:CE:413:VAL:HB   | 29:CE:415:GLU:OE2   | 2.16                     | 0.45              |
| 31:CH:154:GLU:HB2  | 31:CH:193:ASP:OD2   | 2.17                     | 0.45              |
| 31:CH:323:ASP:OD1  | 31:CH:324:ILE:HG12  | 2.16                     | 0.45              |
| 31:CH:429:LYS:NZ   | 31:CH:433:ILE:HA    | 2.31                     | 0.45              |
| 34:CK:511:ASN:OD1  | 34:CK:513:VAL:HG12  | 2.16                     | 0.45              |
| 35:CL:835:HIS:HD2  | 35:CL:837:LYS:H     | 1.64                     | 0.45              |
| 36:CM:192:THR:N    | 36:CM:248:GLN:HE22  | 2.08                     | 0.45              |
| 38:JC:92:LYS:HE3   | 66:D3:407:A:H4'     | 1.97                     | 0.45              |
| 38:JC:339:HIS:HD2  | 38:JC:341:TYR:CZ    | 2.34                     | 0.45              |
| 39:JG:39:LYS:HA    | 39:JG:201:SER:OG    | 2.17                     | 0.45              |
| 42:JJ:119:PRO:HB2  | 42:JJ:175:LEU:CD2   | 2.46                     | 0.45              |
| 43:JK:485:TRP:HB3  | 43:JK:489:GLN:NE2   | 2.32                     | 0.45              |
| 52:DH:141:ARG:HB2  | 52:DH:141:ARG:HH11  | 1.80                     | 0.45              |
| 60:DW:125:ILE:HD12 | 60:DW:125:ILE:N     | 2.29                     | 0.45              |
| 62:DY:131:ARG:NH2  | 66:D3:153:G:H5''    | 2.30                     | 0.45              |
| 65:D2:355:C:H2'    | 65:D2:356:C:H6      | 1.81                     | 0.45              |
| 66:D3:469:C:C4     | 66:D3:470:A:C8      | 3.04                     | 0.45              |
| 66:D3:1171:A:H2'   | 66:D3:1172:G:C8     | 2.49                     | 0.45              |
| 66:D3:1620:C:O2'   | 66:D3:1621:U:OP1    | 2.29                     | 0.45              |
| 66:D3:1661:U:H2'   | 66:D3:1662:G:H8     | 1.82                     | 0.45              |
| 66:D3:1703:C:H2'   | 66:D3:1704:U:C6     | 2.51                     | 0.45              |
| 79:EN:80:MET:N     | 79:EN:125:LEU:H     | 2.14                     | 0.45              |
| 3:JA:32:ARG:C      | 3:JA:34:ARG:H       | 2.19                     | 0.45              |
| 3:JA:121:MET:SD    | 3:JA:147:ILE:HB     | 2.57                     | 0.45              |
| 3:JA:569:PRO:HD3   | 3:JA:583:LEU:CG     | 2.46                     | 0.45              |
| 4:UA:716:ASP:O     | 4:UA:744:ARG:NE     | 2.48                     | 0.45              |
| 6:UC:500:ARG:HD3   | 6:UC:500:ARG:HA     | 1.72                     | 0.45              |
| 7:UD:83:ASN:O      | 7:UD:85:TRP:N       | 2.45                     | 0.45              |
| 7:UD:257:ASP:OD1   | 7:UD:261:SER:HB3    | 2.16                     | 0.45              |
| 7:UD:378:TYR:HH    | 7:UD:632:ASN:HD22   | 1.59                     | 0.45              |
| 9:UF:197:ILE:HD13  | 9:UF:200:ARG:HE     | 1.81                     | 0.45              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 11:UH:652:GLY:O    | 11:UH:656:GLU:HG2   | 2.17                     | 0.45              |
| 13:UJ:550:TYR:OH   | 13:UJ:556:LYS:HD2   | 2.16                     | 0.45              |
| 13:UJ:754:GLU:HA   | 13:UJ:757:ILE:HG12  | 1.97                     | 0.45              |
| 13:UJ:1423:LEU:HA  | 13:UJ:1426:ILE:HG22 | 1.98                     | 0.45              |
| 15:UL:477:TRP:HE1  | 15:UL:493:ALA:HB2   | 1.81                     | 0.45              |
| 15:UL:843:LYS:O    | 15:UL:846:LEU:HB3   | 2.15                     | 0.45              |
| 16:UM:43:ILE:HA    | 16:UM:53:LEU:H      | 1.82                     | 0.45              |
| 16:UM:421:SER:O    | 16:UM:423:LYS:N     | 2.42                     | 0.45              |
| 18:UO:116:ILE:HG23 | 18:UO:116:ILE:O     | 2.16                     | 0.45              |
| 20:UQ:354:TYR:O    | 20:UQ:373:LEU:HD12  | 2.16                     | 0.45              |
| 21:UR:150:TYR:HD2  | 65:D2:313:A:C5      | 2.35                     | 0.45              |
| 22:US:281:LEU:O    | 22:US:286:ILE:HG12  | 2.16                     | 0.45              |
| 22:US:403:TYR:CD2  | 22:US:493:TYR:HE2   | 2.35                     | 0.45              |
| 22:US:427:GLN:OE1  | 22:US:431:GLN:HB2   | 2.15                     | 0.45              |
| 22:US:466:LEU:HD23 | 22:US:466:LEU:HA    | 1.84                     | 0.45              |
| 23:UT:434:LEU:O    | 23:UT:438:GLU:HG2   | 2.16                     | 0.45              |
| 23:UT:552:LEU:HD13 | 23:UT:596:ILE:HA    | 1.99                     | 0.45              |
| 23:UT:839:LYS:HG3  | 23:UT:840:ASN:H     | 1.81                     | 0.45              |
| 23:UT:977:PHE:HB2  | 23:UT:1028:TYR:CD2  | 2.52                     | 0.45              |
| 23:UT:1602:ASP:OD1 | 23:UT:1602:ASP:N    | 2.49                     | 0.45              |
| 24:UU:362:GLN:O    | 24:UU:363:SER:OG    | 2.31                     | 0.45              |
| 25:UV:495:THR:O    | 25:UV:499:LEU:HD23  | 2.16                     | 0.45              |
| 25:UV:894:ARG:HB2  | 25:UV:894:ARG:HH11  | 1.80                     | 0.45              |
| 28:CD:7:LEU:CB     | 28:CD:99:ALA:HB3    | 2.47                     | 0.45              |
| 28:CD:398:ASN:N    | 28:CD:398:ASN:OD1   | 2.49                     | 0.45              |
| 29:CE:358:LYS:HE2  | 67:D4:85:G:OP2      | 2.16                     | 0.45              |
| 30:CF:33:LEU:HD13  | 30:CF:102:ILE:HD13  | 1.98                     | 0.45              |
| 33:CJ:172:MET:O    | 33:CJ:176:ILE:HG13  | 2.17                     | 0.45              |
| 33:CJ:268:ASN:ND2  | 33:CJ:271:ALA:HB2   | 2.30                     | 0.45              |
| 34:CK:304:GLN:HA   | 34:CK:307:ILE:HG22  | 1.97                     | 0.45              |
| 35:CL:134:ILE:HD12 | 35:CL:811:VAL:HG13  | 1.98                     | 0.45              |
| 35:CL:754:GLN:O    | 35:CL:758:ILE:HG12  | 2.16                     | 0.45              |
| 35:CL:975:GLU:OE2  | 35:CL:977:LYS:HE2   | 2.16                     | 0.45              |
| 37:CN:18:PHE:HE1   | 37:CN:156:PHE:HB2   | 1.81                     | 0.45              |
| 37:CN:22:ASP:HB2   | 37:CN:26:LEU:HD22   | 1.98                     | 0.45              |
| 37:CN:225:SER:HB2  | 66:D3:1059:U:C2     | 2.52                     | 0.45              |
| 38:JC:236:PHE:CD2  | 38:JC:240:GLY:HA2   | 2.51                     | 0.45              |
| 45:JN:155:LEU:HD23 | 45:JN:159:LEU:HD13  | 1.98                     | 0.45              |
| 47:JP:15:PRO:HB3   | 47:JP:20:GLN:HE21   | 1.82                     | 0.45              |
| 47:JP:270:ASN:ND2  | 47:JP:273:GLU:HB2   | 2.31                     | 0.45              |
| 47:JP:450:ASP:OD1  | 47:JP:450:ASP:N     | 2.46                     | 0.45              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 48:JQ:182:HIS:CE1   | 48:JQ:183:ARG:HB3   | 2.51                     | 0.45              |
| 51:DG:140:ASN:O     | 51:DG:143:LYS:HG2   | 2.17                     | 0.45              |
| 52:DH:116:ARG:HD3   | 52:DH:116:ARG:HA    | 1.69                     | 0.45              |
| 52:DH:122:HIS:O     | 52:DH:126:LEU:HD23  | 2.17                     | 0.45              |
| 57:DO:41:ARG:NH1    | 66:D3:917:U:C2      | 2.84                     | 0.45              |
| 57:DO:52:ARG:HE     | 66:D3:905:A:C3'     | 2.26                     | 0.45              |
| 58:DQ:15:SER:OG     | 66:D3:1608:U:OP1    | 2.20                     | 0.45              |
| 65:D2:153:U:H3'     | 65:D2:154:A:C8      | 2.51                     | 0.45              |
| 65:D2:165:G:H2'     | 65:D2:166:U:C6      | 2.52                     | 0.45              |
| 65:D2:429:A:H2      | 65:D2:432:C:C4      | 2.35                     | 0.45              |
| 65:D2:448:G:C2      | 65:D2:449:U:N3      | 2.85                     | 0.45              |
| 66:D3:242:U:H2'     | 66:D3:243:G:H8      | 1.80                     | 0.45              |
| 66:D3:843:U:H2'     | 66:D3:844:A:C8      | 2.52                     | 0.45              |
| 66:D3:1164:G:C2     | 66:D3:1165:G:C4     | 3.05                     | 0.45              |
| 66:D3:1586:A:H2'    | 66:D3:1587:A:O4'    | 2.15                     | 0.45              |
| 66:D3:1750:A:H2'    | 66:D3:1751:C:C6     | 2.52                     | 0.45              |
| 71:ED:93:GLY:HA2    | 71:ED:213:LEU:HA    | 1.98                     | 0.45              |
| 3:JA:881:GLN:HA     | 3:JA:912:MET:CE     | 2.46                     | 0.45              |
| 4:UA:496:THR:HG22   | 4:UA:497:ILE:O      | 2.16                     | 0.45              |
| 4:UA:640:SER:O      | 4:UA:642:ASP:N      | 2.49                     | 0.45              |
| 1:CB:228:GLN:CA     | 1:CB:231:ARG:HD2    | 2.47                     | 0.45              |
| 7:UD:354:LYS:O      | 7:UD:374:THR:CA     | 2.61                     | 0.45              |
| 13:UJ:231:LEU:O     | 13:UJ:235:VAL:HG23  | 2.17                     | 0.45              |
| 13:UJ:650:PHE:O     | 13:UJ:654:TRP:HE3   | 1.99                     | 0.45              |
| 13:UJ:1499:ILE:O    | 13:UJ:1503:LEU:HD23 | 2.16                     | 0.45              |
| 13:UJ:1572:LEU:HD12 | 13:UJ:1576:PHE:CE2  | 2.52                     | 0.45              |
| 15:UL:229:TRP:HA    | 15:UL:243:THR:O     | 2.16                     | 0.45              |
| 15:UL:288:LYS:O     | 15:UL:292:ILE:HG12  | 2.16                     | 0.45              |
| 15:UL:538:ARG:HD2   | 15:UL:539:VAL:H     | 1.81                     | 0.45              |
| 16:UM:296:ILE:O     | 16:UM:297:LEU:HG    | 2.16                     | 0.45              |
| 18:UO:52:PRO:HG2    | 18:UO:312:ALA:HA    | 1.99                     | 0.45              |
| 18:UO:360:MET:SD    | 65:D2:234:A:H2'     | 2.57                     | 0.45              |
| 18:UO:383:ARG:HH22  | 18:UO:386:ARG:HH22  | 1.62                     | 0.45              |
| 20:UQ:335:PRO:O     | 20:UQ:336:ARG:HD3   | 2.17                     | 0.45              |
| 20:UQ:634:ASP:OD2   | 20:UQ:635:PHE:N     | 2.50                     | 0.45              |
| 22:US:353:LYS:C     | 22:US:354:TYR:HD1   | 2.20                     | 0.45              |
| 22:US:495:MET:N     | 22:US:495:MET:SD    | 2.90                     | 0.45              |
| 23:UT:991:LEU:HA    | 23:UT:994:ILE:HG12  | 1.97                     | 0.45              |
| 25:UV:121:VAL:HG13  | 25:UV:189:PHE:CE1   | 2.52                     | 0.45              |
| 25:UV:300:TYR:HD1   | 25:UV:341:THR:HG23  | 1.82                     | 0.45              |
| 25:UV:1028:ARG:HA   | 25:UV:1028:ARG:HD3  | 1.76                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:UV:1209:ASP:HA  | 37:CN:9:MET:HG3    | 1.98                     | 0.45              |
| 25:UV:1226:PHE:CZ  | 37:CN:60:LEU:HD13  | 2.51                     | 0.45              |
| 26:UX:93:LYS:NZ    | 26:UX:95:ASN:OD1   | 2.50                     | 0.45              |
| 27:UZ:110:PHE:CZ   | 27:UZ:118:LEU:HD21 | 2.52                     | 0.45              |
| 29:CE:25:SER:HA    | 29:CE:116:ILE:HD11 | 1.98                     | 0.45              |
| 29:CE:49:LYS:HD3   | 29:CE:50:PHE:O     | 2.15                     | 0.45              |
| 30:CF:54:MET:SD    | 30:CF:64:LEU:HD13  | 2.57                     | 0.45              |
| 31:CH:526:VAL:HG12 | 31:CH:539:ILE:HG12 | 1.97                     | 0.45              |
| 32:CI:33:MET:HE3   | 32:CI:41:ARG:HA    | 1.98                     | 0.45              |
| 32:CI:154:MET:HE2  | 32:CI:154:MET:HA   | 1.97                     | 0.45              |
| 37:CN:259:ARG:O    | 37:CN:262:VAL:HG12 | 2.16                     | 0.45              |
| 39:JG:31:LEU:HB3   | 39:JG:40:ARG:HE    | 1.80                     | 0.45              |
| 51:DG:136:LYS:HB3  | 66:D3:168:A:P      | 2.56                     | 0.45              |
| 53:DI:99:ALA:HB3   | 66:D3:329:G:H5'    | 1.98                     | 0.45              |
| 54:DJ:37:LYS:HG3   | 54:DJ:38:ASN:OD1   | 2.15                     | 0.45              |
| 56:DN:98:VAL:O     | 56:DN:102:LEU:HD23 | 2.17                     | 0.45              |
| 57:DO:53:ASP:O     | 57:DO:56:SER:N     | 2.44                     | 0.45              |
| 66:D3:898:A:N3     | 66:D3:899:G:H1'    | 2.31                     | 0.45              |
| 66:D3:974:A:C5     | 66:D3:975:C:C4     | 3.05                     | 0.45              |
| 67:D4:5:A:H2'      | 67:D4:6:C:C6       | 2.52                     | 0.45              |
| 67:D4:321:C:C4     | 67:D4:322:A:C5     | 3.04                     | 0.45              |
| 76:EI:117:ALA:H    | 76:EI:126:VAL:HA   | 1.82                     | 0.45              |
| 79:EN:513:ALA:O    | 79:EN:545:GLY:N    | 2.39                     | 0.45              |
| 1:CA:91:HIS:CD2    | 1:CA:98:ILE:HD11   | 2.51                     | 0.45              |
| 1:CA:236:MET:HG3   | 28:CD:133:LEU:HD12 | 1.99                     | 0.45              |
| 6:UC:546:LYS:HA    | 6:UC:546:LYS:HD2   | 1.61                     | 0.45              |
| 7:UD:64:ASP:HA     | 7:UD:66:ARG:NH1    | 2.31                     | 0.45              |
| 7:UD:230:LYS:HE2   | 7:UD:233:LYS:HZ3   | 1.82                     | 0.45              |
| 8:UE:226:LEU:HD12  | 8:UE:256:PHE:CD1   | 2.50                     | 0.45              |
| 10:UG:546:ILE:O    | 10:UG:550:LEU:HD23 | 2.17                     | 0.45              |
| 12:UI:439:LYS:O    | 12:UI:442:THR:HG22 | 2.16                     | 0.45              |
| 13:UJ:241:ILE:O    | 13:UJ:245:LEU:HD23 | 2.17                     | 0.45              |
| 13:UJ:312:VAL:O    | 13:UJ:312:VAL:HG12 | 2.15                     | 0.45              |
| 13:UJ:562:THR:HG23 | 13:UJ:563:LEU:HD23 | 1.99                     | 0.45              |
| 13:UJ:1723:LEU:O   | 13:UJ:1726:LEU:HG  | 2.17                     | 0.45              |
| 15:UL:288:LYS:HE2  | 15:UL:288:LYS:HB2  | 1.76                     | 0.45              |
| 15:UL:762:GLU:OE2  | 15:UL:763:ILE:HG13 | 2.17                     | 0.45              |
| 16:UM:497:LEU:HG   | 16:UM:506:PHE:HE2  | 1.82                     | 0.45              |
| 16:UM:745:ASP:O    | 16:UM:748:THR:HB   | 2.17                     | 0.45              |
| 18:UO:62:ARG:HG3   | 18:UO:64:GLN:HG3   | 1.98                     | 0.45              |
| 18:UO:82:ASP:CG    | 18:UO:83:VAL:H     | 2.20                     | 0.45              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 18:UO:108:TYR:HB3  | 18:UO:117:LEU:H     | 1.82                     | 0.45              |
| 18:UO:488:LYS:HE3  | 18:UO:492:ARG:CZ    | 2.46                     | 0.45              |
| 20:UQ:318:GLU:O    | 20:UQ:320:VAL:N     | 2.50                     | 0.45              |
| 20:UQ:371:PHE:HB2  | 20:UQ:385:ILE:HB    | 1.98                     | 0.45              |
| 20:UQ:401:GLN:HB2  | 20:UQ:412:ASN:ND2   | 2.31                     | 0.45              |
| 20:UQ:484:VAL:HG23 | 20:UQ:485:ARG:N     | 2.31                     | 0.45              |
| 20:UQ:724:ILE:HG12 | 20:UQ:741:SER:HB2   | 1.98                     | 0.45              |
| 21:UR:364:GLN:NE2  | 21:UR:369:ASN:O     | 2.38                     | 0.45              |
| 22:US:188:PHE:HB2  | 22:US:191:ILE:HG22  | 1.98                     | 0.45              |
| 23:UT:719:LEU:HD23 | 23:UT:754:ASN:HD22  | 1.81                     | 0.45              |
| 23:UT:797:ALA:HB3  | 23:UT:798:PRO:HD3   | 1.98                     | 0.45              |
| 23:UT:1369:HIS:O   | 23:UT:1372:MET:HB2  | 2.16                     | 0.45              |
| 23:UT:2001:ASN:HA  | 23:UT:2004:LYS:HE2  | 1.99                     | 0.45              |
| 24:UU:252:SER:OG   | 24:UU:267:GLY:O     | 2.35                     | 0.45              |
| 24:UU:364:HIS:CD2  | 24:UU:381:ARG:HD2   | 2.52                     | 0.45              |
| 25:UV:174:TYR:CD2  | 25:UV:227:LYS:HE3   | 2.52                     | 0.45              |
| 25:UV:250:SER:HG   | 25:UV:251:PHE:HD1   | 1.63                     | 0.45              |
| 25:UV:847:GLY:HA2  | 25:UV:1132:PHE:CE2  | 2.52                     | 0.45              |
| 25:UV:1194:HIS:CD2 | 25:UV:1200:LEU:HD21 | 2.51                     | 0.45              |
| 27:UZ:73:LEU:HD13  | 27:UZ:122:PHE:CE2   | 2.51                     | 0.45              |
| 30:CF:41:THR:OG1   | 30:CF:67:LEU:HD21   | 2.16                     | 0.45              |
| 31:CH:191:SER:HB3  | 31:CH:195:GLN:HB3   | 1.98                     | 0.45              |
| 32:CI:50:ILE:O     | 32:CI:54:ILE:HG13   | 2.15                     | 0.45              |
| 37:CN:70:PHE:HB2   | 37:CN:158:TRP:HZ3   | 1.81                     | 0.45              |
| 38:JC:115:VAL:HG12 | 38:JC:123:ILE:HD11  | 1.97                     | 0.45              |
| 46:JO:97:ALA:O     | 46:JO:100:LEU:HB3   | 2.16                     | 0.45              |
| 47:JP:302:LYS:O    | 47:JP:302:LYS:HG2   | 2.16                     | 0.45              |
| 49:DE:71:LYS:HA    | 49:DE:76:VAL:HA     | 1.99                     | 0.45              |
| 49:DE:178:GLY:N    | 49:DE:195:ILE:HG13  | 2.32                     | 0.45              |
| 49:DE:200:ARG:HH21 | 66:D3:246:G:P       | 2.39                     | 0.45              |
| 51:DG:38:GLY:O     | 51:DG:45:PHE:HB2    | 2.16                     | 0.45              |
| 51:DG:212:LEU:HA   | 51:DG:215:ARG:HG2   | 1.98                     | 0.45              |
| 54:DJ:109:LEU:HA   | 54:DJ:109:LEU:HD12  | 1.72                     | 0.45              |
| 65:D2:64:U:H2'     | 65:D2:65:U:H6       | 1.82                     | 0.45              |
| 65:D2:82:A:HO2'    | 65:D2:83:U:P        | 2.39                     | 0.45              |
| 65:D2:173:G:H2'    | 65:D2:174:U:C6      | 2.52                     | 0.45              |
| 65:D2:373:U:H2'    | 65:D2:374:U:H6      | 1.81                     | 0.45              |
| 66:D3:300:A:H2'    | 66:D3:301:A:C8      | 2.50                     | 0.45              |
| 66:D3:490:C:C4     | 66:D3:498:G:N1      | 2.85                     | 0.45              |
| 66:D3:651:G:H2'    | 66:D3:652:G:C8      | 2.52                     | 0.45              |
| 66:D3:1575:G:C2    | 66:D3:1576:A:C4     | 3.04                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 67:D4:64:A:H2'     | 67:D4:65:C:C6      | 2.50                     | 0.45              |
| 2:DA:28:GLU:OE1    | 2:DA:50:LYS:HA     | 2.16                     | 0.45              |
| 3:JA:631:SER:H     | 3:JA:721:HIS:HD1   | 1.63                     | 0.45              |
| 4:UA:33:VAL:HG12   | 4:UA:34:GLY:H      | 1.82                     | 0.45              |
| 4:UA:350:SER:OG    | 4:UA:392:ALA:HA    | 2.17                     | 0.45              |
| 4:UA:420:ARG:HG3   | 34:CK:468:ARG:HH22 | 1.82                     | 0.45              |
| 4:UA:713:ASP:OD1   | 4:UA:746:ASN:ND2   | 2.50                     | 0.45              |
| 1:CB:100:ARG:HA    | 1:CB:104:ASP:OD1   | 2.16                     | 0.45              |
| 5:UB:568:PHE:CD2   | 5:UB:643:LEU:HD12  | 2.52                     | 0.45              |
| 5:UB:569:GLN:OE1   | 5:UB:664:ILE:HD13  | 2.17                     | 0.45              |
| 5:UB:699:PRO:HD3   | 22:US:442:TYR:CE2  | 2.52                     | 0.45              |
| 7:UD:40:ASP:N      | 7:UD:40:ASP:OD1    | 2.49                     | 0.45              |
| 7:UD:156:LEU:HD11  | 7:UD:168:ILE:HB    | 1.99                     | 0.45              |
| 7:UD:649:TRP:HB2   | 7:UD:654:ILE:HG13  | 1.99                     | 0.45              |
| 9:UF:9:GLU:CD      | 17:UN:873:ALA:HB2  | 2.37                     | 0.45              |
| 10:UG:106:LEU:O    | 10:UG:397:GLY:HA3  | 2.16                     | 0.45              |
| 10:UG:160:LEU:HD12 | 10:UG:161:GLN:HB3  | 1.98                     | 0.45              |
| 10:UG:475:ASN:O    | 10:UG:479:THR:HG22 | 2.17                     | 0.45              |
| 13:UJ:82:ASP:OD1   | 13:UJ:84:ASN:N     | 2.36                     | 0.45              |
| 15:UL:543:ASP:C    | 15:UL:560:LEU:HD12 | 2.37                     | 0.45              |
| 15:UL:552:ASP:O    | 15:UL:554:THR:HG22 | 2.16                     | 0.45              |
| 18:UO:197:ASP:HB3  | 18:UO:206:ILE:HD11 | 1.99                     | 0.45              |
| 20:UQ:155:THR:OG1  | 20:UQ:172:ARG:HB2  | 2.16                     | 0.45              |
| 20:UQ:440:VAL:HB   | 20:UQ:765:TRP:CD2  | 2.52                     | 0.45              |
| 20:UQ:457:VAL:HG13 | 20:UQ:473:LEU:HD13 | 1.97                     | 0.45              |
| 20:UQ:676:THR:O    | 20:UQ:695:TYR:N    | 2.50                     | 0.45              |
| 21:UR:170:LYS:HD2  | 21:UR:170:LYS:HA   | 1.80                     | 0.45              |
| 23:UT:196:LEU:HA   | 23:UT:199:LEU:HD12 | 1.97                     | 0.45              |
| 23:UT:559:ASN:OD1  | 23:UT:603:LEU:HB2  | 2.16                     | 0.45              |
| 23:UT:605:LYS:HD2  | 23:UT:623:MET:HE1  | 1.99                     | 0.45              |
| 23:UT:643:LYS:HZ2  | 23:UT:683:ASP:HB2  | 1.80                     | 0.45              |
| 23:UT:870:LEU:HD22 | 23:UT:889:LYS:HD3  | 1.99                     | 0.45              |
| 23:UT:918:GLU:O    | 23:UT:922:MET:HG2  | 2.17                     | 0.45              |
| 23:UT:938:THR:OG1  | 23:UT:942:LYS:NZ   | 2.23                     | 0.45              |
| 23:UT:1088:LYS:HB2 | 23:UT:1089:PRO:HD3 | 1.98                     | 0.45              |
| 23:UT:1940:LYS:HD3 | 23:UT:1940:LYS:HA  | 1.75                     | 0.45              |
| 24:UU:135:ASN:HB3  | 24:UU:159:VAL:HB   | 1.98                     | 0.45              |
| 25:UV:363:THR:HA   | 25:UV:393:PHE:CE2  | 2.52                     | 0.45              |
| 25:UV:746:LEU:HD11 | 25:UV:810:ILE:HD11 | 1.98                     | 0.45              |
| 25:UV:865:ARG:NH2  | 66:D3:1060:U:OP2   | 2.39                     | 0.45              |
| 27:UZ:129:TYR:HE1  | 27:UZ:155:ARG:HG3  | 1.82                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:CG:33:LEU:HD12  | 30:CG:101:SER:O    | 2.17                     | 0.45              |
| 31:CH:318:LEU:HD23 | 31:CH:318:LEU:HA   | 1.72                     | 0.45              |
| 31:CH:489:SER:HG   | 31:CH:499:TRP:HE1  | 1.62                     | 0.45              |
| 35:CL:784:LYS:HG2  | 35:CL:785:ALA:N    | 2.32                     | 0.45              |
| 36:CM:115:SER:HG   | 36:CM:167:HIS:HE2  | 1.61                     | 0.45              |
| 37:CN:255:LYS:O    | 37:CN:265:ARG:NH2  | 2.49                     | 0.45              |
| 38:JC:317:ILE:HD13 | 38:JC:331:THR:HB   | 1.98                     | 0.45              |
| 39:JF:105:ASN:OD1  | 39:JF:110:LEU:HD11 | 2.16                     | 0.45              |
| 42:JJ:107:THR:HB   | 42:JJ:108:PRO:HD3  | 1.98                     | 0.45              |
| 44:JM:108:LYS:HE3  | 44:JM:108:LYS:HB2  | 1.71                     | 0.45              |
| 47:JP:17:LYS:HE3   | 47:JP:20:GLN:OE1   | 2.16                     | 0.45              |
| 47:JP:50:LEU:HD23  | 47:JP:50:LEU:HA    | 1.80                     | 0.45              |
| 47:JP:296:ARG:HE   | 47:JP:458:LYS:HE2  | 1.81                     | 0.45              |
| 49:DE:132:GLY:O    | 49:DE:135:GLY:N    | 2.50                     | 0.45              |
| 51:DG:31:ARG:HH12  | 51:DG:32:ILE:HD12  | 1.82                     | 0.45              |
| 51:DG:173:PRO:HG3  | 66:D3:66:U:C6      | 2.51                     | 0.45              |
| 53:DI:86:SER:OG    | 53:DI:87:ASN:N     | 2.48                     | 0.45              |
| 53:DI:164:ARG:HA   | 53:DI:164:ARG:HH21 | 1.77                     | 0.45              |
| 53:DI:172:ARG:HH21 | 53:DI:175:GLN:HE21 | 1.64                     | 0.45              |
| 53:DI:192:TYR:O    | 53:DI:196:LEU:HG   | 2.17                     | 0.45              |
| 57:DO:20:TYR:HB3   | 57:DO:27:PHE:CD2   | 2.51                     | 0.45              |
| 58:DQ:57:LEU:O     | 58:DQ:60:PHE:N     | 2.44                     | 0.45              |
| 60:DW:86:ILE:O     | 60:DW:90:THR:HG23  | 2.16                     | 0.45              |
| 66:D3:1643:U:H2'   | 66:D3:1644:C:C6    | 2.52                     | 0.45              |
| 66:D3:1692:G:N2    | 66:D3:1693:A:N3    | 2.64                     | 0.45              |
| 67:D4:68:A:N3      | 67:D4:69:A:C8      | 2.84                     | 0.45              |
| 67:D4:319:G:C2     | 67:D4:320:G:C4     | 3.05                     | 0.45              |
| 69:EB:163:LYS:HA   | 69:EB:186:PRO:HA   | 1.98                     | 0.45              |
| 69:EB:250:LYS:N    | 70:EC:199:LEU:O    | 2.43                     | 0.45              |
| 76:EI:342:GLU:O    | 76:EI:346:SER:N    | 2.48                     | 0.45              |
| 2:DA:105:PHE:CE2   | 2:DA:213:ARG:HA    | 2.51                     | 0.45              |
| 3:JA:727:TYR:CE2   | 3:JA:760:CYS:HB3   | 2.51                     | 0.45              |
| 3:JA:809:LYS:HA    | 3:JA:812:GLN:HG2   | 1.98                     | 0.45              |
| 4:UA:169:SER:O     | 4:UA:194:VAL:HG21  | 2.17                     | 0.45              |
| 4:UA:327:LEU:HD12  | 4:UA:328:LEU:H     | 1.82                     | 0.45              |
| 4:UA:803:LEU:HD12  | 24:UU:932:VAL:HG22 | 1.99                     | 0.45              |
| 1:CB:107:VAL:CG2   | 1:CB:141:TYR:HB3   | 2.45                     | 0.45              |
| 7:UD:250:THR:O     | 7:UD:252:GLN:N     | 2.50                     | 0.45              |
| 8:UE:47:ASN:ND2    | 20:UQ:826:LEU:O    | 2.50                     | 0.45              |
| 8:UE:120:ILE:HD12  | 8:UE:126:PHE:CD1   | 2.52                     | 0.45              |
| 10:UG:95:VAL:HG12  | 10:UG:96:ASP:N     | 2.31                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:UG:376:ASN:HB3  | 10:UG:394:HIS:HB2  | 1.99                     | 0.45              |
| 13:UJ:270:LEU:HD13 | 13:UJ:274:ILE:HG21 | 1.99                     | 0.45              |
| 13:UJ:497:LEU:O    | 13:UJ:500:GLU:HG3  | 2.17                     | 0.45              |
| 14:UK:16:ARG:HD2   | 66:D3:556:A:C8     | 2.52                     | 0.45              |
| 14:UK:217:ARG:HH21 | 65:D2:260:A:C5'    | 2.30                     | 0.45              |
| 15:UL:491:GLY:HA3  | 15:UL:534:ILE:HD13 | 1.99                     | 0.45              |
| 16:UM:267:PHE:HB3  | 16:UM:281:THR:HG21 | 1.98                     | 0.45              |
| 16:UM:732:ASN:HB2  | 16:UM:735:GLN:CD   | 2.37                     | 0.45              |
| 16:UM:804:TYR:CD2  | 24:UU:928:PHE:HA   | 2.52                     | 0.45              |
| 18:UO:43:THR:HG22  | 18:UO:44:HIS:ND1   | 2.31                     | 0.45              |
| 18:UO:147:ARG:HG2  | 18:UO:170:TYR:H    | 1.82                     | 0.45              |
| 18:UO:231:GLY:O    | 18:UO:255:VAL:HG22 | 2.16                     | 0.45              |
| 22:US:295:LEU:O    | 22:US:299:LEU:HG   | 2.17                     | 0.45              |
| 22:US:417:HIS:O    | 22:US:417:HIS:CG   | 2.69                     | 0.45              |
| 22:US:428:THR:HG23 | 22:US:431:GLN:H    | 1.81                     | 0.45              |
| 23:UT:145:SER:O    | 23:UT:149:GLU:OE1  | 2.33                     | 0.45              |
| 23:UT:325:GLU:OE2  | 23:UT:735:ARG:NH2  | 2.50                     | 0.45              |
| 23:UT:327:GLY:HA2  | 23:UT:330:ILE:HD13 | 1.99                     | 0.45              |
| 23:UT:1096:ASP:OD1 | 23:UT:1096:ASP:N   | 2.49                     | 0.45              |
| 23:UT:1464:ARG:HA  | 23:UT:1467:LYS:HG2 | 1.99                     | 0.45              |
| 23:UT:1614:GLU:HG3 | 23:UT:1661:ILE:CG2 | 2.47                     | 0.45              |
| 24:UU:144:ASP:HB3  | 24:UU:147:ASP:CG   | 2.37                     | 0.45              |
| 25:UV:939:ILE:HD12 | 25:UV:942:PHE:HB2  | 1.99                     | 0.45              |
| 25:UV:1082:GLN:HG2 | 25:UV:1083:GLN:N   | 2.31                     | 0.45              |
| 25:UV:1156:LYS:HG3 | 25:UV:1157:TYR:CD1 | 2.49                     | 0.45              |
| 28:CD:33:GLU:HB3   | 47:JP:384:ASN:OD1  | 2.17                     | 0.45              |
| 28:CD:158:TYR:O    | 28:CD:162:LYS:HG2  | 2.17                     | 0.45              |
| 29:CE:111:ALA:C    | 29:CE:113:THR:H    | 2.20                     | 0.45              |
| 29:CE:191:HIS:CE1  | 29:CE:246:GLU:HA   | 2.52                     | 0.45              |
| 31:CH:541:ALA:O    | 31:CH:543:ILE:HD12 | 2.17                     | 0.45              |
| 32:CI:177:ILE:O    | 58:DQ:8:GLN:NE2    | 2.50                     | 0.45              |
| 44:JM:206:TYR:CZ   | 44:JM:210:LYS:HE2  | 2.51                     | 0.45              |
| 46:JO:64:LEU:HB3   | 46:JO:69:ILE:O     | 2.17                     | 0.45              |
| 49:DE:141:THR:OG1  | 49:DE:143:ASP:OD1  | 2.22                     | 0.45              |
| 49:DE:152:PRO:HD2  | 51:DG:215:ARG:CZ   | 2.47                     | 0.45              |
| 52:DH:57:ALA:O     | 52:DH:88:ARG:NH2   | 2.50                     | 0.45              |
| 53:DI:98:LYS:HD2   | 53:DI:172:ARG:HG3  | 1.98                     | 0.45              |
| 54:DJ:152:SER:O    | 54:DJ:155:HIS:N    | 2.50                     | 0.45              |
| 58:DQ:24:ALA:HA    | 58:DQ:63:ILE:HG22  | 1.99                     | 0.45              |
| 60:DW:124:LYS:NZ   | 66:D3:805:U:O2     | 2.22                     | 0.45              |
| 65:D2:475:G:C2     | 65:D2:476:A:C4     | 3.04                     | 0.45              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 66:D3:45:U:O4'      | 66:D3:359:A:H1'     | 2.17                     | 0.45              |
| 66:D3:202:A:C2      | 66:D3:203:U:H1'     | 2.51                     | 0.45              |
| 66:D3:408:C:H2'     | 66:D3:409:C:C6      | 2.51                     | 0.45              |
| 66:D3:500:C:HO2'    | 66:D3:501:U:P       | 2.40                     | 0.45              |
| 66:D3:1598:U:H2'    | 66:D3:1599:C:H6     | 1.81                     | 0.45              |
| 66:D3:1681:A:H2'    | 66:D3:1682:U:H4'    | 1.98                     | 0.45              |
| 66:D3:1787:C:H2'    | 66:D3:1788:G:C8     | 2.51                     | 0.45              |
| 67:D4:113:G:N3      | 67:D4:256:G:N2      | 2.64                     | 0.45              |
| 77:EJ:223:CYS:HA    | 77:EJ:286:ARG:HA    | 1.99                     | 0.45              |
| 79:EN:971:ALA:O     | 79:EN:975:LYS:N     | 2.39                     | 0.45              |
| 1:CA:144:TRP:CE2    | 1:CA:152:ALA:HB2    | 2.52                     | 0.45              |
| 3:JA:624:ASP:N      | 3:JA:624:ASP:OD1    | 2.50                     | 0.45              |
| 4:UA:348:THR:HG21   | 4:UA:696:ALA:HB1    | 1.99                     | 0.45              |
| 1:CB:218:ILE:HD12   | 1:CB:219:PRO:HD2    | 1.98                     | 0.45              |
| 1:CB:263:ASP:OD1    | 1:CB:264:GLN:N      | 2.49                     | 0.45              |
| 1:CB:303:GLN:HB3    | 1:CB:316:VAL:HG12   | 1.99                     | 0.45              |
| 7:UD:396:GLU:CD     | 7:UD:428:ILE:HG13   | 2.37                     | 0.45              |
| 8:UE:181:VAL:HG23   | 8:UE:182:MET:H      | 1.82                     | 0.45              |
| 8:UE:226:LEU:HD12   | 8:UE:256:PHE:CE1    | 2.52                     | 0.45              |
| 10:UG:384:VAL:HG22  | 10:UG:389:LEU:O     | 2.17                     | 0.45              |
| 13:UJ:1348:LYS:HD2  | 13:UJ:1392:LEU:HD23 | 1.98                     | 0.45              |
| 15:UL:145:ILE:CG1   | 15:UL:159:LEU:HB2   | 2.45                     | 0.45              |
| 15:UL:552:ASP:O     | 15:UL:554:THR:N     | 2.50                     | 0.45              |
| 16:UM:195:GLY:HA3   | 16:UM:246:CYS:SG    | 2.57                     | 0.45              |
| 16:UM:248:PHE:O     | 16:UM:249:LEU:HD22  | 2.17                     | 0.45              |
| 16:UM:514:THR:HA    | 16:UM:529:LEU:O     | 2.16                     | 0.45              |
| 16:UM:532:HIS:HD2   | 16:UM:533:LYS:H     | 1.59                     | 0.45              |
| 20:UQ:18:GLY:HA3    | 20:UQ:781:SER:HB2   | 1.98                     | 0.45              |
| 21:UR:517:THR:HG22  | 21:UR:536:ALA:HB2   | 1.99                     | 0.45              |
| 21:UR:570:PHE:CG    | 21:UR:577:LEU:HD13  | 2.52                     | 0.45              |
| 23:UT:104:GLN:HB2   | 23:UT:150:TRP:CE3   | 2.51                     | 0.45              |
| 23:UT:248:HIS:NE2   | 23:UT:251:ALA:HB2   | 2.31                     | 0.45              |
| 23:UT:493:ASN:OD1   | 23:UT:496:ILE:HB    | 2.17                     | 0.45              |
| 23:UT:1364:ARG:HH22 | 23:UT:1410:LEU:HD22 | 1.82                     | 0.45              |
| 23:UT:1606:ILE:H    | 23:UT:1606:ILE:HD12 | 1.82                     | 0.45              |
| 23:UT:1880:ILE:HD11 | 23:UT:1887:LEU:HA   | 1.98                     | 0.45              |
| 24:UU:232:MET:HE3   | 24:UU:232:MET:HA    | 1.99                     | 0.45              |
| 24:UU:488:ASN:OD1   | 24:UU:489:MET:N     | 2.50                     | 0.45              |
| 24:UU:881:TYR:HA    | 24:UU:884:PHE:HD2   | 1.82                     | 0.45              |
| 25:UV:134:ILE:O     | 25:UV:138:ILE:HG12  | 2.17                     | 0.45              |
| 25:UV:533:LEU:HB3   | 25:UV:606:ASN:ND2   | 2.32                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:UV:703:LYS:HZ2  | 25:UV:1082:GLN:N   | 2.13                     | 0.45              |
| 25:UV:1209:ASP:HB3 | 37:CN:10:LYS:HD2   | 1.99                     | 0.45              |
| 25:UV:1233:ASN:OD1 | 25:UV:1234:PHE:N   | 2.50                     | 0.45              |
| 28:CD:263:ILE:HG21 | 28:CD:267:ASP:OD2  | 2.17                     | 0.45              |
| 29:CE:215:ARG:NH1  | 29:CE:242:SER:HB3  | 2.31                     | 0.45              |
| 29:CE:241:VAL:O    | 29:CE:241:VAL:HG13 | 2.16                     | 0.45              |
| 30:CG:56:ALA:HA    | 30:CG:61:ILE:HD11  | 1.97                     | 0.45              |
| 31:CH:128:GLN:NE2  | 31:CH:129:GLN:HB3  | 2.31                     | 0.45              |
| 31:CH:156:ASN:H    | 31:CH:561:ASN:CG   | 2.20                     | 0.45              |
| 35:CL:831:ARG:HH22 | 35:CL:877:GLU:HA   | 1.81                     | 0.45              |
| 36:CM:22:VAL:O     | 36:CM:25:THR:OG1   | 2.27                     | 0.45              |
| 36:CM:174:ILE:O    | 36:CM:361:ASN:ND2  | 2.31                     | 0.45              |
| 36:CM:185:ARG:NH2  | 36:CM:347:ASN:HD21 | 2.15                     | 0.45              |
| 39:JF:69:ASN:HB3   | 39:JF:72:ASP:HB3   | 1.98                     | 0.45              |
| 39:JG:40:ARG:HH11  | 39:JG:172:PRO:HG3  | 1.82                     | 0.45              |
| 47:JP:147:LEU:HD23 | 47:JP:173:ILE:HB   | 1.98                     | 0.45              |
| 47:JP:276:ASN:HD21 | 66:D3:-7:A:N6      | 2.14                     | 0.45              |
| 47:JP:342:ILE:HD13 | 47:JP:419:VAL:HG12 | 1.98                     | 0.45              |
| 47:JP:378:LYS:HD2  | 47:JP:381:GLU:OE2  | 2.17                     | 0.45              |
| 49:DE:40:GLU:HG2   | 49:DE:40:GLU:O     | 2.17                     | 0.45              |
| 50:DF:180:ARG:HA   | 50:DF:180:ARG:HD2  | 1.65                     | 0.45              |
| 54:DJ:67:PRO:HD2   | 54:DJ:68:LYS:H     | 1.82                     | 0.45              |
| 56:DN:7:ALA:O      | 56:DN:9:LYS:HD3    | 2.16                     | 0.45              |
| 56:DN:98:VAL:HG13  | 56:DN:115:LEU:HD12 | 1.98                     | 0.45              |
| 65:D2:88:U:H2'     | 65:D2:89:C:C6      | 2.52                     | 0.45              |
| 65:D2:195:A:H2'    | 65:D2:196:A:H8     | 1.82                     | 0.45              |
| 66:D3:54:C:O2'     | 66:D3:459:G:N7     | 2.45                     | 0.45              |
| 66:D3:560:U:N3     | 66:D3:568:G:C2     | 2.85                     | 0.45              |
| 66:D3:564:G:H1'    | 66:D3:1596:C:N3    | 2.32                     | 0.45              |
| 66:D3:1026:A:H2'   | 66:D3:1027:A:O4'   | 2.17                     | 0.45              |
| 66:D3:1128:C:C2    | 66:D3:1141:G:C2    | 3.05                     | 0.45              |
| 66:D3:1164:G:C2    | 66:D3:1165:G:C5    | 3.05                     | 0.45              |
| 66:D3:1503:A:H2'   | 66:D3:1504:G:O4'   | 2.17                     | 0.45              |
| 1:CA:231:ARG:NH2   | 28:CD:101:SER:HB3  | 2.31                     | 0.45              |
| 3:JA:191:SER:HB2   | 3:JA:485:TRP:HE1   | 1.82                     | 0.45              |
| 3:JA:567:LEU:HB3   | 3:JA:584:CYS:HB3   | 1.99                     | 0.45              |
| 4:UA:52:TYR:CD2    | 4:UA:80:ILE:HD13   | 2.52                     | 0.45              |
| 4:UA:104:PHE:HD2   | 4:UA:111:PHE:HB3   | 1.82                     | 0.45              |
| 1:CB:254:ALA:O     | 1:CB:258:HIS:CD2   | 2.69                     | 0.45              |
| 5:UB:672:THR:HG23  | 5:UB:682:ARG:HD2   | 1.98                     | 0.45              |
| 7:UD:41:PHE:HD1    | 7:UD:43:PRO:HD3    | 1.81                     | 0.45              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 7:UD:150:ASN:ND2   | 7:UD:198:ASP:OD1    | 2.50                     | 0.45              |
| 7:UD:190:VAL:HA    | 7:UD:205:CYS:HA     | 1.99                     | 0.45              |
| 8:UE:130:ASP:HB2   | 8:UE:137:LEU:HD21   | 1.99                     | 0.45              |
| 8:UE:346:HIS:HB2   | 65:D2:150:G:N3      | 2.32                     | 0.45              |
| 9:UF:152:LYS:CD    | 44:JM:65:LEU:HD11   | 2.42                     | 0.45              |
| 10:UG:477:ALA:HA   | 10:UG:515:ARG:NH2   | 2.31                     | 0.45              |
| 12:UI:430:LEU:HD12 | 12:UI:431:SER:N     | 2.32                     | 0.45              |
| 13:UJ:293:HIS:HA   | 13:UJ:296:LEU:HD12  | 1.99                     | 0.45              |
| 13:UJ:671:LEU:HD23 | 13:UJ:675:ASN:OD1   | 2.17                     | 0.45              |
| 13:UJ:1525:GLU:HB3 | 13:UJ:1529:HIS:CE1  | 2.51                     | 0.45              |
| 13:UJ:1693:GLU:OE2 | 13:UJ:1694:HIS:ND1  | 2.49                     | 0.45              |
| 13:UJ:1725:LEU:O   | 13:UJ:1728:GLN:HG3  | 2.17                     | 0.45              |
| 14:UK:116:LYS:HD3  | 67:D4:323:G:C5'     | 2.47                     | 0.45              |
| 15:UL:498:LYS:HB3  | 15:UL:500:TRP:NE1   | 2.32                     | 0.45              |
| 15:UL:657:GLN:OE1  | 15:UL:657:GLN:N     | 2.50                     | 0.45              |
| 16:UM:126:ILE:HG22 | 16:UM:147:ILE:HD13  | 1.99                     | 0.45              |
| 16:UM:623:LEU:HD12 | 16:UM:633:VAL:O     | 2.16                     | 0.45              |
| 17:UN:294:GLU:HA   | 17:UN:297:LYS:HZ2   | 1.82                     | 0.45              |
| 17:UN:868:GLU:OE1  | 17:UN:868:GLU:N     | 2.50                     | 0.45              |
| 18:UO:186:THR:CG2  | 18:UO:194:ARG:HB2   | 2.47                     | 0.45              |
| 20:UQ:55:TYR:CE1   | 20:UQ:385:ILE:HD12  | 2.51                     | 0.45              |
| 20:UQ:140:LYS:HG3  | 20:UQ:156:THR:HB    | 1.99                     | 0.45              |
| 20:UQ:320:VAL:HG23 | 20:UQ:334:LEU:O     | 2.16                     | 0.45              |
| 20:UQ:598:LYS:HB3  | 20:UQ:638:PHE:CZ    | 2.51                     | 0.45              |
| 21:UR:404:ILE:H    | 21:UR:404:ILE:HD12  | 1.81                     | 0.45              |
| 22:US:411:ASN:O    | 22:US:414:ILE:HG12  | 2.17                     | 0.45              |
| 23:UT:77:LEU:HD22  | 31:CH:67:ALA:HB3    | 1.97                     | 0.45              |
| 23:UT:318:LEU:O    | 23:UT:322:VAL:HG23  | 2.17                     | 0.45              |
| 23:UT:413:GLY:HA2  | 23:UT:416:PHE:HD2   | 1.81                     | 0.45              |
| 23:UT:538:LEU:O    | 23:UT:542:LEU:HG    | 2.17                     | 0.45              |
| 23:UT:700:VAL:HG21 | 23:UT:782:MET:HE3   | 1.99                     | 0.45              |
| 23:UT:1148:GLY:HA2 | 23:UT:1151:ILE:HD12 | 1.99                     | 0.45              |
| 23:UT:1198:PHE:O   | 23:UT:1202:LEU:HG   | 2.17                     | 0.45              |
| 24:UU:902:ASN:HD22 | 24:UU:905:ILE:HG23  | 1.81                     | 0.45              |
| 25:UV:332:TYR:O    | 25:UV:336:VAL:HG12  | 2.17                     | 0.45              |
| 29:CE:145:HIS:HB3  | 29:CE:149:ARG:NH2   | 2.31                     | 0.45              |
| 31:CH:120:ARG:HH12 | 31:CH:532:HIS:CG    | 2.34                     | 0.45              |
| 31:CH:471:GLN:OE1  | 31:CH:471:GLN:N     | 2.50                     | 0.45              |
| 34:CK:335:ARG:HH22 | 35:CL:934:LEU:HD22  | 1.81                     | 0.45              |
| 35:CL:237:TRP:HZ2  | 35:CL:850:GLY:HA2   | 1.81                     | 0.45              |
| 35:CL:778:GLN:HB3  | 35:CL:779:ARG:HD3   | 1.98                     | 0.45              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 36:CM:243:ILE:HG23  | 36:CM:275:VAL:HG21 | 1.99                     | 0.45              |
| 42:JJ:213:LYS:HZ2   | 66:D3:1770:U:H1'   | 1.82                     | 0.45              |
| 45:JN:164:LEU:HD13  | 45:JN:210:THR:HG22 | 1.97                     | 0.45              |
| 45:JN:236:MET:SD    | 66:D3:8:U:C4       | 3.10                     | 0.45              |
| 45:JN:329:ILE:HD11  | 60:DW:89:TRP:CZ2   | 2.51                     | 0.45              |
| 47:JP:301:PHE:CD1   | 47:JP:337:GLY:HA2  | 2.52                     | 0.45              |
| 49:DE:43:PRO:HB2    | 49:DE:45:ILE:HG22  | 1.99                     | 0.45              |
| 49:DE:118:GLU:HG3   | 49:DE:121:TYR:CE1  | 2.52                     | 0.45              |
| 49:DE:118:GLU:HG3   | 49:DE:121:TYR:CZ   | 2.52                     | 0.45              |
| 50:DF:216:GLU:HA    | 50:DF:219:ARG:HG2  | 1.99                     | 0.45              |
| 51:DG:174:LYS:HB2   | 66:D3:79:C:H1'     | 1.99                     | 0.45              |
| 53:DI:26:LYS:HD3    | 66:D3:400:A:C2     | 2.52                     | 0.45              |
| 53:DI:104:ILE:C     | 53:DI:164:ARG:HH12 | 2.19                     | 0.45              |
| 58:DQ:40:GLU:O      | 58:DQ:42:GLU:HG3   | 2.17                     | 0.45              |
| 62:DY:11:LYS:O      | 62:DY:13:ILE:HG12  | 2.17                     | 0.45              |
| 65:D2:97:G:H3'      | 65:D2:98:G:H21     | 1.82                     | 0.45              |
| 65:D2:346:G:H1      | 65:D2:378:C:H42    | 1.64                     | 0.45              |
| 65:D2:415:U:H2'     | 65:D2:416:A:C8     | 2.52                     | 0.45              |
| 65:D2:444:U:H2'     | 65:D2:445:U:O4'    | 2.17                     | 0.45              |
| 66:D3:325:G:H2'     | 66:D3:326:G:C8     | 2.52                     | 0.45              |
| 66:D3:646:C:H2'     | 66:D3:647:G:C8     | 2.52                     | 0.45              |
| 66:D3:793:A:H62     | 66:D3:798:C:H41    | 1.63                     | 0.45              |
| 66:D3:954:G:C6      | 66:D3:955:A:C6     | 3.04                     | 0.45              |
| 70:EC:166:TYR:O     | 70:EC:169:THR:N    | 2.39                     | 0.45              |
| 3:JA:196:PRO:O      | 3:JA:213:ALA:N     | 2.43                     | 0.45              |
| 7:UD:81:PRO:HB3     | 7:UD:85:TRP:CZ3    | 2.51                     | 0.45              |
| 7:UD:396:GLU:O      | 7:UD:398:THR:HG23  | 2.16                     | 0.45              |
| 7:UD:570:ILE:HD12   | 7:UD:584:VAL:HG21  | 1.98                     | 0.45              |
| 8:UE:120:ILE:HG13   | 8:UE:151:LEU:HB2   | 1.99                     | 0.45              |
| 8:UE:354:THR:OG1    | 20:UQ:471:GLN:HG3  | 2.17                     | 0.45              |
| 8:UE:447:SER:OG     | 8:UE:448:ASN:N     | 2.49                     | 0.45              |
| 10:UG:450:GLY:O     | 17:UN:861:LEU:HD11 | 2.17                     | 0.45              |
| 13:UJ:1665:TYR:OH   | 67:D4:144:G:OP2    | 2.34                     | 0.45              |
| 13:UJ:1708:ILE:HG22 | 13:UJ:1712:LYS:HE2 | 1.99                     | 0.45              |
| 15:UL:408:THR:HG21  | 15:UL:447:LEU:CD1  | 2.46                     | 0.45              |
| 16:UM:173:LYS:HB3   | 16:UM:175:TRP:CZ3  | 2.52                     | 0.45              |
| 16:UM:256:ARG:O     | 16:UM:272:SER:HB3  | 2.16                     | 0.45              |
| 16:UM:395:ASP:HB2   | 16:UM:440:VAL:HG23 | 1.99                     | 0.45              |
| 16:UM:590:LEU:O     | 16:UM:601:ILE:HD12 | 2.16                     | 0.45              |
| 18:UO:51:HIS:C      | 18:UO:53:HIS:H     | 2.19                     | 0.45              |
| 18:UO:279:GLY:C     | 18:UO:297:LYS:HA   | 2.38                     | 0.45              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 21:UR:238:LEU:HD23 | 21:UR:279:GLY:HA2   | 1.99                     | 0.45              |
| 22:US:321:ASN:HA   | 22:US:361:LEU:CD2   | 2.46                     | 0.45              |
| 23:UT:44:SER:O     | 31:CH:63:ARG:NH2    | 2.28                     | 0.45              |
| 23:UT:115:HIS:HB2  | 23:UT:161:TYR:CE2   | 2.51                     | 0.45              |
| 23:UT:249:SER:HA   | 23:UT:252:LYS:HG2   | 1.98                     | 0.45              |
| 23:UT:488:TYR:CE2  | 23:UT:490:LYS:HD3   | 2.52                     | 0.45              |
| 23:UT:692:ASP:OD2  | 23:UT:695:LEU:HD12  | 2.17                     | 0.45              |
| 23:UT:886:ASP:HB2  | 38:JC:24:SER:OG     | 2.17                     | 0.45              |
| 23:UT:1127:PHE:HE2 | 23:UT:1169:ASP:HB3  | 1.81                     | 0.45              |
| 23:UT:1309:ASN:HA  | 23:UT:1312:SER:HB2  | 1.99                     | 0.45              |
| 23:UT:1655:ARG:HE  | 23:UT:1693:THR:HG22 | 1.82                     | 0.45              |
| 24:UU:21:SER:OG    | 24:UU:22:LYS:N      | 2.50                     | 0.45              |
| 24:UU:128:LEU:HB3  | 24:UU:140:TYR:HB2   | 1.98                     | 0.45              |
| 24:UU:555:SER:HB3  | 24:UU:557:LEU:HD22  | 1.99                     | 0.45              |
| 25:UV:528:ASP:HA   | 25:UV:614:ARG:NH2   | 2.22                     | 0.45              |
| 25:UV:834:ASN:HD21 | 25:UV:837:ILE:HD11  | 1.82                     | 0.45              |
| 25:UV:932:GLU:O    | 25:UV:936:LEU:HD23  | 2.17                     | 0.45              |
| 25:UV:1228:ASN:OD1 | 25:UV:1229:ASP:N    | 2.47                     | 0.45              |
| 27:UZ:103:VAL:HG11 | 27:UZ:131:VAL:HG11  | 1.99                     | 0.45              |
| 28:CD:183:GLN:NE2  | 28:CD:187:ASP:OD2   | 2.49                     | 0.45              |
| 28:CD:237:LEU:O    | 28:CD:240:LEU:C     | 2.56                     | 0.45              |
| 29:CE:291:VAL:HG22 | 29:CE:295:VAL:HG21  | 1.98                     | 0.45              |
| 30:CF:54:MET:HE1   | 30:CF:67:LEU:HB2    | 1.98                     | 0.45              |
| 31:CH:69:GLN:HA    | 31:CH:72:GLU:CD     | 2.36                     | 0.45              |
| 31:CH:326:GLU:CG   | 31:CH:341:ALA:HB2   | 2.47                     | 0.45              |
| 31:CH:421:ASN:HA   | 31:CH:436:GLU:O     | 2.16                     | 0.45              |
| 36:CM:207:ARG:NE   | 36:CM:268:PRO:HG2   | 2.32                     | 0.45              |
| 39:JF:41:MET:O     | 39:JF:110:LEU:HA    | 2.17                     | 0.45              |
| 39:JF:80:MET:HG3   | 39:JF:82:ARG:HE     | 1.82                     | 0.45              |
| 39:JF:169:ASP:OD1  | 39:JF:169:ASP:N     | 2.50                     | 0.45              |
| 46:JO:258:ARG:CZ   | 56:DN:127:ARG:HH12  | 2.29                     | 0.45              |
| 47:JP:134:ASN:OD1  | 47:JP:152:VAL:HG11  | 2.17                     | 0.45              |
| 47:JP:453:TYR:CE2  | 66:D3:-2:A:C4       | 3.05                     | 0.45              |
| 49:DE:182:TYR:O    | 49:DE:226:PHE:N     | 2.24                     | 0.45              |
| 52:DH:58:LEU:HD21  | 52:DH:90:VAL:HG12   | 1.99                     | 0.45              |
| 53:DI:41:LYS:HD3   | 53:DI:61:GLU:HG2    | 1.98                     | 0.45              |
| 55:DL:111:VAL:HG12 | 55:DL:139:VAL:HG11  | 1.98                     | 0.45              |
| 65:D2:173:G:H2'    | 65:D2:174:U:H6      | 1.82                     | 0.45              |
| 65:D2:191:U:H2'    | 65:D2:192:G:H8      | 1.82                     | 0.45              |
| 65:D2:462:G:C5     | 65:D2:463:A:N7      | 2.85                     | 0.45              |
| 66:D3:279:G:C8     | 66:D3:280:U:H4'     | 2.49                     | 0.45              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 66:D3:762:A:H3'     | 66:D3:763:G:H8      | 1.82                     | 0.45              |
| 66:D3:823:G:H1'     | 66:D3:850:A:N1      | 2.33                     | 0.45              |
| 66:D3:1154:G:N2     | 66:D3:1155:G:C4     | 2.85                     | 0.45              |
| 78:EK:327:LYS:O     | 78:EK:387:GLN:N     | 2.34                     | 0.45              |
| 79:EN:353:PHE:O     | 79:EN:357:MET:N     | 2.42                     | 0.45              |
| 1:CA:233:LEU:O      | 1:CA:234:ILE:HD13   | 2.17                     | 0.44              |
| 3:JA:2:ALA:HB3      | 3:JA:4:LYS:NZ       | 2.32                     | 0.44              |
| 4:UA:521:LEU:HD11   | 4:UA:530:VAL:CG1    | 2.47                     | 0.44              |
| 5:UB:628:PRO:HD2    | 5:UB:631:GLN:HB2    | 1.99                     | 0.44              |
| 5:UB:798:LYS:O      | 5:UB:802:GLU:HG3    | 2.17                     | 0.44              |
| 6:UC:544:ILE:HD13   | 35:CL:834:TRP:CE2   | 2.52                     | 0.44              |
| 6:UC:566:ARG:NH1    | 66:D3:479:C:OP1     | 2.49                     | 0.44              |
| 7:UD:113:ARG:HD3    | 7:UD:174:PRO:HB3    | 2.00                     | 0.44              |
| 7:UD:190:VAL:HG23   | 7:UD:205:CYS:HB3    | 1.99                     | 0.44              |
| 7:UD:757:ARG:HE     | 7:UD:759:PRO:HB3    | 1.82                     | 0.44              |
| 9:UF:68:ALA:O       | 9:UF:72:LYS:HG2     | 2.17                     | 0.44              |
| 10:UG:240:GLN:HB3   | 10:UG:247:MET:CE    | 2.47                     | 0.44              |
| 10:UG:483:ILE:HG13  | 10:UG:516:VAL:HG22  | 1.98                     | 0.44              |
| 10:UG:508:VAL:HG12  | 46:JO:73:LEU:HB3    | 1.99                     | 0.44              |
| 11:UH:679:ILE:HA    | 12:UI:460:LEU:HD11  | 1.99                     | 0.44              |
| 13:UJ:1357:ASN:O    | 13:UJ:1360:GLN:HG2  | 2.17                     | 0.44              |
| 14:UK:229:SER:OG    | 14:UK:245:LYS:HB3   | 2.16                     | 0.44              |
| 15:UL:272:PHE:CZ    | 15:UL:284:PHE:HB2   | 2.53                     | 0.44              |
| 15:UL:408:THR:HG21  | 15:UL:447:LEU:HD11  | 1.98                     | 0.44              |
| 15:UL:416:ILE:HG12  | 15:UL:459:LEU:HD11  | 1.98                     | 0.44              |
| 16:UM:509:ALA:HB2   | 16:UM:515:CYS:HB2   | 1.99                     | 0.44              |
| 18:UO:51:HIS:HD1    | 18:UO:53:HIS:CG     | 2.35                     | 0.44              |
| 20:UQ:47:PRO:HB3    | 20:UQ:52:ILE:HD12   | 1.99                     | 0.44              |
| 20:UQ:414:ILE:H     | 20:UQ:414:ILE:HD12  | 1.82                     | 0.44              |
| 21:UR:562:LEU:O     | 21:UR:581:ASN:ND2   | 2.35                     | 0.44              |
| 22:US:426:PHE:CE2   | 39:JG:250:ASN:HB3   | 2.52                     | 0.44              |
| 23:UT:509:ALA:HA    | 23:UT:547:ASN:HD21  | 1.81                     | 0.44              |
| 23:UT:1914:THR:O    | 23:UT:1918:LEU:HD23 | 2.17                     | 0.44              |
| 25:UV:159:SER:OG    | 25:UV:594:ILE:O     | 2.23                     | 0.44              |
| 25:UV:389:GLY:N     | 25:UV:392:GLU:OE1   | 2.32                     | 0.44              |
| 25:UV:587:GLY:HA3   | 25:UV:611:ASP:N     | 2.32                     | 0.44              |
| 25:UV:723:ASN:O     | 25:UV:724:LEU:HD23  | 2.17                     | 0.44              |
| 25:UV:916:PHE:CE2   | 25:UV:920:LEU:HD11  | 2.52                     | 0.44              |
| 25:UV:1136:LEU:HD13 | 37:CN:174:PRO:HG2   | 1.99                     | 0.44              |
| 28:CD:205:GLU:HG2   | 28:CD:254:ASN:HB3   | 1.99                     | 0.44              |
| 28:CD:389:ILE:HA    | 30:CG:62:GLU:HG2    | 1.98                     | 0.44              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 28:CD:395:GLU:O    | 31:CH:454:GLU:HG3   | 2.17                     | 0.44              |
| 29:CE:98:ILE:O     | 29:CE:101:LEU:HG    | 2.17                     | 0.44              |
| 30:CG:33:LEU:HD11  | 30:CG:100:ALA:HB1   | 1.99                     | 0.44              |
| 31:CH:458:GLU:OE1  | 31:CH:462:ARG:NH1   | 2.50                     | 0.44              |
| 38:JC:293:ASP:C    | 38:JC:295:ARG:H     | 2.21                     | 0.44              |
| 39:JF:190:GLN:O    | 39:JF:193:ILE:N     | 2.50                     | 0.44              |
| 39:JF:196:LEU:HD21 | 39:JF:202:ILE:HD13  | 1.99                     | 0.44              |
| 39:JF:232:LEU:HD23 | 39:JF:236:VAL:HG23  | 1.98                     | 0.44              |
| 39:JG:90:ASP:O     | 39:JG:93:HIS:N      | 2.50                     | 0.44              |
| 45:JN:275:ILE:H    | 45:JN:278:THR:HG22  | 1.81                     | 0.44              |
| 47:JP:314:SER:HB3  | 47:JP:356:TYR:CE2   | 2.51                     | 0.44              |
| 49:DE:195:ILE:HG22 | 49:DE:210:ILE:HG13  | 1.99                     | 0.44              |
| 50:DF:214:LYS:HG2  | 50:DF:218:GLU:OE2   | 2.17                     | 0.44              |
| 51:DG:211:LEU:HD12 | 51:DG:214:LYS:HE2   | 1.99                     | 0.44              |
| 65:D2:270:U:H2'    | 65:D2:271:G:O4'     | 2.17                     | 0.44              |
| 66:D3:0:U:H4'      | 66:D3:1:U:C5'       | 2.47                     | 0.44              |
| 66:D3:95:G:C5      | 66:D3:96:G:C8       | 3.05                     | 0.44              |
| 66:D3:212:U:O4     | 66:D3:213:A:N6      | 2.50                     | 0.44              |
| 66:D3:568:G:C2     | 66:D3:569:C:C2      | 3.06                     | 0.44              |
| 66:D3:905:A:C2     | 66:D3:906:A:H1'     | 2.52                     | 0.44              |
| 66:D3:1260:U:H2'   | 66:D3:1261:G:C8     | 2.52                     | 0.44              |
| 66:D3:1659:A:H2'   | 66:D3:1660:A:H8     | 1.82                     | 0.44              |
| 67:D4:14:A:N7      | 67:D4:15:U:N3       | 2.64                     | 0.44              |
| 67:D4:147:C:N3     | 67:D4:165:G:N1      | 2.42                     | 0.44              |
| 69:EB:286:ASP:O    | 69:EB:290:ARG:N     | 2.43                     | 0.44              |
| 70:EC:164:GLY:O    | 70:EC:171:LEU:N     | 2.43                     | 0.44              |
| 1:CA:109:LYS:HE2   | 1:CA:141:TYR:CE2    | 2.52                     | 0.44              |
| 4:UA:403:PHE:CD1   | 4:UA:438:VAL:HG11   | 2.53                     | 0.44              |
| 4:UA:753:LYS:O     | 4:UA:756:GLU:HG3    | 2.17                     | 0.44              |
| 7:UD:327:LEU:HD23  | 7:UD:327:LEU:H      | 1.82                     | 0.44              |
| 7:UD:773:LYS:NZ    | 65:D2:83:U:H3       | 2.15                     | 0.44              |
| 8:UE:8:SER:O       | 8:UE:293:ASN:ND2    | 2.50                     | 0.44              |
| 10:UG:74:LEU:HD22  | 10:UG:83:THR:HB     | 1.98                     | 0.44              |
| 10:UG:289:MET:HB2  | 10:UG:303:ILE:HD11  | 1.98                     | 0.44              |
| 12:UI:510:ALA:N    | 12:UI:513:ARG:HH21  | 2.15                     | 0.44              |
| 13:UJ:102:LEU:HD13 | 13:UJ:135:LEU:HA    | 1.99                     | 0.44              |
| 13:UJ:564:VAL:HA   | 13:UJ:567:LEU:HG    | 2.00                     | 0.44              |
| 13:UJ:1569:THR:O   | 13:UJ:1573:LEU:HD23 | 2.18                     | 0.44              |
| 15:UL:398:ASP:OD1  | 15:UL:399:ILE:N     | 2.44                     | 0.44              |
| 16:UM:42:ILE:O     | 16:UM:53:LEU:N      | 2.50                     | 0.44              |
| 16:UM:148:SER:O    | 16:UM:194:ARG:NH2   | 2.51                     | 0.44              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 16:UM:463:ILE:HG12  | 16:UM:487:ARG:O    | 2.18                     | 0.44              |
| 16:UM:537:TRP:HD1   | 16:UM:553:GLY:HA2  | 1.76                     | 0.44              |
| 20:UQ:321:MET:CE    | 20:UQ:356:LEU:HD13 | 2.48                     | 0.44              |
| 20:UQ:765:TRP:CG    | 20:UQ:766:ILE:N    | 2.85                     | 0.44              |
| 21:UR:45:ILE:H      | 21:UR:45:ILE:HD12  | 1.83                     | 0.44              |
| 22:US:270:SER:OG    | 22:US:273:GLN:HG2  | 2.16                     | 0.44              |
| 22:US:399:ILE:CD1   | 22:US:480:LEU:HB3  | 2.46                     | 0.44              |
| 23:UT:128:ALA:O     | 23:UT:132:LEU:HG   | 2.17                     | 0.44              |
| 23:UT:498:ILE:CG2   | 23:UT:499:PRO:HD3  | 2.46                     | 0.44              |
| 23:UT:851:HIS:CD2   | 23:UT:924:TYR:HH   | 2.35                     | 0.44              |
| 23:UT:1023:LEU:HD23 | 23:UT:1078:SER:HB3 | 1.97                     | 0.44              |
| 23:UT:1189:LEU:HD23 | 23:UT:1198:PHE:HE2 | 1.81                     | 0.44              |
| 23:UT:1375:ILE:HD13 | 23:UT:1424:MET:HB3 | 1.98                     | 0.44              |
| 25:UV:932:GLU:HA    | 25:UV:935:GLU:OE2  | 2.18                     | 0.44              |
| 25:UV:1160:SER:C    | 25:UV:1187:LYS:HZ2 | 2.21                     | 0.44              |
| 26:UX:84:ARG:NH2    | 60:DW:97:ARG:NH1   | 2.63                     | 0.44              |
| 26:UX:121:ARG:NH1   | 47:JP:369:ASP:O    | 2.26                     | 0.44              |
| 26:UX:121:ARG:O     | 47:JP:67:ARG:NH1   | 2.49                     | 0.44              |
| 29:CE:16:LYS:N      | 29:CE:45:ALA:HB2   | 2.32                     | 0.44              |
| 29:CE:50:PHE:HD2    | 29:CE:51:ASN:O     | 2.00                     | 0.44              |
| 29:CE:84:LYS:HB2    | 29:CE:106:ASN:CG   | 2.37                     | 0.44              |
| 31:CH:458:GLU:OE2   | 31:CH:459:LEU:HG   | 2.17                     | 0.44              |
| 32:CI:90:THR:HG22   | 32:CI:91:LYS:H     | 1.82                     | 0.44              |
| 33:CJ:162:THR:HG23  | 33:CJ:264:GLY:O    | 2.16                     | 0.44              |
| 35:CL:1138:ARG:NH1  | 66:D3:492:A:C8     | 2.84                     | 0.44              |
| 37:CN:4:GLU:O       | 37:CN:149:ALA:HA   | 2.18                     | 0.44              |
| 37:CN:16:VAL:HG13   | 37:CN:144:TYR:CD2  | 2.52                     | 0.44              |
| 38:JC:160:ASN:ND2   | 38:JC:179:ASP:HA   | 2.33                     | 0.44              |
| 39:JF:89:PRO:O      | 39:JF:92:THR:OG1   | 2.31                     | 0.44              |
| 46:JO:190:CYS:HB2   | 46:JO:196:PRO:HG3  | 1.98                     | 0.44              |
| 47:JP:350:HIS:HB2   | 47:JP:368:ASP:HB3  | 2.00                     | 0.44              |
| 50:DF:31:GLU:HA     | 50:DF:34:GLN:OE1   | 2.17                     | 0.44              |
| 50:DF:45:LYS:HE2    | 50:DF:46:TRP:CH2   | 2.52                     | 0.44              |
| 50:DF:200:ASN:ND2   | 50:DF:208:SER:HB3  | 2.32                     | 0.44              |
| 54:DJ:157:ASP:OD2   | 54:DJ:158:PHE:N    | 2.45                     | 0.44              |
| 58:DQ:37:THR:C      | 58:DQ:38:LEU:HD22  | 2.37                     | 0.44              |
| 65:D2:8:A:C5        | 65:D2:9:G:H1'      | 2.52                     | 0.44              |
| 65:D2:415:U:C2      | 65:D2:416:A:C8     | 3.05                     | 0.44              |
| 66:D3:445:A:C8      | 66:D3:525:A:C8     | 3.06                     | 0.44              |
| 66:D3:761:G:H8      | 66:D3:763:G:N7     | 2.15                     | 0.44              |
| 66:D3:892:A:C6      | 66:D3:921:U:N3     | 2.85                     | 0.44              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 66:D3:1035:G:N2    | 66:D3:1083:G:C8     | 2.86                     | 0.44              |
| 66:D3:1170:G:C6    | 66:D3:1574:G:C4     | 3.05                     | 0.44              |
| 66:D3:1658:G:H2'   | 66:D3:1659:A:C8     | 2.52                     | 0.44              |
| 66:D3:1707:A:C5    | 66:D3:1708:U:C4     | 3.05                     | 0.44              |
| 66:D3:1734:U:H2'   | 66:D3:1735:U:C6     | 2.52                     | 0.44              |
| 66:D3:1750:A:H2'   | 66:D3:1751:C:H6     | 1.83                     | 0.44              |
| 1:CA:121:LYS:HE2   | 1:CA:121:LYS:HB3    | 1.60                     | 0.44              |
| 2:DA:33:LYS:HE2    | 2:DA:42:ASN:HB3     | 2.00                     | 0.44              |
| 2:DA:243:LYS:H     | 25:UV:656:ARG:HE    | 1.66                     | 0.44              |
| 3:JA:568:LEU:HD11  | 3:JA:580:PRO:HB2    | 1.99                     | 0.44              |
| 4:UA:585:TYR:CD1   | 4:UA:592:ILE:HG12   | 2.53                     | 0.44              |
| 1:CB:180:SER:O     | 1:CB:184:VAL:HG13   | 2.18                     | 0.44              |
| 5:UB:612:THR:HG23  | 5:UB:614:ILE:N      | 2.32                     | 0.44              |
| 7:UD:127:ASP:N     | 7:UD:132:LEU:O      | 2.33                     | 0.44              |
| 7:UD:561:LYS:NZ    | 7:UD:563:LEU:HA     | 2.33                     | 0.44              |
| 10:UG:134:VAL:HG11 | 10:UG:168:VAL:HG11  | 2.00                     | 0.44              |
| 10:UG:172:LYS:HB3  | 10:UG:173:TYR:CD2   | 2.53                     | 0.44              |
| 11:UH:527:LEU:HB2  | 11:UH:553:GLN:NE2   | 2.33                     | 0.44              |
| 12:UI:437:ILE:HG22 | 12:UI:456:LEU:HD12  | 1.98                     | 0.44              |
| 13:UJ:345:ASP:OD1  | 13:UJ:346:LYS:N     | 2.51                     | 0.44              |
| 13:UJ:1744:ILE:O   | 13:UJ:1748:VAL:HG12 | 2.17                     | 0.44              |
| 14:UK:137:VAL:HG12 | 14:UK:139:SER:H     | 1.82                     | 0.44              |
| 15:UL:167:THR:HG21 | 15:UL:207:CYS:O     | 2.17                     | 0.44              |
| 15:UL:760:ILE:O    | 15:UL:764:GLU:OE1   | 2.35                     | 0.44              |
| 15:UL:821:LEU:HD22 | 15:UL:860:ILE:HD11  | 1.98                     | 0.44              |
| 16:UM:109:ASP:OD2  | 16:UM:109:ASP:N     | 2.50                     | 0.44              |
| 16:UM:464:LYS:HA   | 16:UM:486:THR:HA    | 1.98                     | 0.44              |
| 16:UM:669:LEU:HD12 | 16:UM:684:LEU:HB3   | 2.00                     | 0.44              |
| 18:UO:445:TRP:CZ3  | 18:UO:448:LYS:HD2   | 2.52                     | 0.44              |
| 20:UQ:292:LEU:C    | 20:UQ:293:LEU:HD22  | 2.37                     | 0.44              |
| 20:UQ:665:ILE:HG22 | 20:UQ:669:ASN:HB2   | 1.99                     | 0.44              |
| 20:UQ:745:ILE:O    | 20:UQ:754:LEU:N     | 2.50                     | 0.44              |
| 22:US:156:TRP:CZ3  | 22:US:212:LEU:HA    | 2.52                     | 0.44              |
| 22:US:188:PHE:HA   | 22:US:237:GLU:O     | 2.18                     | 0.44              |
| 23:UT:760:THR:HA   | 23:UT:763:GLU:HG3   | 1.99                     | 0.44              |
| 23:UT:1399:LEU:HG  | 23:UT:1400:PRO:HD3  | 1.98                     | 0.44              |
| 23:UT:1533:MET:O   | 23:UT:1537:LYS:HG2  | 2.18                     | 0.44              |
| 24:UU:51:VAL:HG13  | 24:UU:58:PHE:HD2    | 1.82                     | 0.44              |
| 24:UU:510:LEU:HD23 | 24:UU:511:ASP:O     | 2.17                     | 0.44              |
| 25:UV:122:LEU:HA   | 25:UV:125:GLU:HG3   | 1.98                     | 0.44              |
| 25:UV:316:ARG:HG2  | 66:D3:1697:G:OP1    | 2.17                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:UV:705:HIS:O    | 25:UV:708:LEU:HB2  | 2.17                     | 0.44              |
| 25:UV:1038:GLN:OE1 | 25:UV:1038:GLN:N   | 2.51                     | 0.44              |
| 25:UV:1136:LEU:HB2 | 37:CN:174:PRO:HG2  | 1.99                     | 0.44              |
| 26:UX:60:LYS:HE3   | 54:DJ:100:LYS:NZ   | 2.33                     | 0.44              |
| 26:UX:91:LEU:HD13  | 54:DJ:54:ARG:HH11  | 1.80                     | 0.44              |
| 28:CD:175:ILE:O    | 28:CD:178:ILE:HG22 | 2.18                     | 0.44              |
| 28:CD:195:VAL:HG13 | 28:CD:216:PHE:CE2  | 2.52                     | 0.44              |
| 31:CH:342:ARG:O    | 31:CH:344:ARG:HG3  | 2.17                     | 0.44              |
| 32:CI:141:ASN:OD1  | 32:CI:141:ASN:O    | 2.35                     | 0.44              |
| 33:CJ:89:ILE:HG22  | 33:CJ:91:THR:OG1   | 2.17                     | 0.44              |
| 33:CJ:206:LEU:HB3  | 33:CJ:224:PHE:HE2  | 1.83                     | 0.44              |
| 34:CK:366:GLU:HB3  | 34:CK:370:ARG:NH2  | 2.30                     | 0.44              |
| 35:CL:368:LYS:NZ   | 35:CL:369:ASP:OD2  | 2.36                     | 0.44              |
| 35:CL:760:LYS:O    | 35:CL:764:ILE:HG12 | 2.17                     | 0.44              |
| 38:JC:73:ALA:O     | 38:JC:81:ILE:HA    | 2.18                     | 0.44              |
| 38:JC:100:GLU:CD   | 53:DI:35:ASN:HD21  | 2.20                     | 0.44              |
| 38:JC:171:ARG:HH11 | 43:JK:469:GLN:H    | 1.66                     | 0.44              |
| 38:JC:257:LEU:HG   | 43:JK:493:PHE:CE2  | 2.52                     | 0.44              |
| 39:JF:69:ASN:HB3   | 39:JF:72:ASP:CB    | 2.47                     | 0.44              |
| 39:JG:190:GLN:HE22 | 39:JG:248:ALA:HA   | 1.81                     | 0.44              |
| 42:JJ:193:LEU:HD23 | 42:JJ:193:LEU:HA   | 1.83                     | 0.44              |
| 50:DF:27:THR:O     | 50:DF:29:ILE:HG12  | 2.17                     | 0.44              |
| 57:DO:15:GLY:O     | 57:DO:79:VAL:HA    | 2.17                     | 0.44              |
| 58:DQ:123:ARG:HA   | 58:DQ:123:ARG:NH2  | 2.33                     | 0.44              |
| 65:D2:166:U:C4     | 65:D2:167:U:C4     | 3.05                     | 0.44              |
| 65:D2:292:A:N1     | 67:D4:62:C:C4      | 2.86                     | 0.44              |
| 65:D2:376:U:H2'    | 65:D2:377:U:C6     | 2.52                     | 0.44              |
| 65:D2:423:C:C2     | 65:D2:435:G:C2     | 3.06                     | 0.44              |
| 66:D3:103:A:H2'    | 66:D3:309:C:N4     | 2.31                     | 0.44              |
| 66:D3:336:G:H3'    | 66:D3:338:C:C5     | 2.52                     | 0.44              |
| 66:D3:890:C:H2'    | 66:D3:891:A:H8     | 1.81                     | 0.44              |
| 66:D3:940:A:H2'    | 66:D3:941:A:C8     | 2.53                     | 0.44              |
| 66:D3:1056:U:H3'   | 66:D3:1057:U:H6    | 1.82                     | 0.44              |
| 66:D3:1116:A:C6    | 66:D3:1117:U:C4    | 3.06                     | 0.44              |
| 3:JA:511:SER:OG    | 3:JA:512:GLN:OE1   | 2.35                     | 0.44              |
| 3:JA:841:ARG:NH1   | 3:JA:857:ASP:HB2   | 2.33                     | 0.44              |
| 3:JA:874:SER:HB3   | 3:JA:923:TYR:CE1   | 2.52                     | 0.44              |
| 4:UA:345:PHE:CE2   | 4:UA:677:PRO:HG2   | 2.51                     | 0.44              |
| 4:UA:369:ILE:HD11  | 4:UA:390:VAL:HG11  | 1.99                     | 0.44              |
| 4:UA:478:CYS:SG    | 4:UA:520:ALA:HA    | 2.57                     | 0.44              |
| 4:UA:564:PHE:CE1   | 4:UA:576:ARG:HD2   | 2.53                     | 0.44              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:CB:267:VAL:HG22   | 1:CB:269:ILE:HD11   | 1.98                     | 0.44              |
| 5:UB:588:PHE:HZ     | 5:UB:666:GLN:HB3    | 1.82                     | 0.44              |
| 7:UD:316:LYS:HD3    | 7:UD:316:LYS:HA     | 1.82                     | 0.44              |
| 9:UF:110:TRP:CE3    | 9:UF:136:LEU:HD13   | 2.53                     | 0.44              |
| 9:UF:332:ASP:N      | 9:UF:332:ASP:OD1    | 2.49                     | 0.44              |
| 10:UG:95:VAL:HG12   | 10:UG:96:ASP:H      | 1.83                     | 0.44              |
| 10:UG:113:PRO:HA    | 10:UG:395:GLN:HA    | 2.00                     | 0.44              |
| 10:UG:138:ASP:O     | 10:UG:138:ASP:OD2   | 2.35                     | 0.44              |
| 10:UG:187:LEU:HD21  | 32:CI:21:TRP:HZ3    | 1.83                     | 0.44              |
| 10:UG:449:ILE:HG22  | 10:UG:449:ILE:O     | 2.17                     | 0.44              |
| 13:UJ:340:ASP:OD1   | 13:UJ:340:ASP:N     | 2.50                     | 0.44              |
| 13:UJ:1380:LEU:HD12 | 13:UJ:1380:LEU:HA   | 1.73                     | 0.44              |
| 13:UJ:1605:LEU:HD23 | 13:UJ:1608:PHE:CD2  | 2.52                     | 0.44              |
| 15:UL:40:GLN:HA     | 15:UL:53:ASP:HA     | 2.00                     | 0.44              |
| 15:UL:466:ASP:OD1   | 15:UL:467:THR:N     | 2.50                     | 0.44              |
| 15:UL:521:LYS:HG3   | 15:UL:523:HIS:NE2   | 2.33                     | 0.44              |
| 15:UL:576:VAL:HA    | 15:UL:592:SER:HA    | 1.98                     | 0.44              |
| 15:UL:589:ILE:HD12  | 15:UL:621:VAL:HB    | 1.99                     | 0.44              |
| 15:UL:633:CYS:HB2   | 15:UL:660:VAL:CG1   | 2.47                     | 0.44              |
| 15:UL:767:GLU:HA    | 15:UL:770:ASN:OD1   | 2.16                     | 0.44              |
| 20:UQ:105:HIS:CE1   | 20:UQ:122:LYS:HD2   | 2.53                     | 0.44              |
| 22:US:399:ILE:CG1   | 22:US:400:PRO:HD3   | 2.47                     | 0.44              |
| 23:UT:19:PHE:CZ     | 23:UT:23:ILE:HD11   | 2.52                     | 0.44              |
| 23:UT:233:LEU:HD12  | 23:UT:278:ILE:HG22  | 1.99                     | 0.44              |
| 23:UT:922:MET:O     | 23:UT:926:LEU:N     | 2.40                     | 0.44              |
| 23:UT:1640:CYS:CB   | 23:UT:1680:THR:HG21 | 2.43                     | 0.44              |
| 23:UT:1670:LEU:HA   | 23:UT:1673:VAL:HG12 | 2.00                     | 0.44              |
| 24:UU:882:GLU:OE1   | 24:UU:916:HIS:HE1   | 2.00                     | 0.44              |
| 25:UV:256:TYR:CZ    | 25:UV:594:ILE:HG23  | 2.52                     | 0.44              |
| 25:UV:604:GLY:HA2   | 25:UV:611:ASP:O     | 2.17                     | 0.44              |
| 25:UV:903:SER:O     | 25:UV:906:TYR:N     | 2.50                     | 0.44              |
| 25:UV:1205:LYS:N    | 25:UV:1213:ILE:O    | 2.32                     | 0.44              |
| 27:UZ:176:VAL:HA    | 27:UZ:179:GLN:OE1   | 2.17                     | 0.44              |
| 28:CD:180:LEU:CD2   | 29:CE:183:ARG:HG2   | 2.45                     | 0.44              |
| 29:CE:155:SER:HB3   | 29:CE:158:LYS:CD    | 2.47                     | 0.44              |
| 29:CE:307:ILE:O     | 29:CE:311:LYS:HB2   | 2.18                     | 0.44              |
| 29:CE:309:LEU:HG    | 29:CE:371:LEU:CD2   | 2.43                     | 0.44              |
| 30:CG:39:GLU:O      | 30:CG:43:THR:HG23   | 2.16                     | 0.44              |
| 30:CG:56:ALA:HB2    | 30:CG:80:PHE:HB3    | 1.98                     | 0.44              |
| 31:CH:401:SER:OG    | 31:CH:402:ILE:N     | 2.51                     | 0.44              |
| 31:CH:545:LYS:HD2   | 31:CH:559:ALA:HB3   | 2.00                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:CI:25:GLN:O     | 32:CI:25:GLN:HG2   | 2.18                     | 0.44              |
| 32:CI:113:VAL:CG2  | 32:CI:124:ILE:HD11 | 2.47                     | 0.44              |
| 34:CK:493:GLN:OE1  | 34:CK:493:GLN:N    | 2.49                     | 0.44              |
| 37:CN:18:PHE:HZ    | 37:CN:70:PHE:CE1   | 2.36                     | 0.44              |
| 39:JG:104:ILE:HG23 | 39:JG:110:LEU:HD22 | 1.99                     | 0.44              |
| 45:JN:280:LYS:HE3  | 65:D2:382:U:C5     | 2.52                     | 0.44              |
| 46:JO:90:ASP:O     | 46:JO:93:ILE:N     | 2.50                     | 0.44              |
| 47:JP:240:SER:O    | 47:JP:240:SER:OG   | 2.27                     | 0.44              |
| 51:DG:93:LYS:CD    | 66:D3:405:C:H5''   | 2.48                     | 0.44              |
| 61:DX:48:HIS:HE1   | 66:D3:599:A:N3     | 2.16                     | 0.44              |
| 61:DX:109:ARG:HH22 | 61:DX:118:PRO:HA   | 1.82                     | 0.44              |
| 65:D2:414:G:H2'    | 65:D2:415:U:C6     | 2.53                     | 0.44              |
| 66:D3:413:U:H2'    | 66:D3:414:C:C6     | 2.53                     | 0.44              |
| 66:D3:1590:G:H8    | 66:D3:1590:G:O5'   | 1.99                     | 0.44              |
| 66:D3:1654:G:H2'   | 66:D3:1655:A:C8    | 2.50                     | 0.44              |
| 67:D4:78:G:C6      | 67:D4:330:A:C6     | 3.05                     | 0.44              |
| 67:D4:332:G:H2'    | 67:D4:333:U:O4'    | 2.16                     | 0.44              |
| 79:EN:401:ILE:O    | 79:EN:405:LYS:N    | 2.50                     | 0.44              |
| 3:JA:552:ASP:OD1   | 3:JA:552:ASP:N     | 2.48                     | 0.44              |
| 3:JA:855:ILE:O     | 3:JA:859:ILE:HG23  | 2.17                     | 0.44              |
| 3:JA:884:ILE:O     | 3:JA:888:ILE:HG12  | 2.17                     | 0.44              |
| 4:UA:62:ASP:OD1    | 4:UA:63:LEU:N      | 2.50                     | 0.44              |
| 4:UA:83:ASN:HB2    | 4:UA:90:LEU:CD1    | 2.46                     | 0.44              |
| 3:JB:55:VAL:O      | 3:JB:103:ILE:HA    | 2.17                     | 0.44              |
| 5:UB:476:ASP:HA    | 5:UB:479:ASN:ND2   | 2.32                     | 0.44              |
| 5:UB:605:ASP:HB2   | 5:UB:607:THR:HG23  | 2.00                     | 0.44              |
| 10:UG:409:ALA:HA   | 47:JP:6:ILE:HD13   | 2.00                     | 0.44              |
| 10:UG:511:GLU:O    | 10:UG:515:ARG:HG2  | 2.17                     | 0.44              |
| 11:UH:534:LEU:O    | 11:UH:537:THR:OG1  | 2.33                     | 0.44              |
| 11:UH:564:ASN:HB2  | 11:UH:565:GLU:OE1  | 2.17                     | 0.44              |
| 13:UJ:412:GLU:O    | 13:UJ:416:LEU:HG   | 2.17                     | 0.44              |
| 13:UJ:786:TYR:CZ   | 29:CE:85:SER:HA    | 2.52                     | 0.44              |
| 14:UK:51:LEU:HA    | 14:UK:51:LEU:HD23  | 1.80                     | 0.44              |
| 14:UK:160:ASN:ND2  | 65:D2:206:A:H5''   | 2.32                     | 0.44              |
| 15:UL:100:ASP:O    | 15:UL:100:ASP:OD2  | 2.35                     | 0.44              |
| 15:UL:410:SER:HB2  | 15:UL:432:TYR:CZ   | 2.52                     | 0.44              |
| 15:UL:558:PHE:CD1  | 15:UL:565:PHE:HA   | 2.53                     | 0.44              |
| 15:UL:941:THR:HG22 | 66:D3:1632:C:N4    | 2.33                     | 0.44              |
| 16:UM:362:LEU:HD11 | 16:UM:384:TYR:CD2  | 2.53                     | 0.44              |
| 16:UM:462:THR:HA   | 16:UM:488:HIS:HA   | 2.00                     | 0.44              |
| 20:UQ:363:ASN:ND2  | 20:UQ:366:ASN:O    | 2.48                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:UQ:381:SER:O    | 20:UQ:381:SER:OG   | 2.35                     | 0.44              |
| 20:UQ:390:PRO:HG2  | 20:UQ:392:PHE:CZ   | 2.52                     | 0.44              |
| 20:UQ:628:ASP:H    | 20:UQ:658:GLU:HA   | 1.82                     | 0.44              |
| 20:UQ:715:GLU:CD   | 20:UQ:716:ARG:HD2  | 2.38                     | 0.44              |
| 21:UR:560:THR:HG22 | 65:D2:280:A:OP1    | 2.17                     | 0.44              |
| 22:US:188:PHE:HB3  | 22:US:190:ASP:OD1  | 2.18                     | 0.44              |
| 23:UT:100:GLU:HA   | 23:UT:103:LEU:HD12 | 2.00                     | 0.44              |
| 23:UT:146:ASN:HA   | 23:UT:149:GLU:OE2  | 2.18                     | 0.44              |
| 23:UT:277:ASP:O    | 23:UT:280:MET:HG3  | 2.18                     | 0.44              |
| 23:UT:692:ASP:HB3  | 23:UT:695:LEU:HB2  | 1.99                     | 0.44              |
| 23:UT:863:THR:HG22 | 23:UT:867:LYS:HZ3  | 1.82                     | 0.44              |
| 23:UT:1312:SER:O   | 23:UT:1316:MET:HG2 | 2.17                     | 0.44              |
| 23:UT:1543:GLN:O   | 23:UT:1546:GLN:HG2 | 2.18                     | 0.44              |
| 23:UT:1847:LEU:HA  | 54:DJ:94:ASP:OD2   | 2.17                     | 0.44              |
| 24:UU:166:GLU:O    | 24:UU:184:THR:OG1  | 2.36                     | 0.44              |
| 24:UU:226:VAL:HG23 | 24:UU:250:ARG:HG3  | 1.98                     | 0.44              |
| 24:UU:295:TYR:OH   | 24:UU:351:GLN:OE1  | 2.36                     | 0.44              |
| 25:UV:515:ILE:HG13 | 25:UV:522:LYS:HD2  | 1.98                     | 0.44              |
| 29:CE:16:LYS:HB2   | 29:CE:45:ALA:HB2   | 1.98                     | 0.44              |
| 29:CE:281:LYS:HG2  | 29:CE:288:THR:HG21 | 1.99                     | 0.44              |
| 31:CH:195:GLN:HE21 | 31:CH:196:LEU:C    | 2.21                     | 0.44              |
| 31:CH:322:HIS:HB2  | 31:CH:343:ASP:OD2  | 2.18                     | 0.44              |
| 31:CH:498:VAL:HG12 | 31:CH:511:LEU:HB3  | 1.99                     | 0.44              |
| 37:CN:20:LEU:HD11  | 37:CN:35:HIS:HB2   | 1.99                     | 0.44              |
| 39:JF:167:ILE:HG22 | 39:JF:171:LEU:CD1  | 2.47                     | 0.44              |
| 39:JF:219:GLU:OE1  | 39:JF:219:GLU:N    | 2.35                     | 0.44              |
| 44:JM:184:ASN:HB3  | 44:JM:185:LYS:NZ   | 2.30                     | 0.44              |
| 45:JN:149:LEU:HD12 | 46:JO:198:TYR:CD1  | 2.53                     | 0.44              |
| 45:JN:316:ARG:HD3  | 66:D3:1036:A:N3    | 2.33                     | 0.44              |
| 47:JP:245:VAL:HA   | 47:JP:256:GLN:O    | 2.17                     | 0.44              |
| 49:DE:240:LYS:HE3  | 49:DE:241:GLY:H    | 1.83                     | 0.44              |
| 51:DG:83:CYS:SG    | 66:D3:162:A:H5''   | 2.57                     | 0.44              |
| 52:DH:5:GLN:HE22   | 52:DH:22:GLN:N     | 2.14                     | 0.44              |
| 56:DN:54:LEU:O     | 56:DN:60:VAL:HB    | 2.18                     | 0.44              |
| 60:DW:11:LEU:HD11  | 60:DW:37:PHE:CD1   | 2.52                     | 0.44              |
| 60:DW:31:SER:OG    | 60:DW:34:ILE:N     | 2.34                     | 0.44              |
| 61:DX:85:ALA:CB    | 61:DX:122:PHE:HB2  | 2.48                     | 0.44              |
| 62:DY:37:LYS:HE3   | 66:D3:522:U:H5''   | 2.00                     | 0.44              |
| 65:D2:10:C:H2'     | 65:D2:11:A:C8      | 2.52                     | 0.44              |
| 66:D3:269:G:C6     | 66:D3:287:G:C5     | 3.05                     | 0.44              |
| 66:D3:763:G:C2     | 66:D3:764:U:C4     | 3.05                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 66:D3:845:G:C2     | 66:D3:846:G:H1'    | 2.52                     | 0.44              |
| 66:D3:1202:A:H3'   | 66:D3:1203:A:C8    | 2.52                     | 0.44              |
| 66:D3:1650:U:H2'   | 66:D3:1651:A:C8    | 2.51                     | 0.44              |
| 66:D3:1659:A:H2'   | 66:D3:1660:A:C8    | 2.53                     | 0.44              |
| 67:D4:81:U:H4'     | 67:D4:82:G:OP2     | 2.17                     | 0.44              |
| 79:EN:352:ASN:O    | 79:EN:356:ALA:N    | 2.44                     | 0.44              |
| 2:DA:9:LEU:HD21    | 16:UM:619:ARG:NH1  | 2.33                     | 0.44              |
| 2:DA:87:ARG:HB2    | 2:DA:101:HIS:HD2   | 1.83                     | 0.44              |
| 4:UA:852:THR:HB    | 24:UU:897:HIS:HE1  | 1.82                     | 0.44              |
| 5:UB:546:LEU:O     | 5:UB:550:VAL:HG13  | 2.18                     | 0.44              |
| 10:UG:87:GLN:N     | 10:UG:90:GLU:OE2   | 2.35                     | 0.44              |
| 11:UH:666:VAL:O    | 11:UH:669:ALA:N    | 2.51                     | 0.44              |
| 12:UI:502:ARG:CG   | 18:UO:510:LEU:HD21 | 2.40                     | 0.44              |
| 13:UJ:166:ASN:O    | 13:UJ:166:ASN:ND2  | 2.51                     | 0.44              |
| 13:UJ:180:ILE:HD11 | 20:UQ:876:PHE:CE2  | 2.53                     | 0.44              |
| 13:UJ:308:GLY:H    | 13:UJ:311:ASN:HD21 | 1.63                     | 0.44              |
| 13:UJ:539:LEU:HA   | 13:UJ:539:LEU:HD23 | 1.82                     | 0.44              |
| 14:UK:40:ASP:OD1   | 14:UK:44:LYS:NZ    | 2.39                     | 0.44              |
| 15:UL:276:ASN:O    | 15:UL:338:ILE:HD11 | 2.18                     | 0.44              |
| 15:UL:769:TYR:CZ   | 15:UL:787:LYS:HG2  | 2.53                     | 0.44              |
| 16:UM:84:LEU:HD13  | 16:UM:86:LYS:HZ1   | 1.83                     | 0.44              |
| 16:UM:173:LYS:HB3  | 16:UM:175:TRP:CH2  | 2.53                     | 0.44              |
| 16:UM:199:ILE:O    | 16:UM:209:LEU:HB2  | 2.18                     | 0.44              |
| 16:UM:352:LYS:HG3  | 16:UM:353:LEU:H    | 1.81                     | 0.44              |
| 16:UM:418:ASN:ND2  | 16:UM:423:LYS:HE3  | 2.32                     | 0.44              |
| 16:UM:755:ILE:H    | 16:UM:755:ILE:HD12 | 1.83                     | 0.44              |
| 18:UO:54:ASP:OD1   | 18:UO:67:SER:HA    | 2.18                     | 0.44              |
| 20:UQ:271:LEU:HB2  | 20:UQ:283:VAL:HG23 | 1.98                     | 0.44              |
| 20:UQ:282:ILE:HB   | 20:UQ:291:ARG:HG3  | 2.00                     | 0.44              |
| 21:UR:533:ALA:HB1  | 21:UR:565:VAL:HG21 | 1.99                     | 0.44              |
| 22:US:177:ILE:O    | 22:US:181:THR:HG22 | 2.17                     | 0.44              |
| 23:UT:211:PHE:O    | 23:UT:215:VAL:HG23 | 2.18                     | 0.44              |
| 23:UT:333:TRP:CH2  | 23:UT:369:SER:HA   | 2.52                     | 0.44              |
| 23:UT:943:ARG:HH12 | 66:D3:258:C:N4     | 2.15                     | 0.44              |
| 23:UT:1857:ILE:O   | 47:JP:146:LYS:NZ   | 2.51                     | 0.44              |
| 24:UU:78:SER:OG    | 24:UU:79:SER:N     | 2.51                     | 0.44              |
| 24:UU:287:LEU:HD13 | 24:UU:322:TYR:HE2  | 1.83                     | 0.44              |
| 24:UU:902:ASN:HD21 | 24:UU:904:ASP:HB2  | 1.82                     | 0.44              |
| 25:UV:464:THR:O    | 25:UV:466:THR:HG23 | 2.17                     | 0.44              |
| 25:UV:467:LEU:O    | 25:UV:476:ILE:HG12 | 2.17                     | 0.44              |
| 25:UV:592:PHE:HD2  | 25:UV:596:LYS:HB2  | 1.83                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:UV:679:SER:HA   | 25:UV:682:VAL:HG12 | 1.99                     | 0.44              |
| 25:UV:711:PRO:HB3  | 25:UV:767:GLN:HB2  | 1.99                     | 0.44              |
| 25:UV:960:LYS:HG2  | 25:UV:963:LYS:NZ   | 2.33                     | 0.44              |
| 28:CD:96:ILE:HG22  | 28:CD:115:TYR:O    | 2.18                     | 0.44              |
| 28:CD:213:ASN:O    | 28:CD:216:PHE:HB3  | 2.17                     | 0.44              |
| 29:CE:222:ASP:OD1  | 29:CE:223:LEU:N    | 2.51                     | 0.44              |
| 30:CG:114:ILE:HA   | 30:CG:117:VAL:HG12 | 1.99                     | 0.44              |
| 33:CJ:92:THR:HG22  | 33:CJ:93:SER:H     | 1.82                     | 0.44              |
| 33:CJ:227:ARG:HG3  | 33:CJ:227:ARG:NH1  | 2.33                     | 0.44              |
| 35:CL:170:VAL:HB   | 35:CL:207:LEU:HD23 | 2.00                     | 0.44              |
| 35:CL:830:ARG:NH1  | 61:DX:95:PHE:HZ    | 2.16                     | 0.44              |
| 35:CL:1112:PHE:CG  | 44:JM:178:MET:HE3  | 2.53                     | 0.44              |
| 36:CM:137:LEU:HG   | 36:CM:296:LEU:HD22 | 2.00                     | 0.44              |
| 38:JC:147:ASN:ND2  | 38:JC:150:ASN:HB2  | 2.33                     | 0.44              |
| 38:JC:200:GLU:C    | 38:JC:202:ASN:H    | 2.21                     | 0.44              |
| 39:JF:193:ILE:HA   | 39:JF:196:LEU:HD12 | 1.98                     | 0.44              |
| 39:JG:144:LEU:HD13 | 39:JG:150:ILE:HD12 | 1.99                     | 0.44              |
| 42:JJ:115:LYS:O    | 42:JJ:115:LYS:HD3  | 2.18                     | 0.44              |
| 47:JP:245:VAL:HG12 | 47:JP:257:LYS:HB2  | 1.99                     | 0.44              |
| 49:DE:125:LYS:HB2  | 49:DE:226:PHE:CD1  | 2.52                     | 0.44              |
| 51:DG:31:ARG:HH22  | 51:DG:65:GLN:HA    | 1.82                     | 0.44              |
| 51:DG:190:GLN:O    | 51:DG:193:LEU:HG   | 2.16                     | 0.44              |
| 52:DH:58:LEU:HD23  | 52:DH:88:ARG:HE    | 1.83                     | 0.44              |
| 53:DI:42:ARG:HA    | 53:DI:42:ARG:HH11  | 1.81                     | 0.44              |
| 58:DQ:107:LYS:HD2  | 58:DQ:107:LYS:HA   | 1.60                     | 0.44              |
| 61:DX:85:ALA:HB2   | 61:DX:122:PHE:HD2  | 1.83                     | 0.44              |
| 62:DY:99:LYS:NZ    | 62:DY:101:GLU:HA   | 2.33                     | 0.44              |
| 65:D2:3:G:H2'      | 65:D2:4:C:C6       | 2.53                     | 0.44              |
| 65:D2:24:U:O2      | 65:D2:56:G:N2      | 2.51                     | 0.44              |
| 66:D3:628:G:O6     | 66:D3:969:C:H3'    | 2.17                     | 0.44              |
| 78:EK:845:PRO:HA   | 78:EK:851:ASP:CB   | 2.47                     | 0.44              |
| 3:JA:895:ILE:HA    | 3:JA:898:ILE:HG12  | 2.00                     | 0.44              |
| 4:UA:354:SER:HA    | 4:UA:395:PHE:CE1   | 2.53                     | 0.44              |
| 4:UA:402:MET:HE2   | 4:UA:416:LEU:HD21  | 2.00                     | 0.44              |
| 4:UA:564:PHE:HD1   | 4:UA:567:ASP:OD2   | 2.00                     | 0.44              |
| 1:CB:212:LYS:HD3   | 28:CD:259:MET:CE   | 2.47                     | 0.44              |
| 7:UD:309:GLN:HE21  | 7:UD:318:ASN:HA    | 1.82                     | 0.44              |
| 7:UD:565:ARG:HH11  | 7:UD:567:ASN:N     | 2.16                     | 0.44              |
| 8:UE:280:GLN:NE2   | 8:UE:325:GLU:OE2   | 2.42                     | 0.44              |
| 8:UE:527:HIS:HB3   | 8:UE:531:LYS:HE2   | 1.99                     | 0.44              |
| 9:UF:162:LYS:O     | 9:UF:165:ARG:HG2   | 2.18                     | 0.44              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 9:UF:183:TYR:CE2    | 9:UF:318:ARG:HG2    | 2.52                     | 0.44              |
| 10:UG:213:TRP:CH2   | 65:D2:329:A:N7      | 2.85                     | 0.44              |
| 10:UG:252:SER:HA    | 10:UG:276:PRO:HB3   | 1.99                     | 0.44              |
| 10:UG:445:ASP:N     | 10:UG:445:ASP:OD1   | 2.51                     | 0.44              |
| 13:UJ:1524:ILE:O    | 13:UJ:1528:VAL:HG13 | 2.17                     | 0.44              |
| 13:UJ:1533:ASN:HA   | 13:UJ:1536:VAL:HG22 | 1.99                     | 0.44              |
| 13:UJ:1548:PHE:O    | 13:UJ:1552:VAL:HG23 | 2.18                     | 0.44              |
| 14:UK:45:GLN:O      | 14:UK:46:SER:C      | 2.56                     | 0.44              |
| 14:UK:213:GLN:HE22  | 14:UK:217:ARG:NH1   | 2.14                     | 0.44              |
| 15:UL:10:GLN:NE2    | 15:UL:69:PRO:HG2    | 2.32                     | 0.44              |
| 15:UL:88:HIS:HD2    | 15:UL:91:THR:H      | 1.63                     | 0.44              |
| 15:UL:303:LEU:HD23  | 15:UL:313:ILE:HB    | 2.00                     | 0.44              |
| 15:UL:589:ILE:HG22  | 15:UL:599:ILE:HD13  | 1.99                     | 0.44              |
| 16:UM:36:VAL:HG12   | 16:UM:37:LEU:H      | 1.83                     | 0.44              |
| 16:UM:84:LEU:HD13   | 16:UM:86:LYS:HZ3    | 1.82                     | 0.44              |
| 16:UM:416:ARG:HB2   | 16:UM:427:TYR:CE1   | 2.52                     | 0.44              |
| 16:UM:584:ILE:HG21  | 16:UM:589:GLN:HG3   | 1.99                     | 0.44              |
| 18:UO:57:VAL:HG21   | 18:UO:327:LEU:HD12  | 2.00                     | 0.44              |
| 20:UQ:406:MET:HE3   | 20:UQ:485:ARG:HD3   | 2.00                     | 0.44              |
| 21:UR:257:HIS:HE1   | 21:UR:259:SER:HB3   | 1.83                     | 0.44              |
| 22:US:219:TRP:CE2   | 22:US:223:VAL:HG11  | 2.53                     | 0.44              |
| 22:US:412:CYS:O     | 22:US:415:MET:HG3   | 2.18                     | 0.44              |
| 23:UT:62:LYS:NZ     | 23:UT:97:PHE:HB3    | 2.33                     | 0.44              |
| 23:UT:81:LEU:HD23   | 31:CH:68:LYS:NZ     | 2.33                     | 0.44              |
| 23:UT:280:MET:HE3   | 23:UT:733:VAL:HG11  | 2.00                     | 0.44              |
| 23:UT:887:ASN:HB2   | 23:UT:904:PHE:CE1   | 2.53                     | 0.44              |
| 23:UT:1705:LEU:HB3  | 23:UT:1760:ASN:OD1  | 2.18                     | 0.44              |
| 24:UU:545:PRO:HD2   | 24:UU:563:ASP:HB3   | 2.00                     | 0.44              |
| 24:UU:622:GLY:HA3   | 24:UU:673:PHE:HZ    | 1.82                     | 0.44              |
| 25:UV:349:LEU:HD21  | 25:UV:395:ILE:HD13  | 2.00                     | 0.44              |
| 25:UV:371:GLN:NE2   | 25:UV:372:GLN:HG2   | 2.33                     | 0.44              |
| 25:UV:475:ASN:OD1   | 25:UV:476:ILE:N     | 2.51                     | 0.44              |
| 25:UV:1157:TYR:OH   | 25:UV:1203:ASN:N    | 2.51                     | 0.44              |
| 26:UX:20:LYS:NZ     | 32:CI:31:GLN:HG3    | 2.33                     | 0.44              |
| 27:UZ:142:ARG:NE    | 66:D3:1515:A:N6     | 2.66                     | 0.44              |
| 28:CD:25:ASP:OD2    | 47:JP:383:SER:HB2   | 2.18                     | 0.44              |
| 31:CH:129:GLN:N     | 31:CH:129:GLN:OE1   | 2.51                     | 0.44              |
| 32:CI:70:PHE:CD1    | 34:CK:434:HIS:CD2   | 3.06                     | 0.44              |
| 34:CK:470:GLU:O     | 34:CK:470:GLU:HG2   | 2.17                     | 0.44              |
| 35:CL:256:GLU:HA    | 35:CL:259:GLU:OE2   | 2.18                     | 0.44              |
| 35:CL:1114:GLN:HE22 | 65:D2:412:A:H1'     | 1.81                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:CM:55:LEU:HD12  | 36:CM:88:HIS:ND1   | 2.32                     | 0.44              |
| 39:JF:150:ILE:HG13 | 39:JF:160:LEU:HD12 | 1.99                     | 0.44              |
| 39:JG:96:LEU:HG    | 39:JG:130:ILE:CD1  | 2.48                     | 0.44              |
| 45:JN:316:ARG:NH1  | 66:D3:1036:A:C4    | 2.86                     | 0.44              |
| 47:JP:247:TYR:CE1  | 47:JP:254:PRO:HB3  | 2.52                     | 0.44              |
| 47:JP:306:SER:HB3  | 47:JP:326:ASP:HB2  | 1.99                     | 0.44              |
| 47:JP:320:ILE:O    | 47:JP:331:ILE:HA   | 2.18                     | 0.44              |
| 49:DE:22:LYS:N     | 49:DE:22:LYS:HD3   | 2.33                     | 0.44              |
| 49:DE:162:ILE:HG13 | 49:DE:163:ASP:O    | 2.17                     | 0.44              |
| 50:DF:43:PHE:CE1   | 50:DF:115:LYS:HD3  | 2.53                     | 0.44              |
| 50:DF:111:VAL:HA   | 50:DF:114:ILE:HG22 | 2.00                     | 0.44              |
| 52:DH:51:VAL:HG23  | 52:DH:171:ALA:CB   | 2.48                     | 0.44              |
| 53:DI:26:LYS:HD2   | 53:DI:26:LYS:HA    | 1.80                     | 0.44              |
| 55:DL:45:PRO:HB2   | 55:DL:47:THR:HG22  | 2.00                     | 0.44              |
| 65:D2:112:U:H2'    | 65:D2:113:A:C8     | 2.53                     | 0.44              |
| 65:D2:194:G:N1     | 65:D2:203:C:N3     | 2.49                     | 0.44              |
| 65:D2:248:G:N1     | 65:D2:249:G:C5     | 2.86                     | 0.44              |
| 65:D2:412:A:H2'    | 65:D2:413:C:C6     | 2.53                     | 0.44              |
| 66:D3:753:A:C6     | 66:D3:754:A:H1'    | 2.52                     | 0.44              |
| 66:D3:1272:U:O3'   | 66:D3:1273:G:H8    | 2.01                     | 0.44              |
| 66:D3:1480:G:H1    | 66:D3:1527:C:H42   | 1.66                     | 0.44              |
| 66:D3:1638:G:H4'   | 66:D3:1639:C:OP1   | 2.18                     | 0.44              |
| 66:D3:1752:U:H2'   | 66:D3:1753:A:C8    | 2.53                     | 0.44              |
| 67:D4:78:G:O6      | 67:D4:330:A:N6     | 2.49                     | 0.44              |
| 67:D4:159:C:H2'    | 67:D4:160:G:H8     | 1.82                     | 0.44              |
| 78:EK:634:ALA:HB2  | 78:EK:680:LEU:HA   | 1.99                     | 0.44              |
| 79:EN:660:VAL:O    | 79:EN:664:VAL:N    | 2.43                     | 0.44              |
| 1:CA:212:LYS:HG2   | 29:CE:190:TRP:CZ3  | 2.53                     | 0.44              |
| 2:DA:153:HIS:HB2   | 2:DA:155:TYR:CE1   | 2.52                     | 0.44              |
| 3:JA:86:ARG:HH22   | 3:JA:91:MET:HA     | 1.83                     | 0.44              |
| 5:UB:604:VAL:HG11  | 5:UB:678:PHE:HE1   | 1.83                     | 0.44              |
| 5:UB:614:ILE:HG12  | 5:UB:616:LEU:HD13  | 2.00                     | 0.44              |
| 6:UC:528:LEU:HD11  | 66:D3:579:A:N7     | 2.32                     | 0.44              |
| 7:UD:66:ARG:NH2    | 7:UD:88:GLU:OE2    | 2.45                     | 0.44              |
| 7:UD:487:VAL:HG12  | 7:UD:497:ILE:HG13  | 2.00                     | 0.44              |
| 7:UD:565:ARG:HD2   | 7:UD:565:ARG:C     | 2.38                     | 0.44              |
| 8:UE:54:GLU:H      | 8:UE:54:GLU:CD     | 2.21                     | 0.44              |
| 8:UE:262:SER:O     | 8:UE:270:ASN:ND2   | 2.51                     | 0.44              |
| 9:UF:152:LYS:HA    | 9:UF:152:LYS:HD2   | 1.80                     | 0.44              |
| 9:UF:180:LYS:O     | 9:UF:184:GLU:OE1   | 2.35                     | 0.44              |
| 10:UG:211:THR:HB   | 65:D2:329:A:N3     | 2.32                     | 0.44              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 10:UG:265:GLU:HB3  | 10:UG:266:PRO:HD2   | 1.98                     | 0.44              |
| 10:UG:325:SER:HB2  | 10:UG:383:PHE:CE1   | 2.52                     | 0.44              |
| 14:UK:65:HIS:CG    | 67:D4:55:A:H2       | 2.36                     | 0.44              |
| 15:UL:424:CYS:SG   | 15:UL:425:ILE:N     | 2.91                     | 0.44              |
| 16:UM:15:ILE:HG13  | 16:UM:34:THR:OG1    | 2.18                     | 0.44              |
| 16:UM:732:ASN:O    | 16:UM:736:LEU:HG    | 2.18                     | 0.44              |
| 17:UN:324:ALA:CB   | 28:CD:87:PRO:HA     | 2.48                     | 0.44              |
| 18:UO:229:CYS:SG   | 18:UO:255:VAL:HG23  | 2.57                     | 0.44              |
| 18:UO:319:VAL:HG22 | 18:UO:329:ILE:HG22  | 1.98                     | 0.44              |
| 18:UO:500:GLU:HA   | 18:UO:503:ARG:HG3   | 1.98                     | 0.44              |
| 18:UO:506:GLY:O    | 18:UO:510:LEU:HD23  | 2.18                     | 0.44              |
| 20:UQ:168:LEU:HD23 | 20:UQ:168:LEU:HA    | 1.83                     | 0.44              |
| 20:UQ:270:GLN:O    | 20:UQ:271:LEU:HD22  | 2.18                     | 0.44              |
| 20:UQ:726:GLN:HA   | 20:UQ:739:TYR:HA    | 2.00                     | 0.44              |
| 21:UR:318:ARG:O    | 21:UR:354:SER:HA    | 2.16                     | 0.44              |
| 23:UT:122:LEU:HA   | 23:UT:125:TYR:CB    | 2.46                     | 0.44              |
| 23:UT:193:ALA:HB1  | 23:UT:235:LEU:CA    | 2.48                     | 0.44              |
| 23:UT:279:TRP:CE3  | 23:UT:282:ILE:HD11  | 2.53                     | 0.44              |
| 23:UT:673:ARG:CZ   | 23:UT:771:PRO:HG2   | 2.48                     | 0.44              |
| 23:UT:715:TYR:CD2  | 23:UT:762:ILE:HD11  | 2.53                     | 0.44              |
| 23:UT:921:VAL:HG23 | 23:UT:922:MET:HE2   | 2.00                     | 0.44              |
| 23:UT:939:SER:OG   | 23:UT:942:LYS:HG3   | 2.18                     | 0.44              |
| 23:UT:1083:TYR:HD2 | 23:UT:1124:TYR:HD2  | 1.65                     | 0.44              |
| 23:UT:1206:THR:HB  | 23:UT:1249:LEU:HD13 | 1.99                     | 0.44              |
| 23:UT:1332:ILE:O   | 23:UT:1373:LYS:NZ   | 2.43                     | 0.44              |
| 25:UV:369:TRP:CZ3  | 25:UV:373:ARG:HG3   | 2.52                     | 0.44              |
| 25:UV:627:LEU:HD13 | 25:UV:671:THR:HG23  | 1.99                     | 0.44              |
| 25:UV:844:THR:O    | 25:UV:847:GLY:N     | 2.51                     | 0.44              |
| 27:UZ:13:ALA:O     | 27:UZ:17:LEU:HG     | 2.18                     | 0.44              |
| 27:UZ:77:LYS:HE3   | 27:UZ:77:LYS:HB3    | 1.86                     | 0.44              |
| 27:UZ:86:THR:HG22  | 27:UZ:90:ASP:OD2    | 2.18                     | 0.44              |
| 30:CF:16:LEU:O     | 30:CF:20:ILE:HG12   | 2.18                     | 0.44              |
| 30:CG:50:GLU:HB2   | 30:CG:102:ILE:O     | 2.17                     | 0.44              |
| 31:CH:155:ASN:O    | 31:CH:191:SER:OG    | 2.36                     | 0.44              |
| 31:CH:194:LEU:HD22 | 31:CH:235:HIS:HB3   | 2.00                     | 0.44              |
| 33:CJ:133:LYS:HE2  | 33:CJ:133:LYS:HB3   | 1.60                     | 0.44              |
| 35:CL:1049:ASN:HB3 | 35:CL:1052:SER:HB2  | 2.00                     | 0.44              |
| 45:JN:303:GLU:O    | 45:JN:303:GLU:HG2   | 2.18                     | 0.44              |
| 47:JP:61:GLN:NE2   | 67:D4:31:G:H22      | 2.16                     | 0.44              |
| 47:JP:139:CYS:HB3  | 47:JP:185:ILE:HD12  | 2.00                     | 0.44              |
| 49:DE:181:VAL:HG12 | 49:DE:227:VAL:HA    | 2.00                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 50:DF:24:VAL:O     | 50:DF:24:VAL:HG23  | 2.18                     | 0.44              |
| 56:DN:119:GLU:HA   | 56:DN:122:ILE:HG22 | 1.99                     | 0.44              |
| 56:DN:121:ARG:HH22 | 66:D3:868:G:C5'    | 2.29                     | 0.44              |
| 65:D2:64:U:H2'     | 65:D2:65:U:C6      | 2.53                     | 0.44              |
| 65:D2:426:G:C4     | 65:D2:428:A:H5''   | 2.53                     | 0.44              |
| 65:D2:445:U:H2'    | 65:D2:446:U:O4'    | 2.18                     | 0.44              |
| 65:D2:467:A:O2'    | 65:D2:468:A:H5'    | 2.18                     | 0.44              |
| 66:D3:109:G:C6     | 66:D3:110:U:C4     | 3.05                     | 0.44              |
| 66:D3:319:U:H4'    | 66:D3:323:A:N9     | 2.32                     | 0.44              |
| 66:D3:762:A:H8     | 66:D3:763:G:C8     | 2.36                     | 0.44              |
| 66:D3:874:C:H2'    | 66:D3:875:G:C8     | 2.53                     | 0.44              |
| 66:D3:1064:G:C6    | 66:D3:1065:A:N7    | 2.86                     | 0.44              |
| 66:D3:1594:G:H1    | 66:D3:1602:C:H42   | 1.64                     | 0.44              |
| 66:D3:1676:U:H2'   | 66:D3:1677:C:C6    | 2.53                     | 0.44              |
| 67:D4:54:C:C5      | 67:D4:55:A:C8      | 3.06                     | 0.44              |
| 75:EH:76:ILE:O     | 75:EH:116:GLY:N    | 2.50                     | 0.44              |
| 79:EN:683:SER:HA   | 79:EN:689:ASN:HA   | 2.00                     | 0.44              |
| 1:CA:98:ILE:HG22   | 1:CA:100:ARG:HG2   | 2.00                     | 0.44              |
| 3:JA:34:ARG:O      | 3:JA:94:PHE:HB2    | 2.17                     | 0.44              |
| 3:JA:867:PHE:HZ    | 3:JA:886:LEU:HB2   | 1.83                     | 0.44              |
| 4:UA:324:LEU:HD12  | 4:UA:342:GLN:NE2   | 2.26                     | 0.44              |
| 6:UC:544:ILE:HD13  | 35:CL:834:TRP:CD2  | 2.53                     | 0.44              |
| 7:UD:48:SER:O      | 7:UD:49:LEU:HD23   | 2.17                     | 0.44              |
| 7:UD:55:SER:OG     | 7:UD:340:GLN:O     | 2.26                     | 0.44              |
| 7:UD:389:ARG:CZ    | 7:UD:747:ILE:HD13  | 2.48                     | 0.44              |
| 7:UD:647:TRP:CE3   | 7:UD:656:ARG:HB2   | 2.53                     | 0.44              |
| 8:UE:86:TRP:CD1    | 8:UE:98:LYS:HG2    | 2.53                     | 0.44              |
| 9:UF:336:ASN:O     | 9:UF:340:GLN:HG3   | 2.16                     | 0.44              |
| 10:UG:202:HIS:NE2  | 10:UG:437:LEU:HD12 | 2.33                     | 0.44              |
| 13:UJ:25:ARG:NH1   | 47:JP:16:VAL:HG12  | 2.31                     | 0.44              |
| 13:UJ:717:GLU:HB3  | 13:UJ:751:ILE:HD11 | 2.00                     | 0.44              |
| 13:UJ:800:ASP:OD1  | 13:UJ:800:ASP:N    | 2.49                     | 0.44              |
| 13:UJ:1472:VAL:O   | 13:UJ:1475:SER:OG  | 2.30                     | 0.44              |
| 13:UJ:1501:PHE:O   | 13:UJ:1504:LEU:HG  | 2.17                     | 0.44              |
| 13:UJ:1762:GLU:OE1 | 13:UJ:1766:ARG:HD3 | 2.17                     | 0.44              |
| 15:UL:457:PHE:CE1  | 15:UL:464:LEU:HD13 | 2.53                     | 0.44              |
| 15:UL:756:LEU:O    | 15:UL:760:ILE:HG12 | 2.17                     | 0.44              |
| 16:UM:13:ASN:HA    | 16:UM:640:VAL:HG12 | 2.00                     | 0.44              |
| 16:UM:148:SER:OG   | 16:UM:166:GLY:O    | 2.36                     | 0.44              |
| 16:UM:303:PHE:CE1  | 16:UM:313:LEU:HD21 | 2.52                     | 0.44              |
| 16:UM:392:ASN:ND2  | 16:UM:438:THR:HA   | 2.32                     | 0.44              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 16:UM:655:GLU:OE2  | 16:UM:656:GLN:HG3   | 2.17                     | 0.44              |
| 17:UN:837:LYS:O    | 17:UN:840:LEU:HB3   | 2.17                     | 0.44              |
| 20:UQ:38:SER:N     | 20:UQ:43:ASN:O      | 2.49                     | 0.44              |
| 22:US:357:ARG:N    | 22:US:357:ARG:HE    | 2.16                     | 0.44              |
| 23:UT:140:ILE:CD1  | 23:UT:188:LEU:HD21  | 2.48                     | 0.44              |
| 23:UT:323:PHE:HB2  | 23:UT:364:LEU:HD23  | 1.99                     | 0.44              |
| 23:UT:480:TYR:CE1  | 23:UT:518:MET:HA    | 2.52                     | 0.44              |
| 23:UT:1000:PHE:O   | 23:UT:1003:ILE:HG13 | 2.18                     | 0.44              |
| 23:UT:1090:ARG:O   | 23:UT:1094:PHE:HB2  | 2.17                     | 0.44              |
| 23:UT:1127:PHE:CZ  | 23:UT:1166:HIS:HB3  | 2.52                     | 0.44              |
| 23:UT:1143:LYS:HZ1 | 23:UT:1146:VAL:HG23 | 1.83                     | 0.44              |
| 23:UT:1237:GLU:HG2 | 23:UT:1280:LEU:HD21 | 1.99                     | 0.44              |
| 23:UT:1282:VAL:O   | 23:UT:1285:THR:OG1  | 2.28                     | 0.44              |
| 23:UT:1374:PHE:CE2 | 23:UT:1378:ILE:HD11 | 2.53                     | 0.44              |
| 23:UT:1554:PRO:HA  | 23:UT:1557:GLU:HG2  | 1.99                     | 0.44              |
| 24:UU:174:ALA:O    | 24:UU:175:THR:OG1   | 2.32                     | 0.44              |
| 24:UU:337:VAL:HG12 | 24:UU:338:GLN:O     | 2.17                     | 0.44              |
| 25:UV:300:TYR:CD1  | 25:UV:341:THR:HG23  | 2.53                     | 0.44              |
| 25:UV:468:PHE:HA   | 25:UV:474:VAL:O     | 2.18                     | 0.44              |
| 26:UX:48:SER:OG    | 26:UX:149:LYS:HE2   | 2.17                     | 0.44              |
| 27:UZ:97:PHE:CE2   | 27:UZ:180:LEU:HD11  | 2.52                     | 0.44              |
| 28:CD:253:ASP:O    | 28:CD:257:ILE:HG12  | 2.18                     | 0.44              |
| 30:CG:66:HIS:CE1   | 30:CG:67:LEU:HB2    | 2.53                     | 0.44              |
| 31:CH:489:SER:OG   | 31:CH:497:LYS:HB2   | 2.18                     | 0.44              |
| 33:CJ:92:THR:HG22  | 33:CJ:93:SER:N      | 2.33                     | 0.44              |
| 35:CL:82:LYS:HG2   | 82:CL:2001:GTP:PB   | 2.58                     | 0.44              |
| 35:CL:613:PRO:HB3  | 36:CM:321:ARG:NH2   | 2.33                     | 0.44              |
| 37:CN:121:ARG:HA   | 37:CN:121:ARG:HD2   | 1.84                     | 0.44              |
| 38:JC:146:TYR:HD1  | 38:JC:153:LEU:HD22  | 1.83                     | 0.44              |
| 38:JC:203:VAL:HG11 | 38:JC:217:LYS:HZ1   | 1.83                     | 0.44              |
| 39:JG:42:ILE:HB    | 39:JG:203:CYS:HA    | 1.99                     | 0.44              |
| 39:JG:188:ARG:CZ   | 39:JG:191:ASP:HB2   | 2.48                     | 0.44              |
| 44:JM:173:ILE:HA   | 44:JM:176:THR:HG22  | 2.00                     | 0.44              |
| 47:JP:17:LYS:HZ2   | 47:JP:20:GLN:HB2    | 1.83                     | 0.44              |
| 49:DE:137:PRO:HG2  | 49:DE:149:TYR:HA    | 2.00                     | 0.44              |
| 54:DJ:127:VAL:HA   | 54:DJ:130:THR:HG22  | 2.00                     | 0.44              |
| 57:DO:52:ARG:CZ    | 66:D3:903:U:H3      | 2.31                     | 0.44              |
| 65:D2:171:G:C6     | 65:D2:172:C:C4      | 3.05                     | 0.44              |
| 65:D2:411:A:H2'    | 65:D2:412:A:H8      | 1.83                     | 0.44              |
| 66:D3:61:A:C6      | 66:D3:62:A:C6       | 3.06                     | 0.44              |
| 66:D3:643:G:C6     | 66:D3:644:C:C4      | 3.06                     | 0.44              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 66:D3:1040:G:C2     | 66:D3:1079:U:N3    | 2.85                     | 0.44              |
| 66:D3:1060:U:OP1    | 66:D3:1060:U:H4'   | 2.17                     | 0.44              |
| 3:JA:191:SER:HB2    | 3:JA:485:TRP:NE1   | 2.33                     | 0.43              |
| 3:JA:818:GLU:HB2    | 3:JA:819:LYS:HZ2   | 1.83                     | 0.43              |
| 4:UA:31:SER:OG      | 4:UA:40:PHE:HE2    | 2.01                     | 0.43              |
| 4:UA:560:ILE:O      | 4:UA:599:ASN:HB3   | 2.18                     | 0.43              |
| 5:UB:646:THR:HB     | 5:UB:651:TRP:HZ3   | 1.83                     | 0.43              |
| 7:UD:87:GLN:OE1     | 7:UD:378:TYR:HD2   | 2.00                     | 0.43              |
| 7:UD:144:ILE:HG23   | 7:UD:158:VAL:HB    | 1.99                     | 0.43              |
| 8:UE:118:TRP:CH2    | 8:UE:128:GLN:HB2   | 2.53                     | 0.43              |
| 8:UE:541:LEU:HD23   | 18:UO:495:ILE:HD12 | 2.00                     | 0.43              |
| 9:UF:361:LYS:O      | 9:UF:365:ILE:HG12  | 2.18                     | 0.43              |
| 10:UG:37:THR:HG22   | 10:UG:39:ASP:H     | 1.82                     | 0.43              |
| 11:UH:549:ARG:HH22  | 11:UH:552:LYS:CD   | 2.31                     | 0.43              |
| 11:UH:562:PRO:HB2   | 11:UH:565:GLU:OE1  | 2.17                     | 0.43              |
| 12:UI:473:LYS:HD2   | 12:UI:474:HIS:CE1  | 2.53                     | 0.43              |
| 13:UJ:196:LEU:HD23  | 13:UJ:196:LEU:HA   | 1.73                     | 0.43              |
| 13:UJ:272:LYS:NZ    | 13:UJ:311:ASN:OD1  | 2.51                     | 0.43              |
| 13:UJ:1724:VAL:HG23 | 13:UJ:1725:LEU:HG  | 2.00                     | 0.43              |
| 14:UK:161:ARG:O     | 14:UK:165:ARG:NE   | 2.51                     | 0.43              |
| 15:UL:905:LEU:HG    | 16:UM:782:VAL:CG2  | 2.47                     | 0.43              |
| 16:UM:30:LYS:HG3    | 16:UM:30:LYS:O     | 2.17                     | 0.43              |
| 16:UM:235:LYS:HD2   | 16:UM:237:LEU:HD21 | 2.00                     | 0.43              |
| 16:UM:532:HIS:CD2   | 16:UM:533:LYS:HE2  | 2.52                     | 0.43              |
| 16:UM:532:HIS:NE2   | 16:UM:554:ASP:OD1  | 2.51                     | 0.43              |
| 17:UN:321:HIS:HB3   | 28:CD:89:ALA:HA    | 2.00                     | 0.43              |
| 18:UO:28:ARG:NH2    | 65:D2:142:U:H3     | 2.16                     | 0.43              |
| 22:US:215:ASN:O     | 22:US:218:LYS:HB2  | 2.17                     | 0.43              |
| 22:US:403:TYR:CG    | 22:US:493:TYR:HE2  | 2.36                     | 0.43              |
| 23:UT:1478:ASP:OD1  | 23:UT:1519:SER:N   | 2.38                     | 0.43              |
| 23:UT:1682:LYS:N    | 23:UT:1686:GLN:OE1 | 2.36                     | 0.43              |
| 23:UT:1727:GLY:O    | 23:UT:1731:GLU:HG2 | 2.18                     | 0.43              |
| 24:UU:252:SER:OG    | 24:UU:268:THR:O    | 2.24                     | 0.43              |
| 24:UU:669:ASP:O     | 24:UU:673:PHE:HB2  | 2.18                     | 0.43              |
| 25:UV:177:ASN:HB3   | 25:UV:213:LEU:HD13 | 2.00                     | 0.43              |
| 28:CD:148:GLU:OE1   | 28:CD:148:GLU:N    | 2.34                     | 0.43              |
| 28:CD:246:GLY:HA2   | 28:CD:249:GLN:NE2  | 2.33                     | 0.43              |
| 29:CE:155:SER:HB3   | 29:CE:158:LYS:HD2  | 2.00                     | 0.43              |
| 29:CE:324:LYS:HZ3   | 67:D4:91:C:P       | 2.40                     | 0.43              |
| 31:CH:266:GLU:HG2   | 31:CH:267:SER:N    | 2.33                     | 0.43              |
| 34:CK:454:VAL:O     | 34:CK:456:PHE:CD1  | 2.71                     | 0.43              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 35:CL:198:VAL:HG12 | 35:CL:199:TYR:H     | 1.82                     | 0.43              |
| 35:CL:280:LEU:HD12 | 35:CL:281:PRO:HD2   | 2.00                     | 0.43              |
| 35:CL:769:TYR:HB3  | 35:CL:777:ARG:NH1   | 2.33                     | 0.43              |
| 38:JC:164:ARG:NH2  | 38:JC:174:ASN:O     | 2.51                     | 0.43              |
| 38:JC:237:ARG:NH2  | 38:JC:288:LYS:HG3   | 2.32                     | 0.43              |
| 39:JG:37:ILE:HG13  | 39:JG:38:THR:HG23   | 2.00                     | 0.43              |
| 39:JG:175:CYS:SG   | 39:JG:203:CYS:N     | 2.91                     | 0.43              |
| 44:JM:54:GLU:O     | 44:JM:57:THR:HG22   | 2.17                     | 0.43              |
| 45:JN:257:ALA:O    | 45:JN:260:GLY:C     | 2.57                     | 0.43              |
| 49:DE:11:ARG:HA    | 49:DE:28:ALA:HB2    | 2.00                     | 0.43              |
| 54:DJ:134:ILE:HG23 | 54:DJ:157:ASP:O     | 2.17                     | 0.43              |
| 58:DQ:48:VAL:HG23  | 58:DQ:78:VAL:HG13   | 2.00                     | 0.43              |
| 65:D2:335:G:C2     | 65:D2:390:C:O2      | 2.71                     | 0.43              |
| 66:D3:143:G:H2'    | 66:D3:144:U:C6      | 2.53                     | 0.43              |
| 66:D3:1470:C:H2'   | 66:D3:1573:A:N6     | 2.33                     | 0.43              |
| 66:D3:1667:A:H2'   | 66:D3:1668:G:C8     | 2.52                     | 0.43              |
| 2:DA:98:THR:HG1    | 2:DA:99:ASN:H       | 1.65                     | 0.43              |
| 3:JA:91:MET:CE     | 35:CL:95:LYS:HD3    | 2.48                     | 0.43              |
| 3:JA:617:LEU:O     | 3:JA:620:GLN:HG2    | 2.18                     | 0.43              |
| 7:UD:57:ILE:O      | 7:UD:342:LYS:HG2    | 2.17                     | 0.43              |
| 8:UE:200:GLU:O     | 8:UE:217:ILE:HG22   | 2.19                     | 0.43              |
| 8:UE:513:LEU:HD11  | 18:UO:511:LEU:CG    | 2.39                     | 0.43              |
| 9:UF:173:ARG:NH1   | 28:CD:80:ALA:HA     | 2.33                     | 0.43              |
| 11:UH:310:MET:HA   | 11:UH:326:VAL:HA    | 1.99                     | 0.43              |
| 11:UH:541:LEU:HD11 | 11:UH:551:PHE:HE1   | 1.82                     | 0.43              |
| 13:UJ:270:LEU:HD23 | 13:UJ:270:LEU:HA    | 1.76                     | 0.43              |
| 13:UJ:309:GLN:HE22 | 21:UR:224:ASN:C     | 2.22                     | 0.43              |
| 13:UJ:1601:VAL:HA  | 13:UJ:1604:LEU:HD12 | 2.00                     | 0.43              |
| 13:UJ:1651:LEU:O   | 13:UJ:1654:GLN:HB2  | 2.19                     | 0.43              |
| 14:UK:70:ARG:NH1   | 35:CL:1079:PHE:CZ   | 2.87                     | 0.43              |
| 14:UK:171:LEU:CD2  | 48:JQ:119:ILE:HA    | 2.48                     | 0.43              |
| 15:UL:14:PHE:HB3   | 15:UL:417:TRP:CZ3   | 2.53                     | 0.43              |
| 15:UL:48:ASP:OD1   | 15:UL:49:VAL:N      | 2.51                     | 0.43              |
| 15:UL:406:LEU:HD13 | 15:UL:416:ILE:HG13  | 2.00                     | 0.43              |
| 18:UO:281:VAL:HG13 | 18:UO:296:TRP:HE3   | 1.82                     | 0.43              |
| 18:UO:413:LEU:O    | 18:UO:417:VAL:HG23  | 2.19                     | 0.43              |
| 20:UQ:498:LEU:HD11 | 20:UQ:507:MET:HB2   | 2.00                     | 0.43              |
| 20:UQ:499:LYS:HD3  | 20:UQ:499:LYS:HA    | 1.81                     | 0.43              |
| 21:UR:411:TYR:CE1  | 21:UR:421:THR:HG22  | 2.54                     | 0.43              |
| 22:US:148:PHE:O    | 22:US:152:ILE:HG12  | 2.18                     | 0.43              |
| 22:US:250:GLU:O    | 22:US:253:PHE:HB3   | 2.18                     | 0.43              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 23:UT:177:LEU:HD23  | 23:UT:177:LEU:HA    | 1.83                     | 0.43              |
| 23:UT:391:ASP:OD1   | 23:UT:391:ASP:N     | 2.43                     | 0.43              |
| 23:UT:971:ARG:NH1   | 23:UT:972:LEU:HD21  | 2.33                     | 0.43              |
| 23:UT:1240:THR:O    | 23:UT:1244:LEU:HG   | 2.19                     | 0.43              |
| 23:UT:1351:PHE:CD2  | 23:UT:1367:ALA:HA   | 2.53                     | 0.43              |
| 23:UT:1716:MET:HG2  | 23:UT:1717:ILE:HD12 | 1.99                     | 0.43              |
| 23:UT:1773:VAL:O    | 23:UT:1777:LEU:HD23 | 2.18                     | 0.43              |
| 23:UT:1776:LEU:HD11 | 23:UT:1781:ILE:HD11 | 2.01                     | 0.43              |
| 23:UT:1923:ARG:HH21 | 23:UT:1969:HIS:CD2  | 2.36                     | 0.43              |
| 24:UU:218:LEU:N     | 24:UU:218:LEU:HD12  | 2.33                     | 0.43              |
| 24:UU:375:LEU:HD12  | 24:UU:414:ILE:HD13  | 2.00                     | 0.43              |
| 25:UV:640:THR:O     | 25:UV:644:VAL:HG23  | 2.18                     | 0.43              |
| 25:UV:898:THR:O     | 25:UV:902:ILE:HG12  | 2.18                     | 0.43              |
| 25:UV:956:ASN:HD21  | 25:UV:960:LYS:HE3   | 1.83                     | 0.43              |
| 27:UZ:17:LEU:O      | 27:UZ:20:LEU:HG     | 2.17                     | 0.43              |
| 29:CE:205:TYR:CE2   | 29:CE:209:ILE:HD11  | 2.53                     | 0.43              |
| 29:CE:229:GLU:HA    | 29:CE:232:GLU:HG3   | 2.00                     | 0.43              |
| 29:CE:316:THR:HG22  | 67:D4:324:U:O2'     | 2.18                     | 0.43              |
| 34:CK:297:LEU:HD12  | 34:CK:301:GLU:HG3   | 1.99                     | 0.43              |
| 34:CK:309:LYS:HA    | 34:CK:312:GLU:CD    | 2.39                     | 0.43              |
| 35:CL:92:ARG:C      | 35:CL:92:ARG:HD3    | 2.39                     | 0.43              |
| 35:CL:880:TYR:HB2   | 61:DX:94:ASN:ND2    | 2.33                     | 0.43              |
| 35:CL:1123:LYS:NZ   | 66:D3:487:G:P       | 2.88                     | 0.43              |
| 36:CM:207:ARG:HE    | 36:CM:268:PRO:HG2   | 1.83                     | 0.43              |
| 37:CN:41:ARG:HH21   | 37:CN:138:TRP:HB3   | 1.82                     | 0.43              |
| 38:JC:363:LEU:O     | 38:JC:366:LYS:HB3   | 2.18                     | 0.43              |
| 42:JJ:221:ARG:HB2   | 42:JJ:239:HIS:ND1   | 2.33                     | 0.43              |
| 45:JN:236:MET:SD    | 66:D3:8:U:N3        | 2.91                     | 0.43              |
| 45:JN:320:ILE:HG13  | 60:DW:76:SER:CB     | 2.48                     | 0.43              |
| 46:JO:178:LYS:O     | 46:JO:181:LYS:N     | 2.51                     | 0.43              |
| 50:DF:223:SER:OG    | 50:DF:224:ASN:N     | 2.52                     | 0.43              |
| 51:DG:28:PHE:HE1    | 51:DG:102:VAL:HG22  | 1.84                     | 0.43              |
| 51:DG:33:GLY:HA2    | 51:DG:51:LYS:NZ     | 2.33                     | 0.43              |
| 53:DI:48:THR:OG1    | 53:DI:52:ASN:HB3    | 2.17                     | 0.43              |
| 60:DW:6:VAL:HG23    | 60:DW:29:PRO:HG2    | 2.00                     | 0.43              |
| 66:D3:494:U:H3'     | 66:D3:494:U:H6      | 1.83                     | 0.43              |
| 66:D3:520:A:C6      | 66:D3:521:A:C6      | 3.06                     | 0.43              |
| 66:D3:647:G:H1      | 66:D3:687:G:H1      | 1.67                     | 0.43              |
| 66:D3:887:A:H61     | 66:D3:925:G:H1      | 1.65                     | 0.43              |
| 66:D3:1489:U:H4'    | 66:D3:1490:C:C6     | 2.52                     | 0.43              |
| 66:D3:1672:G:N2     | 66:D3:1730:A:H1'    | 2.33                     | 0.43              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 67:D4:55:A:O2'      | 67:D4:56:A:OP2      | 2.34                     | 0.43              |
| 67:D4:250:C:N4      | 67:D4:251:G:O6      | 2.51                     | 0.43              |
| 1:CA:239:CYS:SG     | 1:CA:240:VAL:N      | 2.91                     | 0.43              |
| 2:DA:187:LYS:HG2    | 2:DA:192:VAL:HG21   | 2.00                     | 0.43              |
| 3:JA:19:GLN:NE2     | 3:JA:219:LEU:HD22   | 2.34                     | 0.43              |
| 3:JA:34:ARG:HB3     | 3:JA:94:PHE:CD2     | 2.52                     | 0.43              |
| 4:UA:561:SER:OG     | 4:UA:577:SER:OG     | 1.97                     | 0.43              |
| 1:CB:172:TYR:CE1    | 1:CB:241:PHE:CD2    | 3.06                     | 0.43              |
| 1:CB:236:MET:CE     | 29:CE:118:ARG:HG3   | 2.49                     | 0.43              |
| 5:UB:552:GLN:NE2    | 5:UB:555:ARG:HE     | 2.17                     | 0.43              |
| 6:UC:595:LYS:HD2    | 6:UC:595:LYS:H      | 1.84                     | 0.43              |
| 7:UD:106:ASN:O      | 7:UD:106:ASN:ND2    | 2.52                     | 0.43              |
| 7:UD:115:PHE:CD1    | 7:UD:125:GLU:HB3    | 2.54                     | 0.43              |
| 7:UD:210:ILE:HD12   | 7:UD:265:TRP:HZ3    | 1.83                     | 0.43              |
| 7:UD:282:ASP:OD1    | 7:UD:282:ASP:N      | 2.51                     | 0.43              |
| 7:UD:443:GLY:HA2    | 7:UD:448:THR:HG22   | 2.00                     | 0.43              |
| 7:UD:588:ASP:HB3    | 7:UD:590:LYS:HB2    | 2.01                     | 0.43              |
| 8:UE:74:VAL:HG23    | 8:UE:90:VAL:HG21    | 2.00                     | 0.43              |
| 10:UG:475:ASN:OD1   | 10:UG:478:LYS:HB2   | 2.19                     | 0.43              |
| 11:UH:551:PHE:HE2   | 11:UH:578:LEU:HD21  | 1.83                     | 0.43              |
| 11:UH:676:TRP:CD1   | 11:UH:676:TRP:C     | 2.91                     | 0.43              |
| 13:UJ:200:ILE:HD13  | 13:UJ:205:THR:HG21  | 2.00                     | 0.43              |
| 13:UJ:538:ALA:O     | 13:UJ:541:LEU:HG    | 2.19                     | 0.43              |
| 13:UJ:1573:LEU:HD22 | 13:UJ:1618:LEU:HD13 | 2.00                     | 0.43              |
| 14:UK:169:ASP:OD2   | 14:UK:169:ASP:N     | 2.50                     | 0.43              |
| 15:UL:640:LYS:HD3   | 15:UL:652:LYS:NZ    | 2.33                     | 0.43              |
| 16:UM:12:LEU:O      | 16:UM:640:VAL:HA    | 2.19                     | 0.43              |
| 16:UM:140:PHE:HZ    | 16:UM:180:ARG:HA    | 1.83                     | 0.43              |
| 16:UM:230:LYS:HD2   | 16:UM:230:LYS:O     | 2.18                     | 0.43              |
| 18:UO:86:SER:O      | 18:UO:98:ALA:HA     | 2.18                     | 0.43              |
| 18:UO:209:LEU:HD13  | 18:UO:237:TRP:CD2   | 2.53                     | 0.43              |
| 20:UQ:90:LYS:HG2    | 20:UQ:144:VAL:O     | 2.18                     | 0.43              |
| 20:UQ:509:THR:CG2   | 20:UQ:530:LYS:HB2   | 2.48                     | 0.43              |
| 21:UR:164:LEU:HD23  | 24:UU:175:THR:HG22  | 2.00                     | 0.43              |
| 21:UR:165:ARG:HE    | 24:UU:218:LEU:CD2   | 2.24                     | 0.43              |
| 21:UR:405:THR:OG1   | 21:UR:428:ALA:HB2   | 2.18                     | 0.43              |
| 22:US:197:SER:HA    | 22:US:256:ASN:ND2   | 2.33                     | 0.43              |
| 22:US:360:ARG:O     | 22:US:363:ASP:HB2   | 2.18                     | 0.43              |
| 23:UT:395:GLU:HA    | 23:UT:398:GLN:HG3   | 2.00                     | 0.43              |
| 23:UT:844:VAL:HG22  | 23:UT:845:TYR:H     | 1.83                     | 0.43              |
| 23:UT:969:SER:HA    | 23:UT:972:LEU:HB2   | 1.99                     | 0.43              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 23:UT:1281:ARG:O   | 23:UT:1285:THR:HG23 | 2.18                     | 0.43              |
| 23:UT:1958:MET:O   | 23:UT:1958:MET:HG2  | 2.17                     | 0.43              |
| 24:UU:605:LEU:HD13 | 24:UU:628:VAL:HG11  | 2.00                     | 0.43              |
| 25:UV:255:GLU:OE1  | 25:UV:269:ARG:NH2   | 2.51                     | 0.43              |
| 25:UV:351:LYS:HA   | 25:UV:354:LYS:HZ3   | 1.82                     | 0.43              |
| 25:UV:754:LEU:HD23 | 25:UV:785:GLU:OE2   | 2.18                     | 0.43              |
| 28:CD:201:TRP:CZ2  | 29:CE:161:VAL:HG21  | 2.53                     | 0.43              |
| 28:CD:411:ARG:O    | 28:CD:414:PHE:HB3   | 2.17                     | 0.43              |
| 29:CE:144:ALA:O    | 29:CE:147:ILE:HG22  | 2.18                     | 0.43              |
| 30:CG:93:VAL:O     | 31:CH:552:TRP:NE1   | 2.40                     | 0.43              |
| 31:CH:198:LYS:HE3  | 31:CH:211:LEU:HB2   | 2.00                     | 0.43              |
| 31:CH:437:ARG:HD3  | 31:CH:437:ARG:HA    | 1.67                     | 0.43              |
| 33:CJ:118:ASN:HD22 | 33:CJ:118:ASN:C     | 2.13                     | 0.43              |
| 35:CL:254:HIS:O    | 35:CL:258:ILE:HG12  | 2.18                     | 0.43              |
| 35:CL:808:PHE:CD2  | 35:CL:1026:LYS:HD2  | 2.53                     | 0.43              |
| 35:CL:835:HIS:CD2  | 35:CL:836:LYS:N     | 2.86                     | 0.43              |
| 36:CM:90:CYS:SG    | 36:CM:120:GLY:HA3   | 2.58                     | 0.43              |
| 38:JC:85:ASP:HB3   | 38:JC:88:ASN:OD1    | 2.18                     | 0.43              |
| 38:JC:343:ILE:HD11 | 38:JC:345:SER:HB2   | 2.01                     | 0.43              |
| 45:JN:274:LYS:HB3  | 45:JN:274:LYS:HE3   | 1.70                     | 0.43              |
| 47:JP:345:THR:HG23 | 47:JP:347:ARG:H     | 1.83                     | 0.43              |
| 49:DE:130:GLN:HE21 | 49:DE:131:LEU:H     | 1.65                     | 0.43              |
| 53:DI:98:LYS:HZ3   | 53:DI:99:ALA:HB2    | 1.83                     | 0.43              |
| 60:DW:93:LEU:HA    | 60:DW:93:LEU:HD23   | 1.79                     | 0.43              |
| 66:D3:542:A:HO2'   | 66:D3:543:C:P       | 2.34                     | 0.43              |
| 66:D3:837:G:H2'    | 66:D3:838:G:C8      | 2.52                     | 0.43              |
| 66:D3:1149:G:H2'   | 66:D3:1150:G:H8     | 1.82                     | 0.43              |
| 66:D3:1155:G:C6    | 66:D3:1156:C:C4     | 3.07                     | 0.43              |
| 67:D4:64:A:H2'     | 67:D4:65:C:H6       | 1.83                     | 0.43              |
| 3:JA:805:ILE:O     | 3:JA:808:SER:OG     | 2.24                     | 0.43              |
| 4:UA:396:ALA:C     | 4:UA:398:ARG:H      | 2.22                     | 0.43              |
| 4:UA:564:PHE:CE2   | 4:UA:678:GLU:HG2    | 2.54                     | 0.43              |
| 4:UA:710:ILE:HG13  | 4:UA:711:LEU:N      | 2.33                     | 0.43              |
| 8:UE:498:LEU:O     | 8:UE:502:VAL:HG12   | 2.18                     | 0.43              |
| 10:UG:90:GLU:O     | 10:UG:93:SER:OG     | 2.31                     | 0.43              |
| 10:UG:139:TRP:O    | 10:UG:139:TRP:CG    | 2.71                     | 0.43              |
| 10:UG:482:ASP:OD1  | 10:UG:483:ILE:N     | 2.52                     | 0.43              |
| 10:UG:529:ARG:NH1  | 10:UG:542:HIS:O     | 2.21                     | 0.43              |
| 11:UH:596:LYS:HZ3  | 11:UH:600:LYS:HD3   | 1.84                     | 0.43              |
| 12:UI:415:GLU:N    | 12:UI:415:GLU:OE1   | 2.51                     | 0.43              |
| 13:UJ:119:GLU:O    | 13:UJ:122:VAL:HG12  | 2.18                     | 0.43              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 13:UJ:1583:GLN:HE22 | 13:UJ:1629:SER:HB3 | 1.83                     | 0.43              |
| 14:UK:185:MET:O     | 14:UK:189:SER:OG   | 2.35                     | 0.43              |
| 15:UL:226:VAL:CG2   | 15:UL:248:PHE:HB3  | 2.48                     | 0.43              |
| 15:UL:472:HIS:HB3   | 15:UL:494:ASP:OD2  | 2.17                     | 0.43              |
| 16:UM:19:SER:OG     | 16:UM:20:SER:N     | 2.51                     | 0.43              |
| 16:UM:279:LYS:HB3   | 16:UM:327:ILE:HD11 | 2.01                     | 0.43              |
| 19:UP:171:VAL:O     | 19:UP:177:ARG:NH1  | 2.51                     | 0.43              |
| 20:UQ:409:LYS:H     | 20:UQ:409:LYS:HG2  | 1.58                     | 0.43              |
| 21:UR:141:ASN:ND2   | 65:D2:307:C:H5'    | 2.33                     | 0.43              |
| 23:UT:546:GLU:O     | 23:UT:549:LYS:HE3  | 2.19                     | 0.43              |
| 23:UT:917:ASP:O     | 23:UT:921:VAL:HG22 | 2.18                     | 0.43              |
| 23:UT:1932:GLU:O    | 23:UT:1936:ASN:ND2 | 2.52                     | 0.43              |
| 24:UU:511:ASP:O     | 24:UU:513:MET:N    | 2.52                     | 0.43              |
| 24:UU:580:GLN:C     | 24:UU:581:LEU:HD12 | 2.38                     | 0.43              |
| 25:UV:339:SER:HA    | 25:UV:342:HIS:NE2  | 2.33                     | 0.43              |
| 25:UV:578:ILE:HA    | 25:UV:619:VAL:HA   | 1.99                     | 0.43              |
| 25:UV:905:SER:C     | 25:UV:906:TYR:HD2  | 2.21                     | 0.43              |
| 25:UV:934:ALA:O     | 25:UV:937:ILE:HG22 | 2.17                     | 0.43              |
| 27:UZ:19:ALA:O      | 27:UZ:22:LEU:HG    | 2.18                     | 0.43              |
| 28:CD:31:LEU:HD23   | 28:CD:31:LEU:HA    | 1.79                     | 0.43              |
| 28:CD:86:LEU:HD23   | 28:CD:86:LEU:HA    | 1.82                     | 0.43              |
| 29:CE:53:ALA:O      | 29:CE:57:LEU:HG    | 2.18                     | 0.43              |
| 29:CE:145:HIS:O     | 29:CE:149:ARG:HG3  | 2.18                     | 0.43              |
| 29:CE:160:ASP:HA    | 29:CE:163:ILE:HB   | 2.00                     | 0.43              |
| 35:CL:124:ASP:HB2   | 35:CL:808:PHE:HE1  | 1.84                     | 0.43              |
| 35:CL:1113:ILE:HD13 | 35:CL:1113:ILE:HA  | 1.88                     | 0.43              |
| 39:JF:214:ASP:OD2   | 39:JF:224:LYS:NZ   | 2.32                     | 0.43              |
| 39:JG:110:LEU:H     | 39:JG:110:LEU:HD23 | 1.84                     | 0.43              |
| 46:JO:103:LEU:HD12  | 46:JO:116:ILE:HG21 | 2.01                     | 0.43              |
| 49:DE:53:LYS:HD2    | 49:DE:53:LYS:HA    | 1.76                     | 0.43              |
| 50:DF:185:ARG:HA    | 50:DF:185:ARG:CZ   | 2.48                     | 0.43              |
| 52:DH:73:VAL:O      | 52:DH:77:LEU:HD23  | 2.18                     | 0.43              |
| 56:DN:114:ARG:O     | 56:DN:118:ILE:HG12 | 2.18                     | 0.43              |
| 61:DX:52:ILE:O      | 61:DX:75:GLN:N     | 2.49                     | 0.43              |
| 62:DY:20:ARG:O      | 62:DY:21:LYS:HD3   | 2.17                     | 0.43              |
| 62:DY:106:GLN:OE1   | 62:DY:106:GLN:HA   | 2.19                     | 0.43              |
| 66:D3:96:G:H21      | 66:D3:426:G:H5'    | 1.83                     | 0.43              |
| 66:D3:111:U:H2'     | 66:D3:112:A:C8     | 2.44                     | 0.43              |
| 66:D3:147:A:H2'     | 66:D3:148:A:H8     | 1.83                     | 0.43              |
| 66:D3:548:G:C5      | 66:D3:549:G:C8     | 3.06                     | 0.43              |
| 66:D3:1592:A:N3     | 66:D3:1605:G:N2    | 2.66                     | 0.43              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 66:D3:1623:C:H2'    | 66:D3:1624:C:H6     | 1.83                     | 0.43              |
| 67:D4:172:U:H2'     | 67:D4:173:A:H8      | 1.81                     | 0.43              |
| 69:EB:101:GLU:O     | 69:EB:105:SER:N     | 2.51                     | 0.43              |
| 77:EJ:211:ARG:HA    | 77:EJ:248:ALA:HA    | 2.00                     | 0.43              |
| 1:CA:222:GLU:HB2    | 28:CD:162:LYS:NZ    | 2.33                     | 0.43              |
| 2:DA:131:ASP:OD2    | 2:DA:180:THR:HB     | 2.18                     | 0.43              |
| 3:JA:74:GLU:O       | 3:JA:78:LYS:HG2     | 2.18                     | 0.43              |
| 3:JA:130:LEU:HB3    | 3:JA:135:LEU:HD21   | 1.99                     | 0.43              |
| 3:JA:747:LEU:HD12   | 3:JA:759:THR:O      | 2.18                     | 0.43              |
| 3:JA:769:ARG:HH22   | 3:JA:771:SER:HB2    | 1.82                     | 0.43              |
| 3:JA:888:ILE:HD11   | 3:JA:898:ILE:HG21   | 2.01                     | 0.43              |
| 4:UA:162:LEU:HB2    | 4:UA:172:ILE:HG22   | 2.01                     | 0.43              |
| 4:UA:218:TRP:CZ3    | 4:UA:250:ILE:HG13   | 2.53                     | 0.43              |
| 1:CB:218:ILE:CD1    | 29:CE:141:LEU:HA    | 2.48                     | 0.43              |
| 1:CB:221:ILE:O      | 1:CB:221:ILE:HG22   | 2.18                     | 0.43              |
| 5:UB:562:PRO:HA     | 5:UB:565:VAL:HG12   | 2.00                     | 0.43              |
| 8:UE:111:ASP:OD1    | 8:UE:153:ILE:N      | 2.52                     | 0.43              |
| 8:UE:318:GLN:O      | 8:UE:322:ILE:HG23   | 2.18                     | 0.43              |
| 9:UF:127:LYS:O      | 9:UF:130:HIS:HB2    | 2.18                     | 0.43              |
| 10:UG:160:LEU:HD12  | 10:UG:161:GLN:N     | 2.34                     | 0.43              |
| 11:UH:545:ARG:HG2   | 11:UH:574:ARG:HH22  | 1.83                     | 0.43              |
| 11:UH:596:LYS:HD3   | 11:UH:600:LYS:NZ    | 2.32                     | 0.43              |
| 11:UH:670:GLU:O     | 11:UH:674:GLU:OE1   | 2.37                     | 0.43              |
| 13:UJ:669:VAL:HA    | 13:UJ:672:ASP:OD2   | 2.18                     | 0.43              |
| 13:UJ:763:LEU:HB3   | 13:UJ:768:LYS:NZ    | 2.33                     | 0.43              |
| 15:UL:120:HIS:CE1   | 15:UL:146:ILE:HG13  | 2.53                     | 0.43              |
| 15:UL:337:LYS:HD2   | 15:UL:358:SER:HB3   | 2.01                     | 0.43              |
| 21:UR:142:LYS:HB3   | 65:D2:309:A:C2      | 2.53                     | 0.43              |
| 23:UT:37:ARG:NE     | 23:UT:40:ASP:OD2    | 2.49                     | 0.43              |
| 23:UT:270:ARG:O     | 23:UT:273:SER:OG    | 2.36                     | 0.43              |
| 23:UT:1024:GLN:OE1  | 23:UT:1024:GLN:N    | 2.50                     | 0.43              |
| 23:UT:1613:ALA:O    | 23:UT:1617:VAL:HG13 | 2.18                     | 0.43              |
| 23:UT:1625:ASN:OD1  | 23:UT:1626:ASP:N    | 2.49                     | 0.43              |
| 23:UT:1636:LEU:HD12 | 23:UT:1676:GLU:OE2  | 2.19                     | 0.43              |
| 23:UT:1870:LYS:HB2  | 23:UT:1910:VAL:HG12 | 2.01                     | 0.43              |
| 24:UU:522:LEU:HD23  | 24:UU:546:ILE:O     | 2.18                     | 0.43              |
| 25:UV:222:PHE:HD2   | 25:UV:225:LEU:HD11  | 1.84                     | 0.43              |
| 25:UV:713:LEU:HD23  | 25:UV:713:LEU:HA    | 1.82                     | 0.43              |
| 25:UV:940:LYS:HG2   | 25:UV:964:PHE:CZ    | 2.54                     | 0.43              |
| 27:UZ:72:ILE:CG2    | 27:UZ:97:PHE:HA     | 2.48                     | 0.43              |
| 28:CD:108:SER:O     | 28:CD:111:GLU:HG3   | 2.18                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:CD:323:THR:OG1  | 28:CD:324:ASN:N    | 2.51                     | 0.43              |
| 29:CE:159:VAL:HG23 | 29:CE:162:MET:CG   | 2.49                     | 0.43              |
| 30:CF:17:THR:O     | 30:CF:21:LEU:HG    | 2.17                     | 0.43              |
| 31:CH:312:PHE:O    | 62:DY:2:SER:HA     | 2.19                     | 0.43              |
| 31:CH:546:GLU:CD   | 31:CH:551:ARG:HG2  | 2.38                     | 0.43              |
| 32:CI:13:LEU:O     | 32:CI:16:VAL:N     | 2.47                     | 0.43              |
| 32:CI:156:ASP:OD2  | 33:CJ:7:ARG:NH2    | 2.48                     | 0.43              |
| 35:CL:45:ARG:NE    | 35:CL:45:ARG:HA    | 2.34                     | 0.43              |
| 35:CL:828:ARG:NH1  | 61:DX:94:ASN:OD1   | 2.51                     | 0.43              |
| 35:CL:904:ASN:HA   | 35:CL:907:THR:HG23 | 2.00                     | 0.43              |
| 35:CL:1161:PHE:HB3 | 66:D3:1111:G:C6    | 2.54                     | 0.43              |
| 37:CN:233:LYS:HB2  | 37:CN:233:LYS:HE3  | 1.88                     | 0.43              |
| 39:JG:95:CYS:O     | 39:JG:99:LEU:HD23  | 2.19                     | 0.43              |
| 43:JK:460:LYS:HZ3  | 66:D3:342:C:H41    | 1.66                     | 0.43              |
| 45:JN:155:LEU:HD21 | 46:JO:197:ILE:HD11 | 2.01                     | 0.43              |
| 47:JP:322:THR:OG1  | 47:JP:330:ARG:HB2  | 2.18                     | 0.43              |
| 51:DG:49:VAL:CG2   | 51:DG:115:LYS:HE3  | 2.49                     | 0.43              |
| 51:DG:54:GLY:O     | 51:DG:110:ALA:N    | 2.52                     | 0.43              |
| 52:DH:45:SER:O     | 52:DH:46:ILE:HD13  | 2.19                     | 0.43              |
| 52:DH:112:ARG:NH2  | 66:D3:638:U:H1'    | 2.33                     | 0.43              |
| 53:DI:33:PRO:HB3   | 66:D3:330:G:O2'    | 2.18                     | 0.43              |
| 53:DI:110:ARG:NH2  | 53:DI:160:PHE:HB3  | 2.34                     | 0.43              |
| 53:DI:195:ARG:NH1  | 55:DL:11:ARG:O     | 2.51                     | 0.43              |
| 56:DN:54:LEU:HD13  | 56:DN:54:LEU:HA    | 1.89                     | 0.43              |
| 62:DY:86:GLU:HB2   | 62:DY:91:LEU:HD21  | 2.00                     | 0.43              |
| 62:DY:112:LYS:HD2  | 66:D3:57:G:P       | 2.58                     | 0.43              |
| 65:D2:184:U:H3     | 65:D2:213:G:H1     | 1.65                     | 0.43              |
| 66:D3:117:U:H3     | 66:D3:299:A:H61    | 1.65                     | 0.43              |
| 66:D3:353:A:H3'    | 66:D3:354:C:C6     | 2.53                     | 0.43              |
| 66:D3:541:A:H2'    | 66:D3:541:A:N3     | 2.34                     | 0.43              |
| 66:D3:752:A:H2     | 66:D3:797:G:H22    | 1.66                     | 0.43              |
| 66:D3:1474:G:H8    | 66:D3:1474:G:OP2   | 2.01                     | 0.43              |
| 2:DA:86:LEU:HB3    | 2:DA:98:THR:OG1    | 2.18                     | 0.43              |
| 2:DA:98:THR:HG1    | 2:DA:99:ASN:N      | 2.17                     | 0.43              |
| 3:JA:188:PHE:O     | 3:JA:192:LEU:HG    | 2.19                     | 0.43              |
| 3:JA:887:ALA:O     | 3:JA:892:ARG:N     | 2.52                     | 0.43              |
| 4:UA:164:THR:HG22  | 4:UA:194:VAL:O     | 2.18                     | 0.43              |
| 4:UA:337:TYR:CE1   | 24:UU:746:PRO:HB3  | 2.52                     | 0.43              |
| 4:UA:405:SER:HB2   | 4:UA:436:LEU:HD23  | 1.99                     | 0.43              |
| 4:UA:450:LEU:HD12  | 4:UA:451:ASP:OD1   | 2.18                     | 0.43              |
| 4:UA:592:ILE:O     | 4:UA:603:LEU:HD12  | 2.19                     | 0.43              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 3:JB:201:VAL:HA     | 3:JB:207:VAL:HA     | 2.00                     | 0.43              |
| 7:UD:100:GLU:N      | 7:UD:117:ILE:O      | 2.50                     | 0.43              |
| 9:UF:23:LEU:HG      | 9:UF:24:PHE:HD1     | 1.83                     | 0.43              |
| 9:UF:138:LYS:HZ3    | 28:CD:85:ASN:ND2    | 2.15                     | 0.43              |
| 9:UF:138:LYS:HB3    | 28:CD:52:SER:OG     | 2.19                     | 0.43              |
| 9:UF:266:ARG:O      | 9:UF:269:ILE:HG12   | 2.18                     | 0.43              |
| 13:UJ:706:CYS:SG    | 13:UJ:711:THR:OG1   | 2.72                     | 0.43              |
| 13:UJ:1375:PRO:HA   | 13:UJ:1378:ILE:HG12 | 2.00                     | 0.43              |
| 13:UJ:1627:THR:HG22 | 13:UJ:1669:ALA:HA   | 1.99                     | 0.43              |
| 14:UK:195:LEU:O     | 14:UK:199:LYS:HG2   | 2.19                     | 0.43              |
| 15:UL:624:LEU:HD23  | 15:UL:624:LEU:HA    | 1.89                     | 0.43              |
| 18:UO:30:TYR:CD2    | 18:UO:332:LYS:HB2   | 2.53                     | 0.43              |
| 18:UO:212:ASP:OD1   | 18:UO:212:ASP:N     | 2.51                     | 0.43              |
| 20:UQ:174:TYR:HD1   | 20:UQ:189:HIS:HA    | 1.82                     | 0.43              |
| 20:UQ:665:ILE:CG2   | 20:UQ:669:ASN:HB2   | 2.49                     | 0.43              |
| 21:UR:253:SER:HA    | 21:UR:567:SER:OG    | 2.18                     | 0.43              |
| 21:UR:374:ILE:HD11  | 21:UR:386:ILE:CG2   | 2.48                     | 0.43              |
| 22:US:355:ARG:HA    | 22:US:355:ARG:HD3   | 1.74                     | 0.43              |
| 23:UT:291:LEU:HA    | 23:UT:294:VAL:HG12  | 2.01                     | 0.43              |
| 23:UT:666:LEU:HG    | 23:UT:681:VAL:HG13  | 2.01                     | 0.43              |
| 23:UT:699:LEU:O     | 23:UT:702:SER:OG    | 2.34                     | 0.43              |
| 23:UT:874:LEU:HD13  | 23:UT:874:LEU:HA    | 1.84                     | 0.43              |
| 23:UT:887:ASN:HB2   | 23:UT:904:PHE:CZ    | 2.53                     | 0.43              |
| 23:UT:1147:ILE:O    | 23:UT:1150:ILE:HB   | 2.19                     | 0.43              |
| 23:UT:1502:ASN:O    | 23:UT:1506:GLU:HG3  | 2.18                     | 0.43              |
| 23:UT:1632:LEU:O    | 23:UT:1636:LEU:HD23 | 2.18                     | 0.43              |
| 23:UT:1957:GLN:HE22 | 23:UT:1995:ARG:C    | 2.20                     | 0.43              |
| 24:UU:83:LEU:HD23   | 24:UU:83:LEU:HA     | 1.80                     | 0.43              |
| 24:UU:570:ILE:HD12  | 24:UU:577:VAL:HA    | 2.00                     | 0.43              |
| 25:UV:188:SER:O     | 25:UV:193:ALA:N     | 2.41                     | 0.43              |
| 25:UV:440:LEU:HA    | 25:UV:457:TYR:HA    | 2.00                     | 0.43              |
| 25:UV:741:ILE:HA    | 25:UV:744:MET:HG2   | 2.00                     | 0.43              |
| 25:UV:895:HIS:NE2   | 25:UV:899:LEU:HD11  | 2.32                     | 0.43              |
| 25:UV:1205:LYS:NZ   | 25:UV:1215:ASN:HA   | 2.32                     | 0.43              |
| 26:UX:69:THR:HG22   | 26:UX:102:VAL:HG13  | 2.00                     | 0.43              |
| 27:UZ:217:GLN:HA    | 27:UZ:220:ILE:HG12  | 2.00                     | 0.43              |
| 28:CD:172:ASN:HA    | 28:CD:175:ILE:HD12  | 2.01                     | 0.43              |
| 32:CI:138:VAL:HG22  | 32:CI:158:VAL:HG12  | 2.00                     | 0.43              |
| 32:CI:171:LEU:O     | 32:CI:174:ARG:N     | 2.52                     | 0.43              |
| 33:CJ:7:ARG:HG2     | 33:CJ:11:GLU:OE2    | 2.18                     | 0.43              |
| 35:CL:93:MET:HE1    | 35:CL:227:ILE:HD11  | 2.01                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:CM:207:ARG:HB3  | 36:CM:269:GLU:CD   | 2.38                     | 0.43              |
| 36:CM:248:GLN:HB2  | 36:CM:250:LYS:NZ   | 2.33                     | 0.43              |
| 38:JC:139:LYS:HG2  | 38:JC:163:TYR:OH   | 2.18                     | 0.43              |
| 38:JC:247:THR:HG23 | 38:JC:251:TYR:HB3  | 2.00                     | 0.43              |
| 38:JC:276:LYS:O    | 38:JC:290:VAL:HA   | 2.19                     | 0.43              |
| 39:JG:121:LEU:HD13 | 39:JG:121:LEU:HA   | 1.91                     | 0.43              |
| 47:JP:350:HIS:HB2  | 47:JP:368:ASP:CB   | 2.49                     | 0.43              |
| 49:DE:137:PRO:HD2  | 49:DE:149:TYR:CD1  | 2.53                     | 0.43              |
| 50:DF:69:PHE:CD1   | 58:DQ:46:PHE:HD2   | 2.36                     | 0.43              |
| 50:DF:211:ILE:HD12 | 50:DF:214:LYS:HE3  | 2.01                     | 0.43              |
| 53:DI:193:LEU:HD23 | 53:DI:196:LEU:HD12 | 2.01                     | 0.43              |
| 54:DJ:86:LEU:HA    | 54:DJ:90:LYS:HD2   | 2.01                     | 0.43              |
| 54:DJ:143:ILE:HG21 | 66:D3:767:U:C2     | 2.54                     | 0.43              |
| 65:D2:182:G:C2     | 65:D2:216:U:C2     | 3.06                     | 0.43              |
| 66:D3:556:A:H3'    | 66:D3:557:G:H5''   | 1.99                     | 0.43              |
| 66:D3:1126:G:H2'   | 66:D3:1127:G:C4    | 2.53                     | 0.43              |
| 66:D3:1129:U:C2    | 66:D3:1140:G:C2    | 3.07                     | 0.43              |
| 66:D3:1140:G:H2'   | 66:D3:1141:G:C8    | 2.48                     | 0.43              |
| 66:D3:1483:A:C2    | 66:D3:1524:A:C6    | 3.07                     | 0.43              |
| 69:EB:260:THR:O    | 69:EB:264:CYS:N    | 2.48                     | 0.43              |
| 75:EH:119:VAL:HA   | 75:EH:149:ILE:HA   | 2.00                     | 0.43              |
| 1:CA:208:ILE:HD11  | 28:CD:159:SER:HB2  | 2.01                     | 0.43              |
| 3:JA:201:VAL:HG12  | 3:JA:202:ASP:O     | 2.18                     | 0.43              |
| 3:JA:280:ALA:HB3   | 3:JA:467:GLU:HA    | 2.00                     | 0.43              |
| 3:JA:473:PRO:HB2   | 3:JA:476:TYR:O     | 2.18                     | 0.43              |
| 3:JA:860:PRO:HD2   | 3:JA:861:MET:HE3   | 2.01                     | 0.43              |
| 4:UA:88:ASN:HD21   | 24:UU:659:GLN:NE2  | 2.08                     | 0.43              |
| 4:UA:323:LYS:HE3   | 4:UA:323:LYS:HB3   | 1.89                     | 0.43              |
| 5:UB:527:GLN:OE1   | 5:UB:531:GLN:HB2   | 2.17                     | 0.43              |
| 6:UC:433:ARG:CD    | 39:JF:231:PRO:HG2  | 2.41                     | 0.43              |
| 6:UC:544:ILE:HD12  | 6:UC:544:ILE:HA    | 1.77                     | 0.43              |
| 7:UD:479:LYS:NZ    | 7:UD:535:GLU:HA    | 2.34                     | 0.43              |
| 7:UD:535:GLU:HB2   | 7:UD:542:VAL:HG12  | 2.00                     | 0.43              |
| 8:UE:198:THR:HB    | 8:UE:201:PHE:HD1   | 1.82                     | 0.43              |
| 8:UE:301:LEU:HD23  | 8:UE:317:LEU:HD11  | 1.99                     | 0.43              |
| 8:UE:489:ALA:C     | 18:UO:16:LEU:HD21  | 2.39                     | 0.43              |
| 8:UE:539:ARG:HH11  | 20:UQ:524:ASP:CG   | 2.20                     | 0.43              |
| 9:UF:311:TYR:O     | 9:UF:314:SER:OG    | 2.29                     | 0.43              |
| 10:UG:122:GLY:CA   | 10:UG:385:PRO:HG2  | 2.49                     | 0.43              |
| 12:UI:501:GLY:C    | 12:UI:505:MET:HE2  | 2.39                     | 0.43              |
| 13:UJ:136:LEU:O    | 13:UJ:140:LEU:HB2  | 2.18                     | 0.43              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 13:UJ:272:LYS:HG2   | 13:UJ:306:LEU:HD21  | 2.00                     | 0.43              |
| 13:UJ:601:SER:O     | 13:UJ:611:ILE:HG22  | 2.18                     | 0.43              |
| 13:UJ:622:TRP:HB2   | 13:UJ:650:PHE:CE2   | 2.54                     | 0.43              |
| 13:UJ:680:TYR:CG    | 13:UJ:681:ALA:N     | 2.87                     | 0.43              |
| 13:UJ:1710:ALA:O    | 13:UJ:1714:ILE:HG12 | 2.18                     | 0.43              |
| 13:UJ:1743:GLU:OE2  | 13:UJ:1744:ILE:HG13 | 2.19                     | 0.43              |
| 14:UK:116:LYS:HE2   | 14:UK:116:LYS:HB2   | 1.79                     | 0.43              |
| 15:UL:321:TYR:HA    | 15:UL:324:PHE:HB3   | 2.00                     | 0.43              |
| 15:UL:403:ASN:O     | 15:UL:419:ILE:HG12  | 2.17                     | 0.43              |
| 15:UL:655:ALA:HB3   | 15:UL:656:HIS:HD1   | 1.83                     | 0.43              |
| 16:UM:74:GLN:O      | 16:UM:89:HIS:HD2    | 2.02                     | 0.43              |
| 16:UM:152:PHE:CE2   | 16:UM:163:LEU:HD13  | 2.53                     | 0.43              |
| 16:UM:732:ASN:HB2   | 16:UM:735:GLN:NE2   | 2.34                     | 0.43              |
| 18:UO:192:LEU:HD13  | 18:UO:210:ASN:HA    | 2.00                     | 0.43              |
| 18:UO:368:GLY:O     | 18:UO:374:ILE:HD11  | 2.18                     | 0.43              |
| 20:UQ:51:GLN:HB3    | 20:UQ:67:LYS:HA     | 2.00                     | 0.43              |
| 20:UQ:78:PHE:CD1    | 20:UQ:87:SER:HA     | 2.54                     | 0.43              |
| 20:UQ:421:LYS:HE2   | 20:UQ:421:LYS:HB3   | 1.81                     | 0.43              |
| 21:UR:174:ARG:NE    | 21:UR:179:ASP:OD1   | 2.52                     | 0.43              |
| 21:UR:252:GLN:HE22  | 65:D2:234:A:H61     | 1.66                     | 0.43              |
| 22:US:197:SER:HA    | 22:US:256:ASN:HD21  | 1.83                     | 0.43              |
| 22:US:199:PHE:CZ    | 22:US:212:LEU:HD22  | 2.54                     | 0.43              |
| 23:UT:452:ASN:OD1   | 23:UT:490:LYS:HE3   | 2.18                     | 0.43              |
| 23:UT:774:ILE:HG13  | 23:UT:775:ARG:N     | 2.34                     | 0.43              |
| 23:UT:1091:ILE:H    | 23:UT:1091:ILE:HD12 | 1.82                     | 0.43              |
| 23:UT:1651:ARG:NH1  | 23:UT:1744:GLU:OE2  | 2.48                     | 0.43              |
| 23:UT:1740:THR:HG23 | 23:UT:1742:VAL:H    | 1.83                     | 0.43              |
| 24:UU:115:ASP:N     | 24:UU:115:ASP:OD1   | 2.48                     | 0.43              |
| 24:UU:192:ASN:O     | 24:UU:196:GLY:N     | 2.43                     | 0.43              |
| 25:UV:612:PHE:CD2   | 25:UV:614:ARG:NH2   | 2.84                     | 0.43              |
| 26:UX:91:LEU:HD21   | 54:DJ:53:ARG:HB3    | 2.00                     | 0.43              |
| 27:UZ:90:ASP:O      | 27:UZ:92:HIS:ND1    | 2.51                     | 0.43              |
| 27:UZ:155:ARG:HB3   | 27:UZ:175:TYR:HE2   | 1.83                     | 0.43              |
| 30:CG:8:ALA:O       | 30:CG:80:PHE:CD2    | 2.71                     | 0.43              |
| 30:CG:18:GLN:OE1    | 30:CG:18:GLN:HA     | 2.18                     | 0.43              |
| 31:CH:66:LEU:HA     | 31:CH:69:GLN:OE1    | 2.19                     | 0.43              |
| 31:CH:189:THR:OG1   | 31:CH:197:THR:OG1   | 1.99                     | 0.43              |
| 31:CH:310:ASN:OD1   | 31:CH:310:ASN:N     | 2.50                     | 0.43              |
| 31:CH:399:GLU:OE2   | 31:CH:402:ILE:HG12  | 2.19                     | 0.43              |
| 31:CH:489:SER:OG    | 31:CH:499:TRP:NE1   | 2.33                     | 0.43              |
| 32:CI:57:LEU:HD12   | 32:CI:57:LEU:HA     | 1.79                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:CK:308:ARG:O    | 34:CK:312:GLU:OE1  | 2.36                     | 0.43              |
| 34:CK:508:ARG:HG3  | 34:CK:514:ALA:HB2  | 2.00                     | 0.43              |
| 35:CL:45:ARG:O     | 35:CL:49:VAL:HG22  | 2.19                     | 0.43              |
| 35:CL:148:PHE:CE2  | 35:CL:190:LEU:HD13 | 2.54                     | 0.43              |
| 36:CM:244:THR:HG22 | 36:CM:259:GLU:CB   | 2.48                     | 0.43              |
| 37:CN:263:ARG:HA   | 37:CN:266:LYS:HE2  | 2.00                     | 0.43              |
| 37:CN:267:LYS:HE3  | 37:CN:267:LYS:HB3  | 1.87                     | 0.43              |
| 38:JC:55:PHE:HZ    | 38:JC:77:TYR:O     | 2.02                     | 0.43              |
| 38:JC:56:SER:O     | 38:JC:336:ILE:HG23 | 2.19                     | 0.43              |
| 38:JC:69:GLN:HA    | 38:JC:86:PHE:CD2   | 2.54                     | 0.43              |
| 38:JC:109:ASP:OD1  | 38:JC:110:ASP:N    | 2.51                     | 0.43              |
| 38:JC:185:HIS:CD2  | 38:JC:233:THR:HA   | 2.53                     | 0.43              |
| 47:JP:330:ARG:HD2  | 47:JP:339:SER:OG   | 2.18                     | 0.43              |
| 51:DG:28:PHE:HD1   | 51:DG:102:VAL:HG13 | 1.83                     | 0.43              |
| 51:DG:171:LYS:HD3  | 66:D3:66:U:O2'     | 2.19                     | 0.43              |
| 53:DI:47:ARG:NH1   | 66:D3:398:G:OP2    | 2.30                     | 0.43              |
| 53:DI:79:ALA:CB    | 53:DI:164:ARG:HH11 | 2.28                     | 0.43              |
| 55:DL:72:THR:H     | 55:DL:88:ARG:NH2   | 2.17                     | 0.43              |
| 56:DN:20:ARG:HE    | 60:DW:56:HIS:CE1   | 2.35                     | 0.43              |
| 60:DW:57:ARG:O     | 60:DW:58:SER:OG    | 2.35                     | 0.43              |
| 65:D2:68:U:H5'     | 65:D2:69:U:OP2     | 2.19                     | 0.43              |
| 65:D2:427:A:H8     | 65:D2:428:A:H1'    | 1.82                     | 0.43              |
| 66:D3:627:C:N4     | 66:D3:628:G:C2     | 2.86                     | 0.43              |
| 66:D3:760:A:H2'    | 66:D3:761:G:O3'    | 2.19                     | 0.43              |
| 67:D4:20:U:H2'     | 67:D4:21:C:C6      | 2.53                     | 0.43              |
| 67:D4:319:G:H2'    | 67:D4:320:G:O4'    | 2.19                     | 0.43              |
| 67:D4:320:G:C2     | 67:D4:321:C:C2     | 3.07                     | 0.43              |
| 1:CA:225:ARG:HA    | 1:CA:252:ILE:CD1   | 2.48                     | 0.43              |
| 3:JA:540:LEU:HD11  | 3:JA:641:ASN:N     | 2.34                     | 0.43              |
| 3:JA:709:LEU:HD23  | 3:JA:709:LEU:H     | 1.83                     | 0.43              |
| 4:UA:711:LEU:HG    | 4:UA:712:PHE:H     | 1.83                     | 0.43              |
| 4:UA:820:ALA:O     | 4:UA:824:ILE:HG12  | 2.19                     | 0.43              |
| 5:UB:522:LEU:HD21  | 5:UB:553:TYR:CD2   | 2.53                     | 0.43              |
| 6:UC:496:GLN:HG2   | 6:UC:497:GLN:N     | 2.33                     | 0.43              |
| 6:UC:576:LEU:HD11  | 6:UC:580:ARG:CD    | 2.49                     | 0.43              |
| 7:UD:587:ALA:C     | 7:UD:589:ASN:H     | 2.21                     | 0.43              |
| 8:UE:148:LEU:HD23  | 8:UE:149:ASN:N     | 2.33                     | 0.43              |
| 9:UF:4:THR:O       | 9:UF:8:LEU:HD23    | 2.19                     | 0.43              |
| 9:UF:31:LEU:HD12   | 9:UF:32:ILE:N      | 2.33                     | 0.43              |
| 10:UG:140:ARG:NH1  | 13:UJ:20:LEU:HD21  | 2.16                     | 0.43              |
| 11:UH:549:ARG:HA   | 11:UH:549:ARG:NH2  | 2.33                     | 0.43              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 12:UI:416:ILE:HA   | 12:UI:419:PHE:CD1   | 2.53                     | 0.43              |
| 13:UJ:765:ASN:O    | 13:UJ:768:LYS:HB3   | 2.18                     | 0.43              |
| 13:UJ:1574:ALA:HA  | 13:UJ:1577:LYS:HG2  | 2.01                     | 0.43              |
| 15:UL:105:VAL:HG21 | 15:UL:115:LEU:HD23  | 2.01                     | 0.43              |
| 15:UL:677:HIS:C    | 15:UL:679:HIS:H     | 2.22                     | 0.43              |
| 15:UL:941:THR:HG22 | 66:D3:1632:C:H42    | 1.82                     | 0.43              |
| 16:UM:363:ARG:HG2  | 16:UM:383:ILE:HG22  | 2.01                     | 0.43              |
| 16:UM:513:LYS:HZ1  | 16:UM:534:ARG:N     | 2.17                     | 0.43              |
| 18:UO:40:ASN:CG    | 18:UO:41:SER:H      | 2.20                     | 0.43              |
| 20:UQ:10:TYR:HB2   | 20:UQ:757:PHE:CZ    | 2.54                     | 0.43              |
| 20:UQ:598:LYS:NZ   | 20:UQ:636:ASP:HA    | 2.34                     | 0.43              |
| 22:US:242:ASN:O    | 22:US:244:PRO:HD3   | 2.19                     | 0.43              |
| 23:UT:593:ASP:O    | 23:UT:597:ARG:HG2   | 2.18                     | 0.43              |
| 23:UT:706:LEU:HA   | 23:UT:706:LEU:HD23  | 1.68                     | 0.43              |
| 23:UT:859:GLY:O    | 23:UT:930:PHE:HD2   | 2.02                     | 0.43              |
| 23:UT:1341:GLU:CD  | 23:UT:1389:LYS:HZ3  | 2.21                     | 0.43              |
| 23:UT:1657:THR:HA  | 23:UT:1660:LYS:HG2  | 1.99                     | 0.43              |
| 23:UT:1816:HIS:HB2 | 23:UT:1895:PHE:CE1  | 2.54                     | 0.43              |
| 23:UT:1919:ILE:O   | 23:UT:1922:ILE:HG22 | 2.19                     | 0.43              |
| 23:UT:1928:ASP:O   | 23:UT:1931:SER:OG   | 2.35                     | 0.43              |
| 24:UU:230:VAL:CG1  | 24:UU:244:ILE:HB    | 2.48                     | 0.43              |
| 24:UU:567:ILE:HB   | 24:UU:581:LEU:HB2   | 2.00                     | 0.43              |
| 25:UV:401:LEU:O    | 25:UV:410:LYS:NZ    | 2.30                     | 0.43              |
| 25:UV:429:LEU:O    | 25:UV:489:LYS:NZ    | 2.48                     | 0.43              |
| 25:UV:762:TYR:CE2  | 25:UV:900:GLU:HG2   | 2.50                     | 0.43              |
| 25:UV:1048:SER:HB3 | 25:UV:1051:LEU:HD11 | 2.00                     | 0.43              |
| 27:UZ:191:PRO:C    | 27:UZ:192:ASN:HD22  | 2.22                     | 0.43              |
| 27:UZ:192:ASN:OD1  | 66:D3:1510:U:H5'    | 2.18                     | 0.43              |
| 28:CD:189:ASN:O    | 28:CD:193:MET:HE2   | 2.19                     | 0.43              |
| 28:CD:388:ARG:NH2  | 30:CG:66:HIS:CE1    | 2.87                     | 0.43              |
| 31:CH:168:ASN:HB3  | 31:CH:171:THR:O     | 2.19                     | 0.43              |
| 36:CM:56:ILE:O     | 36:CM:60:THR:OG1    | 2.24                     | 0.43              |
| 36:CM:263:ASP:OD1  | 36:CM:264:ALA:N     | 2.39                     | 0.43              |
| 36:CM:302:VAL:HG21 | 36:CM:329:ILE:HD11  | 2.00                     | 0.43              |
| 38:JC:209:PRO:C    | 38:JC:211:SER:H     | 2.22                     | 0.43              |
| 39:JG:171:LEU:HD22 | 39:JG:203:CYS:SG    | 2.59                     | 0.43              |
| 42:JJ:117:TYR:CG   | 42:JJ:118:PRO:HD3   | 2.54                     | 0.43              |
| 42:JJ:172:ILE:HB   | 42:JJ:176:ARG:NH1   | 2.33                     | 0.43              |
| 46:JO:42:MET:HB2   | 46:JO:81:THR:HG22   | 2.00                     | 0.43              |
| 47:JP:301:PHE:HB3  | 47:JP:332:TYR:CE2   | 2.54                     | 0.43              |
| 50:DF:221:ALA:O    | 50:DF:225:ARG:HG3   | 2.18                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:DG:78:THR:H     | 51:DG:81:VAL:CG2   | 2.31                     | 0.43              |
| 54:DJ:66:ASP:O     | 54:DJ:70:LEU:HD23  | 2.19                     | 0.43              |
| 54:DJ:106:GLU:OE2  | 54:DJ:115:LYS:HE3  | 2.19                     | 0.43              |
| 54:DJ:107:ARG:HD2  | 54:DJ:107:ARG:HA   | 1.71                     | 0.43              |
| 57:DO:26:THR:O     | 57:DO:43:THR:HG23  | 2.19                     | 0.43              |
| 58:DQ:48:VAL:CG2   | 58:DQ:78:VAL:HG13  | 2.48                     | 0.43              |
| 65:D2:97:G:C6      | 65:D2:98:G:C6      | 3.07                     | 0.43              |
| 65:D2:134:A:H2'    | 65:D2:135:G:H8     | 1.84                     | 0.43              |
| 65:D2:224:G:C5     | 65:D2:225:U:C4     | 3.07                     | 0.43              |
| 66:D3:243:G:H2'    | 66:D3:244:A:C8     | 2.53                     | 0.43              |
| 66:D3:299:A:C6     | 66:D3:300:A:C5     | 3.07                     | 0.43              |
| 66:D3:1114:G:C2    | 66:D3:1115:U:C4    | 3.06                     | 0.43              |
| 66:D3:1271:G:C6    | 66:D3:1272:U:C2    | 3.06                     | 0.43              |
| 66:D3:1529:C:H6    | 66:D3:1529:C:O5'   | 2.02                     | 0.43              |
| 66:D3:1616:G:C6    | 66:D3:1617:U:C2    | 3.07                     | 0.43              |
| 66:D3:1702:A:H3'   | 66:D3:1703:C:O4'   | 2.19                     | 0.43              |
| 71:ED:348:SER:O    | 71:ED:361:THR:N    | 2.51                     | 0.43              |
| 79:EN:567:VAL:O    | 79:EN:571:MET:N    | 2.41                     | 0.43              |
| 1:CA:109:LYS:HG3   | 1:CA:110:ASN:N     | 2.33                     | 0.43              |
| 1:CA:320:TYR:CE2   | 1:CA:322:ARG:HD2   | 2.54                     | 0.43              |
| 2:DA:119:THR:OG1   | 2:DA:155:TYR:HA    | 2.19                     | 0.43              |
| 3:JA:734:HIS:O     | 3:JA:738:LYS:HG2   | 2.19                     | 0.43              |
| 3:JA:846:SER:HB2   | 3:JA:918:ARG:NH1   | 2.32                     | 0.43              |
| 4:UA:109:ARG:NH1   | 4:UA:109:ARG:HB2   | 2.34                     | 0.43              |
| 4:UA:493:TRP:CH2   | 32:CI:140:PRO:HD3  | 2.54                     | 0.43              |
| 4:UA:524:ARG:HG3   | 4:UA:585:TYR:HD2   | 1.84                     | 0.43              |
| 4:UA:542:PHE:CE2   | 4:UA:549:GLN:HB2   | 2.54                     | 0.43              |
| 5:UB:573:LEU:HA    | 5:UB:573:LEU:HD23  | 1.74                     | 0.43              |
| 5:UB:657:PHE:O     | 5:UB:661:ILE:HG12  | 2.18                     | 0.43              |
| 7:UD:322:ASN:CB    | 20:UQ:329:ASN:HD22 | 2.28                     | 0.43              |
| 8:UE:15:GLN:O      | 8:UE:34:THR:HG22   | 2.19                     | 0.43              |
| 8:UE:126:PHE:HB2   | 8:UE:140:PHE:HD2   | 1.84                     | 0.43              |
| 8:UE:129:PHE:CZ    | 8:UE:136:LEU:HB2   | 2.54                     | 0.43              |
| 8:UE:300:LEU:H     | 8:UE:319:TRP:HE1   | 1.66                     | 0.43              |
| 9:UF:6:TYR:O       | 9:UF:9:GLU:HG3     | 2.18                     | 0.43              |
| 10:UG:246:VAL:HG23 | 10:UG:259:TRP:O    | 2.19                     | 0.43              |
| 10:UG:263:MET:CE   | 17:UN:836:ASN:HA   | 2.49                     | 0.43              |
| 10:UG:409:ALA:O    | 47:JP:8:ARG:NH2    | 2.47                     | 0.43              |
| 13:UJ:526:LEU:O    | 13:UJ:530:THR:HG23 | 2.18                     | 0.43              |
| 13:UJ:1461:TRP:HB2 | 13:UJ:1477:PHE:CZ  | 2.54                     | 0.43              |
| 13:UJ:1601:VAL:O   | 13:UJ:1605:LEU:HG  | 2.19                     | 0.43              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 14:UK:223:GLU:OE2   | 14:UK:223:GLU:HA    | 2.18                     | 0.43              |
| 15:UL:39:GLY:O      | 15:UL:54:ILE:HG12   | 2.18                     | 0.43              |
| 15:UL:611:LEU:HA    | 15:UL:611:LEU:HD23  | 1.74                     | 0.43              |
| 15:UL:658:SER:HB2   | 15:UL:677:HIS:HB3   | 2.01                     | 0.43              |
| 15:UL:829:VAL:O     | 15:UL:833:LEU:HD23  | 2.19                     | 0.43              |
| 16:UM:39:GLU:O      | 16:UM:40:ILE:HD13   | 2.19                     | 0.43              |
| 16:UM:365:ILE:HG22  | 16:UM:381:VAL:HG22  | 2.00                     | 0.43              |
| 16:UM:552:SER:OG    | 16:UM:553:GLY:N     | 2.51                     | 0.43              |
| 16:UM:662:GLN:O     | 16:UM:666:GLU:OE1   | 2.37                     | 0.43              |
| 18:UO:77:PHE:CD1    | 18:UO:113:PRO:HB3   | 2.53                     | 0.43              |
| 18:UO:117:LEU:HD12  | 50:DF:192:GLU:OE1   | 2.17                     | 0.43              |
| 18:UO:179:ALA:HB2   | 18:UO:223:PRO:HB3   | 1.99                     | 0.43              |
| 18:UO:360:MET:HE1   | 65:D2:234:A:H2'     | 2.00                     | 0.43              |
| 19:UP:172:LYS:HA    | 19:UP:177:ARG:HD2   | 1.99                     | 0.43              |
| 20:UQ:29:THR:HA     | 20:UQ:32:LYS:HE2    | 2.01                     | 0.43              |
| 23:UT:146:ASN:HA    | 23:UT:149:GLU:CD    | 2.39                     | 0.43              |
| 23:UT:193:ALA:HB1   | 23:UT:235:LEU:HA    | 2.00                     | 0.43              |
| 23:UT:296:GLU:HG2   | 23:UT:300:GLN:NE2   | 2.17                     | 0.43              |
| 23:UT:523:LEU:O     | 23:UT:526:TYR:HB3   | 2.18                     | 0.43              |
| 23:UT:863:THR:HA    | 23:UT:866:GLN:HB2   | 2.01                     | 0.43              |
| 23:UT:1112:TRP:CD1  | 23:UT:1118:LEU:HD13 | 2.52                     | 0.43              |
| 23:UT:1203:VAL:HG21 | 23:UT:1242:LYS:HB3  | 2.01                     | 0.43              |
| 23:UT:1383:ASN:OD1  | 23:UT:1384:LEU:N    | 2.52                     | 0.43              |
| 23:UT:1401:ASN:HA   | 23:UT:1404:ILE:HG12 | 1.99                     | 0.43              |
| 23:UT:1591:TYR:HB3  | 23:UT:1592:PRO:HD3  | 2.00                     | 0.43              |
| 23:UT:1653:ALA:O    | 23:UT:1656:VAL:HG22 | 2.19                     | 0.43              |
| 23:UT:1661:ILE:HG13 | 23:UT:1662:SER:N    | 2.33                     | 0.43              |
| 24:UU:30:ILE:HD11   | 24:UU:653:ILE:HG13  | 2.01                     | 0.43              |
| 24:UU:570:ILE:CD1   | 24:UU:577:VAL:HA    | 2.48                     | 0.43              |
| 25:UV:1144:ASP:OD2  | 25:UV:1146:THR:HG22 | 2.18                     | 0.43              |
| 25:UV:1190:PHE:HA   | 25:UV:1194:HIS:CE1  | 2.54                     | 0.43              |
| 25:UV:1227:GLY:HA3  | 25:UV:1231:VAL:CG2  | 2.49                     | 0.43              |
| 26:UX:182:ILE:HG22  | 26:UX:183:GLU:N     | 2.34                     | 0.43              |
| 28:CD:392:TYR:HB3   | 30:CG:62:GLU:OE1    | 2.18                     | 0.43              |
| 29:CE:70:SER:HA     | 29:CE:73:GLU:CD     | 2.39                     | 0.43              |
| 35:CL:608:LEU:HB2   | 36:CM:16:ASN:OD1    | 2.18                     | 0.43              |
| 35:CL:825:VAL:O     | 35:CL:884:ALA:HA    | 2.19                     | 0.43              |
| 35:CL:833:ARG:HD2   | 61:DX:138:GLU:HB3   | 2.01                     | 0.43              |
| 35:CL:867:THR:OG1   | 35:CL:868:ARG:NH2   | 2.52                     | 0.43              |
| 36:CM:260:ASP:HB3   | 36:CM:271:LEU:HD11  | 2.00                     | 0.43              |
| 37:CN:140:ALA:HA    | 37:CN:143:LYS:HE2   | 1.99                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:JO:197:ILE:HD12 | 46:JO:197:ILE:HA   | 1.90                     | 0.43              |
| 47:JP:5:THR:HG23   | 47:JP:6:ILE:O      | 2.19                     | 0.43              |
| 47:JP:428:GLU:O    | 47:JP:432:ILE:HG13 | 2.19                     | 0.43              |
| 49:DE:101:LEU:HD11 | 49:DE:109:PHE:HB3  | 2.00                     | 0.43              |
| 50:DF:72:HIS:HE2   | 58:DQ:75:VAL:HG13  | 1.84                     | 0.43              |
| 51:DG:46:LYS:HB2   | 51:DG:119:GLN:NE2  | 2.33                     | 0.43              |
| 52:DH:14:THR:O     | 52:DH:18:LEU:HG    | 2.19                     | 0.43              |
| 53:DI:40:ALA:HA    | 53:DI:61:GLU:OE1   | 2.18                     | 0.43              |
| 53:DI:172:ARG:HG2  | 66:D3:330:G:OP1    | 2.19                     | 0.43              |
| 55:DL:63:LEU:HD11  | 66:D3:249:U:N3     | 2.33                     | 0.43              |
| 60:DW:31:SER:O     | 60:DW:35:ILE:HG12  | 2.19                     | 0.43              |
| 65:D2:82:A:O2'     | 65:D2:83:U:P       | 2.77                     | 0.43              |
| 65:D2:185:A:C6     | 65:D2:186:C:C4     | 3.07                     | 0.43              |
| 66:D3:26:A:H61     | 66:D3:600:U:H3     | 1.67                     | 0.43              |
| 66:D3:350:U:O3'    | 66:D3:352:A:H5''   | 2.18                     | 0.43              |
| 66:D3:547:U:O2'    | 66:D3:548:G:OP1    | 2.33                     | 0.43              |
| 66:D3:579:A:O2'    | 66:D3:580:A:OP2    | 2.29                     | 0.43              |
| 66:D3:956:C:O2'    | 66:D3:1047:G:N3    | 2.48                     | 0.43              |
| 67:D4:12:U:O2'     | 67:D4:13:C:H5'     | 2.19                     | 0.43              |
| 76:EI:238:GLN:O    | 76:EI:242:ALA:N    | 2.49                     | 0.43              |
| 78:EK:928:VAL:O    | 78:EK:936:GLU:HA   | 2.18                     | 0.43              |
| 1:CA:171:LEU:HD12  | 1:CA:172:TYR:H     | 1.84                     | 0.43              |
| 2:DA:8:ARG:HH22    | 66:D3:907:A:H3'    | 1.84                     | 0.43              |
| 2:DA:9:LEU:HD21    | 16:UM:619:ARG:CZ   | 2.49                     | 0.43              |
| 2:DA:43:VAL:O      | 2:DA:43:VAL:HG13   | 2.19                     | 0.43              |
| 3:JA:734:HIS:HE1   | 3:JA:803:SER:C     | 2.22                     | 0.43              |
| 3:JA:803:SER:O     | 3:JA:806:GLU:HG3   | 2.18                     | 0.43              |
| 3:JA:895:ILE:H     | 3:JA:895:ILE:HD12  | 1.83                     | 0.43              |
| 4:UA:162:LEU:HD22  | 4:UA:199:PHE:CZ    | 2.54                     | 0.43              |
| 4:UA:273:ARG:O     | 4:UA:273:ARG:HG2   | 2.19                     | 0.43              |
| 4:UA:319:PHE:O     | 4:UA:327:LEU:HD12  | 2.19                     | 0.43              |
| 5:UB:573:LEU:HD12  | 5:UB:591:ILE:HG21  | 2.00                     | 0.43              |
| 5:UB:680:LYS:HD2   | 5:UB:681:PRO:HD3   | 1.99                     | 0.43              |
| 7:UD:33:VAL:HG12   | 7:UD:752:LEU:HB2   | 2.01                     | 0.43              |
| 7:UD:53:HIS:CE1    | 7:UD:64:ASP:OD2    | 2.72                     | 0.43              |
| 7:UD:231:VAL:HG13  | 7:UD:263:LYS:HE2   | 2.01                     | 0.43              |
| 8:UE:307:GLN:HG2   | 8:UE:313:TYR:CD2   | 2.54                     | 0.43              |
| 8:UE:368:ASN:O     | 20:UQ:596:LEU:HD21 | 2.18                     | 0.43              |
| 9:UF:154:GLU:OE2   | 9:UF:160:ASN:HB2   | 2.19                     | 0.43              |
| 10:UG:245:ALA:HB2  | 47:JP:35:PHE:HZ    | 1.83                     | 0.43              |
| 10:UG:494:ASN:O    | 65:D2:354:G:O2'    | 2.26                     | 0.43              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 11:UH:552:LYS:HA   | 11:UH:576:ARG:HH22  | 1.82                     | 0.43              |
| 13:UJ:65:LYS:HZ1   | 21:UR:45:ILE:HB     | 1.84                     | 0.43              |
| 13:UJ:172:LYS:NZ   | 29:CE:402:GLU:OE1   | 2.35                     | 0.43              |
| 13:UJ:177:LEU:O    | 13:UJ:181:LYS:HG2   | 2.18                     | 0.43              |
| 13:UJ:1481:LEU:O   | 13:UJ:1485:VAL:HG23 | 2.19                     | 0.43              |
| 13:UJ:1587:ARG:HA  | 13:UJ:1632:PHE:CD2  | 2.54                     | 0.43              |
| 14:UK:22:ARG:HD3   | 14:UK:22:ARG:HA     | 1.64                     | 0.43              |
| 15:UL:17:ILE:H     | 15:UL:360:ASN:CG    | 2.22                     | 0.43              |
| 15:UL:409:ALA:HB3  | 15:UL:413:SER:OG    | 2.18                     | 0.43              |
| 15:UL:810:LEU:HD11 | 15:UL:849:HIS:NE2   | 2.34                     | 0.43              |
| 16:UM:16:TYR:OH    | 16:UM:21:ALA:O      | 2.37                     | 0.43              |
| 16:UM:195:GLY:O    | 16:UM:214:GLY:N     | 2.31                     | 0.43              |
| 16:UM:500:SER:HA   | 16:UM:541:PHE:HD2   | 1.83                     | 0.43              |
| 18:UO:21:THR:OG1   | 18:UO:24:GLN:HG2    | 2.19                     | 0.43              |
| 18:UO:156:ASN:OD1  | 50:DF:203:LYS:HE3   | 2.19                     | 0.43              |
| 18:UO:411:LYS:HE3  | 18:UO:411:LYS:HB2   | 1.68                     | 0.43              |
| 21:UR:227:LEU:HD12 | 21:UR:227:LEU:HA    | 1.92                     | 0.43              |
| 23:UT:229:TYR:CE2  | 23:UT:274:LEU:HD13  | 2.54                     | 0.43              |
| 23:UT:461:ILE:HA   | 23:UT:464:PHE:HB3   | 1.99                     | 0.43              |
| 23:UT:597:ARG:NH1  | 23:UT:668:GLY:HA3   | 2.33                     | 0.43              |
| 23:UT:705:LYS:HZ1  | 23:UT:799:PHE:HE2   | 1.66                     | 0.43              |
| 23:UT:844:VAL:HG22 | 23:UT:845:TYR:N     | 2.33                     | 0.43              |
| 23:UT:897:PHE:O    | 23:UT:901:ILE:HG12  | 2.19                     | 0.43              |
| 23:UT:1471:GLU:HB2 | 23:UT:1517:HIS:CE1  | 2.54                     | 0.43              |
| 24:UU:190:LEU:HD13 | 24:UU:200:PHE:CD2   | 2.47                     | 0.43              |
| 24:UU:595:PRO:HB3  | 24:UU:636:PRO:O     | 2.19                     | 0.43              |
| 25:UV:256:TYR:HD2  | 25:UV:592:PHE:CE2   | 2.36                     | 0.43              |
| 25:UV:532:PRO:HG2  | 25:UV:693:LYS:HE2   | 2.01                     | 0.43              |
| 25:UV:1148:GLN:HA  | 25:UV:1151:LYS:NZ   | 2.32                     | 0.43              |
| 25:UV:1206:PRO:HA  | 25:UV:1212:VAL:HA   | 2.00                     | 0.43              |
| 25:UV:1208:ASP:OD1 | 25:UV:1211:ASN:N    | 2.42                     | 0.43              |
| 27:UZ:33:ASP:HB2   | 27:UZ:247:SER:HB2   | 2.01                     | 0.43              |
| 29:CE:87:LEU:HB3   | 29:CE:107:VAL:HG23  | 2.00                     | 0.43              |
| 29:CE:380:ARG:NH1  | 29:CE:382:ASP:OD1   | 2.45                     | 0.43              |
| 33:CJ:14:TYR:CZ    | 33:CJ:18:GLN:NE2    | 2.87                     | 0.43              |
| 33:CJ:59:ASP:O     | 33:CJ:62:LEU:HB2    | 2.19                     | 0.43              |
| 33:CJ:157:PHE:O    | 33:CJ:159:HIS:N     | 2.48                     | 0.43              |
| 35:CL:170:VAL:HA   | 35:CL:205:PHE:O     | 2.19                     | 0.43              |
| 39:JF:65:TYR:CD1   | 39:JF:146:HIS:NE2   | 2.87                     | 0.43              |
| 39:JF:176:ARG:O    | 39:JF:202:ILE:HD12  | 2.18                     | 0.43              |
| 42:JJ:205:ILE:HD11 | 42:JJ:251:ILE:HG23  | 1.99                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 42:JJ:246:SER:O   | 42:JJ:250:LEU:HG   | 2.19                     | 0.43              |
| 42:JJ:272:GLU:HG2 | 42:JJ:273:ARG:H    | 1.83                     | 0.43              |
| 46:JO:58:ASN:ND2  | 65:D2:347:U:H5''   | 2.19                     | 0.43              |
| 46:JO:94:ILE:HD12 | 46:JO:97:ALA:HB3   | 2.01                     | 0.43              |
| 47:JP:147:LEU:O   | 47:JP:148:TRP:HD1  | 2.02                     | 0.43              |
| 49:DE:18:TRP:CZ2  | 49:DE:43:PRO:HD3   | 2.54                     | 0.43              |
| 52:DH:51:VAL:HG12 | 52:DH:55:LYS:O     | 2.19                     | 0.43              |
| 53:DI:34:ALA:HB2  | 53:DI:56:ARG:HB3   | 2.00                     | 0.43              |
| 55:DL:53:TYR:OH   | 55:DL:114:ALA:HB2  | 2.19                     | 0.43              |
| 58:DQ:36:ILE:HG23 | 58:DQ:49:TYR:HE1   | 1.83                     | 0.43              |
| 65:D2:448:G:C2    | 65:D2:449:U:C2     | 3.06                     | 0.43              |
| 66:D3:330:G:H2'   | 66:D3:331:A:H8     | 1.83                     | 0.43              |
| 66:D3:397:A:C6    | 66:D3:398:G:C5     | 3.07                     | 0.43              |
| 66:D3:626:U:O2'   | 66:D3:627:C:O5'    | 2.37                     | 0.43              |
| 66:D3:685:A:N3    | 66:D3:685:A:H2'    | 2.34                     | 0.43              |
| 66:D3:910:C:H2'   | 66:D3:911:U:O4'    | 2.19                     | 0.43              |
| 66:D3:1148:C:H2'  | 66:D3:1149:G:H8    | 1.83                     | 0.43              |
| 66:D3:1721:A:N1   | 66:D3:1722:A:C5    | 2.87                     | 0.43              |
| 67:D4:164:C:H2'   | 67:D4:165:G:H8     | 1.84                     | 0.43              |
| 2:DA:83:LYS:HE3   | 2:DA:83:LYS:HB2    | 1.71                     | 0.42              |
| 3:JA:115:LEU:HD21 | 3:JA:137:ARG:NE    | 2.34                     | 0.42              |
| 3:JA:188:PHE:CE2  | 3:JA:192:LEU:HD11  | 2.54                     | 0.42              |
| 3:JA:790:SER:OG   | 3:JA:891:GLN:HG3   | 2.19                     | 0.42              |
| 4:UA:113:LEU:HD23 | 4:UA:114:ALA:N     | 2.34                     | 0.42              |
| 4:UA:361:VAL:HG22 | 4:UA:371:VAL:HG22  | 2.01                     | 0.42              |
| 4:UA:789:SER:OG   | 4:UA:790:GLN:N     | 2.52                     | 0.42              |
| 4:UA:802:LEU:HD23 | 4:UA:802:LEU:HA    | 1.80                     | 0.42              |
| 4:UA:853:ASP:OD1  | 4:UA:854:GLY:N     | 2.52                     | 0.42              |
| 1:CB:286:PHE:CE2  | 1:CB:314:CYS:HB3   | 2.53                     | 0.42              |
| 7:UD:122:VAL:HG21 | 7:UD:136:ASN:HB2   | 1.99                     | 0.42              |
| 7:UD:270:ALA:HB3  | 21:UR:446:ARG:NH2  | 2.34                     | 0.42              |
| 14:UK:162:SER:OG  | 14:UK:163:GLU:OE1  | 2.36                     | 0.42              |
| 15:UL:253:LYS:HZ1 | 66:D3:1741:U:H5''  | 1.83                     | 0.42              |
| 15:UL:658:SER:HB2 | 15:UL:677:HIS:HD1  | 1.84                     | 0.42              |
| 16:UM:189:HIS:CD2 | 16:UM:189:HIS:N    | 2.87                     | 0.42              |
| 16:UM:529:LEU:HG  | 16:UM:560:TRP:CD2  | 2.54                     | 0.42              |
| 16:UM:648:THR:O   | 16:UM:652:ILE:HG12 | 2.19                     | 0.42              |
| 18:UO:500:GLU:O   | 18:UO:504:ILE:HG12 | 2.19                     | 0.42              |
| 20:UQ:226:SER:HA  | 20:UQ:237:LEU:O    | 2.19                     | 0.42              |
| 21:UR:528:GLN:NE2 | 21:UR:546:LEU:O    | 2.52                     | 0.42              |
| 23:UT:174:CYS:O   | 23:UT:178:ILE:HG12 | 2.19                     | 0.42              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 23:UT:1680:THR:HG23 | 23:UT:1681:LEU:CD1 | 2.44                     | 0.42              |
| 24:UU:587:ARG:HH21  | 24:UU:605:LEU:HD21 | 1.83                     | 0.42              |
| 25:UV:141:TRP:CZ3   | 25:UV:144:LYS:HD2  | 2.54                     | 0.42              |
| 25:UV:328:ALA:O     | 25:UV:554:LYS:NZ   | 2.49                     | 0.42              |
| 25:UV:558:LEU:HD23  | 25:UV:562:LEU:HD23 | 2.00                     | 0.42              |
| 25:UV:968:TRP:NE1   | 25:UV:973:ASP:O    | 2.39                     | 0.42              |
| 25:UV:1043:SER:OG   | 25:UV:1046:ASP:OD2 | 2.25                     | 0.42              |
| 26:UX:182:ILE:HD12  | 26:UX:182:ILE:HG23 | 1.78                     | 0.42              |
| 28:CD:119:ILE:HD13  | 28:CD:119:ILE:HA   | 1.82                     | 0.42              |
| 29:CE:138:LYS:H     | 29:CE:138:LYS:HE2  | 1.84                     | 0.42              |
| 29:CE:230:GLU:O     | 29:CE:233:GLU:HG3  | 2.18                     | 0.42              |
| 33:CJ:77:TYR:HE1    | 33:CJ:156:HIS:CE1  | 2.37                     | 0.42              |
| 37:CN:136:ASN:HA    | 37:CN:139:ASN:ND2  | 2.32                     | 0.42              |
| 38:JC:50:ILE:HG13   | 38:JC:89:LEU:O     | 2.19                     | 0.42              |
| 38:JC:233:THR:O     | 38:JC:245:CYS:HA   | 2.19                     | 0.42              |
| 39:JF:89:PRO:HG2    | 39:JF:134:PHE:HZ   | 1.84                     | 0.42              |
| 39:JG:110:LEU:HD23  | 39:JG:110:LEU:N    | 2.34                     | 0.42              |
| 43:JK:487:ASP:HA    | 43:JK:490:ILE:HB   | 2.00                     | 0.42              |
| 47:JP:94:TYR:HD2    | 47:JP:150:ILE:CG2  | 2.26                     | 0.42              |
| 47:JP:109:HIS:NE2   | 47:JP:138:SER:OG   | 2.31                     | 0.42              |
| 49:DE:35:PRO:HG3    | 66:D3:122:U:O2'    | 2.19                     | 0.42              |
| 49:DE:154:ILE:HA    | 49:DE:174:LYS:NZ   | 2.34                     | 0.42              |
| 49:DE:181:VAL:HA    | 49:DE:228:ILE:H    | 1.84                     | 0.42              |
| 50:DF:207:THR:HA    | 50:DF:212:LYS:HZ3  | 1.83                     | 0.42              |
| 52:DH:15:GLU:HG2    | 52:DH:16:LEU:HD22  | 2.01                     | 0.42              |
| 52:DH:38:LEU:HD11   | 52:DH:77:LEU:HD11  | 2.00                     | 0.42              |
| 52:DH:45:SER:OG     | 52:DH:46:ILE:N     | 2.52                     | 0.42              |
| 57:DO:61:MET:O      | 57:DO:65:GLN:HG2   | 2.18                     | 0.42              |
| 58:DQ:60:PHE:CE1    | 58:DQ:89:LEU:HD13  | 2.53                     | 0.42              |
| 60:DW:111:MET:CE    | 60:DW:116:ALA:HA   | 2.48                     | 0.42              |
| 61:DX:114:LYS:NZ    | 66:D3:568:G:O3'    | 2.52                     | 0.42              |
| 61:DX:135:LEU:N     | 61:DX:135:LEU:HD12 | 2.33                     | 0.42              |
| 62:DY:125:LEU:HA    | 62:DY:128:LYS:HG3  | 2.00                     | 0.42              |
| 65:D2:202:U:H2'     | 65:D2:203:C:H6     | 1.84                     | 0.42              |
| 66:D3:-4:A:N6       | 66:D3:1:U:C2       | 2.87                     | 0.42              |
| 66:D3:69:G:C6       | 66:D3:70:C:C4      | 3.07                     | 0.42              |
| 66:D3:93:A:C6       | 66:D3:398:G:C6     | 3.07                     | 0.42              |
| 66:D3:195:G:H2'     | 66:D3:196:G:H8     | 1.84                     | 0.42              |
| 66:D3:557:G:N1      | 66:D3:558:U:C2     | 2.87                     | 0.42              |
| 66:D3:1150:G:C2     | 66:D3:1151:A:C4    | 3.07                     | 0.42              |
| 66:D3:1219:A:N1     | 66:D3:1265:G:H1'   | 2.34                     | 0.42              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 66:D3:1649:G:H2'   | 66:D3:1650:U:H6     | 1.83                     | 0.42              |
| 66:D3:1679:G:N2    | 66:D3:1722:A:H62    | 2.16                     | 0.42              |
| 67:D4:265:C:C2     | 67:D4:307:G:C2      | 3.07                     | 0.42              |
| 1:CA:226:HIS:O     | 1:CA:229:LYS:N      | 2.51                     | 0.42              |
| 2:DA:30:PHE:CE1    | 2:DA:94:LYS:HA      | 2.53                     | 0.42              |
| 3:JA:81:ILE:CD1    | 3:JA:88:VAL:HA      | 2.49                     | 0.42              |
| 3:JA:724:GLY:HA2   | 3:JA:763:LEU:HA     | 2.01                     | 0.42              |
| 5:UB:605:ASP:OD1   | 5:UB:610:ARG:HD3    | 2.19                     | 0.42              |
| 7:UD:147:ILE:O     | 7:UD:148:SER:OG     | 2.30                     | 0.42              |
| 8:UE:182:MET:HB3   | 8:UE:184:PHE:CE2    | 2.54                     | 0.42              |
| 9:UF:6:TYR:CD2     | 65:D2:487:A:C6      | 3.07                     | 0.42              |
| 9:UF:126:TYR:HA    | 9:UF:129:ILE:HD12   | 1.99                     | 0.42              |
| 9:UF:273:ILE:HD13  | 17:UN:341:LYS:NZ    | 2.35                     | 0.42              |
| 10:UG:98:SER:HB2   | 13:UJ:84:ASN:O      | 2.19                     | 0.42              |
| 13:UJ:330:VAL:O    | 13:UJ:333:LEU:HG    | 2.19                     | 0.42              |
| 13:UJ:362:LYS:HB3  | 13:UJ:365:ILE:HD13  | 2.00                     | 0.42              |
| 13:UJ:615:ASN:HB3  | 13:UJ:618:ASP:OD2   | 2.19                     | 0.42              |
| 13:UJ:741:LEU:HA   | 13:UJ:742:ASN:HA    | 1.61                     | 0.42              |
| 13:UJ:1483:SER:O   | 13:UJ:1487:ASN:ND2  | 2.52                     | 0.42              |
| 14:UK:130:SER:O    | 14:UK:130:SER:OG    | 2.31                     | 0.42              |
| 14:UK:223:GLU:HA   | 14:UK:226:LYS:HG3   | 2.02                     | 0.42              |
| 15:UL:298:LYS:O    | 15:UL:302:ARG:HG3   | 2.19                     | 0.42              |
| 15:UL:500:TRP:CZ3  | 15:UL:524:HIS:HB3   | 2.55                     | 0.42              |
| 16:UM:529:LEU:HG   | 16:UM:560:TRP:CE3   | 2.55                     | 0.42              |
| 16:UM:536:LEU:HA   | 16:UM:552:SER:HA    | 2.00                     | 0.42              |
| 16:UM:556:THR:HB   | 16:UM:572:GLU:OE1   | 2.19                     | 0.42              |
| 16:UM:625:THR:HA   | 16:UM:632:ILE:HA    | 2.00                     | 0.42              |
| 16:UM:628:ASP:N    | 16:UM:628:ASP:OD1   | 2.51                     | 0.42              |
| 18:UO:440:GLU:CG   | 18:UO:441:PRO:HD3   | 2.49                     | 0.42              |
| 20:UQ:215:VAL:O    | 20:UQ:219:ASP:HB2   | 2.19                     | 0.42              |
| 20:UQ:240:PRO:O    | 20:UQ:244:ILE:HG12  | 2.19                     | 0.42              |
| 20:UQ:396:ILE:HG22 | 20:UQ:397:LYS:N     | 2.35                     | 0.42              |
| 20:UQ:410:ASN:ND2  | 20:UQ:488:LEU:O     | 2.53                     | 0.42              |
| 22:US:415:MET:HB2  | 22:US:461:SER:O     | 2.19                     | 0.42              |
| 23:UT:323:PHE:CE2  | 23:UT:736:LEU:HB2   | 2.55                     | 0.42              |
| 23:UT:555:LEU:HD12 | 23:UT:596:ILE:HG13  | 2.00                     | 0.42              |
| 23:UT:904:PHE:HA   | 23:UT:910:SER:O     | 2.18                     | 0.42              |
| 23:UT:1661:ILE:O   | 23:UT:1665:LEU:HB2  | 2.19                     | 0.42              |
| 23:UT:1710:LEU:HB2 | 23:UT:1760:ASN:HD22 | 1.84                     | 0.42              |
| 24:UU:232:MET:HA   | 24:UU:232:MET:CE    | 2.48                     | 0.42              |
| 29:CE:215:ARG:HH12 | 29:CE:242:SER:HB3   | 1.85                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:CF:50:GLU:N     | 30:CF:102:ILE:O    | 2.52                     | 0.42              |
| 31:CH:443:LEU:N    | 31:CH:471:GLN:O    | 2.52                     | 0.42              |
| 32:CI:33:MET:HG2   | 32:CI:38:ILE:CG1   | 2.49                     | 0.42              |
| 32:CI:61:LEU:HD23  | 32:CI:61:LEU:HA    | 1.80                     | 0.42              |
| 33:CJ:287:LYS:HG2  | 33:CJ:288:ASP:N    | 2.33                     | 0.42              |
| 35:CL:69:PRO:HG3   | 35:CL:274:TYR:CD2  | 2.54                     | 0.42              |
| 35:CL:767:ILE:HG13 | 35:CL:768:GLU:OE1  | 2.19                     | 0.42              |
| 35:CL:976:ILE:HG13 | 35:CL:987:TYR:CD2  | 2.54                     | 0.42              |
| 35:CL:1025:GLU:N   | 35:CL:1025:GLU:OE1 | 2.40                     | 0.42              |
| 35:CL:1093:THR:OG1 | 35:CL:1094:TYR:N   | 2.52                     | 0.42              |
| 39:JF:213:LYS:HZ1  | 39:JF:215:ASN:HD22 | 1.66                     | 0.42              |
| 39:JG:37:ILE:HG13  | 39:JG:38:THR:N     | 2.34                     | 0.42              |
| 39:JG:188:ARG:NH1  | 39:JG:191:ASP:HB2  | 2.35                     | 0.42              |
| 44:JM:65:LEU:HD12  | 44:JM:66:GLU:N     | 2.34                     | 0.42              |
| 47:JP:280:ALA:HB1  | 47:JP:308:VAL:HG12 | 2.01                     | 0.42              |
| 49:DE:126:VAL:HG13 | 49:DE:139:VAL:HG21 | 2.02                     | 0.42              |
| 50:DF:92:ARG:NH2   | 66:D3:1613:U:OP1   | 2.52                     | 0.42              |
| 54:DJ:56:ALA:O     | 54:DJ:60:LEU:HD23  | 2.20                     | 0.42              |
| 55:DL:124:THR:CG2  | 55:DL:141:LYS:HE2  | 2.49                     | 0.42              |
| 60:DW:71:LYS:HB3   | 60:DW:130:TYR:CZ   | 2.54                     | 0.42              |
| 65:D2:90:G:C2      | 65:D2:91:U:C2      | 3.07                     | 0.42              |
| 65:D2:202:U:H2'    | 65:D2:203:C:C6     | 2.54                     | 0.42              |
| 65:D2:300:C:C2     | 65:D2:301:U:C5     | 3.07                     | 0.42              |
| 66:D3:172:C:H2'    | 66:D3:173:A:C8     | 2.55                     | 0.42              |
| 66:D3:364:G:H2'    | 66:D3:365:G:H8     | 1.84                     | 0.42              |
| 66:D3:514:G:O2'    | 66:D3:515:A:H8     | 2.02                     | 0.42              |
| 66:D3:549:G:C2     | 66:D3:550:A:C5     | 3.08                     | 0.42              |
| 66:D3:655:G:H5''   | 66:D3:679:U:H3     | 1.83                     | 0.42              |
| 66:D3:769:A:H5'    | 66:D3:770:A:OP2    | 2.19                     | 0.42              |
| 66:D3:867:G:H2'    | 66:D3:868:G:H8     | 1.83                     | 0.42              |
| 66:D3:915:A:C5     | 66:D3:916:U:C4     | 3.08                     | 0.42              |
| 66:D3:1055:U:H2'   | 66:D3:1056:U:O4'   | 2.19                     | 0.42              |
| 67:D4:54:C:C4      | 67:D4:55:A:N7      | 2.87                     | 0.42              |
| 67:D4:199:G:H2'    | 67:D4:200:C:C6     | 2.54                     | 0.42              |
| 71:ED:345:SER:HA   | 71:ED:365:GLY:H    | 1.84                     | 0.42              |
| 4:UA:492:SER:C     | 4:UA:494:ASP:N     | 2.72                     | 0.42              |
| 7:UD:79:TRP:HH2    | 7:UD:376:GLU:HG3   | 1.82                     | 0.42              |
| 7:UD:113:ARG:HD3   | 7:UD:174:PRO:HA    | 2.01                     | 0.42              |
| 8:UE:139:HIS:CG    | 8:UE:140:PHE:N     | 2.87                     | 0.42              |
| 10:UG:256:VAL:HB   | 10:UG:270:LEU:HB2  | 1.99                     | 0.42              |
| 10:UG:502:ARG:HG3  | 65:D2:370:U:H5     | 1.84                     | 0.42              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 11:UH:548:PRO:HB2  | 11:UH:549:ARG:H     | 1.57                     | 0.42              |
| 13:UJ:637:ILE:HG22 | 13:UJ:637:ILE:O     | 2.19                     | 0.42              |
| 13:UJ:651:LEU:HD21 | 13:UJ:683:SER:HB2   | 2.00                     | 0.42              |
| 13:UJ:1478:LEU:HA  | 13:UJ:1481:LEU:HG   | 2.01                     | 0.42              |
| 13:UJ:1688:ASN:O   | 13:UJ:1691:ILE:HG12 | 2.19                     | 0.42              |
| 14:UK:13:HIS:CE1   | 66:D3:555:A:N1      | 2.87                     | 0.42              |
| 14:UK:109:THR:O    | 14:UK:113:ILE:HG12  | 2.19                     | 0.42              |
| 14:UK:135:ILE:CG2  | 19:UP:178:VAL:HG22  | 2.49                     | 0.42              |
| 16:UM:387:HIS:HD2  | 16:UM:413:ILE:HD11  | 1.84                     | 0.42              |
| 16:UM:442:LEU:HD12 | 16:UM:442:LEU:O     | 2.19                     | 0.42              |
| 17:UN:849:PHE:CE1  | 66:D3:-4:A:C4       | 3.07                     | 0.42              |
| 18:UO:100:ASP:CG   | 18:UO:101:ALA:H     | 2.22                     | 0.42              |
| 18:UO:439:LEU:O    | 18:UO:442:LEU:HB3   | 2.20                     | 0.42              |
| 20:UQ:249:THR:O    | 20:UQ:257:ARG:NH1   | 2.47                     | 0.42              |
| 20:UQ:347:LEU:HD21 | 20:UQ:355:SER:HB2   | 2.00                     | 0.42              |
| 23:UT:52:ASP:O     | 23:UT:56:GLU:OE1    | 2.38                     | 0.42              |
| 23:UT:140:ILE:HD13 | 23:UT:140:ILE:HA    | 1.83                     | 0.42              |
| 23:UT:654:THR:OG1  | 23:UT:659:SER:OG    | 2.35                     | 0.42              |
| 23:UT:727:VAL:HG12 | 23:UT:728:LEU:HD23  | 2.01                     | 0.42              |
| 23:UT:901:ILE:HG21 | 23:UT:952:VAL:CG2   | 2.50                     | 0.42              |
| 23:UT:1002:ASN:HA  | 23:UT:1005:ASN:ND2  | 2.34                     | 0.42              |
| 23:UT:1241:GLN:HB3 | 23:UT:1245:LYS:NZ   | 2.34                     | 0.42              |
| 23:UT:1688:HIS:CG  | 23:UT:1745:ILE:HG12 | 2.54                     | 0.42              |
| 24:UU:58:PHE:CE1   | 24:UU:101:TYR:HD2   | 2.37                     | 0.42              |
| 24:UU:226:VAL:O    | 24:UU:250:ARG:HA    | 2.19                     | 0.42              |
| 25:UV:481:THR:N    | 25:UV:484:SER:OG    | 2.52                     | 0.42              |
| 27:UZ:249:SER:O    | 66:D3:1497:U:O2'    | 2.35                     | 0.42              |
| 28:CD:104:ASN:O    | 28:CD:107:PRO:HD2   | 2.20                     | 0.42              |
| 28:CD:222:PHE:HE2  | 28:CD:240:LEU:HB2   | 1.84                     | 0.42              |
| 29:CE:214:ILE:HG23 | 29:CE:217:LYS:H     | 1.84                     | 0.42              |
| 31:CH:205:SER:OG   | 31:CH:206:LYS:N     | 2.52                     | 0.42              |
| 32:CI:67:THR:O     | 32:CI:67:THR:HG22   | 2.18                     | 0.42              |
| 32:CI:93:LYS:HB3   | 32:CI:96:ASP:CG     | 2.39                     | 0.42              |
| 33:CJ:23:SER:O     | 33:CJ:26:GLN:HB2    | 2.19                     | 0.42              |
| 34:CK:305:ILE:HG22 | 34:CK:309:LYS:NZ    | 2.34                     | 0.42              |
| 35:CL:51:GLU:HA    | 35:CL:54:LEU:CD2    | 2.49                     | 0.42              |
| 35:CL:1086:MET:CE  | 65:D2:408:U:H1'     | 2.47                     | 0.42              |
| 36:CM:26:LEU:HD23  | 36:CM:26:LEU:HA     | 1.82                     | 0.42              |
| 38:JC:63:LYS:HE3   | 38:JC:66:ARG:HH22   | 1.83                     | 0.42              |
| 38:JC:200:GLU:HG2  | 38:JC:230:GLN:HA    | 2.01                     | 0.42              |
| 42:JJ:221:ARG:HB2  | 42:JJ:239:HIS:HD1   | 1.85                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 47:JP:92:ILE:HD11 | 47:JP:148:TRP:CZ3  | 2.54                     | 0.42              |
| 47:JP:244:ILE:HB  | 47:JP:258:ILE:CG2  | 2.50                     | 0.42              |
| 47:JP:433:GLU:O   | 47:JP:436:SER:OG   | 2.28                     | 0.42              |
| 49:DE:177:ALA:HA  | 49:DE:195:ILE:HG13 | 2.00                     | 0.42              |
| 50:DF:81:ARG:HD3  | 50:DF:82:PHE:CZ    | 2.54                     | 0.42              |
| 50:DF:197:GLU:OE1 | 50:DF:208:SER:HB2  | 2.19                     | 0.42              |
| 55:DL:133:LYS:HB2 | 66:D3:338:C:P      | 2.60                     | 0.42              |
| 62:DY:76:TYR:OH   | 62:DY:86:GLU:OE2   | 2.32                     | 0.42              |
| 65:D2:316:U:C4    | 65:D2:317:C:N4     | 2.87                     | 0.42              |
| 66:D3:206:A:H1'   | 66:D3:262:U:C2     | 2.54                     | 0.42              |
| 66:D3:312:A:H62   | 66:D3:352:A:H1'    | 1.83                     | 0.42              |
| 66:D3:488:G:C6    | 66:D3:489:C:C4     | 3.08                     | 0.42              |
| 66:D3:648:G:H2'   | 66:D3:648:G:N3     | 2.34                     | 0.42              |
| 66:D3:887:A:H2'   | 66:D3:888:U:C6     | 2.53                     | 0.42              |
| 66:D3:1642:G:C6   | 66:D3:1643:U:C4    | 3.07                     | 0.42              |
| 66:D3:1667:A:H2'  | 66:D3:1668:G:H8    | 1.84                     | 0.42              |
| 66:D3:1736:G:C2   | 66:D3:1737:G:C4    | 3.08                     | 0.42              |
| 66:D3:1781:A:H5'' | 66:D3:1782:A:C8    | 2.54                     | 0.42              |
| 67:D4:138:A:H2'   | 67:D4:139:G:O4'    | 2.19                     | 0.42              |
| 1:CA:295:GLU:OE2  | 1:CA:295:GLU:HA    | 2.18                     | 0.42              |
| 2:DA:129:THR:HG22 | 2:DA:133:TYR:O     | 2.19                     | 0.42              |
| 3:JA:561:ALA:O    | 3:JA:589:ALA:HA    | 2.19                     | 0.42              |
| 3:JA:617:LEU:HA   | 3:JA:620:GLN:HG2   | 2.01                     | 0.42              |
| 3:JA:651:SER:HA   | 3:JA:654:ILE:HG22  | 2.00                     | 0.42              |
| 3:JA:773:TRP:HB2  | 3:JA:777:PHE:CZ    | 2.55                     | 0.42              |
| 3:JA:856:GLY:HA2  | 3:JA:859:ILE:HG12  | 2.01                     | 0.42              |
| 4:UA:153:THR:O    | 4:UA:162:LEU:HD23  | 2.19                     | 0.42              |
| 4:UA:255:PHE:CE1  | 65:D2:323:A:C5     | 3.08                     | 0.42              |
| 5:UB:478:ILE:HA   | 5:UB:481:MET:CG    | 2.49                     | 0.42              |
| 7:UD:399:VAL:HG12 | 7:UD:401:ILE:HD11  | 2.02                     | 0.42              |
| 7:UD:467:ASN:O    | 7:UD:470:LEU:HG    | 2.19                     | 0.42              |
| 7:UD:580:LYS:O    | 7:UD:596:MET:HG3   | 2.20                     | 0.42              |
| 9:UF:161:PHE:CD2  | 9:UF:192:PHE:CD2   | 3.08                     | 0.42              |
| 10:UG:42:LEU:HD13 | 17:UN:850:PRO:O    | 2.20                     | 0.42              |
| 10:UG:531:HIS:HE1 | 65:D2:365:G:H4'    | 1.78                     | 0.42              |
| 11:UH:544:LEU:HB3 | 11:UH:551:PHE:HD1  | 1.83                     | 0.42              |
| 14:UK:106:TYR:CE1 | 14:UK:110:LEU:HD21 | 2.54                     | 0.42              |
| 15:UL:57:GLY:HA3  | 15:UL:385:ILE:CD1  | 2.49                     | 0.42              |
| 15:UL:169:PHE:N   | 15:UL:210:LEU:HD12 | 2.35                     | 0.42              |
| 15:UL:211:ALA:O   | 15:UL:217:LEU:HD12 | 2.19                     | 0.42              |
| 15:UL:538:ARG:O   | 15:UL:546:LEU:HD12 | 2.20                     | 0.42              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 15:UL:661:TRP:CD1   | 15:UL:677:HIS:HB2   | 2.54                     | 0.42              |
| 16:UM:426:ILE:O     | 16:UM:426:ILE:HG13  | 2.20                     | 0.42              |
| 16:UM:754:THR:OG1   | 16:UM:755:ILE:HD12  | 2.18                     | 0.42              |
| 18:UO:28:ARG:NH1    | 65:D2:142:U:O2      | 2.52                     | 0.42              |
| 18:UO:149:THR:CG2   | 18:UO:164:LEU:HB3   | 2.50                     | 0.42              |
| 18:UO:193:ILE:O     | 18:UO:208:SER:HA    | 2.19                     | 0.42              |
| 18:UO:273:ILE:HA    | 18:UO:282:LYS:O     | 2.19                     | 0.42              |
| 18:UO:280:HIS:HB3   | 18:UO:282:LYS:HZ3   | 1.85                     | 0.42              |
| 20:UQ:282:ILE:HD11  | 20:UQ:312:LEU:HD13  | 2.01                     | 0.42              |
| 22:US:285:ILE:HD13  | 22:US:285:ILE:HA    | 1.84                     | 0.42              |
| 23:UT:519:VAL:HG11  | 23:UT:548:TYR:CE2   | 2.54                     | 0.42              |
| 23:UT:520:GLY:HA3   | 23:UT:553:ASN:HB3   | 2.01                     | 0.42              |
| 23:UT:1017:LEU:HD23 | 23:UT:1017:LEU:HA   | 1.77                     | 0.42              |
| 23:UT:1280:LEU:O    | 23:UT:1284:LEU:HD23 | 2.19                     | 0.42              |
| 23:UT:1610:MET:N    | 23:UT:1611:PRO:HD2  | 2.34                     | 0.42              |
| 24:UU:622:GLY:HA3   | 24:UU:673:PHE:CZ    | 2.54                     | 0.42              |
| 25:UV:129:HIS:O     | 25:UV:132:TYR:HB2   | 2.19                     | 0.42              |
| 25:UV:751:LYS:HB3   | 25:UV:785:GLU:O     | 2.20                     | 0.42              |
| 25:UV:906:TYR:HD1   | 25:UV:942:PHE:CD1   | 2.38                     | 0.42              |
| 25:UV:1163:LEU:HD12 | 25:UV:1183:THR:O    | 2.18                     | 0.42              |
| 26:UX:141:LEU:O     | 26:UX:144:ARG:N     | 2.52                     | 0.42              |
| 28:CD:139:PHE:C     | 28:CD:141:GLY:H     | 2.23                     | 0.42              |
| 28:CD:173:HIS:HE1   | 29:CE:190:TRP:NE1   | 2.18                     | 0.42              |
| 28:CD:203:PHE:CE2   | 28:CD:206:LEU:HB2   | 2.54                     | 0.42              |
| 30:CG:57:ASP:HB3    | 31:CH:469:LEU:HD11  | 2.01                     | 0.42              |
| 31:CH:141:LEU:HB3   | 31:CH:144:GLU:OE2   | 2.18                     | 0.42              |
| 31:CH:260:LEU:HA    | 31:CH:260:LEU:HD23  | 1.80                     | 0.42              |
| 33:CJ:236:HIS:ND1   | 33:CJ:249:GLU:HA    | 2.34                     | 0.42              |
| 35:CL:94:THR:HG23   | 35:CL:96:SER:N      | 2.35                     | 0.42              |
| 36:CM:132:ALA:HB1   | 36:CM:257:PHE:HE2   | 1.83                     | 0.42              |
| 37:CN:82:SER:HA     | 37:CN:133:SER:HA    | 2.01                     | 0.42              |
| 38:JC:106:ILE:HG23  | 38:JC:111:TRP:HA    | 2.00                     | 0.42              |
| 38:JC:238:ASN:HB3   | 38:JC:279:TRP:CZ3   | 2.55                     | 0.42              |
| 38:JC:254:ILE:O     | 38:JC:263:SER:OG    | 2.24                     | 0.42              |
| 39:JG:77:LEU:HD22   | 39:JG:84:ILE:HG13   | 2.01                     | 0.42              |
| 39:JG:93:HIS:NE2    | 39:JG:132:ARG:O     | 2.41                     | 0.42              |
| 42:JJ:272:GLU:HG2   | 42:JJ:273:ARG:N     | 2.34                     | 0.42              |
| 44:JM:114:ARG:HA    | 44:JM:117:VAL:HG12  | 2.02                     | 0.42              |
| 47:JP:91:VAL:HG23   | 47:JP:106:PHE:O     | 2.20                     | 0.42              |
| 47:JP:330:ARG:CZ    | 47:JP:342:ILE:HD12  | 2.49                     | 0.42              |
| 47:JP:425:LYS:HA    | 47:JP:425:LYS:HD3   | 1.52                     | 0.42              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 51:DG:1:MET:HG2     | 51:DG:107:ALA:O    | 2.20                     | 0.42              |
| 52:DH:75:THR:O      | 52:DH:79:ARG:HG2   | 2.18                     | 0.42              |
| 53:DI:110:ARG:HH21  | 53:DI:160:PHE:HB3  | 1.84                     | 0.42              |
| 55:DL:140:VAL:O     | 55:DL:141:LYS:HD3  | 2.19                     | 0.42              |
| 56:DN:72:MET:HA     | 56:DN:75:LEU:HB2   | 2.00                     | 0.42              |
| 60:DW:84:GLY:O      | 60:DW:88:LYS:HG2   | 2.20                     | 0.42              |
| 61:DX:76:LEU:O      | 61:DX:80:GLY:N     | 2.52                     | 0.42              |
| 65:D2:180:G:H2'     | 65:D2:181:A:H8     | 1.83                     | 0.42              |
| 65:D2:252:A:O5'     | 65:D2:254:C:H5'    | 2.19                     | 0.42              |
| 66:D3:16:G:N2       | 67:D4:16:A:C4      | 2.87                     | 0.42              |
| 66:D3:187:G:C5      | 66:D3:197:A:N6     | 2.86                     | 0.42              |
| 66:D3:192:U:O2'     | 66:D3:193:U:O4'    | 2.31                     | 0.42              |
| 66:D3:230:C:H1'     | 66:D3:238:U:O4     | 2.18                     | 0.42              |
| 66:D3:487:G:H8      | 66:D3:487:G:O5'    | 2.02                     | 0.42              |
| 66:D3:760:A:C3'     | 66:D3:761:G:H4'    | 2.44                     | 0.42              |
| 66:D3:1049:U:N3     | 66:D3:1050:G:N7    | 2.67                     | 0.42              |
| 66:D3:1270:G:H2'    | 66:D3:1271:G:C8    | 2.54                     | 0.42              |
| 79:EN:846:LEU:O     | 79:EN:850:TYR:N    | 2.51                     | 0.42              |
| 2:DA:240:LYS:HE3    | 2:DA:240:LYS:HB2   | 1.94                     | 0.42              |
| 3:JA:748:ARG:NH2    | 3:JA:757:GLU:O     | 2.53                     | 0.42              |
| 4:UA:288:ASP:OD2    | 4:UA:290:PRO:HD2   | 2.19                     | 0.42              |
| 1:CB:102:LYS:HA     | 1:CB:102:LYS:HD2   | 1.81                     | 0.42              |
| 1:CB:190:PRO:HA     | 1:CB:216:ASN:HD21  | 1.84                     | 0.42              |
| 5:UB:284:ALA:O      | 5:UB:286:SER:N     | 2.52                     | 0.42              |
| 5:UB:488:ASN:N      | 5:UB:488:ASN:OD1   | 2.51                     | 0.42              |
| 5:UB:488:ASN:ND2    | 5:UB:491:ASP:HB2   | 2.35                     | 0.42              |
| 5:UB:789:ASN:OD1    | 61:DX:117:ILE:HG23 | 2.20                     | 0.42              |
| 6:UC:548:LYS:HA     | 61:DX:139:LYS:HZ3  | 1.83                     | 0.42              |
| 7:UD:467:ASN:O      | 7:UD:471:LEU:HG    | 2.20                     | 0.42              |
| 7:UD:769:PHE:CE1    | 19:UP:211:LEU:HB2  | 2.54                     | 0.42              |
| 8:UE:90:VAL:HG23    | 8:UE:91:LEU:N      | 2.35                     | 0.42              |
| 8:UE:253:LEU:HD21   | 8:UE:255:ILE:HD11  | 2.01                     | 0.42              |
| 11:UH:671:ARG:NH2   | 12:UI:453:PRO:HG2  | 2.35                     | 0.42              |
| 13:UJ:169:ARG:NH1   | 65:D2:469:C:C5     | 2.87                     | 0.42              |
| 13:UJ:190:LYS:HE2   | 13:UJ:237:ILE:HG12 | 2.01                     | 0.42              |
| 13:UJ:492:LYS:HE2   | 13:UJ:710:LYS:NZ   | 2.34                     | 0.42              |
| 13:UJ:1573:LEU:HD21 | 13:UJ:1618:LEU:HB2 | 2.01                     | 0.42              |
| 14:UK:49:LYS:O      | 14:UK:52:ARG:N     | 2.52                     | 0.42              |
| 14:UK:118:LEU:HD13  | 14:UK:204:HIS:CB   | 2.49                     | 0.42              |
| 15:UL:164:ASP:HB3   | 15:UL:183:ASP:H    | 1.84                     | 0.42              |
| 15:UL:908:VAL:HG12  | 16:UM:769:ILE:HG23 | 2.01                     | 0.42              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 16:UM:43:ILE:HA    | 16:UM:52:ILE:HA     | 2.00                     | 0.42              |
| 16:UM:231:CYS:O    | 16:UM:232:LYS:HD3   | 2.20                     | 0.42              |
| 16:UM:779:VAL:O    | 16:UM:782:VAL:HG12  | 2.19                     | 0.42              |
| 17:UN:307:ARG:CZ   | 66:D3:-6:A:C8       | 3.02                     | 0.42              |
| 18:UO:404:ALA:HB2  | 18:UO:417:VAL:HG11  | 2.00                     | 0.42              |
| 20:UQ:141:LEU:HA   | 20:UQ:155:THR:HG22  | 2.01                     | 0.42              |
| 20:UQ:213:LYS:O    | 20:UQ:217:THR:HG23  | 2.20                     | 0.42              |
| 20:UQ:776:PHE:CZ   | 20:UQ:784:GLY:HA3   | 2.54                     | 0.42              |
| 20:UQ:862:LYS:HD3  | 20:UQ:863:LYS:N     | 2.35                     | 0.42              |
| 22:US:397:THR:O    | 22:US:400:PRO:HD2   | 2.20                     | 0.42              |
| 23:UT:184:SER:HA   | 23:UT:227:ASN:ND2   | 2.35                     | 0.42              |
| 23:UT:951:SER:O    | 23:UT:954:PRO:HD2   | 2.20                     | 0.42              |
| 23:UT:972:LEU:HD11 | 23:UT:1000:PHE:CB   | 2.49                     | 0.42              |
| 23:UT:1143:LYS:NZ  | 23:UT:1145:ALA:HB3  | 2.34                     | 0.42              |
| 23:UT:1186:TYR:CE2 | 23:UT:1227:ILE:HA   | 2.54                     | 0.42              |
| 23:UT:1935:LYS:CB  | 23:UT:1939:ARG:HH11 | 2.33                     | 0.42              |
| 24:UU:176:TYR:HB3  | 24:UU:179:LYS:HG3   | 2.01                     | 0.42              |
| 24:UU:272:ASP:OD1  | 24:UU:288:LYS:HA    | 2.19                     | 0.42              |
| 27:UZ:36:ILE:HB    | 27:UZ:201:VAL:O     | 2.19                     | 0.42              |
| 27:UZ:49:ASN:HA    | 27:UZ:193:ASN:OD1   | 2.19                     | 0.42              |
| 29:CE:117:TYR:HA   | 29:CE:120:ILE:HG12  | 2.01                     | 0.42              |
| 31:CH:164:GLN:HG3  | 31:CH:185:LEU:HD11  | 2.00                     | 0.42              |
| 31:CH:327:ASP:HB2  | 31:CH:403:ASP:O     | 2.19                     | 0.42              |
| 32:CI:7:HIS:NE2    | 32:CI:11:LYS:HE3    | 2.35                     | 0.42              |
| 32:CI:108:ARG:NH1  | 65:D2:394:U:OP1     | 2.51                     | 0.42              |
| 35:CL:236:LYS:HA   | 35:CL:236:LYS:HD3   | 1.84                     | 0.42              |
| 35:CL:831:ARG:CZ   | 35:CL:831:ARG:HB3   | 2.46                     | 0.42              |
| 38:JC:171:ARG:NH1  | 43:JK:469:GLN:H     | 2.17                     | 0.42              |
| 38:JC:227:ARG:NH2  | 38:JC:249:ASN:HD21  | 2.17                     | 0.42              |
| 39:JF:106:LYS:O    | 39:JF:106:LYS:HG2   | 2.19                     | 0.42              |
| 39:JF:164:LYS:HE3  | 39:JF:164:LYS:HB3   | 1.88                     | 0.42              |
| 39:JG:147:LYS:O    | 39:JG:148:LEU:HB2   | 2.19                     | 0.42              |
| 39:JG:186:VAL:HG23 | 39:JG:227:LEU:C     | 2.39                     | 0.42              |
| 47:JP:228:ASN:OD1  | 47:JP:228:ASN:N     | 2.44                     | 0.42              |
| 47:JP:281:ASN:ND2  | 47:JP:283:ASP:OD1   | 2.52                     | 0.42              |
| 49:DE:66:MET:O     | 49:DE:68:ARG:HG3    | 2.19                     | 0.42              |
| 52:DH:33:GLU:O     | 52:DH:37:GLU:HG2    | 2.19                     | 0.42              |
| 52:DH:113:PRO:HD2  | 52:DH:116:ARG:HB2   | 2.01                     | 0.42              |
| 55:DL:111:VAL:HA   | 55:DL:139:VAL:HG22  | 2.02                     | 0.42              |
| 57:DO:37:GLU:CD    | 66:D3:895:G:H4'     | 2.40                     | 0.42              |
| 58:DQ:23:LYS:HD2   | 65:D2:267:U:C5      | 2.54                     | 0.42              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 61:DX:68:ILE:HG13  | 61:DX:69:ARG:N      | 2.33                     | 0.42              |
| 65:D2:144:C:H2'    | 65:D2:145:A:H8      | 1.84                     | 0.42              |
| 66:D3:425:A:H2'    | 66:D3:425:A:N3      | 2.35                     | 0.42              |
| 66:D3:1169:G:H8    | 66:D3:1169:G:O5'    | 2.03                     | 0.42              |
| 66:D3:1215:C:H2'   | 66:D3:1216:C:C6     | 2.55                     | 0.42              |
| 66:D3:1478:G:N2    | 66:D3:1530:C:C2     | 2.87                     | 0.42              |
| 66:D3:1663:G:H2'   | 66:D3:1664:C:O4'    | 2.20                     | 0.42              |
| 66:D3:1694:A:H2'   | 66:D3:1695:G:C8     | 2.54                     | 0.42              |
| 67:D4:52:U:H2'     | 67:D4:53:U:H6       | 1.83                     | 0.42              |
| 67:D4:115:G:N2     | 67:D4:116:A:H1'     | 2.34                     | 0.42              |
| 1:CA:225:ARG:O     | 1:CA:226:HIS:ND1    | 2.51                     | 0.42              |
| 2:DA:241:GLY:C     | 2:DA:242:LYS:HD3    | 2.40                     | 0.42              |
| 3:JA:563:LYS:H     | 3:JA:587:GLN:HE22   | 1.67                     | 0.42              |
| 3:JA:727:TYR:HB2   | 3:JA:733:LEU:HD21   | 2.02                     | 0.42              |
| 4:UA:314:GLY:O     | 4:UA:332:TRP:NE1    | 2.44                     | 0.42              |
| 5:UB:433:ILE:O     | 5:UB:436:LEU:HG     | 2.19                     | 0.42              |
| 5:UB:447:SER:HA    | 5:UB:450:ARG:HH21   | 1.84                     | 0.42              |
| 5:UB:448:PHE:O     | 5:UB:452:GLN:HG2    | 2.20                     | 0.42              |
| 7:UD:168:ILE:HD12  | 7:UD:179:HIS:HA     | 2.01                     | 0.42              |
| 7:UD:372:MET:HA    | 7:UD:373:PRO:HD3    | 1.85                     | 0.42              |
| 7:UD:441:VAL:HG11  | 7:UD:478:VAL:HG21   | 2.02                     | 0.42              |
| 8:UE:537:LEU:HD22  | 18:UO:498:SER:HB2   | 2.02                     | 0.42              |
| 9:UF:278:MET:HE2   | 9:UF:316:SER:HB3    | 2.01                     | 0.42              |
| 10:UG:116:ILE:CD1  | 10:UG:398:ILE:HG23  | 2.49                     | 0.42              |
| 10:UG:321:ASN:HB2  | 10:UG:333:SER:OG    | 2.19                     | 0.42              |
| 10:UG:550:LEU:HD11 | 25:UV:806:PHE:CE1   | 2.55                     | 0.42              |
| 11:UH:574:ARG:HB2  | 11:UH:578:LEU:HD12  | 2.01                     | 0.42              |
| 11:UH:660:LEU:C    | 11:UH:664:LYS:HZ2   | 2.23                     | 0.42              |
| 13:UJ:564:VAL:O    | 13:UJ:568:ILE:HG12  | 2.20                     | 0.42              |
| 13:UJ:677:SER:HA   | 13:UJ:678:PRO:HA    | 1.78                     | 0.42              |
| 13:UJ:1434:SER:N   | 13:UJ:1437:ARG:HH21 | 2.17                     | 0.42              |
| 13:UJ:1709:ARG:O   | 13:UJ:1712:LYS:HB2  | 2.19                     | 0.42              |
| 14:UK:158:MET:SD   | 14:UK:165:ARG:HA    | 2.60                     | 0.42              |
| 15:UL:14:PHE:HB3   | 15:UL:417:TRP:HZ3   | 1.84                     | 0.42              |
| 15:UL:17:ILE:N     | 15:UL:360:ASN:OD1   | 2.52                     | 0.42              |
| 15:UL:22:ASN:HD21  | 15:UL:85:LEU:N      | 2.16                     | 0.42              |
| 15:UL:42:ILE:HG12  | 15:UL:51:ILE:CG2    | 2.50                     | 0.42              |
| 15:UL:197:ILE:O    | 16:UM:667:GLN:NE2   | 2.51                     | 0.42              |
| 15:UL:391:ARG:CZ   | 15:UL:391:ARG:HB3   | 2.50                     | 0.42              |
| 15:UL:437:LYS:HB2  | 15:UL:479:LEU:HD11  | 2.02                     | 0.42              |
| 16:UM:30:LYS:HD2   | 16:UM:45:LEU:N      | 2.34                     | 0.42              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 16:UM:89:HIS:HB3   | 16:UM:92:THR:OG1    | 2.20                     | 0.42              |
| 16:UM:622:ALA:HB3  | 16:UM:635:ALA:HB3   | 2.01                     | 0.42              |
| 17:UN:861:LEU:HA   | 47:JP:403:ARG:NH2   | 2.35                     | 0.42              |
| 18:UO:391:ASN:HD21 | 18:UO:399:GLU:HG3   | 1.85                     | 0.42              |
| 20:UQ:86:GLU:HG2   | 20:UQ:113:ASN:OD1   | 2.20                     | 0.42              |
| 20:UQ:724:ILE:HG21 | 20:UQ:762:TYR:CD2   | 2.53                     | 0.42              |
| 20:UQ:749:ASP:OD1  | 20:UQ:750:LEU:N     | 2.53                     | 0.42              |
| 21:UR:209:THR:O    | 21:UR:213:SER:OG    | 2.24                     | 0.42              |
| 21:UR:277:ILE:HA   | 21:UR:282:ASN:OD1   | 2.19                     | 0.42              |
| 22:US:216:VAL:HG12 | 22:US:264:LEU:HD22  | 2.02                     | 0.42              |
| 22:US:345:ILE:HA   | 22:US:349:LEU:HD13  | 2.01                     | 0.42              |
| 22:US:486:GLN:HB3  | 22:US:487:PRO:HD2   | 2.02                     | 0.42              |
| 23:UT:95:ILE:HG13  | 23:UT:135:LEU:HD12  | 2.01                     | 0.42              |
| 23:UT:151:GLY:O    | 23:UT:155:LEU:HD23  | 2.20                     | 0.42              |
| 23:UT:196:LEU:HG   | 23:UT:199:LEU:HD12  | 2.00                     | 0.42              |
| 23:UT:422:LYS:HA   | 23:UT:422:LYS:HD2   | 1.78                     | 0.42              |
| 23:UT:454:PRO:O    | 23:UT:458:ILE:HG12  | 2.20                     | 0.42              |
| 23:UT:861:ARG:HB3  | 23:UT:934:GLN:CD    | 2.39                     | 0.42              |
| 23:UT:937:PRO:HD3  | 23:UT:946:LYS:NZ    | 2.34                     | 0.42              |
| 23:UT:1557:GLU:O   | 23:UT:1561:ILE:HG12 | 2.19                     | 0.42              |
| 24:UU:141:LYS:HE2  | 24:UU:154:TYR:CE1   | 2.55                     | 0.42              |
| 24:UU:198:LEU:HD11 | 24:UU:200:PHE:O     | 2.19                     | 0.42              |
| 24:UU:501:HIS:ND1  | 24:UU:521:GLY:HA3   | 2.34                     | 0.42              |
| 24:UU:885:MET:HE1  | 24:UU:912:TRP:CE3   | 2.54                     | 0.42              |
| 24:UU:905:ILE:HG13 | 24:UU:906:ALA:N     | 2.35                     | 0.42              |
| 25:UV:104:LYS:HA   | 25:UV:104:LYS:HD3   | 1.80                     | 0.42              |
| 25:UV:361:GLU:HB2  | 25:UV:418:SER:OG    | 2.19                     | 0.42              |
| 25:UV:713:LEU:HD21 | 25:UV:770:PRO:HD2   | 2.01                     | 0.42              |
| 25:UV:1135:ASN:HB3 | 25:UV:1138:ASP:H    | 1.84                     | 0.42              |
| 27:UZ:77:LYS:HB2   | 27:UZ:83:TYR:HE2    | 1.84                     | 0.42              |
| 28:CD:185:ASP:OD2  | 28:CD:285:ARG:NH2   | 2.53                     | 0.42              |
| 28:CD:382:LYS:O    | 28:CD:385:MET:HB3   | 2.19                     | 0.42              |
| 31:CH:253:THR:HG22 | 31:CH:263:TRP:HE1   | 1.84                     | 0.42              |
| 31:CH:359:PHE:HE2  | 31:CH:413:PHE:HE1   | 1.66                     | 0.42              |
| 31:CH:439:ALA:O    | 31:CH:497:LYS:HE3   | 2.20                     | 0.42              |
| 32:CI:28:ARG:NH1   | 65:D2:393:C:O5'     | 2.52                     | 0.42              |
| 32:CI:78:LEU:CD2   | 32:CI:97:LEU:HD21   | 2.48                     | 0.42              |
| 33:CJ:253:ARG:HG3  | 33:CJ:253:ARG:O     | 2.19                     | 0.42              |
| 35:CL:991:PHE:HB3  | 35:CL:992:GLU:H     | 1.73                     | 0.42              |
| 35:CL:1034:LEU:O   | 35:CL:1038:ILE:HG12 | 2.19                     | 0.42              |
| 37:CN:63:ASN:N     | 37:CN:66:HIS:HB2    | 2.34                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:JC:53:PHE:HA    | 38:JC:84:TYR:CE2   | 2.55                     | 0.42              |
| 39:JG:193:ILE:HA   | 39:JG:196:LEU:HD12 | 2.02                     | 0.42              |
| 42:JJ:97:ARG:O     | 42:JJ:139:LEU:HD23 | 2.19                     | 0.42              |
| 45:JN:267:VAL:HG13 | 45:JN:268:LYS:O    | 2.19                     | 0.42              |
| 46:JO:156:LEU:HD21 | 46:JO:183:VAL:HG22 | 2.00                     | 0.42              |
| 47:JP:347:ARG:NH2  | 67:D4:31:G:C8      | 2.88                     | 0.42              |
| 51:DG:214:LYS:HG3  | 51:DG:215:ARG:N    | 2.35                     | 0.42              |
| 52:DH:39:ARG:O     | 52:DH:39:ARG:NE    | 2.50                     | 0.42              |
| 54:DJ:87:SER:O     | 54:DJ:90:LYS:HG2   | 2.19                     | 0.42              |
| 54:DJ:90:LYS:HB2   | 54:DJ:95:TYR:CG    | 2.55                     | 0.42              |
| 55:DL:124:THR:HG21 | 55:DL:141:LYS:HE2  | 2.01                     | 0.42              |
| 65:D2:158:G:C2     | 65:D2:159:A:C4     | 3.07                     | 0.42              |
| 65:D2:382:U:O5'    | 65:D2:382:U:H6     | 2.02                     | 0.42              |
| 66:D3:70:C:H2'     | 66:D3:71:A:H8      | 1.84                     | 0.42              |
| 66:D3:109:G:N2     | 66:D3:305:C:C2     | 2.87                     | 0.42              |
| 66:D3:645:C:N4     | 66:D3:690:G:O6     | 2.53                     | 0.42              |
| 66:D3:872:G:H2'    | 66:D3:873:U:O4'    | 2.20                     | 0.42              |
| 66:D3:1602:C:N4    | 66:D3:1603:U:O4    | 2.53                     | 0.42              |
| 66:D3:1748:G:C2    | 66:D3:1749:A:C4    | 3.07                     | 0.42              |
| 67:D4:4:G:O2'      | 67:D4:5:A:H5'      | 2.20                     | 0.42              |
| 67:D4:14:A:C8      | 67:D4:15:U:C4      | 3.08                     | 0.42              |
| 67:D4:202:G:C6     | 67:D4:248:G:C6     | 3.07                     | 0.42              |
| 76:EI:339:ASN:O    | 76:EI:343:SER:N    | 2.50                     | 0.42              |
| 79:EN:998:MET:O    | 79:EN:1002:TYR:N   | 2.52                     | 0.42              |
| 1:CA:272:LYS:HD3   | 1:CA:313:HIS:NE2   | 2.34                     | 0.42              |
| 2:DA:148:ASN:ND2   | 66:D3:1066:C:O2    | 2.52                     | 0.42              |
| 3:JA:49:LEU:HA     | 3:JA:53:LYS:NZ     | 2.34                     | 0.42              |
| 3:JA:72:LYS:NZ     | 66:D3:158:U:H5'    | 2.35                     | 0.42              |
| 3:JA:121:MET:HE2   | 3:JA:147:ILE:H     | 1.85                     | 0.42              |
| 3:JA:140:GLU:HA    | 3:JA:475:ARG:HH12  | 1.85                     | 0.42              |
| 3:JA:140:GLU:HA    | 3:JA:475:ARG:NH1   | 2.35                     | 0.42              |
| 4:UA:104:PHE:CD2   | 4:UA:111:PHE:HB3   | 2.54                     | 0.42              |
| 4:UA:146:PHE:N     | 4:UA:167:ASP:OD2   | 2.53                     | 0.42              |
| 4:UA:412:ARG:HH21  | 4:UA:424:THR:HB    | 1.84                     | 0.42              |
| 1:CB:256:ASN:O     | 1:CB:260:PHE:HB2   | 2.19                     | 0.42              |
| 5:UB:525:MET:HB2   | 5:UB:546:LEU:HD11  | 2.01                     | 0.42              |
| 5:UB:618:THR:HB    | 5:UB:622:MET:HE1   | 2.01                     | 0.42              |
| 7:UD:167:LEU:HD11  | 7:UD:183:LEU:HD11  | 2.02                     | 0.42              |
| 7:UD:300:VAL:O     | 7:UD:332:ASP:HB2   | 2.20                     | 0.42              |
| 7:UD:635:GLY:HA3   | 7:UD:649:TRP:NE1   | 2.34                     | 0.42              |
| 8:UE:285:ASP:CG    | 8:UE:287:ARG:HG3   | 2.40                     | 0.42              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 8:UE:487:ARG:HD2    | 8:UE:487:ARG:HA     | 1.83                     | 0.42              |
| 10:UG:116:ILE:HD11  | 10:UG:398:ILE:HG23  | 2.02                     | 0.42              |
| 11:UH:541:LEU:HD12  | 11:UH:541:LEU:HA    | 1.77                     | 0.42              |
| 12:UI:466:GLU:OE1   | 12:UI:466:GLU:N     | 2.28                     | 0.42              |
| 13:UJ:1370:TYR:HA   | 13:UJ:1373:ILE:HG12 | 2.02                     | 0.42              |
| 13:UJ:1405:ALA:O    | 13:UJ:1408:ILE:HG22 | 2.20                     | 0.42              |
| 13:UJ:1705:LEU:HA   | 13:UJ:1708:ILE:HD12 | 2.00                     | 0.42              |
| 14:UK:9:GLN:HG3     | 66:D3:572:C:H5'     | 2.02                     | 0.42              |
| 15:UL:341:ALA:HA    | 15:UL:354:VAL:O     | 2.18                     | 0.42              |
| 15:UL:482:THR:HG23  | 15:UL:485:GLY:H     | 1.85                     | 0.42              |
| 16:UM:283:LYS:HB2   | 16:UM:283:LYS:HE2   | 1.86                     | 0.42              |
| 16:UM:306:LEU:HB2   | 16:UM:310:THR:OG1   | 2.20                     | 0.42              |
| 18:UO:248:ARG:NE    | 18:UO:290:PHE:O     | 2.53                     | 0.42              |
| 18:UO:356:ASN:O     | 18:UO:360:MET:HB2   | 2.19                     | 0.42              |
| 18:UO:503:ARG:HG2   | 18:UO:503:ARG:H     | 1.70                     | 0.42              |
| 20:UQ:111:THR:HB    | 20:UQ:115:HIS:HB2   | 2.02                     | 0.42              |
| 20:UQ:133:LYS:H     | 20:UQ:183:LYS:HE3   | 1.84                     | 0.42              |
| 20:UQ:334:LEU:HA    | 20:UQ:335:PRO:HD3   | 1.79                     | 0.42              |
| 22:US:462:SER:HB2   | 22:US:464:TRP:CZ2   | 2.55                     | 0.42              |
| 23:UT:567:PRO:HB3   | 23:UT:610:LEU:HA    | 2.02                     | 0.42              |
| 23:UT:1355:ILE:HD12 | 23:UT:1364:ARG:HB3  | 2.02                     | 0.42              |
| 24:UU:128:LEU:HB2   | 24:UU:150:PRO:HG2   | 2.00                     | 0.42              |
| 25:UV:214:PHE:CE2   | 25:UV:299:PRO:HD2   | 2.55                     | 0.42              |
| 25:UV:684:PHE:CZ    | 25:UV:688:LYS:HD3   | 2.55                     | 0.42              |
| 26:UX:51:LEU:HD12   | 26:UX:51:LEU:HA     | 1.82                     | 0.42              |
| 26:UX:121:ARG:NH1   | 47:JP:369:ASP:OD1   | 2.52                     | 0.42              |
| 28:CD:109:ILE:HD13  | 28:CD:109:ILE:HA    | 1.91                     | 0.42              |
| 29:CE:18:SER:H      | 29:CE:42:PHE:HE2    | 1.68                     | 0.42              |
| 29:CE:319:ILE:O     | 29:CE:319:ILE:HG13  | 2.20                     | 0.42              |
| 30:CF:115:TYR:HD1   | 30:CF:118:LYS:HD3   | 1.81                     | 0.42              |
| 30:CG:50:GLU:HG2    | 30:CG:104:THR:HA    | 2.00                     | 0.42              |
| 34:CK:332:ALA:HA    | 34:CK:335:ARG:NH1   | 2.32                     | 0.42              |
| 35:CL:101:ILE:H     | 35:CL:101:ILE:HD12  | 1.85                     | 0.42              |
| 38:JC:227:ARG:NH1   | 38:JC:229:PHE:HA    | 2.34                     | 0.42              |
| 39:JG:91:ILE:HG13   | 39:JG:92:THR:H      | 1.84                     | 0.42              |
| 42:JJ:121:VAL:HG12  | 42:JJ:126:LEU:O     | 2.19                     | 0.42              |
| 42:JJ:166:PHE:HB3   | 42:JJ:170:ASP:HB2   | 2.01                     | 0.42              |
| 42:JJ:251:ILE:HG13  | 42:JJ:252:LEU:N     | 2.35                     | 0.42              |
| 47:JP:91:VAL:HA     | 47:JP:106:PHE:O     | 2.20                     | 0.42              |
| 47:JP:278:VAL:HG13  | 47:JP:313:PHE:CZ    | 2.52                     | 0.42              |
| 47:JP:291:MET:HE3   | 47:JP:291:MET:HB3   | 1.87                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 49:DE:130:GLN:HG3  | 49:DE:131:LEU:N    | 2.34                     | 0.42              |
| 50:DF:100:ASN:HD22 | 50:DF:103:ASN:ND2  | 2.18                     | 0.42              |
| 51:DG:14:LYS:HG2   | 51:DG:15:THR:H     | 1.85                     | 0.42              |
| 51:DG:85:ARG:HH12  | 51:DG:87:ARG:NH2   | 2.18                     | 0.42              |
| 56:DN:25:TRP:HA    | 56:DN:27:LYS:NZ    | 2.34                     | 0.42              |
| 65:D2:100:G:H1     | 65:D2:144:C:H42    | 1.68                     | 0.42              |
| 66:D3:551:G:N1     | 66:D3:588:U:N3     | 2.67                     | 0.42              |
| 66:D3:686:C:C2     | 66:D3:687:G:C8     | 3.08                     | 0.42              |
| 66:D3:765:G:N2     | 66:D3:772:G:C2     | 2.87                     | 0.42              |
| 66:D3:1057:U:HO2'  | 66:D3:1058:U:P     | 2.41                     | 0.42              |
| 66:D3:1654:G:N2    | 66:D3:1747:G:C2    | 2.88                     | 0.42              |
| 67:D4:199:G:C2     | 67:D4:200:C:C2     | 3.07                     | 0.42              |
| 2:DA:183:GLN:HG2   | 25:UV:754:LEU:HD11 | 2.02                     | 0.42              |
| 2:DA:228:LEU:HD23  | 2:DA:228:LEU:HA    | 1.81                     | 0.42              |
| 3:JA:10:ILE:HD12   | 3:JA:10:ILE:H      | 1.84                     | 0.42              |
| 3:JA:391:ALA:HA    | 3:JA:754:LEU:HD12  | 2.01                     | 0.42              |
| 3:JA:637:ARG:HD2   | 3:JA:638:ILE:N     | 2.34                     | 0.42              |
| 4:UA:162:LEU:HB3   | 4:UA:172:ILE:HG22  | 2.00                     | 0.42              |
| 4:UA:164:THR:HG21  | 4:UA:196:GLY:N     | 2.35                     | 0.42              |
| 4:UA:285:ARG:NE    | 4:UA:297:GLN:OE1   | 2.53                     | 0.42              |
| 4:UA:354:SER:O     | 4:UA:688:PRO:HG3   | 2.19                     | 0.42              |
| 4:UA:610:VAL:HG22  | 4:UA:611:LEU:N     | 2.35                     | 0.42              |
| 1:CB:271:ILE:HD13  | 1:CB:314:CYS:SG    | 2.59                     | 0.42              |
| 7:UD:527:TYR:HA    | 7:UD:530:ARG:HG2   | 2.00                     | 0.42              |
| 8:UE:318:GLN:O     | 8:UE:321:GLU:HG3   | 2.20                     | 0.42              |
| 9:UF:118:LYS:HE2   | 9:UF:153:TYR:CD1   | 2.54                     | 0.42              |
| 9:UF:197:ILE:CD1   | 9:UF:200:ARG:HE    | 2.32                     | 0.42              |
| 13:UJ:54:LYS:HE3   | 13:UJ:54:LYS:HB2   | 1.89                     | 0.42              |
| 13:UJ:560:ILE:HD13 | 13:UJ:592:ARG:NH1  | 2.35                     | 0.42              |
| 13:UJ:1554:TRP:CZ2 | 13:UJ:1571:ARG:HD2 | 2.55                     | 0.42              |
| 13:UJ:1644:PHE:CZ  | 13:UJ:1683:HIS:HB3 | 2.55                     | 0.42              |
| 15:UL:300:GLU:O    | 15:UL:304:LYS:HE3  | 2.19                     | 0.42              |
| 15:UL:472:HIS:HE2  | 15:UL:498:LYS:HB2  | 1.84                     | 0.42              |
| 15:UL:923:GLU:HA   | 42:JJ:264:ARG:NH2  | 2.35                     | 0.42              |
| 16:UM:353:LEU:O    | 16:UM:364:ILE:HA   | 2.20                     | 0.42              |
| 16:UM:453:PHE:HE2  | 16:UM:455:LEU:HB2  | 1.85                     | 0.42              |
| 16:UM:736:LEU:HD21 | 16:UM:767:HIS:CE1  | 2.55                     | 0.42              |
| 16:UM:760:ILE:O    | 16:UM:763:ILE:HG22 | 2.20                     | 0.42              |
| 17:UN:342:VAL:HA   | 17:UN:345:VAL:HG22 | 2.01                     | 0.42              |
| 18:UO:47:PHE:CD1   | 18:UO:55:PHE:HB3   | 2.55                     | 0.42              |
| 20:UQ:107:ILE:HD11 | 20:UQ:119:LEU:HB2  | 2.00                     | 0.42              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 20:UQ:110:PHE:CD1   | 20:UQ:116:VAL:HG22  | 2.55                     | 0.42              |
| 20:UQ:335:PRO:C     | 20:UQ:336:ARG:HD3   | 2.40                     | 0.42              |
| 20:UQ:890:ARG:O     | 20:UQ:894:VAL:HG23  | 2.19                     | 0.42              |
| 21:UR:205:ILE:HG23  | 21:UR:206:ASN:OD1   | 2.20                     | 0.42              |
| 21:UR:295:ILE:HD12  | 21:UR:314:THR:HG23  | 2.02                     | 0.42              |
| 21:UR:383:TRP:HA    | 21:UR:398:CYS:O     | 2.20                     | 0.42              |
| 22:US:270:SER:O     | 22:US:274:TYR:HB2   | 2.19                     | 0.42              |
| 23:UT:414:LEU:O     | 23:UT:417:LEU:HG    | 2.20                     | 0.42              |
| 23:UT:520:GLY:O     | 23:UT:524:LYS:HG2   | 2.19                     | 0.42              |
| 23:UT:600:THR:O     | 23:UT:604:MET:HG2   | 2.20                     | 0.42              |
| 23:UT:603:LEU:HG    | 23:UT:607:LEU:HD23  | 2.00                     | 0.42              |
| 23:UT:1199:LEU:HD22 | 23:UT:1239:ASP:OD1  | 2.20                     | 0.42              |
| 23:UT:1423:TYR:O    | 23:UT:1427:ASN:HB2  | 2.19                     | 0.42              |
| 23:UT:1777:LEU:HD21 | 23:UT:1789:LEU:HD22 | 2.01                     | 0.42              |
| 24:UU:881:TYR:HA    | 24:UU:884:PHE:CD2   | 2.55                     | 0.42              |
| 25:UV:592:PHE:HB3   | 25:UV:599:VAL:HG22  | 2.01                     | 0.42              |
| 25:UV:656:ARG:HH11  | 25:UV:668:VAL:HG21  | 1.84                     | 0.42              |
| 25:UV:1081:ASN:HD21 | 25:UV:1083:GLN:HE22 | 1.67                     | 0.42              |
| 25:UV:1220:PHE:HA   | 25:UV:1223:ILE:HD12 | 2.02                     | 0.42              |
| 29:CE:73:GLU:HA     | 29:CE:76:LEU:CG     | 2.48                     | 0.42              |
| 31:CH:168:ASN:O     | 31:CH:172:PHE:HD1   | 2.02                     | 0.42              |
| 32:CI:29:ASP:OD2    | 32:CI:41:ARG:NH1    | 2.52                     | 0.42              |
| 34:CK:442:ALA:O     | 34:CK:445:VAL:HG12  | 2.20                     | 0.42              |
| 35:CL:58:MET:HG3    | 35:CL:236:LYS:NZ    | 2.35                     | 0.42              |
| 35:CL:282:SER:HB3   | 35:CL:782:GLY:HA2   | 2.00                     | 0.42              |
| 36:CM:295:PRO:HB3   | 36:CM:325:LEU:HD22  | 2.02                     | 0.42              |
| 38:JC:89:LEU:HD12   | 51:DG:69:LEU:HD11   | 2.01                     | 0.42              |
| 38:JC:232:THR:HG21  | 38:JC:275:LYS:HZ1   | 1.85                     | 0.42              |
| 38:JC:232:THR:HG21  | 38:JC:275:LYS:NZ    | 2.34                     | 0.42              |
| 42:JJ:127:GLN:O     | 42:JJ:140:ARG:HG2   | 2.19                     | 0.42              |
| 50:DF:81:ARG:HG2    | 50:DF:82:PHE:CE1    | 2.54                     | 0.42              |
| 56:DN:72:MET:HE1    | 66:D3:961:U:O3'     | 2.19                     | 0.42              |
| 56:DN:114:ARG:HA    | 56:DN:114:ARG:HD3   | 1.85                     | 0.42              |
| 60:DW:55:ASP:O      | 60:DW:57:ARG:HD2    | 2.20                     | 0.42              |
| 65:D2:9:G:H2'       | 65:D2:10:C:C6       | 2.55                     | 0.42              |
| 65:D2:211:G:H2'     | 65:D2:212:U:C6      | 2.55                     | 0.42              |
| 65:D2:243:A:C5      | 65:D2:271:G:N1      | 2.88                     | 0.42              |
| 66:D3:75:U:H3'      | 66:D3:76:A:C5'      | 2.50                     | 0.42              |
| 66:D3:107:C:H2'     | 66:D3:108:A:H8      | 1.84                     | 0.42              |
| 66:D3:319:U:H5'     | 66:D3:320:U:H5''    | 2.01                     | 0.42              |
| 66:D3:529:A:H2'     | 66:D3:530:C:H6      | 1.84                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 66:D3:645:C:H2'    | 66:D3:646:C:H6     | 1.85                     | 0.42              |
| 66:D3:793:A:N6     | 66:D3:798:C:H5     | 2.18                     | 0.42              |
| 66:D3:940:A:C4     | 66:D3:941:A:C8     | 3.08                     | 0.42              |
| 66:D3:942:G:C2     | 66:D3:943:C:O2     | 2.73                     | 0.42              |
| 66:D3:1151:A:H61   | 66:D3:1627:U:H3    | 1.67                     | 0.42              |
| 66:D3:1158:C:N4    | 66:D3:1582:U:C5    | 2.85                     | 0.42              |
| 66:D3:1462:G:H2'   | 66:D3:1463:C:C6    | 2.54                     | 0.42              |
| 66:D3:1785:U:H2'   | 66:D3:1786:G:C8    | 2.55                     | 0.42              |
| 67:D4:42:U:C4      | 67:D4:43:C:C4      | 3.07                     | 0.42              |
| 67:D4:317:A:O2'    | 67:D4:318:U:H3'    | 2.20                     | 0.42              |
| 2:DA:8:ARG:NH1     | 66:D3:907:A:H5''   | 2.35                     | 0.42              |
| 3:JA:115:LEU:HD11  | 3:JA:137:ARG:HG2   | 2.02                     | 0.42              |
| 3:JA:510:PRO:HA    | 3:JA:513:CYS:SG    | 2.59                     | 0.42              |
| 3:JA:627:PHE:HA    | 3:JA:630:LEU:HD12  | 2.02                     | 0.42              |
| 4:UA:31:SER:HG     | 4:UA:40:PHE:HE2    | 1.66                     | 0.42              |
| 4:UA:81:LEU:HD22   | 4:UA:136:PHE:HE1   | 1.85                     | 0.42              |
| 4:UA:363:ALA:HB1   | 4:UA:390:VAL:CG1   | 2.50                     | 0.42              |
| 1:CB:102:LYS:HE2   | 14:UK:193:LYS:HB3  | 2.00                     | 0.42              |
| 1:CB:179:THR:OG1   | 1:CB:180:SER:N     | 2.53                     | 0.42              |
| 1:CB:227:PRO:HB2   | 1:CB:259:MET:SD    | 2.60                     | 0.42              |
| 5:UB:739:LYS:HD3   | 5:UB:739:LYS:HA    | 1.78                     | 0.42              |
| 5:UB:766:ARG:O     | 5:UB:769:GLU:HG2   | 2.20                     | 0.42              |
| 6:UC:529:ALA:O     | 6:UC:532:VAL:HG13  | 2.20                     | 0.42              |
| 7:UD:36:CYS:HA     | 11:UH:716:TYR:CD1  | 2.55                     | 0.42              |
| 7:UD:36:CYS:HA     | 11:UH:716:TYR:HD1  | 1.84                     | 0.42              |
| 7:UD:42:THR:HG23   | 7:UD:42:THR:O      | 2.20                     | 0.42              |
| 7:UD:96:ASP:HB2    | 19:UP:193:LYS:HD3  | 2.00                     | 0.42              |
| 8:UE:150:LYS:O     | 8:UE:165:VAL:HA    | 2.20                     | 0.42              |
| 9:UF:110:TRP:CE3   | 9:UF:136:LEU:HD22  | 2.55                     | 0.42              |
| 10:UG:126:LEU:HB2  | 10:UG:159:TYR:HE2  | 1.85                     | 0.42              |
| 10:UG:394:HIS:ND1  | 10:UG:396:THR:HG22 | 2.34                     | 0.42              |
| 12:UI:492:ILE:HD13 | 12:UI:492:ILE:HG21 | 1.84                     | 0.42              |
| 13:UJ:127:ILE:HG22 | 13:UJ:131:ASN:HD21 | 1.85                     | 0.42              |
| 13:UJ:576:ILE:H    | 13:UJ:576:ILE:HD12 | 1.85                     | 0.42              |
| 13:UJ:1484:THR:HA  | 13:UJ:1487:ASN:OD1 | 2.20                     | 0.42              |
| 15:UL:186:ILE:HD11 | 15:UL:202:ALA:HB2  | 2.02                     | 0.42              |
| 15:UL:303:LEU:HB3  | 15:UL:313:ILE:HD12 | 2.02                     | 0.42              |
| 15:UL:498:LYS:HG2  | 15:UL:527:THR:HG22 | 2.01                     | 0.42              |
| 15:UL:681:ILE:O    | 15:UL:682:ARG:HD3  | 2.20                     | 0.42              |
| 16:UM:30:LYS:HD2   | 16:UM:45:LEU:H     | 1.84                     | 0.42              |
| 16:UM:408:LYS:HA   | 16:UM:436:ALA:HB1  | 2.02                     | 0.42              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 18:UO:5:ARG:NH1    | 65:D2:87:C:OP2      | 2.53                     | 0.42              |
| 18:UO:415:LEU:HD23 | 18:UO:415:LEU:HA    | 1.83                     | 0.42              |
| 20:UQ:30:GLY:HA2   | 20:UQ:199:SER:O     | 2.19                     | 0.42              |
| 20:UQ:282:ILE:HD11 | 20:UQ:312:LEU:CD1   | 2.50                     | 0.42              |
| 20:UQ:305:PHE:HB3  | 20:UQ:309:GLY:HA2   | 2.01                     | 0.42              |
| 20:UQ:721:ALA:C    | 20:UQ:722:LEU:HD12  | 2.40                     | 0.42              |
| 20:UQ:862:LYS:HE2  | 20:UQ:863:LYS:HG2   | 2.02                     | 0.42              |
| 23:UT:54:TRP:CA    | 23:UT:57:ILE:HG22   | 2.44                     | 0.42              |
| 23:UT:119:PRO:HG3  | 23:UT:165:PHE:HZ    | 1.85                     | 0.42              |
| 23:UT:357:LYS:HG2  | 23:UT:728:LEU:HD13  | 2.02                     | 0.42              |
| 23:UT:855:MET:HA   | 23:UT:924:TYR:CE1   | 2.55                     | 0.42              |
| 23:UT:858:LEU:HD12 | 23:UT:866:GLN:HG2   | 2.00                     | 0.42              |
| 23:UT:988:LYS:HD2  | 23:UT:990:THR:HG23  | 2.02                     | 0.42              |
| 23:UT:1258:TRP:NE1 | 23:UT:1262:GLU:OE2  | 2.53                     | 0.42              |
| 23:UT:1372:MET:HE1 | 23:UT:1420:VAL:HA   | 2.02                     | 0.42              |
| 23:UT:1660:LYS:O   | 23:UT:1664:ILE:HG12 | 2.20                     | 0.42              |
| 23:UT:1677:LEU:HA  | 23:UT:1680:THR:HG22 | 2.01                     | 0.42              |
| 23:UT:1907:ASN:O   | 23:UT:1910:VAL:HG22 | 2.20                     | 0.42              |
| 23:UT:1926:PHE:CE2 | 23:UT:1929:GLU:HB2  | 2.55                     | 0.42              |
| 23:UT:1957:GLN:HG2 | 23:UT:1998:LEU:HB2  | 2.02                     | 0.42              |
| 24:UU:247:PRO:HB2  | 24:UU:248:GLN:OE1   | 2.20                     | 0.42              |
| 24:UU:371:LYS:C    | 24:UU:373:ARG:H     | 2.23                     | 0.42              |
| 25:UV:369:TRP:CE3  | 25:UV:370:LEU:HD22  | 2.54                     | 0.42              |
| 25:UV:480:MET:N    | 25:UV:480:MET:SD    | 2.93                     | 0.42              |
| 25:UV:796:ILE:HG21 | 37:CN:100:LEU:CD1   | 2.49                     | 0.42              |
| 25:UV:971:LYS:HA   | 25:UV:1028:ARG:NH2  | 2.35                     | 0.42              |
| 26:UX:115:ILE:HG23 | 26:UX:116:ALA:N     | 2.35                     | 0.42              |
| 26:UX:145:VAL:HG11 | 26:UX:170:ILE:HG21  | 2.02                     | 0.42              |
| 28:CD:75:SER:OG    | 28:CD:76:GLU:N      | 2.53                     | 0.42              |
| 28:CD:79:LYS:HB2   | 28:CD:79:LYS:HE2    | 1.80                     | 0.42              |
| 29:CE:212:MET:CE   | 29:CE:218:ALA:HB2   | 2.50                     | 0.42              |
| 29:CE:280:MET:HG3  | 29:CE:288:THR:OG1   | 2.20                     | 0.42              |
| 30:CF:67:LEU:HB2   | 30:CF:68:PRO:HD3    | 2.02                     | 0.42              |
| 30:CG:34:LYS:HE2   | 30:CG:103:THR:HG21  | 2.02                     | 0.42              |
| 31:CH:240:LEU:HA   | 31:CH:240:LEU:HD23  | 1.81                     | 0.42              |
| 32:CI:63:LEU:HA    | 32:CI:63:LEU:HD23   | 1.83                     | 0.42              |
| 35:CL:864:ASP:O    | 35:CL:865:SER:OG    | 2.30                     | 0.42              |
| 35:CL:992:GLU:HG3  | 66:D3:565:C:H5      | 1.85                     | 0.42              |
| 36:CM:215:VAL:HG21 | 36:CM:273:GLU:HA    | 2.02                     | 0.42              |
| 37:CN:78:TYR:CG    | 37:CN:143:LYS:HE3   | 2.55                     | 0.42              |
| 38:JC:60:ASN:ND2   | 38:JC:101:ASN:O     | 2.52                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:JC:144:LEU:HD12 | 38:JC:154:TYR:O    | 2.20                     | 0.42              |
| 38:JC:223:ASN:ND2  | 38:JC:227:ARG:O    | 2.52                     | 0.42              |
| 39:JF:193:ILE:HD13 | 39:JF:245:ALA:HA   | 2.02                     | 0.42              |
| 39:JG:136:ARG:O    | 39:JG:140:LEU:HD23 | 2.20                     | 0.42              |
| 44:JM:175:GLU:O    | 44:JM:178:MET:HB2  | 2.20                     | 0.42              |
| 46:JO:52:TYR:CE2   | 46:JO:56:ILE:HD13  | 2.54                     | 0.42              |
| 46:JO:186:VAL:HG22 | 46:JO:199:HIS:CG   | 2.55                     | 0.42              |
| 47:JP:289:TYR:CE1  | 47:JP:297:SER:HB3  | 2.54                     | 0.42              |
| 49:DE:127:LYS:HE3  | 49:DE:127:LYS:HB2  | 1.88                     | 0.42              |
| 50:DF:186:ASN:OD1  | 50:DF:188:LYS:N    | 2.53                     | 0.42              |
| 56:DN:48:SER:O     | 56:DN:52:VAL:HG23  | 2.19                     | 0.42              |
| 57:DO:81:VAL:CG2   | 57:DO:115:ILE:HG22 | 2.50                     | 0.42              |
| 65:D2:68:U:H5      | 65:D2:70:A:H2'     | 1.83                     | 0.42              |
| 65:D2:117:G:C6     | 65:D2:130:G:C5     | 3.08                     | 0.42              |
| 65:D2:125:G:H2'    | 65:D2:126:A:C8     | 2.55                     | 0.42              |
| 65:D2:169:A:C8     | 65:D2:171:G:C8     | 3.08                     | 0.42              |
| 66:D3:103:A:H2'    | 66:D3:309:C:H41    | 1.84                     | 0.42              |
| 66:D3:477:A:H2'    | 66:D3:478:A:C8     | 2.55                     | 0.42              |
| 66:D3:1694:A:O2'   | 66:D3:1695:G:H5'   | 2.20                     | 0.42              |
| 66:D3:1711:C:H2'   | 66:D3:1712:A:H5''  | 2.02                     | 0.42              |
| 3:JA:63:LEU:HD13   | 3:JA:66:PHE:CE2    | 2.54                     | 0.42              |
| 3:JA:133:ASN:OD1   | 3:JA:551:ASN:HB2   | 2.20                     | 0.42              |
| 3:JA:747:LEU:HD11  | 3:JA:758:HIS:HB2   | 2.01                     | 0.42              |
| 3:JA:783:LYS:O     | 3:JA:786:LEU:HG    | 2.20                     | 0.42              |
| 4:UA:684:VAL:HG12  | 4:UA:695:ALA:CB    | 2.50                     | 0.42              |
| 1:CB:103:GLU:HA    | 14:UK:194:LYS:HE3  | 2.01                     | 0.42              |
| 1:CB:248:ASP:OD1   | 1:CB:248:ASP:N     | 2.51                     | 0.42              |
| 3:JB:771:SER:C     | 3:JB:773:TRP:H     | 2.23                     | 0.42              |
| 7:UD:141:SER:OG    | 7:UD:162:ASN:OD1   | 2.36                     | 0.42              |
| 7:UD:163:GLY:HA2   | 7:UD:188:ALA:O     | 2.19                     | 0.42              |
| 7:UD:519:THR:N     | 7:UD:522:SER:HB2   | 2.35                     | 0.42              |
| 7:UD:564:ALA:HA    | 13:UJ:636:ASP:OD2  | 2.20                     | 0.42              |
| 7:UD:689:ASN:C     | 7:UD:689:ASN:ND2   | 2.73                     | 0.42              |
| 8:UE:519:LEU:HA    | 8:UE:519:LEU:HD23  | 1.87                     | 0.42              |
| 8:UE:531:LYS:O     | 8:UE:534:SER:OG    | 2.29                     | 0.42              |
| 9:UF:276:VAL:HG11  | 17:UN:338:LEU:HD11 | 2.01                     | 0.42              |
| 10:UG:378:VAL:O    | 10:UG:378:VAL:HG13 | 2.18                     | 0.42              |
| 11:UH:674:GLU:O    | 11:UH:678:LEU:HD23 | 2.19                     | 0.42              |
| 13:UJ:732:PHE:HB3  | 13:UJ:735:ASP:HB2  | 2.02                     | 0.42              |
| 14:UK:247:GLN:NE2  | 21:UR:515:THR:HB   | 2.33                     | 0.42              |
| 15:UL:5:TYR:OH     | 15:UL:643:ASP:OD2  | 2.27                     | 0.42              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 15:UL:208:TRP:CZ3   | 15:UL:222:THR:HG22  | 2.55                     | 0.42              |
| 15:UL:211:ALA:HB2   | 15:UL:259:ILE:HG22  | 2.02                     | 0.42              |
| 15:UL:269:THR:HB    | 15:UL:288:LYS:NZ    | 2.35                     | 0.42              |
| 15:UL:365:TYR:OH    | 15:UL:381:LYS:HD3   | 2.19                     | 0.42              |
| 15:UL:390:GLN:HG2   | 15:UL:394:VAL:CG2   | 2.50                     | 0.42              |
| 15:UL:801:PRO:O     | 15:UL:804:TYR:HB3   | 2.19                     | 0.42              |
| 15:UL:824:MET:HA    | 15:UL:825:PRO:HD3   | 1.91                     | 0.42              |
| 16:UM:24:THR:OG1    | 16:UM:69:LEU:HD23   | 2.20                     | 0.42              |
| 16:UM:54:HIS:CE1    | 16:UM:56:ILE:HD11   | 2.55                     | 0.42              |
| 16:UM:293:VAL:HG13  | 16:UM:293:VAL:O     | 2.20                     | 0.42              |
| 16:UM:436:ALA:HB3   | 16:UM:459:ASN:HB2   | 2.02                     | 0.42              |
| 16:UM:758:ARG:HA    | 16:UM:758:ARG:HD2   | 1.86                     | 0.42              |
| 20:UQ:182:LYS:HD3   | 20:UQ:182:LYS:HA    | 1.76                     | 0.42              |
| 20:UQ:553:ILE:O     | 20:UQ:555:VAL:HG23  | 2.20                     | 0.42              |
| 20:UQ:631:GLN:NE2   | 20:UQ:652:GLU:OE2   | 2.52                     | 0.42              |
| 21:UR:365:ASN:HB2   | 21:UR:368:THR:HG23  | 2.02                     | 0.42              |
| 22:US:185:TYR:CD1   | 22:US:192:GLN:HG2   | 2.54                     | 0.42              |
| 22:US:324:PHE:HB2   | 22:US:365:PHE:HZ    | 1.85                     | 0.42              |
| 23:UT:139:ALA:HA    | 23:UT:142:PHE:HB2   | 2.02                     | 0.42              |
| 23:UT:457:PHE:CZ    | 23:UT:485:ILE:HD13  | 2.55                     | 0.42              |
| 23:UT:704:ILE:HD13  | 23:UT:704:ILE:HA    | 1.88                     | 0.42              |
| 23:UT:707:PRO:HG3   | 23:UT:711:GLN:NE2   | 2.35                     | 0.42              |
| 23:UT:971:ARG:HH11  | 23:UT:972:LEU:HD21  | 1.85                     | 0.42              |
| 23:UT:1243:ILE:HD13 | 23:UT:1246:ILE:HD12 | 2.02                     | 0.42              |
| 23:UT:1667:ALA:O    | 23:UT:1670:LEU:HB2  | 2.19                     | 0.42              |
| 23:UT:1983:LEU:HA   | 23:UT:1986:VAL:HG22 | 2.00                     | 0.42              |
| 24:UU:87:PHE:CD1    | 65:D2:308:A:C6      | 3.07                     | 0.42              |
| 24:UU:277:ASP:OD2   | 24:UU:280:ARG:HD2   | 2.20                     | 0.42              |
| 24:UU:856:GLU:O     | 24:UU:858:PHE:CD1   | 2.73                     | 0.42              |
| 25:UV:351:LYS:HA    | 25:UV:354:LYS:NZ    | 2.35                     | 0.42              |
| 25:UV:439:HIS:NE2   | 25:UV:458:ILE:HB    | 2.34                     | 0.42              |
| 25:UV:1136:LEU:HD12 | 25:UV:1137:ASN:N    | 2.35                     | 0.42              |
| 28:CD:148:GLU:H     | 28:CD:148:GLU:CD    | 2.12                     | 0.42              |
| 29:CE:122:GLU:O     | 29:CE:125:PRO:HD2   | 2.20                     | 0.42              |
| 29:CE:206:ALA:HA    | 29:CE:209:ILE:HD12  | 2.01                     | 0.42              |
| 31:CH:224:SER:HB3   | 31:CH:229:GLU:OE2   | 2.19                     | 0.42              |
| 32:CI:33:MET:HG2    | 32:CI:38:ILE:HG13   | 2.01                     | 0.42              |
| 33:CJ:155:SER:HB2   | 33:CJ:266:LEU:HD23  | 2.01                     | 0.42              |
| 35:CL:58:MET:SD     | 35:CL:58:MET:N      | 2.93                     | 0.42              |
| 38:JC:205:GLU:HG2   | 38:JC:214:ARG:NH1   | 2.35                     | 0.42              |
| 38:JC:206:PHE:HE1   | 38:JC:218:LEU:HD21  | 1.84                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 42:JJ:117:TYR:CD2  | 42:JJ:118:PRO:HD3  | 2.55                     | 0.42              |
| 46:JO:179:GLY:O    | 46:JO:183:VAL:HG23 | 2.20                     | 0.42              |
| 47:JP:32:LEU:O     | 47:JP:34:PRO:HD3   | 2.19                     | 0.42              |
| 49:DE:87:MET:HA    | 49:DE:101:LEU:O    | 2.20                     | 0.42              |
| 50:DF:121:ILE:HD11 | 50:DF:195:ALA:HA   | 2.02                     | 0.42              |
| 55:DL:109:VAL:HG13 | 55:DL:137:PHE:C    | 2.40                     | 0.42              |
| 56:DN:119:GLU:O    | 56:DN:122:ILE:HG22 | 2.20                     | 0.42              |
| 65:D2:105:G:C2     | 65:D2:140:U:C2     | 3.07                     | 0.42              |
| 66:D3:81:G:H2'     | 66:D3:82:U:O4'     | 2.20                     | 0.42              |
| 66:D3:90:C:H2'     | 66:D3:91:G:C8      | 2.55                     | 0.42              |
| 66:D3:332:U:H2'    | 66:D3:333:A:H3'    | 2.02                     | 0.42              |
| 66:D3:384:G:H2'    | 66:D3:385:A:C8     | 2.55                     | 0.42              |
| 66:D3:557:G:C6     | 66:D3:558:U:C4     | 3.08                     | 0.42              |
| 66:D3:682:C:H2'    | 66:D3:683:C:C6     | 2.55                     | 0.42              |
| 66:D3:953:G:H2'    | 66:D3:954:G:C8     | 2.48                     | 0.42              |
| 66:D3:1621:U:N3    | 66:D3:1622:G:C5    | 2.88                     | 0.42              |
| 66:D3:1731:A:H2'   | 66:D3:1732:A:O4'   | 2.19                     | 0.42              |
| 67:D4:19:A:N1      | 67:D4:20:U:C4      | 2.88                     | 0.42              |
| 67:D4:100:U:H2'    | 67:D4:101:G:H8     | 1.84                     | 0.42              |
| 78:EK:81:ALA:CB    | 78:EK:82:PRO:HA    | 2.45                     | 0.42              |
| 79:EN:957:PRO:HA   | 79:EN:960:ALA:HB3  | 2.02                     | 0.42              |
| 3:JA:219:LEU:O     | 3:JA:221:PRO:HD3   | 2.20                     | 0.41              |
| 1:CB:111:MET:CE    | 1:CB:186:ASP:HA    | 2.49                     | 0.41              |
| 3:JB:28:ILE:HA     | 3:JB:201:VAL:O     | 2.20                     | 0.41              |
| 5:UB:498:LEU:HD11  | 5:UB:545:VAL:CG1   | 2.46                     | 0.41              |
| 5:UB:592:ARG:HD2   | 22:US:348:ASP:OD2  | 2.20                     | 0.41              |
| 7:UD:213:TRP:CD1   | 7:UD:225:LEU:HB3   | 2.55                     | 0.41              |
| 7:UD:298:ALA:HA    | 7:UD:304:ILE:HD13  | 2.02                     | 0.41              |
| 8:UE:4:PRO:O       | 8:UE:21:THR:OG1    | 2.16                     | 0.41              |
| 8:UE:85:ILE:HB     | 8:UE:99:PHE:HB2    | 2.01                     | 0.41              |
| 8:UE:477:ALA:O     | 8:UE:480:LEU:HB3   | 2.20                     | 0.41              |
| 10:UG:130:ARG:HG3  | 10:UG:130:ARG:O    | 2.21                     | 0.41              |
| 10:UG:140:ARG:HE   | 13:UJ:20:LEU:CG    | 2.33                     | 0.41              |
| 10:UG:358:MET:H    | 10:UG:364:ARG:HD3  | 1.84                     | 0.41              |
| 10:UG:414:LEU:HD12 | 47:JP:26:ARG:NH2   | 2.35                     | 0.41              |
| 10:UG:451:SER:OG   | 10:UG:452:VAL:N    | 2.50                     | 0.41              |
| 12:UI:452:LEU:HB3  | 12:UI:453:PRO:HD3  | 2.02                     | 0.41              |
| 12:UI:461:THR:HG23 | 12:UI:462:LEU:HD12 | 2.01                     | 0.41              |
| 13:UJ:92:LYS:HG3   | 13:UJ:92:LYS:H     | 1.72                     | 0.41              |
| 13:UJ:1475:SER:O   | 13:UJ:1478:LEU:HG  | 2.20                     | 0.41              |
| 14:UK:118:LEU:HD11 | 14:UK:201:VAL:HG13 | 2.01                     | 0.41              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 15:UL:59:LEU:HD21   | 15:UL:62:LYS:HB3    | 2.00                     | 0.41              |
| 15:UL:337:LYS:O     | 15:UL:357:THR:HB    | 2.20                     | 0.41              |
| 15:UL:763:ILE:HD13  | 15:UL:838:THR:HG21  | 2.02                     | 0.41              |
| 15:UL:857:LEU:HD21  | 16:UM:806:LEU:HD11  | 2.01                     | 0.41              |
| 16:UM:33:ALA:HA     | 16:UM:41:ASN:O      | 2.20                     | 0.41              |
| 18:UO:52:PRO:HG2    | 18:UO:311:THR:O     | 2.19                     | 0.41              |
| 18:UO:97:CYS:HB2    | 18:UO:107:VAL:HG22  | 2.00                     | 0.41              |
| 20:UQ:210:HIS:NE2   | 20:UQ:226:SER:OG    | 2.53                     | 0.41              |
| 20:UQ:214:ASP:OD1   | 20:UQ:214:ASP:N     | 2.53                     | 0.41              |
| 20:UQ:323:LEU:O     | 20:UQ:331:GLN:HA    | 2.19                     | 0.41              |
| 20:UQ:474:THR:HG21  | 20:UQ:493:PRO:HB2   | 2.02                     | 0.41              |
| 20:UQ:742:ARG:O     | 20:UQ:743:ILE:HD13  | 2.20                     | 0.41              |
| 21:UR:229:PRO:HA    | 21:UR:230:PRO:HD3   | 1.85                     | 0.41              |
| 23:UT:498:ILE:O     | 23:UT:501:LEU:HB2   | 2.19                     | 0.41              |
| 23:UT:986:SER:O     | 23:UT:986:SER:OG    | 2.37                     | 0.41              |
| 23:UT:1364:ARG:NH2  | 23:UT:1413:VAL:HB   | 2.35                     | 0.41              |
| 23:UT:1463:GLN:HA   | 23:UT:1466:ILE:HD12 | 2.01                     | 0.41              |
| 23:UT:1818:LEU:HD23 | 23:UT:1872:ALA:HB2  | 2.01                     | 0.41              |
| 23:UT:1967:ILE:HG22 | 23:UT:2009:LYS:HE3  | 2.01                     | 0.41              |
| 25:UV:222:PHE:CD2   | 25:UV:225:LEU:HD21  | 2.55                     | 0.41              |
| 25:UV:888:LYS:HG2   | 25:UV:889:TYR:CD1   | 2.54                     | 0.41              |
| 25:UV:923:HIS:NE2   | 25:UV:1088:LEU:O    | 2.47                     | 0.41              |
| 25:UV:1024:PHE:HB2  | 25:UV:1040:PHE:CE2  | 2.55                     | 0.41              |
| 25:UV:1197:ARG:HD2  | 25:UV:1200:LEU:HD13 | 2.02                     | 0.41              |
| 27:UZ:23:GLN:HA     | 27:UZ:26:GLU:HG3    | 2.01                     | 0.41              |
| 27:UZ:67:PRO:CB     | 27:UZ:96:LEU:HD11   | 2.50                     | 0.41              |
| 28:CD:249:GLN:OE1   | 28:CD:249:GLN:N     | 2.43                     | 0.41              |
| 34:CK:531:ALA:HA    | 34:CK:534:ARG:HG2   | 2.02                     | 0.41              |
| 35:CL:67:PRO:HA     | 35:CL:68:PRO:HD3    | 1.94                     | 0.41              |
| 35:CL:89:LEU:HD22   | 35:CL:117:PHE:HE2   | 1.84                     | 0.41              |
| 35:CL:300:GLN:HB2   | 35:CL:792:VAL:CG1   | 2.50                     | 0.41              |
| 38:JC:58:ALA:HB3    | 38:JC:76:THR:OG1    | 2.19                     | 0.41              |
| 38:JC:116:HIS:CE1   | 38:JC:126:GLN:NE2   | 2.86                     | 0.41              |
| 38:JC:163:TYR:HE1   | 43:JK:464:LEU:HD22  | 1.84                     | 0.41              |
| 38:JC:185:HIS:CE1   | 38:JC:234:THR:H     | 2.38                     | 0.41              |
| 38:JC:245:CYS:SG    | 38:JC:253:TYR:HB2   | 2.59                     | 0.41              |
| 38:JC:356:LEU:HA    | 38:JC:359:ILE:CG1   | 2.50                     | 0.41              |
| 39:JF:41:MET:HB3    | 39:JF:110:LEU:HB3   | 2.02                     | 0.41              |
| 39:JF:67:LEU:CD2    | 39:JF:142:VAL:HB    | 2.50                     | 0.41              |
| 44:JM:62:LEU:HD23   | 44:JM:63:PRO:O      | 2.20                     | 0.41              |
| 46:JO:103:LEU:HA    | 46:JO:103:LEU:HD23  | 1.75                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:JO:186:VAL:HG22 | 46:JO:199:HIS:ND1  | 2.35                     | 0.41              |
| 47:JP:48:THR:O     | 47:JP:51:GLU:HG2   | 2.19                     | 0.41              |
| 47:JP:92:ILE:HD11  | 47:JP:148:TRP:CE3  | 2.55                     | 0.41              |
| 47:JP:282:GLU:C    | 47:JP:284:HIS:H    | 2.22                     | 0.41              |
| 49:DE:195:ILE:O    | 49:DE:195:ILE:HG13 | 2.19                     | 0.41              |
| 51:DG:173:PRO:HA   | 66:D3:66:U:P       | 2.60                     | 0.41              |
| 51:DG:180:THR:OG1  | 51:DG:183:ARG:HG3  | 2.19                     | 0.41              |
| 52:DH:23:ALA:O     | 52:DH:27:LEU:HG    | 2.20                     | 0.41              |
| 52:DH:27:LEU:HD11  | 52:DH:81:LEU:HD21  | 2.01                     | 0.41              |
| 54:DJ:85:VAL:HG23  | 54:DJ:86:LEU:HB2   | 2.02                     | 0.41              |
| 54:DJ:86:LEU:HG    | 54:DJ:90:LYS:HG3   | 2.02                     | 0.41              |
| 56:DN:32:SER:HA    | 56:DN:35:GLU:OE1   | 2.19                     | 0.41              |
| 57:DO:81:VAL:HG23  | 57:DO:115:ILE:HA   | 2.01                     | 0.41              |
| 62:DY:124:ARG:NH2  | 66:D3:151:G:O6     | 2.53                     | 0.41              |
| 66:D3:23:G:OP2     | 66:D3:23:G:H8      | 2.03                     | 0.41              |
| 66:D3:636:A:C6     | 66:D3:637:C:C4     | 3.08                     | 0.41              |
| 66:D3:1686:C:H2'   | 66:D3:1687:U:C6    | 2.55                     | 0.41              |
| 67:D4:199:G:C6     | 67:D4:200:C:C4     | 3.07                     | 0.41              |
| 67:D4:318:U:H4'    | 67:D4:319:G:C5'    | 2.51                     | 0.41              |
| 78:EK:368:LYS:O    | 78:EK:372:LEU:CB   | 2.67                     | 0.41              |
| 78:EK:663:ASP:O    | 78:EK:664:LYS:CB   | 2.66                     | 0.41              |
| 79:EN:790:VAL:O    | 79:EN:794:LEU:N    | 2.43                     | 0.41              |
| 1:CA:250:ALA:HB2   | 1:CA:289:GLU:OE1   | 2.20                     | 0.41              |
| 3:JA:45:MET:HG2    | 3:JA:53:LYS:NZ     | 2.35                     | 0.41              |
| 3:JA:131:THR:O     | 3:JA:135:LEU:HG    | 2.20                     | 0.41              |
| 3:JA:779:LYS:HG3   | 3:JA:783:LYS:NZ    | 2.34                     | 0.41              |
| 3:JA:877:LEU:HB2   | 3:JA:881:GLN:OE1   | 2.20                     | 0.41              |
| 4:UA:311:ASN:ND2   | 4:UA:316:TRP:HB2   | 2.35                     | 0.41              |
| 4:UA:514:VAL:HG12  | 4:UA:515:TYR:N     | 2.35                     | 0.41              |
| 5:UB:737:ILE:O     | 5:UB:740:MET:HG3   | 2.20                     | 0.41              |
| 7:UD:159:GLY:HA3   | 7:UD:193:LEU:HD11  | 2.01                     | 0.41              |
| 7:UD:427:ASN:HB2   | 7:UD:444:ARG:HE    | 1.85                     | 0.41              |
| 7:UD:576:ASN:HB3   | 7:UD:578:SER:O     | 2.20                     | 0.41              |
| 8:UE:91:LEU:HG     | 20:UQ:822:PHE:HE2  | 1.85                     | 0.41              |
| 8:UE:305:TRP:O     | 8:UE:306:LEU:HD23  | 2.21                     | 0.41              |
| 9:UF:81:ASN:N      | 9:UF:81:ASN:OD1    | 2.53                     | 0.41              |
| 9:UF:173:ARG:HH12  | 28:CD:83:ASP:HB3   | 1.84                     | 0.41              |
| 9:UF:204:GLY:HA2   | 9:UF:207:ASN:OD1   | 2.21                     | 0.41              |
| 10:UG:125:LEU:HA   | 10:UG:125:LEU:HD12 | 1.85                     | 0.41              |
| 13:UJ:49:PHE:CD2   | 13:UJ:79:ILE:HD11  | 2.55                     | 0.41              |
| 13:UJ:561:PHE:O    | 13:UJ:564:VAL:HG22 | 2.20                     | 0.41              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 13:UJ:684:TYR:CE2  | 13:UJ:723:LEU:HA    | 2.56                     | 0.41              |
| 13:UJ:800:ASP:OD1  | 13:UJ:801:ILE:HD12  | 2.20                     | 0.41              |
| 13:UJ:1522:SER:OG  | 67:D4:141:U:H4'     | 2.20                     | 0.41              |
| 13:UJ:1590:ILE:HA  | 13:UJ:1593:TYR:HD2  | 1.85                     | 0.41              |
| 13:UJ:1652:VAL:HA  | 13:UJ:1655:LEU:HD12 | 2.02                     | 0.41              |
| 13:UJ:1712:LYS:NZ  | 13:UJ:1752:LEU:HD22 | 2.35                     | 0.41              |
| 14:UK:22:ARG:HH12  | 35:CL:937:PHE:CB    | 2.32                     | 0.41              |
| 14:UK:62:GLU:HA    | 32:CI:119:LYS:O     | 2.20                     | 0.41              |
| 15:UL:46:LEU:HD12  | 15:UL:657:GLN:HE22  | 1.85                     | 0.41              |
| 15:UL:137:ILE:HG22 | 15:UL:169:PHE:HZ    | 1.85                     | 0.41              |
| 15:UL:574:LEU:HD23 | 15:UL:574:LEU:HA    | 1.87                     | 0.41              |
| 15:UL:606:ASP:OD1  | 15:UL:606:ASP:N     | 2.51                     | 0.41              |
| 16:UM:212:LEU:HD23 | 16:UM:213:SER:N     | 2.35                     | 0.41              |
| 16:UM:433:HIS:CE1  | 16:UM:437:VAL:HG12  | 2.55                     | 0.41              |
| 16:UM:513:LYS:NZ   | 16:UM:535:GLY:N     | 2.68                     | 0.41              |
| 16:UM:655:GLU:HA   | 16:UM:658:LYS:NZ    | 2.35                     | 0.41              |
| 17:UN:861:LEU:O    | 17:UN:863:MET:N     | 2.54                     | 0.41              |
| 20:UQ:229:SER:HB2  | 20:UQ:235:VAL:HG12  | 2.01                     | 0.41              |
| 20:UQ:252:LEU:HD11 | 65:D2:81:A:H8       | 1.84                     | 0.41              |
| 20:UQ:290:ILE:HD12 | 20:UQ:292:LEU:HD21  | 2.01                     | 0.41              |
| 21:UR:242:ASN:HD22 | 21:UR:585:LYS:HA    | 1.85                     | 0.41              |
| 21:UR:271:THR:HG22 | 21:UR:289:HIS:HB2   | 2.01                     | 0.41              |
| 21:UR:345:LEU:HD23 | 21:UR:345:LEU:HA    | 1.89                     | 0.41              |
| 21:UR:366:SER:N    | 21:UR:368:THR:O     | 2.53                     | 0.41              |
| 21:UR:374:ILE:HD13 | 21:UR:374:ILE:HG21  | 1.77                     | 0.41              |
| 21:UR:477:LYS:HA   | 21:UR:477:LYS:HD3   | 1.94                     | 0.41              |
| 22:US:185:TYR:CE1  | 22:US:192:GLN:HG2   | 2.55                     | 0.41              |
| 23:UT:464:PHE:O    | 23:UT:468:ALA:HB2   | 2.20                     | 0.41              |
| 23:UT:510:SER:HA   | 23:UT:511:PRO:HD3   | 1.94                     | 0.41              |
| 23:UT:634:ASN:O    | 23:UT:638:LEU:HD23  | 2.20                     | 0.41              |
| 23:UT:863:THR:C    | 23:UT:867:LYS:HZ3   | 2.23                     | 0.41              |
| 23:UT:873:LEU:O    | 23:UT:876:TYR:HB2   | 2.20                     | 0.41              |
| 23:UT:1236:GLN:O   | 23:UT:1240:THR:HG23 | 2.20                     | 0.41              |
| 23:UT:1436:ASP:O   | 23:UT:1476:LEU:HD22 | 2.20                     | 0.41              |
| 23:UT:1488:MET:SD  | 23:UT:1489:ILE:HG13 | 2.59                     | 0.41              |
| 23:UT:1728:PHE:HE1 | 60:DW:119:LYS:HD2   | 1.85                     | 0.41              |
| 23:UT:1975:LYS:O   | 23:UT:1979:LEU:HG   | 2.20                     | 0.41              |
| 24:UU:51:VAL:HG21  | 24:UU:90:VAL:HG11   | 2.02                     | 0.41              |
| 24:UU:416:ALA:HB3  | 24:UU:433:ALA:HB3   | 2.03                     | 0.41              |
| 24:UU:860:GLU:HA   | 24:UU:863:TRP:CE3   | 2.54                     | 0.41              |
| 25:UV:331:LEU:HD23 | 25:UV:331:LEU:H     | 1.85                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:UV:562:LEU:O    | 25:UV:566:ILE:HG12 | 2.20                     | 0.41              |
| 25:UV:749:SER:OG   | 25:UV:787:GLU:OE2  | 2.34                     | 0.41              |
| 25:UV:808:LEU:O    | 25:UV:812:GLU:OE1  | 2.38                     | 0.41              |
| 27:UZ:90:ASP:C     | 27:UZ:92:HIS:H     | 2.23                     | 0.41              |
| 27:UZ:129:TYR:HB2  | 27:UZ:153:MET:CE   | 2.50                     | 0.41              |
| 28:CD:17:VAL:O     | 28:CD:51:VAL:HG12  | 2.20                     | 0.41              |
| 30:CG:52:ILE:O     | 30:CG:78:TYR:HA    | 2.20                     | 0.41              |
| 31:CH:504:ASN:HB2  | 31:CH:506:ARG:NH2  | 2.35                     | 0.41              |
| 32:CI:7:HIS:ND1    | 67:D4:34:A:C6      | 2.88                     | 0.41              |
| 35:CL:140:LEU:O    | 35:CL:169:GLY:HA2  | 2.20                     | 0.41              |
| 35:CL:607:ASP:OD2  | 35:CL:609:GLU:HG2  | 2.20                     | 0.41              |
| 35:CL:778:GLN:CB   | 35:CL:779:ARG:HD3  | 2.50                     | 0.41              |
| 35:CL:993:ASP:OD1  | 66:D3:565:C:N4     | 2.53                     | 0.41              |
| 35:CL:1146:GLU:HA  | 35:CL:1146:GLU:OE2 | 2.20                     | 0.41              |
| 38:JC:200:GLU:HG2  | 38:JC:230:GLN:HG3  | 2.01                     | 0.41              |
| 39:JF:55:ILE:O     | 39:JF:63:ASP:CA    | 2.60                     | 0.41              |
| 39:JF:205:PHE:HE2  | 39:JF:221:VAL:HA   | 1.84                     | 0.41              |
| 47:JP:416:HIS:CE1  | 66:D3:5:U:N3       | 2.88                     | 0.41              |
| 49:DE:65:LEU:HD13  | 49:DE:79:ASP:O     | 2.20                     | 0.41              |
| 49:DE:102:VAL:HG21 | 49:DE:239:PRO:HG3  | 2.01                     | 0.41              |
| 49:DE:125:LYS:O    | 49:DE:141:THR:HA   | 2.19                     | 0.41              |
| 49:DE:179:LYS:O    | 49:DE:194:THR:HA   | 2.19                     | 0.41              |
| 50:DF:56:ALA:O     | 50:DF:57:SER:HB2   | 2.19                     | 0.41              |
| 50:DF:160:VAL:HG22 | 50:DF:161:ASP:N    | 2.34                     | 0.41              |
| 50:DF:175:LEU:HD23 | 50:DF:175:LEU:HA   | 1.75                     | 0.41              |
| 51:DG:85:ARG:HH12  | 51:DG:87:ARG:CZ    | 2.33                     | 0.41              |
| 53:DI:8:ARG:HD2    | 53:DI:21:PHE:CD1   | 2.55                     | 0.41              |
| 65:D2:352:U:C4     | 65:D2:353:A:C5     | 3.08                     | 0.41              |
| 65:D2:412:A:C6     | 65:D2:413:C:C4     | 3.08                     | 0.41              |
| 65:D2:479:G:N2     | 67:D4:40:A:C4      | 2.88                     | 0.41              |
| 66:D3:252:U:H2'    | 66:D3:253:A:C8     | 2.54                     | 0.41              |
| 66:D3:270:C:C4     | 66:D3:271:A:N7     | 2.88                     | 0.41              |
| 66:D3:876:G:C5     | 66:D3:936:G:C2     | 3.08                     | 0.41              |
| 66:D3:1124:A:H1'   | 67:D4:1:G:C2       | 2.54                     | 0.41              |
| 66:D3:1152:A:H2'   | 66:D3:1153:G:H8    | 1.85                     | 0.41              |
| 66:D3:1586:A:C4    | 66:D3:1611:A:C6    | 3.08                     | 0.41              |
| 66:D3:1603:U:C6    | 66:D3:1604:U:H5    | 2.37                     | 0.41              |
| 67:D4:60:A:H4'     | 67:D4:61:G:O5'     | 2.19                     | 0.41              |
| 2:DA:46:THR:HG22   | 2:DA:47:LEU:N      | 2.35                     | 0.41              |
| 3:JA:36:GLN:O      | 3:JA:40:LEU:HG     | 2.21                     | 0.41              |
| 3:JA:167:ASP:OD1   | 3:JA:169:HIS:ND1   | 2.46                     | 0.41              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 3:JA:614:ILE:HG13   | 3:JA:761:VAL:HG21   | 2.02                     | 0.41              |
| 4:UA:566:GLN:OE1    | 4:UA:675:MET:HE1    | 2.20                     | 0.41              |
| 4:UA:613:LYS:HG3    | 4:UA:614:ARG:H      | 1.85                     | 0.41              |
| 1:CB:243:ASP:HA     | 1:CB:270:SER:OG     | 2.20                     | 0.41              |
| 1:CB:291:GLN:HA     | 1:CB:294:ARG:HB3    | 2.01                     | 0.41              |
| 7:UD:62:PRO:HB2     | 7:UD:64:ASP:OD1     | 2.20                     | 0.41              |
| 7:UD:161:ASP:C      | 7:UD:163:GLY:H      | 2.23                     | 0.41              |
| 7:UD:385:ASN:ND2    | 7:UD:387:GLU:HB2    | 2.33                     | 0.41              |
| 7:UD:516:VAL:HG22   | 7:UD:517:THR:O      | 2.21                     | 0.41              |
| 8:UE:140:PHE:HE1    | 8:UE:178:LYS:HG2    | 1.85                     | 0.41              |
| 8:UE:148:LEU:HD23   | 8:UE:150:LYS:H      | 1.85                     | 0.41              |
| 8:UE:213:ASN:HB3    | 8:UE:215:TYR:CZ     | 2.56                     | 0.41              |
| 12:UI:509:GLN:C     | 12:UI:513:ARG:HE    | 2.19                     | 0.41              |
| 13:UJ:22:ARG:NH1    | 47:JP:20:GLN:O      | 2.37                     | 0.41              |
| 13:UJ:89:GLU:OE1    | 13:UJ:92:LYS:NZ     | 2.25                     | 0.41              |
| 13:UJ:127:ILE:HB    | 13:UJ:131:ASN:OD1   | 2.20                     | 0.41              |
| 13:UJ:672:ASP:OD1   | 13:UJ:673:ASN:N     | 2.53                     | 0.41              |
| 13:UJ:765:ASN:O     | 13:UJ:769:LEU:HG    | 2.20                     | 0.41              |
| 13:UJ:1450:LEU:O    | 13:UJ:1454:LEU:HG   | 2.19                     | 0.41              |
| 13:UJ:1550:ILE:HD12 | 13:UJ:1553:ARG:HB2  | 2.02                     | 0.41              |
| 13:UJ:1626:LEU:HD12 | 13:UJ:1627:THR:N    | 2.36                     | 0.41              |
| 13:UJ:1715:TYR:OH   | 13:UJ:1726:LEU:HD23 | 2.19                     | 0.41              |
| 14:UK:45:GLN:O      | 14:UK:48:LEU:N      | 2.53                     | 0.41              |
| 14:UK:167:THR:OG1   | 14:UK:169:ASP:OD2   | 2.26                     | 0.41              |
| 15:UL:532:ASP:OD1   | 15:UL:533:ASP:N     | 2.42                     | 0.41              |
| 15:UL:614:HIS:HB3   | 15:UL:634:SER:CB    | 2.50                     | 0.41              |
| 16:UM:463:ILE:HG12  | 16:UM:487:ARG:H     | 1.85                     | 0.41              |
| 16:UM:517:ILE:HG23  | 16:UM:526:GLU:HB2   | 2.01                     | 0.41              |
| 16:UM:560:TRP:CD1   | 16:UM:567:VAL:HA    | 2.55                     | 0.41              |
| 17:UN:849:PHE:CZ    | 66:D3:-4:A:C4       | 3.07                     | 0.41              |
| 20:UQ:89:VAL:N      | 20:UQ:110:PHE:O     | 2.21                     | 0.41              |
| 20:UQ:168:LEU:HD12  | 20:UQ:195:ASN:HB2   | 2.02                     | 0.41              |
| 20:UQ:408:THR:OG1   | 20:UQ:409:LYS:N     | 2.52                     | 0.41              |
| 20:UQ:462:PHE:HE2   | 20:UQ:463:TYR:CZ    | 2.38                     | 0.41              |
| 20:UQ:507:MET:CG    | 20:UQ:532:TRP:HB2   | 2.49                     | 0.41              |
| 21:UR:233:LEU:H     | 21:UR:554:ASN:HD21  | 1.68                     | 0.41              |
| 21:UR:474:SER:O     | 21:UR:477:LYS:NZ    | 2.53                     | 0.41              |
| 23:UT:1194:SER:HB3  | 23:UT:1198:PHE:CE2  | 2.55                     | 0.41              |
| 23:UT:1217:ARG:O    | 23:UT:1221:ILE:HG23 | 2.20                     | 0.41              |
| 24:UU:836:THR:HA    | 24:UU:839:ASN:OD1   | 2.20                     | 0.41              |
| 24:UU:860:GLU:HG2   | 24:UU:861:ILE:N     | 2.35                     | 0.41              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 25:UV:598:LYS:HE3   | 25:UV:600:TYR:CD1  | 2.55                     | 0.41              |
| 25:UV:1169:ILE:HG12 | 25:UV:1177:GLY:O   | 2.20                     | 0.41              |
| 27:UZ:55:ARG:HH11   | 27:UZ:56:ILE:HG13  | 1.84                     | 0.41              |
| 27:UZ:226:LYS:O     | 27:UZ:229:ARG:HG2  | 2.20                     | 0.41              |
| 28:CD:265:GLU:O     | 28:CD:269:GLU:OE1  | 2.38                     | 0.41              |
| 30:CG:59:GLU:HA     | 30:CG:60:PRO:HA    | 1.80                     | 0.41              |
| 31:CH:279:ARG:H     | 31:CH:279:ARG:HG2  | 1.59                     | 0.41              |
| 32:CI:47:TYR:HB2    | 32:CI:103:VAL:HG23 | 2.01                     | 0.41              |
| 33:CJ:54:LYS:HE3    | 33:CJ:54:LYS:HB3   | 1.86                     | 0.41              |
| 35:CL:612:VAL:HG22  | 35:CL:615:PHE:HE2  | 1.85                     | 0.41              |
| 38:JC:355:PHE:CE2   | 38:JC:359:ILE:HD11 | 2.55                     | 0.41              |
| 39:JG:217:ALA:O     | 39:JG:221:VAL:HG13 | 2.20                     | 0.41              |
| 42:JJ:190:VAL:HG21  | 42:JJ:251:ILE:HD12 | 2.02                     | 0.41              |
| 45:JN:238:ILE:HD13  | 65:D2:339:A:C2     | 2.56                     | 0.41              |
| 47:JP:92:ILE:HD12   | 47:JP:136:MET:HE2  | 2.02                     | 0.41              |
| 49:DE:80:THR:HG23   | 49:DE:81:THR:HG23  | 2.01                     | 0.41              |
| 49:DE:115:THR:HG1   | 49:DE:117:GLU:CD   | 2.24                     | 0.41              |
| 49:DE:183:VAL:HG13  | 49:DE:190:GLY:H    | 1.85                     | 0.41              |
| 49:DE:185:GLY:O     | 49:DE:189:LEU:HB3  | 2.19                     | 0.41              |
| 50:DF:76:ARG:O      | 50:DF:83:ARG:HG2   | 2.21                     | 0.41              |
| 52:DH:27:LEU:O      | 52:DH:31:SER:CB    | 2.66                     | 0.41              |
| 52:DH:51:VAL:HG13   | 52:DH:53:GLY:N     | 2.36                     | 0.41              |
| 52:DH:134:GLU:OE1   | 52:DH:134:GLU:N    | 2.53                     | 0.41              |
| 52:DH:144:VAL:CA    | 60:DW:42:GLN:HE21  | 2.30                     | 0.41              |
| 53:DI:87:ASN:O      | 53:DI:91:VAL:HG23  | 2.19                     | 0.41              |
| 53:DI:172:ARG:HE    | 53:DI:175:GLN:CG   | 2.33                     | 0.41              |
| 58:DQ:24:ALA:HB2    | 58:DQ:92:TYR:OH    | 2.19                     | 0.41              |
| 65:D2:433:C:H2'     | 65:D2:434:G:H8     | 1.85                     | 0.41              |
| 65:D2:471:C:H1'     | 67:D4:48:A:H2      | 1.84                     | 0.41              |
| 66:D3:34:G:N2       | 66:D3:475:A:N3     | 2.68                     | 0.41              |
| 66:D3:464:A:C6      | 66:D3:465:G:C6     | 3.08                     | 0.41              |
| 66:D3:761:G:H2'     | 66:D3:762:A:C8     | 2.56                     | 0.41              |
| 66:D3:955:A:C5      | 66:D3:956:C:C2     | 3.07                     | 0.41              |
| 66:D3:1167:G:H1     | 66:D3:1578:U:H3    | 1.67                     | 0.41              |
| 66:D3:1496:U:H2'    | 66:D3:1497:U:H6    | 1.84                     | 0.41              |
| 67:D4:6:C:H2'       | 67:D4:7:G:H8       | 1.86                     | 0.41              |
| 67:D4:100:U:H2'     | 67:D4:101:G:C8     | 2.55                     | 0.41              |
| 78:EK:140:ASP:C     | 78:EK:142:HIS:H    | 2.23                     | 0.41              |
| 79:EN:850:TYR:O     | 79:EN:854:SER:N    | 2.50                     | 0.41              |
| 2:DA:21:VAL:HG23    | 2:DA:23:PRO:HD3    | 2.03                     | 0.41              |
| 2:DA:61:LEU:HD22    | 2:DA:96:LEU:HD21   | 2.02                     | 0.41              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:DA:62:LYS:NZ      | 2:DA:90:GLU:OE1     | 2.39                     | 0.41              |
| 3:JA:651:SER:O      | 3:JA:652:ARG:C      | 2.59                     | 0.41              |
| 3:JA:840:LYS:HG3    | 3:JA:841:ARG:N      | 2.36                     | 0.41              |
| 4:UA:346:ASP:OD2    | 4:UA:666:ARG:NH2    | 2.53                     | 0.41              |
| 4:UA:674:LYS:O      | 4:UA:674:LYS:HD2    | 2.20                     | 0.41              |
| 1:CB:234:ILE:HB     | 1:CB:260:PHE:CZ     | 2.55                     | 0.41              |
| 1:CB:287:ALA:O      | 1:CB:291:GLN:OE1    | 2.38                     | 0.41              |
| 5:UB:698:ILE:HG22   | 5:UB:699:PRO:O      | 2.19                     | 0.41              |
| 8:UE:504:TRP:CZ3    | 12:UI:512:LEU:HD21  | 2.55                     | 0.41              |
| 10:UG:111:PHE:CZ    | 10:UG:149:PHE:CE1   | 3.08                     | 0.41              |
| 10:UG:259:TRP:CH2   | 10:UG:266:PRO:HD3   | 2.55                     | 0.41              |
| 10:UG:260:SER:HB3   | 10:UG:267:LEU:HD11  | 2.03                     | 0.41              |
| 10:UG:530:ASN:O     | 10:UG:534:LYS:HE3   | 2.20                     | 0.41              |
| 10:UG:553:PHE:CD2   | 25:UV:806:PHE:HZ    | 2.38                     | 0.41              |
| 13:UJ:218:ILE:HD12  | 13:UJ:263:VAL:HG21  | 2.02                     | 0.41              |
| 13:UJ:665:TYR:O     | 13:UJ:668:THR:OG1   | 2.32                     | 0.41              |
| 13:UJ:684:TYR:HE2   | 13:UJ:723:LEU:HA    | 1.86                     | 0.41              |
| 13:UJ:755:ARG:O     | 13:UJ:759:ILE:HG12  | 2.20                     | 0.41              |
| 13:UJ:1349:ILE:O    | 13:UJ:1352:LEU:HG   | 2.20                     | 0.41              |
| 13:UJ:1644:PHE:CE2  | 13:UJ:1683:HIS:HB3  | 2.56                     | 0.41              |
| 14:UK:14:ARG:NE     | 66:D3:583:C:HO2'    | 2.15                     | 0.41              |
| 15:UL:187:LYS:HG2   | 15:UL:199:THR:HG23  | 2.02                     | 0.41              |
| 15:UL:275:GLN:HE22  | 15:UL:339:LYS:C     | 2.24                     | 0.41              |
| 15:UL:432:TYR:CD2   | 66:D3:1657:U:C5     | 3.08                     | 0.41              |
| 20:UQ:42:ARG:O      | 20:UQ:57:VAL:HG23   | 2.20                     | 0.41              |
| 20:UQ:48:PHE:HB2    | 20:UQ:51:GLN:O      | 2.21                     | 0.41              |
| 20:UQ:98:VAL:HA     | 20:UQ:99:PRO:HD3    | 1.94                     | 0.41              |
| 20:UQ:293:LEU:HB3   | 20:UQ:324:TRP:CZ3   | 2.55                     | 0.41              |
| 21:UR:257:HIS:HD1   | 21:UR:260:LYS:H     | 1.67                     | 0.41              |
| 21:UR:487:GLU:OE2   | 21:UR:517:THR:OG1   | 2.29                     | 0.41              |
| 23:UT:114:CYS:O     | 23:UT:117:LEU:O     | 2.39                     | 0.41              |
| 23:UT:786:PRO:HD2   | 23:UT:787:GLN:OE1   | 2.21                     | 0.41              |
| 23:UT:1012:ARG:HG3  | 23:UT:1013:THR:HG23 | 2.01                     | 0.41              |
| 23:UT:1402:ILE:HG13 | 23:UT:1417:TYR:CD1  | 2.51                     | 0.41              |
| 23:UT:1856:THR:HG21 | 47:JP:110:TYR:HE1   | 1.85                     | 0.41              |
| 24:UU:257:ARG:HH12  | 24:UU:261:SER:HB2   | 1.83                     | 0.41              |
| 24:UU:469:SER:OG    | 24:UU:470:GLN:N     | 2.53                     | 0.41              |
| 24:UU:579:ARG:HH12  | 24:UU:615:PRO:HA    | 1.86                     | 0.41              |
| 25:UV:141:TRP:CE3   | 25:UV:144:LYS:HD2   | 2.56                     | 0.41              |
| 25:UV:306:LYS:HA    | 25:UV:306:LYS:HD3   | 1.91                     | 0.41              |
| 25:UV:485:TYR:O     | 25:UV:488:LEU:HG    | 2.20                     | 0.41              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 25:UV:521:LEU:HD12 | 25:UV:963:LYS:HZ2   | 1.85                     | 0.41              |
| 25:UV:703:LYS:HD2  | 25:UV:1085:ILE:HD11 | 2.02                     | 0.41              |
| 26:UX:16:THR:OG1   | 32:CI:34:ARG:NH2    | 2.53                     | 0.41              |
| 26:UX:27:LYS:HB3   | 26:UX:27:LYS:HE2    | 1.76                     | 0.41              |
| 26:UX:97:LEU:HD22  | 26:UX:128:LEU:HD23  | 2.01                     | 0.41              |
| 27:UZ:119:TYR:CD1  | 27:UZ:149:LYS:HD2   | 2.55                     | 0.41              |
| 28:CD:149:ARG:O    | 28:CD:152:LEU:HG    | 2.20                     | 0.41              |
| 28:CD:291:TYR:OH   | 29:CE:251:ASP:OD1   | 2.30                     | 0.41              |
| 29:CE:71:GLN:O     | 29:CE:75:LEU:HD23   | 2.20                     | 0.41              |
| 29:CE:201:ASP:OD1  | 29:CE:203:VAL:N     | 2.49                     | 0.41              |
| 31:CH:288:PHE:CE1  | 31:CH:295:LEU:HB2   | 2.55                     | 0.41              |
| 31:CH:413:PHE:CE1  | 31:CH:425:TRP:HB2   | 2.55                     | 0.41              |
| 31:CH:464:LEU:HD23 | 31:CH:464:LEU:HA    | 1.83                     | 0.41              |
| 32:CI:71:ARG:NH2   | 33:CJ:61:SER:HB2    | 2.35                     | 0.41              |
| 33:CJ:42:LEU:O     | 45:JN:222:ASN:HB3   | 2.20                     | 0.41              |
| 33:CJ:182:GLN:H    | 66:D3:1159:C:H42    | 1.67                     | 0.41              |
| 34:CK:366:GLU:HB3  | 34:CK:370:ARG:NH1   | 2.34                     | 0.41              |
| 35:CL:635:PHE:CZ   | 36:CM:221:CYS:HB2   | 2.56                     | 0.41              |
| 35:CL:1034:LEU:HB2 | 35:CL:1037:GLN:NE2  | 2.36                     | 0.41              |
| 36:CM:189:SER:OG   | 36:CM:250:LYS:HG2   | 2.19                     | 0.41              |
| 37:CN:84:VAL:HB    | 37:CN:126:LEU:HD11  | 2.01                     | 0.41              |
| 38:JC:163:TYR:CD1  | 38:JC:175:PRO:HB3   | 2.56                     | 0.41              |
| 38:JC:295:ARG:HD2  | 38:JC:314:SER:C     | 2.41                     | 0.41              |
| 39:JF:102:SER:OG   | 39:JF:104:ILE:HG22  | 2.20                     | 0.41              |
| 39:JF:233:SER:HB2  | 39:JG:101:ASP:OD2   | 2.20                     | 0.41              |
| 39:JF:240:LYS:O    | 39:JG:243:HIS:CE1   | 2.73                     | 0.41              |
| 44:JM:110:ASP:O    | 44:JM:114:ARG:HD3   | 2.21                     | 0.41              |
| 45:JN:155:LEU:HD23 | 45:JN:155:LEU:C     | 2.40                     | 0.41              |
| 47:JP:217:TRP:HE3  | 47:JP:254:PRO:HB2   | 1.86                     | 0.41              |
| 55:DL:12:ALA:C     | 55:DL:14:GLN:HE21   | 2.21                     | 0.41              |
| 56:DN:26:PHE:CZ    | 56:DN:28:LEU:HB2    | 2.55                     | 0.41              |
| 56:DN:89:TYR:CZ    | 56:DN:93:LYS:HD2    | 2.55                     | 0.41              |
| 60:DW:115:GLU:HG2  | 60:DW:118:ARG:NH1   | 2.35                     | 0.41              |
| 65:D2:195:A:H2'    | 65:D2:196:A:C8      | 2.55                     | 0.41              |
| 65:D2:217:C:H2'    | 65:D2:218:U:C6      | 2.55                     | 0.41              |
| 65:D2:357:G:C6     | 65:D2:369:G:C5      | 3.09                     | 0.41              |
| 66:D3:155:U:H2'    | 66:D3:157:A:OP2     | 2.21                     | 0.41              |
| 66:D3:194:U:O2'    | 66:D3:195:G:O4'     | 2.29                     | 0.41              |
| 66:D3:686:C:H2'    | 66:D3:687:G:C8      | 2.56                     | 0.41              |
| 66:D3:1203:A:H8    | 66:D3:1203:A:OP2    | 2.03                     | 0.41              |
| 67:D4:331:A:C2     | 67:D4:332:G:C4      | 3.09                     | 0.41              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 3:JA:214:LYS:HB3    | 3:JA:214:LYS:HE2    | 1.85                     | 0.41              |
| 3:JA:480:ASP:OD2    | 3:JA:482:ILE:HB     | 2.20                     | 0.41              |
| 3:JA:510:PRO:HB3    | 3:JA:649:TYR:CD1    | 2.55                     | 0.41              |
| 3:JA:512:GLN:O      | 3:JA:512:GLN:HG2    | 2.20                     | 0.41              |
| 4:UA:220:PHE:HD1    | 4:UA:248:TRP:H      | 1.69                     | 0.41              |
| 4:UA:340:LYS:HB3    | 34:CK:479:ALA:HB3   | 2.03                     | 0.41              |
| 4:UA:414:TRP:HA     | 4:UA:421:ASN:HA     | 2.02                     | 0.41              |
| 4:UA:660:SER:O      | 4:UA:660:SER:OG     | 2.36                     | 0.41              |
| 1:CB:236:MET:N      | 29:CE:121:LYS:HZ2   | 2.18                     | 0.41              |
| 3:JB:494:VAL:HA     | 3:JB:539:ALA:HB1    | 2.02                     | 0.41              |
| 7:UD:434:SER:HB3    | 7:UD:440:LEU:HD13   | 2.02                     | 0.41              |
| 8:UE:184:PHE:HE1    | 8:UE:202:PHE:HE1    | 1.69                     | 0.41              |
| 8:UE:364:THR:O      | 20:UQ:547:VAL:HA    | 2.21                     | 0.41              |
| 8:UE:461:ASP:OD2    | 8:UE:464:VAL:HG23   | 2.21                     | 0.41              |
| 9:UF:357:GLU:O      | 9:UF:360:LEU:HG     | 2.19                     | 0.41              |
| 10:UG:111:PHE:CD2   | 10:UG:133:HIS:HB2   | 2.55                     | 0.41              |
| 10:UG:274:ARG:NH2   | 65:D2:321:G:C2      | 2.89                     | 0.41              |
| 13:UJ:300:CYS:O     | 13:UJ:304:GLN:HG2   | 2.20                     | 0.41              |
| 13:UJ:329:THR:HA    | 13:UJ:332:ILE:HD13  | 2.03                     | 0.41              |
| 13:UJ:332:ILE:O     | 13:UJ:336:LEU:HD23  | 2.21                     | 0.41              |
| 13:UJ:550:TYR:HA    | 13:UJ:553:SER:OG    | 2.20                     | 0.41              |
| 13:UJ:648:LYS:HE2   | 13:UJ:648:LYS:HB2   | 1.89                     | 0.41              |
| 13:UJ:1380:LEU:HD21 | 13:UJ:1400:ILE:HA   | 2.02                     | 0.41              |
| 13:UJ:1435:SER:HA   | 13:UJ:1438:LEU:HD13 | 2.02                     | 0.41              |
| 13:UJ:1751:GLY:O    | 13:UJ:1755:VAL:HG22 | 2.20                     | 0.41              |
| 15:UL:880:ILE:HG23  | 16:UM:806:LEU:HD22  | 2.02                     | 0.41              |
| 16:UM:200:GLU:HA    | 16:UM:209:LEU:HB2   | 2.02                     | 0.41              |
| 16:UM:416:ARG:HB3   | 16:UM:425:ASP:HB3   | 2.02                     | 0.41              |
| 16:UM:591:ILE:HA    | 16:UM:600:LYS:O     | 2.20                     | 0.41              |
| 16:UM:756:ALA:O     | 16:UM:760:ILE:HG22  | 2.21                     | 0.41              |
| 17:UN:330:THR:HB    | 28:CD:88:LYS:HE2    | 2.02                     | 0.41              |
| 18:UO:378:LYS:HD2   | 21:UR:292:GLY:O     | 2.20                     | 0.41              |
| 20:UQ:64:LYS:NZ     | 20:UQ:122:LYS:HA    | 2.36                     | 0.41              |
| 21:UR:208:LEU:HA    | 21:UR:211:ILE:HG22  | 2.03                     | 0.41              |
| 21:UR:426:VAL:CG2   | 21:UR:458:ILE:HG13  | 2.48                     | 0.41              |
| 21:UR:464:THR:O     | 21:UR:479:ASN:ND2   | 2.50                     | 0.41              |
| 21:UR:570:PHE:CE2   | 21:UR:577:LEU:HD22  | 2.56                     | 0.41              |
| 22:US:381:LYS:CE    | 22:US:461:SER:HB2   | 2.48                     | 0.41              |
| 23:UT:306:LEU:HG    | 23:UT:346:GLN:NE2   | 2.35                     | 0.41              |
| 23:UT:521:THR:O     | 23:UT:525:ILE:HG12  | 2.21                     | 0.41              |
| 23:UT:852:ASP:O     | 23:UT:855:MET:HB3   | 2.21                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:UT:1335:GLY:O   | 23:UT:1337:LYS:NZ  | 2.54                     | 0.41              |
| 23:UT:1431:PHE:O   | 23:UT:1435:GLU:HG2 | 2.19                     | 0.41              |
| 23:UT:1556:ARG:NH1 | 23:UT:1618:ASN:OD1 | 2.54                     | 0.41              |
| 24:UU:511:ASP:C    | 24:UU:513:MET:H    | 2.24                     | 0.41              |
| 25:UV:795:GLU:O    | 25:UV:798:SER:OG   | 2.25                     | 0.41              |
| 29:CE:87:LEU:HD12  | 29:CE:88:ILE:H     | 1.84                     | 0.41              |
| 29:CE:183:ARG:HA   | 29:CE:183:ARG:HD3  | 1.81                     | 0.41              |
| 29:CE:316:THR:HA   | 29:CE:319:ILE:HG22 | 2.01                     | 0.41              |
| 30:CF:54:MET:HE1   | 30:CF:68:PRO:HD3   | 2.03                     | 0.41              |
| 31:CH:412:HIS:CE1  | 31:CH:505:LEU:HD23 | 2.56                     | 0.41              |
| 32:CI:114:ILE:HD12 | 32:CI:114:ILE:HG23 | 1.80                     | 0.41              |
| 33:CJ:196:THR:HG23 | 33:CJ:199:GLY:H    | 1.86                     | 0.41              |
| 34:CK:306:GLU:OE1  | 34:CK:309:LYS:HD2  | 2.21                     | 0.41              |
| 34:CK:538:LYS:HE2  | 66:D3:1628:U:C2    | 2.56                     | 0.41              |
| 35:CL:53:LYS:HE2   | 66:D3:433:C:C4     | 2.56                     | 0.41              |
| 35:CL:774:PRO:HA   | 35:CL:778:GLN:NE2  | 2.36                     | 0.41              |
| 35:CL:818:THR:OG1  | 36:CM:362:THR:HG21 | 2.20                     | 0.41              |
| 35:CL:836:LYS:HE2  | 35:CL:836:LYS:HA   | 2.02                     | 0.41              |
| 38:JC:194:LEU:HD11 | 38:JC:243:PHE:CZ   | 2.55                     | 0.41              |
| 46:JO:42:MET:HG2   | 46:JO:43:THR:N     | 2.35                     | 0.41              |
| 46:JO:153:LEU:HD12 | 46:JO:153:LEU:HA   | 1.73                     | 0.41              |
| 47:JP:201:ILE:HG22 | 47:JP:215:LEU:O    | 2.19                     | 0.41              |
| 49:DE:100:ARG:HH11 | 49:DE:100:ARG:HG2  | 1.85                     | 0.41              |
| 52:DH:107:ARG:HA   | 52:DH:107:ARG:NE   | 2.35                     | 0.41              |
| 53:DI:45:SER:HB3   | 53:DI:53:LYS:HE3   | 2.02                     | 0.41              |
| 54:DJ:68:LYS:O     | 54:DJ:72:GLU:OE1   | 2.39                     | 0.41              |
| 60:DW:97:ARG:HB2   | 60:DW:98:GLN:OE1   | 2.20                     | 0.41              |
| 65:D2:178:G:C6     | 65:D2:179:A:C5     | 3.08                     | 0.41              |
| 65:D2:185:A:C6     | 65:D2:213:G:C6     | 3.08                     | 0.41              |
| 65:D2:405:A:H1'    | 65:D2:452:A:N6     | 2.35                     | 0.41              |
| 66:D3:273:G:N2     | 66:D3:284:G:H1'    | 2.36                     | 0.41              |
| 66:D3:486:G:H4'    | 66:D3:487:G:OP1    | 2.20                     | 0.41              |
| 66:D3:548:G:C2     | 66:D3:591:A:C2     | 3.09                     | 0.41              |
| 66:D3:1168:U:O2'   | 66:D3:1465:C:OP2   | 2.36                     | 0.41              |
| 66:D3:1178:G:C2    | 66:D3:1462:G:C2    | 3.08                     | 0.41              |
| 66:D3:1706:C:H2'   | 66:D3:1707:A:N9    | 2.35                     | 0.41              |
| 74:EG:94:SER:O     | 74:EG:137:ILE:N    | 2.54                     | 0.41              |
| 79:EN:699:ALA:O    | 79:EN:718:ILE:N    | 2.43                     | 0.41              |
| 2:DA:145:LYS:HB2   | 2:DA:149:GLN:CG    | 2.50                     | 0.41              |
| 3:JA:899:ALA:HB1   | 3:JA:904:LEU:O     | 2.20                     | 0.41              |
| 4:UA:499:ILE:HD12  | 4:UA:544:ILE:HD11  | 2.03                     | 0.41              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 5:UB:672:THR:CG2    | 5:UB:682:ARG:HD2    | 2.50                     | 0.41              |
| 7:UD:84:ASN:ND2     | 7:UD:630:LYS:HD2    | 2.36                     | 0.41              |
| 7:UD:436:ASP:N      | 7:UD:436:ASP:OD1    | 2.54                     | 0.41              |
| 7:UD:580:LYS:HE2    | 7:UD:580:LYS:HB2    | 1.92                     | 0.41              |
| 7:UD:742:LEU:HD23   | 7:UD:742:LEU:HA     | 1.87                     | 0.41              |
| 10:UG:508:VAL:HA    | 46:JO:73:LEU:O      | 2.21                     | 0.41              |
| 13:UJ:82:ASP:HB2    | 47:JP:11:ASP:OD2    | 2.19                     | 0.41              |
| 13:UJ:413:ASP:HB2   | 13:UJ:417:LYS:NZ    | 2.35                     | 0.41              |
| 13:UJ:1609:ILE:HG21 | 13:UJ:1653:ASN:HD21 | 1.85                     | 0.41              |
| 13:UJ:1713:LEU:O    | 13:UJ:1717:LYS:HG2  | 2.20                     | 0.41              |
| 13:UJ:1741:ASP:CB   | 13:UJ:1744:ILE:HD12 | 2.49                     | 0.41              |
| 14:UK:196:LYS:HD2   | 65:D2:424:G:OP2     | 2.20                     | 0.41              |
| 15:UL:105:VAL:HG21  | 15:UL:115:LEU:CD2   | 2.50                     | 0.41              |
| 15:UL:168:GLY:HA3   | 15:UL:180:THR:OG1   | 2.20                     | 0.41              |
| 15:UL:170:TRP:CG    | 15:UL:212:VAL:HG21  | 2.55                     | 0.41              |
| 15:UL:554:THR:OG1   | 15:UL:555:VAL:N     | 2.54                     | 0.41              |
| 15:UL:811:ARG:HH11  | 15:UL:811:ARG:HG3   | 1.86                     | 0.41              |
| 16:UM:78:TYR:CZ     | 16:UM:86:LYS:HB2    | 2.55                     | 0.41              |
| 16:UM:191:SER:OG    | 16:UM:192:ALA:N     | 2.53                     | 0.41              |
| 16:UM:353:LEU:HB2   | 16:UM:365:ILE:HG13  | 2.01                     | 0.41              |
| 16:UM:463:ILE:N     | 16:UM:487:ARG:O     | 2.48                     | 0.41              |
| 16:UM:632:ILE:CG1   | 16:UM:644:TRP:HB2   | 2.51                     | 0.41              |
| 16:UM:684:LEU:O     | 16:UM:687:THR:OG1   | 2.31                     | 0.41              |
| 18:UO:8:ILE:O       | 18:UO:8:ILE:HG13    | 2.20                     | 0.41              |
| 19:UP:163:LEU:O     | 19:UP:167:ARG:HG2   | 2.21                     | 0.41              |
| 20:UQ:60:ARG:HG2    | 20:UQ:382:LYS:O     | 2.21                     | 0.41              |
| 20:UQ:148:GLU:OE2   | 20:UQ:148:GLU:N     | 2.48                     | 0.41              |
| 21:UR:433:TRP:NE1   | 21:UR:446:ARG:HD2   | 2.35                     | 0.41              |
| 22:US:424:ASN:HB3   | 22:US:427:GLN:CG    | 2.51                     | 0.41              |
| 23:UT:500:LEU:HB3   | 23:UT:503:ARG:NH1   | 2.36                     | 0.41              |
| 23:UT:1202:LEU:O    | 23:UT:1206:THR:HG23 | 2.20                     | 0.41              |
| 23:UT:1952:SER:CB   | 23:UT:1995:ARG:HD2  | 2.50                     | 0.41              |
| 24:UU:125:GLY:O     | 24:UU:142:LYS:HE3   | 2.21                     | 0.41              |
| 24:UU:217:VAL:HG23  | 24:UU:220:ILE:HG13  | 2.03                     | 0.41              |
| 24:UU:225:THR:OG1   | 24:UU:229:GLU:O     | 2.38                     | 0.41              |
| 24:UU:255:SER:HB2   | 24:UU:302:THR:HA    | 2.03                     | 0.41              |
| 24:UU:449:ARG:HG2   | 24:UU:450:VAL:O     | 2.21                     | 0.41              |
| 25:UV:1138:ASP:HA   | 25:UV:1141:GLU:OE1  | 2.20                     | 0.41              |
| 27:UZ:225:ASP:OD2   | 27:UZ:228:LYS:NZ    | 2.39                     | 0.41              |
| 29:CE:121:LYS:O     | 29:CE:124:LEU:HG    | 2.21                     | 0.41              |
| 29:CE:299:LEU:HD22  | 29:CE:341:LEU:HD23  | 2.02                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:CE:327:PHE:CD2  | 67:D4:323:G:C5     | 3.08                     | 0.41              |
| 33:CJ:29:ARG:HD3   | 33:CJ:59:ASP:HB3   | 2.01                     | 0.41              |
| 35:CL:846:VAL:HA   | 35:CL:855:GLN:HA   | 2.02                     | 0.41              |
| 36:CM:130:ILE:O    | 36:CM:133:ILE:HG22 | 2.20                     | 0.41              |
| 36:CM:133:ILE:HG13 | 36:CM:137:LEU:HD13 | 2.02                     | 0.41              |
| 38:JC:84:TYR:HD1   | 38:JC:91:LEU:HA    | 1.85                     | 0.41              |
| 38:JC:101:ASN:OD1  | 38:JC:116:HIS:HB2  | 2.20                     | 0.41              |
| 44:JM:57:THR:HG23  | 44:JM:61:LYS:NZ    | 2.35                     | 0.41              |
| 45:JN:287:ILE:HG23 | 45:JN:287:ILE:HD12 | 1.83                     | 0.41              |
| 47:JP:61:GLN:HE21  | 67:D4:31:G:H22     | 1.69                     | 0.41              |
| 47:JP:208:ARG:HD2  | 47:JP:212:VAL:HG22 | 2.02                     | 0.41              |
| 49:DE:122:LYS:C    | 49:DE:123:LEU:HD12 | 2.41                     | 0.41              |
| 49:DE:132:GLY:HA2  | 66:D3:252:U:H5'    | 2.01                     | 0.41              |
| 49:DE:207:LEU:HD12 | 49:DE:219:VAL:CG1  | 2.51                     | 0.41              |
| 51:DG:136:LYS:HB3  | 66:D3:168:A:O5'    | 2.21                     | 0.41              |
| 57:DO:24:ASN:HD22  | 57:DO:24:ASN:C     | 2.18                     | 0.41              |
| 57:DO:43:THR:HG22  | 57:DO:45:GLY:H     | 1.85                     | 0.41              |
| 58:DQ:65:ILE:HG21  | 58:DQ:85:ILE:CD1   | 2.51                     | 0.41              |
| 58:DQ:83:GLN:OE1   | 58:DQ:119:ALA:HB2  | 2.21                     | 0.41              |
| 62:DY:91:LEU:HA    | 62:DY:91:LEU:HD23  | 1.87                     | 0.41              |
| 65:D2:443:G:N2     | 65:D2:444:U:C2     | 2.88                     | 0.41              |
| 65:D2:458:A:C6     | 65:D2:459:U:C4     | 3.08                     | 0.41              |
| 65:D2:476:A:C2     | 65:D2:477:G:C4     | 3.09                     | 0.41              |
| 66:D3:59:C:C4      | 66:D3:452:A:C6     | 3.09                     | 0.41              |
| 66:D3:103:A:O3'    | 66:D3:308:C:N4     | 2.54                     | 0.41              |
| 66:D3:523:G:C8     | 66:D3:524:U:C5     | 3.09                     | 0.41              |
| 66:D3:555:A:C6     | 66:D3:557:G:C4     | 3.08                     | 0.41              |
| 66:D3:1499:G:H1    | 66:D3:1508:U:H3    | 1.68                     | 0.41              |
| 66:D3:1533:C:H2'   | 66:D3:1534:G:C8    | 2.56                     | 0.41              |
| 66:D3:1586:A:C2    | 66:D3:1611:A:C5    | 3.08                     | 0.41              |
| 79:EN:329:TYR:N    | 79:EN:555:VAL:O    | 2.51                     | 0.41              |
| 4:UA:217:VAL:HB    | 4:UA:252:LYS:HB3   | 2.03                     | 0.41              |
| 4:UA:417:ILE:HD13  | 4:UA:417:ILE:HA    | 1.88                     | 0.41              |
| 4:UA:743:PHE:HZ    | 4:UA:778:ILE:HD13  | 1.85                     | 0.41              |
| 4:UA:753:LYS:HA    | 24:UU:710:TYR:CE2  | 2.56                     | 0.41              |
| 1:CB:103:GLU:N     | 1:CB:103:GLU:OE1   | 2.54                     | 0.41              |
| 7:UD:291:ASP:OD2   | 7:UD:293:ASN:ND2   | 2.52                     | 0.41              |
| 7:UD:581:SER:OG    | 7:UD:582:VAL:N     | 2.53                     | 0.41              |
| 8:UE:552:ASN:O     | 8:UE:556:THR:HG23  | 2.20                     | 0.41              |
| 9:UF:128:LYS:O     | 9:UF:132:ILE:HG22  | 2.20                     | 0.41              |
| 10:UG:160:LEU:HD13 | 10:UG:219:VAL:HG21 | 2.02                     | 0.41              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 10:UG:335:GLY:O     | 10:UG:378:VAL:HG12  | 2.20                     | 0.41              |
| 10:UG:401:LEU:HA    | 10:UG:401:LEU:HD23  | 1.66                     | 0.41              |
| 11:UH:567:LEU:HD12  | 11:UH:598:GLU:CG    | 2.51                     | 0.41              |
| 12:UI:420:ILE:O     | 12:UI:424:ILE:HG13  | 2.21                     | 0.41              |
| 13:UJ:1499:ILE:H    | 13:UJ:1499:ILE:HD12 | 1.85                     | 0.41              |
| 13:UJ:1573:LEU:HD13 | 13:UJ:1621:LEU:HD12 | 2.03                     | 0.41              |
| 13:UJ:1651:LEU:O    | 13:UJ:1655:LEU:HG   | 2.21                     | 0.41              |
| 13:UJ:1670:ILE:HA   | 13:UJ:1673:LEU:CD2  | 2.51                     | 0.41              |
| 13:UJ:1670:ILE:HA   | 13:UJ:1673:LEU:HD21 | 2.03                     | 0.41              |
| 13:UJ:1764:PHE:HE2  | 13:UJ:1768:LEU:HD13 | 1.86                     | 0.41              |
| 15:UL:25:TRP:HA     | 15:UL:41:LEU:HD12   | 2.03                     | 0.41              |
| 15:UL:367:ILE:HD11  | 15:UL:379:PRO:HB3   | 2.01                     | 0.41              |
| 15:UL:426:ARG:HG3   | 15:UL:428:PHE:CE2   | 2.55                     | 0.41              |
| 15:UL:502:PHE:HZ    | 15:UL:520:LEU:HD23  | 1.85                     | 0.41              |
| 16:UM:679:THR:HG21  | 16:UM:723:GLU:CG    | 2.51                     | 0.41              |
| 17:UN:306:ARG:O     | 17:UN:306:ARG:HG2   | 2.20                     | 0.41              |
| 18:UO:281:VAL:O     | 18:UO:295:GLY:HA2   | 2.21                     | 0.41              |
| 20:UQ:115:HIS:HD2   | 20:UQ:131:HIS:CE1   | 2.38                     | 0.41              |
| 20:UQ:141:LEU:HD23  | 20:UQ:142:ALA:N     | 2.35                     | 0.41              |
| 20:UQ:208:LEU:O     | 20:UQ:227:VAL:HA    | 2.21                     | 0.41              |
| 20:UQ:346:VAL:C     | 20:UQ:347:LEU:HD22  | 2.41                     | 0.41              |
| 20:UQ:424:GLN:O     | 20:UQ:428:LEU:HD23  | 2.19                     | 0.41              |
| 21:UR:216:TYR:OH    | 24:UU:246:ILE:HA    | 2.21                     | 0.41              |
| 21:UR:426:VAL:HG11  | 21:UR:455:ILE:HG21  | 2.01                     | 0.41              |
| 21:UR:449:ASP:OD1   | 21:UR:450:GLN:N     | 2.53                     | 0.41              |
| 21:UR:462:GLY:HA2   | 21:UR:527:GLY:HA3   | 2.02                     | 0.41              |
| 22:US:273:GLN:O     | 22:US:276:SER:N     | 2.54                     | 0.41              |
| 23:UT:27:LYS:HZ3    | 23:UT:29:GLU:HB2    | 1.84                     | 0.41              |
| 23:UT:269:GLU:O     | 23:UT:272:VAL:HG22  | 2.20                     | 0.41              |
| 23:UT:446:GLN:N     | 23:UT:449:ARG:HH21  | 2.18                     | 0.41              |
| 23:UT:465:PHE:CD1   | 23:UT:500:LEU:HD13  | 2.55                     | 0.41              |
| 23:UT:1074:ASP:OD1  | 23:UT:1074:ASP:N    | 2.54                     | 0.41              |
| 23:UT:1106:LEU:HD11 | 23:UT:1150:ILE:HG12 | 2.01                     | 0.41              |
| 23:UT:1405:GLY:O    | 23:UT:1408:ASP:HB2  | 2.20                     | 0.41              |
| 23:UT:1431:PHE:HB3  | 23:UT:1434:PHE:CD2  | 2.55                     | 0.41              |
| 23:UT:1602:ASP:OD2  | 23:UT:1609:ARG:HB2  | 2.21                     | 0.41              |
| 24:UU:85:ALA:HB2    | 24:UU:90:VAL:HG12   | 2.03                     | 0.41              |
| 24:UU:93:ALA:HB2    | 24:UU:121:LEU:HD12  | 2.02                     | 0.41              |
| 24:UU:120:HIS:HB2   | 24:UU:131:SER:OG    | 2.21                     | 0.41              |
| 24:UU:814:GLU:OE1   | 24:UU:814:GLU:N     | 2.54                     | 0.41              |
| 25:UV:141:TRP:HD1   | 25:UV:178:TYR:HD2   | 1.68                     | 0.41              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 25:UV:164:ASP:HA   | 25:UV:165:PRO:HA    | 1.91                     | 0.41              |
| 25:UV:442:PHE:CE1  | 25:UV:469:ASP:HB2   | 2.56                     | 0.41              |
| 25:UV:708:LEU:HD13 | 25:UV:721:VAL:HG21  | 2.02                     | 0.41              |
| 25:UV:1081:ASN:ND2 | 25:UV:1083:GLN:HE22 | 2.19                     | 0.41              |
| 28:CD:100:ILE:HG12 | 28:CD:102:ASP:H     | 1.85                     | 0.41              |
| 28:CD:194:ARG:NH1  | 29:CE:165:GLN:HE22  | 2.17                     | 0.41              |
| 32:CI:93:LYS:HG2   | 32:CI:95:SER:HG     | 1.85                     | 0.41              |
| 34:CK:491:ALA:N    | 34:CK:494:GLU:OE1   | 2.29                     | 0.41              |
| 35:CL:831:ARG:NH2  | 35:CL:838:ILE:HG22  | 2.35                     | 0.41              |
| 35:CL:966:ILE:HG22 | 35:CL:1003:LEU:HD12 | 2.02                     | 0.41              |
| 35:CL:991:PHE:CD1  | 35:CL:995:ILE:HG21  | 2.56                     | 0.41              |
| 36:CM:189:SER:HB2  | 36:CM:250:LYS:H     | 1.86                     | 0.41              |
| 38:JC:227:ARG:NH2  | 38:JC:227:ARG:HB3   | 2.36                     | 0.41              |
| 39:JF:125:ASN:OD1  | 39:JF:125:ASN:N     | 2.54                     | 0.41              |
| 39:JG:176:ARG:HA   | 39:JG:176:ARG:NE    | 2.36                     | 0.41              |
| 42:JJ:181:TYR:O    | 42:JJ:234:LEU:HA    | 2.20                     | 0.41              |
| 47:JP:229:GLN:HG3  | 47:JP:271:PRO:HB3   | 2.02                     | 0.41              |
| 47:JP:415:ARG:NH2  | 66:D3:4:C:N4        | 2.69                     | 0.41              |
| 49:DE:57:ASN:ND2   | 49:DE:59:ARG:HG2    | 2.35                     | 0.41              |
| 49:DE:163:ASP:OD1  | 49:DE:166:SER:N     | 2.53                     | 0.41              |
| 50:DF:42:LEU:HB2   | 50:DF:48:PHE:HE1    | 1.86                     | 0.41              |
| 50:DF:82:PHE:O     | 50:DF:85:ALA:N      | 2.54                     | 0.41              |
| 53:DI:174:GLY:HA3  | 66:D3:331:A:OP1     | 2.19                     | 0.41              |
| 58:DQ:52:LEU:HD13  | 58:DQ:60:PHE:CE2    | 2.56                     | 0.41              |
| 60:DW:37:PHE:CE2   | 60:DW:103:ILE:HD12  | 2.56                     | 0.41              |
| 60:DW:81:VAL:HG13  | 60:DW:85:ASP:HB2    | 2.02                     | 0.41              |
| 61:DX:98:GLU:N     | 61:DX:100:ASP:OD2   | 2.46                     | 0.41              |
| 65:D2:163:G:H21    | 65:D2:164:G:H1'     | 1.85                     | 0.41              |
| 66:D3:104:A:N6     | 66:D3:308:C:O4'     | 2.54                     | 0.41              |
| 66:D3:158:U:H2'    | 66:D3:160:C:C5'     | 2.48                     | 0.41              |
| 66:D3:765:G:N2     | 66:D3:771:A:N6      | 2.68                     | 0.41              |
| 66:D3:882:U:H2'    | 66:D3:883:C:C6      | 2.55                     | 0.41              |
| 66:D3:955:A:C6     | 66:D3:956:C:N3      | 2.88                     | 0.41              |
| 66:D3:1634:C:N4    | 66:D3:1635:A:C6     | 2.88                     | 0.41              |
| 66:D3:1784:C:H2'   | 66:D3:1785:U:H6     | 1.86                     | 0.41              |
| 67:D4:44:U:C2      | 67:D4:45:U:C4       | 3.09                     | 0.41              |
| 74:EG:70:GLN:O     | 74:EG:145:LYS:N     | 2.41                     | 0.41              |
| 2:DA:16:GLN:O      | 16:UM:358:ASN:ND2   | 2.39                     | 0.41              |
| 2:DA:208:GLN:HG3   | 2:DA:209:ASN:N      | 2.36                     | 0.41              |
| 3:JA:616:TRP:HE1   | 51:DG:22:HIS:CE1    | 2.39                     | 0.41              |
| 3:JA:796:PHE:CZ    | 3:JA:801:ALA:HB2    | 2.56                     | 0.41              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 4:UA:83:ASN:HB2    | 4:UA:90:LEU:HD11    | 2.03                     | 0.41              |
| 4:UA:653:LEU:HD13  | 4:UA:653:LEU:HA     | 1.81                     | 0.41              |
| 4:UA:653:LEU:O     | 4:UA:656:ARG:N      | 2.40                     | 0.41              |
| 4:UA:804:SER:HB2   | 16:UM:811:VAL:HG11  | 2.02                     | 0.41              |
| 1:CB:246:GLN:HB3   | 1:CB:248:ASP:OD1    | 2.20                     | 0.41              |
| 1:CB:311:ARG:NH2   | 1:CB:312:ASP:OD2    | 2.53                     | 0.41              |
| 5:UB:617:HIS:O     | 5:UB:621:THR:HG23   | 2.20                     | 0.41              |
| 7:UD:383:LEU:HD13  | 7:UD:433:LEU:HA     | 2.01                     | 0.41              |
| 9:UF:357:GLU:CD    | 9:UF:357:GLU:H      | 2.24                     | 0.41              |
| 10:UG:15:ARG:HD2   | 10:UG:61:ALA:HB3    | 2.03                     | 0.41              |
| 10:UG:88:GLN:O     | 10:UG:91:ILE:N      | 2.54                     | 0.41              |
| 10:UG:498:ARG:O    | 10:UG:502:ARG:HG2   | 2.20                     | 0.41              |
| 11:UH:676:TRP:NE1  | 12:UI:487:ARG:NH2   | 2.68                     | 0.41              |
| 12:UI:479:CYS:O    | 12:UI:482:LEU:HG    | 2.20                     | 0.41              |
| 12:UI:493:LEU:O    | 12:UI:496:LEU:HB3   | 2.21                     | 0.41              |
| 13:UJ:345:ASP:HB2  | 13:UJ:375:LEU:HD13  | 2.02                     | 0.41              |
| 13:UJ:571:LEU:HD22 | 13:UJ:630:TYR:OH    | 2.20                     | 0.41              |
| 13:UJ:1375:PRO:HB2 | 13:UJ:1379:LYS:NZ   | 2.36                     | 0.41              |
| 13:UJ:1456:VAL:O   | 13:UJ:1459:ARG:HG2  | 2.20                     | 0.41              |
| 13:UJ:1476:LEU:O   | 13:UJ:1480:THR:HG23 | 2.20                     | 0.41              |
| 13:UJ:1519:ASN:OD1 | 13:UJ:1520:THR:N    | 2.51                     | 0.41              |
| 13:UJ:1568:GLU:O   | 13:UJ:1572:LEU:HD23 | 2.21                     | 0.41              |
| 13:UJ:1726:LEU:N   | 13:UJ:1727:PRO:HD2  | 2.36                     | 0.41              |
| 14:UK:231:LYS:O    | 14:UK:242:PHE:HA    | 2.20                     | 0.41              |
| 15:UL:139:GLY:HA2  | 15:UL:145:ILE:HG22  | 2.03                     | 0.41              |
| 15:UL:334:SER:OG   | 15:UL:335:LEU:N     | 2.53                     | 0.41              |
| 15:UL:754:GLU:HG2  | 15:UL:755:ALA:N     | 2.34                     | 0.41              |
| 15:UL:760:ILE:O    | 15:UL:761:ALA:C     | 2.59                     | 0.41              |
| 16:UM:341:ALA:HA   | 16:UM:621:TRP:CD1   | 2.56                     | 0.41              |
| 18:UO:437:SER:O    | 18:UO:440:GLU:HG2   | 2.21                     | 0.41              |
| 18:UO:453:VAL:HG23 | 18:UO:454:ARG:N     | 2.22                     | 0.41              |
| 20:UQ:483:LYS:HA   | 20:UQ:487:GLU:OE2   | 2.21                     | 0.41              |
| 20:UQ:633:LEU:HA   | 20:UQ:639:LYS:O     | 2.21                     | 0.41              |
| 23:UT:95:ILE:HD11  | 23:UT:107:LEU:HD22  | 2.01                     | 0.41              |
| 23:UT:118:GLY:O    | 23:UT:120:ASP:N     | 2.54                     | 0.41              |
| 23:UT:687:ASN:OD1  | 23:UT:688:VAL:HG13  | 2.21                     | 0.41              |
| 23:UT:990:THR:O    | 23:UT:994:ILE:HG23  | 2.20                     | 0.41              |
| 24:UU:542:LEU:HD13 | 24:UU:542:LEU:HA    | 1.97                     | 0.41              |
| 25:UV:303:PHE:HB3  | 25:UV:307:LYS:NZ    | 2.35                     | 0.41              |
| 25:UV:492:ALA:O    | 25:UV:496:LEU:HD23  | 2.21                     | 0.41              |
| 25:UV:1220:PHE:HB3 | 25:UV:1234:PHE:CE2  | 2.56                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:UZ:243:PHE:HD1  | 27:UZ:253:PRO:HA   | 1.86                     | 0.41              |
| 28:CD:300:ALA:HA   | 28:CD:390:ASP:OD1  | 2.21                     | 0.41              |
| 30:CF:62:GLU:O     | 30:CF:65:LEU:N     | 2.54                     | 0.41              |
| 31:CH:140:LEU:HD12 | 31:CH:568:ILE:HG22 | 2.03                     | 0.41              |
| 31:CH:304:ILE:HG21 | 31:CH:338:THR:HG21 | 2.03                     | 0.41              |
| 31:CH:308:SER:HB2  | 31:CH:315:LEU:HD11 | 2.03                     | 0.41              |
| 31:CH:330:ALA:C    | 31:CH:331:LEU:HD12 | 2.42                     | 0.41              |
| 31:CH:443:LEU:HD23 | 31:CH:471:GLN:HE21 | 1.85                     | 0.41              |
| 33:CJ:192:ASP:OD1  | 33:CJ:193:ASN:N    | 2.54                     | 0.41              |
| 34:CK:442:ALA:HA   | 34:CK:445:VAL:HG12 | 2.02                     | 0.41              |
| 35:CL:107:VAL:HG12 | 35:CL:108:VAL:N    | 2.36                     | 0.41              |
| 35:CL:772:MET:O    | 35:CL:776:GLN:HB3  | 2.20                     | 0.41              |
| 36:CM:91:PRO:HD2   | 36:CM:99:PHE:CE2   | 2.54                     | 0.41              |
| 37:CN:224:ASN:OD1  | 37:CN:227:ARG:NH2  | 2.54                     | 0.41              |
| 38:JC:286:GLU:OE1  | 38:JC:302:ARG:NH1  | 2.54                     | 0.41              |
| 39:JG:151:ARG:HH21 | 66:D3:1572:G:H21   | 1.67                     | 0.41              |
| 44:JM:177:LEU:HD12 | 44:JM:177:LEU:HA   | 1.91                     | 0.41              |
| 45:JN:264:LEU:HD22 | 45:JN:273:ARG:NH2  | 2.36                     | 0.41              |
| 50:DF:68:ILE:HD12  | 50:DF:68:ILE:HA    | 1.89                     | 0.41              |
| 50:DF:186:ASN:ND2  | 50:DF:188:LYS:HB2  | 2.36                     | 0.41              |
| 51:DG:65:GLN:OE1   | 51:DG:65:GLN:N     | 2.54                     | 0.41              |
| 51:DG:93:LYS:HD2   | 66:D3:405:C:H5''   | 2.02                     | 0.41              |
| 51:DG:102:VAL:HG23 | 51:DG:106:LEU:HD13 | 2.02                     | 0.41              |
| 51:DG:132:ARG:HD2  | 51:DG:132:ARG:HA   | 1.90                     | 0.41              |
| 52:DH:140:VAL:CG1  | 60:DW:52:TYR:HB3   | 2.51                     | 0.41              |
| 56:DN:110:ASP:O    | 56:DN:114:ARG:HG2  | 2.19                     | 0.41              |
| 57:DO:92:LYS:NZ    | 57:DO:121:VAL:HG23 | 2.35                     | 0.41              |
| 65:D2:243:A:C4     | 65:D2:271:G:N1     | 2.88                     | 0.41              |
| 65:D2:341:G:C6     | 65:D2:342:C:C4     | 3.09                     | 0.41              |
| 66:D3:121:U:C4     | 66:D3:122:U:C4     | 3.08                     | 0.41              |
| 66:D3:379:U:H2'    | 66:D3:380:U:C6     | 2.56                     | 0.41              |
| 66:D3:386:G:C2     | 66:D3:387:A:C2     | 3.09                     | 0.41              |
| 66:D3:912:U:H4'    | 66:D3:913:G:O5'    | 2.21                     | 0.41              |
| 66:D3:1503:A:H8    | 66:D3:1503:A:OP1   | 2.03                     | 0.41              |
| 66:D3:1528:U:H6    | 66:D3:1528:U:O5'   | 2.04                     | 0.41              |
| 66:D3:1638:G:O2'   | 66:D3:1639:C:O5'   | 2.20                     | 0.41              |
| 66:D3:1645:G:H2'   | 66:D3:1646:C:C6    | 2.56                     | 0.41              |
| 66:D3:1658:G:H2'   | 66:D3:1659:A:H8    | 1.86                     | 0.41              |
| 66:D3:1661:U:H2'   | 66:D3:1662:G:C8    | 2.55                     | 0.41              |
| 66:D3:1785:U:H2'   | 66:D3:1786:G:O4'   | 2.21                     | 0.41              |
| 73:EF:65:LYS:O     | 73:EF:123:LYS:N    | 2.52                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 78:EK:567:GLY:HA2  | 78:EK:627:ILE:HA   | 2.02                     | 0.41              |
| 1:CA:172:TYR:CE2   | 1:CA:241:PHE:CD2   | 3.09                     | 0.41              |
| 1:CA:236:MET:HG3   | 28:CD:133:LEU:CD1  | 2.51                     | 0.41              |
| 3:JA:36:GLN:HG3    | 3:JA:205:LEU:HD21  | 2.03                     | 0.41              |
| 3:JA:45:MET:HG2    | 3:JA:53:LYS:CE     | 2.51                     | 0.41              |
| 3:JA:97:PHE:CE1    | 3:JA:101:GLN:HG3   | 2.56                     | 0.41              |
| 3:JA:159:LYS:HA    | 3:JA:159:LYS:HD2   | 1.85                     | 0.41              |
| 4:UA:155:SER:OG    | 4:UA:156:GLN:N     | 2.53                     | 0.41              |
| 4:UA:380:LEU:HD23  | 4:UA:380:LEU:C     | 2.41                     | 0.41              |
| 4:UA:458:TRP:CD1   | 4:UA:465:LEU:HB3   | 2.56                     | 0.41              |
| 4:UA:477:SER:HB2   | 4:UA:493:TRP:NE1   | 2.36                     | 0.41              |
| 4:UA:491:ALA:HB1   | 4:UA:518:VAL:CG2   | 2.48                     | 0.41              |
| 1:CB:142:ARG:NH2   | 1:CB:183:HIS:CE1   | 2.89                     | 0.41              |
| 1:CB:272:LYS:HD3   | 1:CB:275:CYS:HB2   | 2.01                     | 0.41              |
| 3:JB:790:SER:CB    | 3:JB:891:GLN:HA    | 2.50                     | 0.41              |
| 5:UB:511:SER:OG    | 5:UB:556:ILE:O     | 2.24                     | 0.41              |
| 6:UC:502:LYS:O     | 6:UC:505:LYS:HG2   | 2.21                     | 0.41              |
| 6:UC:538:ARG:HB3   | 35:CL:150:MET:CE   | 2.50                     | 0.41              |
| 6:UC:596:THR:CG2   | 44:JM:137:LYS:HG3  | 2.50                     | 0.41              |
| 7:UD:55:SER:HB3    | 7:UD:290:THR:HG22  | 2.03                     | 0.41              |
| 7:UD:82:ARG:NH2    | 7:UD:685:SER:O     | 2.49                     | 0.41              |
| 7:UD:100:GLU:OE2   | 7:UD:119:GLY:HA2   | 2.21                     | 0.41              |
| 7:UD:163:GLY:HA3   | 7:UD:186:GLN:O     | 2.20                     | 0.41              |
| 7:UD:197:LYS:C     | 7:UD:199:ASP:H     | 2.24                     | 0.41              |
| 7:UD:438:GLN:HB2   | 7:UD:453:LEU:O     | 2.21                     | 0.41              |
| 7:UD:569:PHE:HB2   | 7:UD:687:PHE:CZ    | 2.55                     | 0.41              |
| 7:UD:768:ALA:HA    | 19:UP:213:LYS:HZ2  | 1.86                     | 0.41              |
| 8:UE:11:ASP:HB3    | 8:UE:65:TRP:CZ3    | 2.56                     | 0.41              |
| 8:UE:238:SER:OG    | 8:UE:243:SER:N     | 2.51                     | 0.41              |
| 10:UG:40:LYS:HE2   | 66:D3:-5:G:N7      | 2.36                     | 0.41              |
| 10:UG:218:ASP:OD1  | 10:UG:220:SER:N    | 2.34                     | 0.41              |
| 10:UG:394:HIS:NE2  | 10:UG:399:THR:OG1  | 2.42                     | 0.41              |
| 10:UG:431:ARG:NH1  | 67:D4:37:G:C4      | 2.89                     | 0.41              |
| 10:UG:485:ASP:HA   | 10:UG:519:GLN:HE22 | 1.86                     | 0.41              |
| 10:UG:553:PHE:HZ   | 25:UV:792:TRP:CE3  | 2.39                     | 0.41              |
| 11:UH:551:PHE:HZ   | 11:UH:569:GLU:HG2  | 1.86                     | 0.41              |
| 12:UI:483:LYS:HG2  | 12:UI:487:ARG:NH2  | 2.36                     | 0.41              |
| 12:UI:499:ILE:HD13 | 12:UI:502:ARG:HD2  | 2.02                     | 0.41              |
| 13:UJ:160:LEU:HD21 | 24:UU:328:LEU:HG   | 2.03                     | 0.41              |
| 13:UJ:238:LEU:O    | 13:UJ:241:ILE:HG22 | 2.20                     | 0.41              |
| 13:UJ:362:LYS:O    | 13:UJ:366:ILE:HG13 | 2.21                     | 0.41              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 14:UK:134:THR:HA    | 19:UP:177:ARG:O     | 2.21                     | 0.41              |
| 14:UK:156:SER:OG    | 14:UK:157:GLU:N     | 2.54                     | 0.41              |
| 15:UL:52:TRP:HA     | 15:UL:60:VAL:HG22   | 2.03                     | 0.41              |
| 15:UL:68:PRO:HG2    | 15:UL:71:ALA:HB2    | 2.03                     | 0.41              |
| 15:UL:88:HIS:NE2    | 15:UL:90:ASP:HB2    | 2.36                     | 0.41              |
| 15:UL:632:SER:OG    | 15:UL:640:LYS:HB2   | 2.21                     | 0.41              |
| 15:UL:826:PHE:O     | 15:UL:829:VAL:HB    | 2.21                     | 0.41              |
| 15:UL:888:ARG:HH11  | 15:UL:888:ARG:HD2   | 1.74                     | 0.41              |
| 16:UM:25:VAL:HG23   | 16:UM:31:ILE:O      | 2.21                     | 0.41              |
| 16:UM:268:GLN:HE22  | 16:UM:280:ARG:NE    | 2.19                     | 0.41              |
| 16:UM:540:SER:OG    | 16:UM:549:ALA:HB3   | 2.20                     | 0.41              |
| 16:UM:555:LYS:HE3   | 16:UM:572:GLU:OE2   | 2.21                     | 0.41              |
| 16:UM:593:CYS:HB3   | 16:UM:620:LEU:CB    | 2.51                     | 0.41              |
| 16:UM:610:LEU:HD23  | 16:UM:611:LYS:HG3   | 2.03                     | 0.41              |
| 18:UO:2:SER:HA      | 20:UQ:336:ARG:O     | 2.21                     | 0.41              |
| 19:UP:170:SER:HA    | 19:UP:178:VAL:O     | 2.21                     | 0.41              |
| 20:UQ:179:ASP:HA    | 20:UQ:181:ALA:O     | 2.21                     | 0.41              |
| 20:UQ:408:THR:HG23  | 20:UQ:410:ASN:N     | 2.27                     | 0.41              |
| 20:UQ:558:THR:OG1   | 20:UQ:576:ALA:O     | 2.29                     | 0.41              |
| 21:UR:15:PRO:CB     | 21:UR:20:GLN:HE21   | 2.31                     | 0.41              |
| 21:UR:421:THR:OG1   | 21:UR:437:LEU:HB2   | 2.20                     | 0.41              |
| 22:US:149:ARG:NE    | 22:US:198:GLU:OE1   | 2.54                     | 0.41              |
| 22:US:186:THR:O     | 22:US:186:THR:HG22  | 2.21                     | 0.41              |
| 23:UT:27:LYS:HZ1    | 23:UT:32:ARG:HB2    | 1.86                     | 0.41              |
| 23:UT:42:VAL:HG21   | 62:DY:49:LYS:NZ     | 2.36                     | 0.41              |
| 23:UT:94:PHE:O      | 23:UT:97:PHE:HB2    | 2.21                     | 0.41              |
| 23:UT:337:THR:HA    | 23:UT:340:ILE:HG22  | 2.03                     | 0.41              |
| 23:UT:572:LYS:HE2   | 23:UT:572:LYS:HB3   | 1.89                     | 0.41              |
| 23:UT:649:PHE:CE1   | 23:UT:659:SER:HA    | 2.56                     | 0.41              |
| 23:UT:667:PHE:HB3   | 23:UT:703:PHE:CZ    | 2.56                     | 0.41              |
| 23:UT:795:ASP:O     | 23:UT:798:PRO:HD2   | 2.21                     | 0.41              |
| 23:UT:900:GLU:OE1   | 23:UT:904:PHE:HE1   | 2.04                     | 0.41              |
| 23:UT:914:LYS:HA    | 23:UT:914:LYS:HD3   | 1.67                     | 0.41              |
| 23:UT:943:ARG:HH22  | 66:D3:258:C:H41     | 1.69                     | 0.41              |
| 23:UT:999:GLY:O     | 23:UT:1003:ILE:HG12 | 2.21                     | 0.41              |
| 23:UT:1015:PHE:CZ   | 23:UT:1065:VAL:HG23 | 2.55                     | 0.41              |
| 23:UT:1023:LEU:O    | 23:UT:1027:ILE:HG12 | 2.21                     | 0.41              |
| 23:UT:1415:SER:HA   | 23:UT:1418:VAL:HG12 | 2.03                     | 0.41              |
| 23:UT:1476:LEU:O    | 23:UT:1477:LYS:HB3  | 2.21                     | 0.41              |
| 23:UT:1482:SER:HA   | 23:UT:1486:ILE:HG23 | 2.02                     | 0.41              |
| 23:UT:1725:ILE:HG12 | 23:UT:1792:LEU:HD21 | 2.02                     | 0.41              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 24:UU:24:PHE:CZ     | 24:UU:641:LEU:HD22 | 2.56                     | 0.41              |
| 24:UU:491:SER:OG    | 24:UU:493:ILE:HG13 | 2.20                     | 0.41              |
| 24:UU:581:LEU:HD23  | 24:UU:612:TRP:CE3  | 2.56                     | 0.41              |
| 25:UV:365:LEU:HD12  | 25:UV:368:LEU:HD11 | 2.03                     | 0.41              |
| 25:UV:378:ASN:O     | 25:UV:387:GLY:HA2  | 2.21                     | 0.41              |
| 25:UV:626:LYS:HG3   | 25:UV:628:VAL:O    | 2.21                     | 0.41              |
| 25:UV:918:ARG:O     | 25:UV:922:THR:HG23 | 2.21                     | 0.41              |
| 25:UV:947:PRO:HD2   | 25:UV:948:TYR:CE2  | 2.56                     | 0.41              |
| 25:UV:960:LYS:HA    | 25:UV:963:LYS:NZ   | 2.35                     | 0.41              |
| 25:UV:966:SER:O     | 25:UV:1069:LYS:HE3 | 2.20                     | 0.41              |
| 25:UV:1201:ASP:CG   | 37:CN:121:ARG:HE   | 2.24                     | 0.41              |
| 26:UX:65:VAL:HA     | 26:UX:152:ILE:O    | 2.20                     | 0.41              |
| 26:UX:85:GLY:O      | 26:UX:88:ASP:OD1   | 2.39                     | 0.41              |
| 28:CD:281:LEU:HD12  | 28:CD:281:LEU:HA   | 1.81                     | 0.41              |
| 28:CD:296:MET:HG3   | 28:CD:304:SER:HB2  | 2.03                     | 0.41              |
| 28:CD:385:MET:SD    | 30:CG:63:ILE:HD12  | 2.60                     | 0.41              |
| 29:CE:128:LEU:HG    | 29:CE:132:SER:HG   | 1.86                     | 0.41              |
| 29:CE:192:PHE:HE1   | 29:CE:239:ALA:HA   | 1.86                     | 0.41              |
| 30:CF:58:CYS:SG     | 30:CF:61:ILE:HA    | 2.61                     | 0.41              |
| 31:CH:79:ASN:O      | 31:CH:82:LEU:HG    | 2.21                     | 0.41              |
| 31:CH:144:GLU:OE1   | 31:CH:144:GLU:N    | 2.52                     | 0.41              |
| 31:CH:364:GLU:OE1   | 31:CH:364:GLU:N    | 2.54                     | 0.41              |
| 33:CJ:56:PHE:CG     | 33:CJ:56:PHE:O     | 2.72                     | 0.41              |
| 33:CJ:120:GLY:O     | 66:D3:1585:U:OP1   | 2.39                     | 0.41              |
| 33:CJ:172:MET:HE3   | 33:CJ:172:MET:HB3  | 1.82                     | 0.41              |
| 34:CK:457:VAL:HA    | 34:CK:458:PRO:HD3  | 1.87                     | 0.41              |
| 34:CK:501:ALA:HB2   | 34:CK:508:ARG:HB2  | 2.03                     | 0.41              |
| 34:CK:505:GLY:O     | 34:CK:517:LYS:HG2  | 2.21                     | 0.41              |
| 34:CK:516:SER:O     | 34:CK:519:GLU:HG3  | 2.21                     | 0.41              |
| 35:CL:54:LEU:HD12   | 61:DX:77:ILE:CG2   | 2.50                     | 0.41              |
| 35:CL:69:PRO:CD     | 35:CL:274:TYR:HD2  | 2.33                     | 0.41              |
| 35:CL:71:ILE:HD11   | 35:CL:276:HIS:CD2  | 2.56                     | 0.41              |
| 35:CL:216:PRO:HB2   | 35:CL:219:GLU:HG3  | 2.01                     | 0.41              |
| 35:CL:631:ILE:HD12  | 35:CL:631:ILE:HA   | 1.91                     | 0.41              |
| 35:CL:802:LYS:NZ    | 35:CL:803:ASN:OD1  | 2.40                     | 0.41              |
| 35:CL:1071:LYS:HD3  | 35:CL:1071:LYS:HA  | 1.77                     | 0.41              |
| 35:CL:1117:LEU:HD23 | 35:CL:1117:LEU:HA  | 1.81                     | 0.41              |
| 35:CL:1142:LEU:CD2  | 66:D3:493:U:H5"    | 2.45                     | 0.41              |
| 36:CM:18:ARG:HD3    | 36:CM:98:TYR:HE1   | 1.84                     | 0.41              |
| 36:CM:343:ASP:OD1   | 36:CM:344:GLU:N    | 2.53                     | 0.41              |
| 38:JC:169:LYS:O     | 38:JC:171:ARG:NH1  | 2.54                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:JC:207:TRP:HE1  | 38:JC:214:ARG:NH1  | 2.19                     | 0.41              |
| 38:JC:223:ASN:OD1  | 38:JC:226:ASN:N    | 2.53                     | 0.41              |
| 38:JC:227:ARG:NH1  | 38:JC:248:SER:HG   | 2.16                     | 0.41              |
| 38:JC:252:SER:OG   | 38:JC:266:LYS:HG3  | 2.21                     | 0.41              |
| 39:JF:45:LEU:HB2   | 39:JF:114:ILE:HG13 | 2.02                     | 0.41              |
| 39:JF:99:LEU:HD23  | 39:JF:99:LEU:HA    | 1.87                     | 0.41              |
| 39:JF:219:GLU:HG2  | 39:JF:220:TYR:N    | 2.36                     | 0.41              |
| 42:JJ:269:ARG:N    | 42:JJ:269:ARG:HD2  | 2.36                     | 0.41              |
| 43:JK:489:GLN:OE1  | 43:JK:489:GLN:N    | 2.54                     | 0.41              |
| 45:JN:165:LEU:HD13 | 45:JN:165:LEU:HA   | 1.91                     | 0.41              |
| 47:JP:26:ARG:HH21  | 47:JP:26:ARG:HG2   | 1.86                     | 0.41              |
| 47:JP:133:GLN:OE1  | 47:JP:151:ASN:HA   | 2.20                     | 0.41              |
| 47:JP:221:ASN:OD1  | 47:JP:221:ASN:N    | 2.45                     | 0.41              |
| 49:DE:139:VAL:CG1  | 49:DE:147:ILE:HB   | 2.51                     | 0.41              |
| 50:DF:25:LEU:HD11  | 58:DQ:57:LEU:HD12  | 2.02                     | 0.41              |
| 50:DF:65:ARG:HD2   | 50:DF:65:ARG:N     | 2.36                     | 0.41              |
| 50:DF:68:ILE:HD11  | 50:DF:73:THR:OG1   | 2.21                     | 0.41              |
| 50:DF:114:ILE:O    | 50:DF:117:THR:OG1  | 2.31                     | 0.41              |
| 50:DF:165:LEU:CD1  | 50:DF:169:ASN:HD21 | 2.34                     | 0.41              |
| 51:DG:25:ARG:HA    | 51:DG:28:PHE:CD2   | 2.56                     | 0.41              |
| 51:DG:121:LEU:HD23 | 51:DG:121:LEU:HA   | 1.84                     | 0.41              |
| 53:DI:77:ARG:O     | 53:DI:104:ILE:HG23 | 2.20                     | 0.41              |
| 54:DJ:49:LEU:HA    | 54:DJ:49:LEU:HD12  | 1.61                     | 0.41              |
| 54:DJ:64:GLU:HG2   | 54:DJ:65:LYS:N     | 2.35                     | 0.41              |
| 55:DL:57:LYS:CE    | 66:D3:326:G:H5''   | 2.50                     | 0.41              |
| 55:DL:63:LEU:HD11  | 66:D3:249:U:H3     | 1.86                     | 0.41              |
| 58:DQ:12:LYS:HA    | 58:DQ:12:LYS:HD3   | 1.85                     | 0.41              |
| 65:D2:219:U:H2'    | 65:D2:220:U:H6     | 1.86                     | 0.41              |
| 65:D2:246:G:N3     | 65:D2:268:G:C2     | 2.89                     | 0.41              |
| 65:D2:264:C:H2'    | 65:D2:265:A:C8     | 2.56                     | 0.41              |
| 65:D2:450:G:H5''   | 65:D2:451:G:OP2    | 2.20                     | 0.41              |
| 66:D3:7:G:C4       | 67:D4:28:A:N7      | 2.88                     | 0.41              |
| 66:D3:345:U:O3'    | 66:D3:346:G:H8     | 2.04                     | 0.41              |
| 66:D3:497:G:C4     | 66:D3:498:G:C8     | 3.09                     | 0.41              |
| 66:D3:782:U:H5''   | 66:D3:783:G:N7     | 2.36                     | 0.41              |
| 66:D3:784:C:H3'    | 66:D3:785:U:H6     | 1.85                     | 0.41              |
| 66:D3:1268:G:C2    | 66:D3:1270:G:C4    | 3.09                     | 0.41              |
| 66:D3:1268:G:O2'   | 66:D3:1270:G:O4'   | 2.39                     | 0.41              |
| 66:D3:1690:G:H2'   | 66:D3:1691:A:H8    | 1.86                     | 0.41              |
| 67:D4:98:U:H2'     | 67:D4:99:U:H6      | 1.86                     | 0.41              |
| 67:D4:159:C:H2'    | 67:D4:160:G:C8     | 2.56                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:EN:792:LYS:O    | 79:EN:796:GLU:N    | 2.49                     | 0.41              |
| 1:CA:246:GLN:N     | 1:CA:246:GLN:OE1   | 2.54                     | 0.41              |
| 3:JA:94:PHE:O      | 3:JA:97:PHE:HB3    | 2.20                     | 0.41              |
| 4:UA:11:LEU:HD11   | 4:UA:373:ASP:O     | 2.20                     | 0.41              |
| 4:UA:308:VAL:HG13  | 4:UA:319:PHE:HE1   | 1.85                     | 0.41              |
| 4:UA:454:ASP:N     | 4:UA:454:ASP:OD1   | 2.52                     | 0.41              |
| 4:UA:521:LEU:HA    | 4:UA:521:LEU:HD12  | 1.61                     | 0.41              |
| 1:CB:144:TRP:NE1   | 1:CB:183:HIS:HB3   | 2.36                     | 0.41              |
| 5:UB:440:ASN:OD1   | 5:UB:441:TYR:N     | 2.46                     | 0.41              |
| 7:UD:157:SER:HB3   | 7:UD:195:TRP:CZ2   | 2.54                     | 0.41              |
| 7:UD:230:LYS:NZ    | 65:D2:166:U:OP1    | 2.43                     | 0.41              |
| 7:UD:288:THR:HG22  | 7:UD:295:VAL:HG23  | 2.03                     | 0.41              |
| 10:UG:178:ASP:OD1  | 10:UG:179:HIS:ND1  | 2.49                     | 0.41              |
| 10:UG:292:THR:OG1  | 10:UG:319:GLY:O    | 2.27                     | 0.41              |
| 11:UH:636:GLN:O    | 11:UH:640:LEU:HG   | 2.21                     | 0.41              |
| 12:UI:436:THR:HA   | 12:UI:439:LYS:HG2  | 2.02                     | 0.41              |
| 13:UJ:384:ILE:HG12 | 13:UJ:407:PHE:CE2  | 2.56                     | 0.41              |
| 13:UJ:588:LEU:HA   | 13:UJ:591:LYS:HG2  | 2.03                     | 0.41              |
| 16:UM:65:THR:OG1   | 16:UM:79:VAL:HG13  | 2.21                     | 0.41              |
| 16:UM:136:ILE:O    | 66:D3:1777:G:O2'   | 2.39                     | 0.41              |
| 16:UM:748:THR:HG21 | 34:CK:498:VAL:HG23 | 2.03                     | 0.41              |
| 20:UQ:312:LEU:HB3  | 20:UQ:324:TRP:HB2  | 2.03                     | 0.41              |
| 20:UQ:336:ARG:C    | 20:UQ:337:LEU:HD22 | 2.42                     | 0.41              |
| 20:UQ:703:LYS:HE3  | 20:UQ:706:HIS:HE2  | 1.85                     | 0.41              |
| 21:UR:406:ASP:CG   | 21:UR:407:PHE:H    | 2.24                     | 0.41              |
| 21:UR:557:THR:OG1  | 21:UR:558:SER:N    | 2.52                     | 0.41              |
| 23:UT:195:ALA:O    | 23:UT:198:PHE:HB3  | 2.21                     | 0.41              |
| 23:UT:295:TYR:HA   | 23:UT:298:MET:CE   | 2.51                     | 0.41              |
| 23:UT:486:PHE:O    | 23:UT:525:ILE:HG23 | 2.21                     | 0.41              |
| 23:UT:523:LEU:HB3  | 23:UT:557:GLY:HA3  | 2.02                     | 0.41              |
| 23:UT:796:ILE:H    | 23:UT:796:ILE:HD12 | 1.86                     | 0.41              |
| 23:UT:797:ALA:HB1  | 23:UT:801:TYR:CZ   | 2.56                     | 0.41              |
| 23:UT:1334:ASP:HA  | 23:UT:1335:GLY:HA3 | 1.65                     | 0.41              |
| 23:UT:1381:LYS:NZ  | 23:UT:1390:SER:HB2 | 2.36                     | 0.41              |
| 23:UT:1668:GLU:HG2 | 23:UT:1669:TYR:CD1 | 2.56                     | 0.41              |
| 24:UU:66:LEU:HD23  | 24:UU:66:LEU:HA    | 1.67                     | 0.41              |
| 24:UU:142:LYS:HA   | 24:UU:150:PRO:HA   | 2.03                     | 0.41              |
| 24:UU:343:LEU:HG   | 24:UU:344:ARG:HG3  | 2.02                     | 0.41              |
| 25:UV:439:HIS:HE1  | 25:UV:460:GLU:HB2  | 1.82                     | 0.41              |
| 25:UV:547:PHE:HD1  | 25:UV:551:GLU:HB3  | 1.86                     | 0.41              |
| 25:UV:738:TYR:CE1  | 25:UV:753:ILE:HD13 | 2.56                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:UV:945:PRO:O    | 25:UV:948:TYR:N    | 2.54                     | 0.41              |
| 27:UZ:88:THR:O     | 27:UZ:94:SER:HB3   | 2.21                     | 0.41              |
| 28:CD:196:LYS:HG3  | 28:CD:216:PHE:CE1  | 2.56                     | 0.41              |
| 29:CE:201:ASP:CG   | 29:CE:204:ALA:H    | 2.25                     | 0.41              |
| 31:CH:257:ASP:C    | 31:CH:258:ARG:HG2  | 2.40                     | 0.41              |
| 31:CH:417:SER:OG   | 31:CH:421:ASN:N    | 2.54                     | 0.41              |
| 31:CH:440:HIS:CE1  | 31:CH:491:SER:HG   | 2.35                     | 0.41              |
| 32:CI:5:LEU:HD12   | 32:CI:5:LEU:O      | 2.20                     | 0.41              |
| 33:CJ:28:LYS:HG2   | 33:CJ:46:LEU:HD21  | 2.03                     | 0.41              |
| 33:CJ:268:ASN:C    | 33:CJ:270:ASP:H    | 2.23                     | 0.41              |
| 35:CL:231:LYS:HE3  | 35:CL:231:LYS:HB2  | 1.93                     | 0.41              |
| 35:CL:634:ARG:HE   | 35:CL:634:ARG:HB3  | 1.76                     | 0.41              |
| 35:CL:823:GLY:O    | 35:CL:886:TYR:HD1  | 2.03                     | 0.41              |
| 35:CL:833:ARG:HD3  | 61:DX:141:GLU:OE2  | 2.21                     | 0.41              |
| 35:CL:921:GLU:OE2  | 36:CM:365:LYS:HD2  | 2.21                     | 0.41              |
| 38:JC:160:ASN:HD21 | 38:JC:179:ASP:HA   | 1.85                     | 0.41              |
| 38:JC:277:ILE:HA   | 38:JC:289:ILE:O    | 2.21                     | 0.41              |
| 39:JG:105:ASN:HB2  | 39:JG:110:LEU:HD21 | 2.03                     | 0.41              |
| 45:JN:217:ARG:HB3  | 45:JN:217:ARG:NH1  | 2.36                     | 0.41              |
| 47:JP:365:SER:O    | 47:JP:365:SER:OG   | 2.39                     | 0.41              |
| 52:DH:102:PRO:HG2  | 66:D3:810:G:N2     | 2.36                     | 0.41              |
| 54:DJ:118:LEU:HA   | 54:DJ:118:LEU:HD23 | 1.81                     | 0.41              |
| 58:DQ:91:ALA:O     | 58:DQ:94:GLN:HG3   | 2.20                     | 0.41              |
| 60:DW:4:SER:O      | 66:D3:634:G:H4'    | 2.21                     | 0.41              |
| 60:DW:107:SER:HA   | 66:D3:804:A:C5     | 2.56                     | 0.41              |
| 65:D2:97:G:C2      | 65:D2:148:G:N3     | 2.89                     | 0.41              |
| 65:D2:134:A:H2'    | 65:D2:135:G:O4'    | 2.21                     | 0.41              |
| 65:D2:375:C:N4     | 65:D2:376:U:H3     | 2.19                     | 0.41              |
| 65:D2:436:G:C4     | 65:D2:437:G:C8     | 3.09                     | 0.41              |
| 66:D3:32:U:N3      | 66:D3:595:G:C6     | 2.89                     | 0.41              |
| 66:D3:457:G:C4     | 66:D3:458:G:C8     | 3.09                     | 0.41              |
| 66:D3:883:C:H1'    | 66:D3:946:U:O2     | 2.21                     | 0.41              |
| 66:D3:1120:U:C4    | 66:D3:1121:C:C4    | 3.08                     | 0.41              |
| 66:D3:1149:G:C6    | 66:D3:1642:G:C6    | 3.09                     | 0.41              |
| 66:D3:1504:G:C6    | 66:D3:1505:A:C6    | 3.09                     | 0.41              |
| 66:D3:1641:C:H2'   | 66:D3:1642:G:C8    | 2.56                     | 0.41              |
| 67:D4:43:C:H2'     | 67:D4:44:U:C6      | 2.52                     | 0.41              |
| 67:D4:65:C:C4      | 67:D4:66:U:C4      | 3.09                     | 0.41              |
| 1:CA:98:ILE:H      | 1:CA:98:ILE:HD12   | 1.86                     | 0.40              |
| 3:JA:707:PRO:HB2   | 3:JA:709:LEU:HD23  | 2.03                     | 0.40              |
| 4:UA:41:ASP:OD1    | 4:UA:44:ASN:HB2    | 2.20                     | 0.40              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 4:UA:576:ARG:HB3    | 32:CI:142:LEU:CD2   | 2.48                     | 0.40              |
| 1:CB:121:LYS:HG2    | 1:CB:143:VAL:HG11   | 2.03                     | 0.40              |
| 1:CB:211:ALA:HB1    | 29:CE:145:HIS:NE2   | 2.35                     | 0.40              |
| 1:CB:241:PHE:HD1    | 1:CB:268:VAL:CG1    | 2.33                     | 0.40              |
| 5:UB:520:PRO:HG3    | 22:US:510:GLU:CG    | 2.51                     | 0.40              |
| 6:UC:558:ASN:ND2    | 66:D3:546:U:O4      | 2.53                     | 0.40              |
| 7:UD:347:LEU:HD23   | 7:UD:359:ASN:O      | 2.21                     | 0.40              |
| 8:UE:189:SER:OG     | 8:UE:190:PRO:O      | 2.40                     | 0.40              |
| 11:UH:592:ARG:NH1   | 20:UQ:603:ASN:HB2   | 2.35                     | 0.40              |
| 11:UH:665:GLN:OE1   | 12:UI:496:LEU:HD21  | 2.21                     | 0.40              |
| 13:UJ:269:PRO:HG2   | 21:UR:219:LYS:HG3   | 2.03                     | 0.40              |
| 13:UJ:583:LYS:HE2   | 13:UJ:630:TYR:HD2   | 1.85                     | 0.40              |
| 13:UJ:1545:ARG:O    | 13:UJ:1549:VAL:HG23 | 2.21                     | 0.40              |
| 13:UJ:1712:LYS:HZ3  | 13:UJ:1751:GLY:HA3  | 1.84                     | 0.40              |
| 14:UK:191:ASP:OD1   | 14:UK:192:LYS:N     | 2.53                     | 0.40              |
| 15:UL:174:GLU:C     | 15:UL:191:LEU:HD12  | 2.41                     | 0.40              |
| 15:UL:337:LYS:CD    | 15:UL:358:SER:HB3   | 2.50                     | 0.40              |
| 15:UL:453:GLU:OE2   | 15:UL:455:GLN:NE2   | 2.55                     | 0.40              |
| 16:UM:46:THR:O      | 16:UM:50:ARG:NE     | 2.48                     | 0.40              |
| 16:UM:510:SER:HB3   | 16:UM:512:ASP:OD1   | 2.21                     | 0.40              |
| 16:UM:649:GLU:HG2   | 16:UM:650:GLN:N     | 2.35                     | 0.40              |
| 16:UM:702:LEU:HD23  | 16:UM:702:LEU:HA    | 1.87                     | 0.40              |
| 17:UN:313:PHE:CE2   | 17:UN:883:ILE:HB    | 2.56                     | 0.40              |
| 18:UO:217:ASN:OD1   | 18:UO:218:VAL:N     | 2.52                     | 0.40              |
| 18:UO:462:TRP:O     | 18:UO:465:VAL:HG12  | 2.21                     | 0.40              |
| 21:UR:155:ILE:HD13  | 21:UR:163:ARG:CZ    | 2.51                     | 0.40              |
| 22:US:210:ASP:O     | 22:US:213:LEU:HG    | 2.22                     | 0.40              |
| 23:UT:19:PHE:HA     | 23:UT:22:ARG:HE     | 1.86                     | 0.40              |
| 23:UT:117:LEU:HD13  | 23:UT:117:LEU:HA    | 1.98                     | 0.40              |
| 23:UT:232:LEU:HB2   | 23:UT:274:LEU:HD21  | 2.03                     | 0.40              |
| 23:UT:953:LEU:O     | 23:UT:961:ILE:HD11  | 2.21                     | 0.40              |
| 23:UT:1033:ALA:HB2  | 23:UT:1054:LEU:HD22 | 2.03                     | 0.40              |
| 23:UT:1187:VAL:HG23 | 23:UT:1188:LYS:HG3  | 2.02                     | 0.40              |
| 23:UT:1559:LEU:HA   | 23:UT:1562:VAL:HG22 | 2.03                     | 0.40              |
| 23:UT:1777:LEU:HD13 | 23:UT:1777:LEU:HA   | 1.89                     | 0.40              |
| 25:UV:99:LYS:HD2    | 25:UV:100:SER:N     | 2.37                     | 0.40              |
| 25:UV:715:SER:HB2   | 25:UV:718:LYS:HD2   | 2.03                     | 0.40              |
| 25:UV:834:ASN:ND2   | 25:UV:837:ILE:HD11  | 2.35                     | 0.40              |
| 25:UV:891:ALA:O     | 25:UV:895:HIS:HB2   | 2.21                     | 0.40              |
| 25:UV:897:ARG:HG3   | 25:UV:898:THR:N     | 2.37                     | 0.40              |
| 25:UV:1146:THR:OG1  | 25:UV:1180:ASN:ND2  | 2.55                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 28:CD:9:PHE:HE2   | 28:CD:11:GLU:HG3   | 1.86                     | 0.40              |
| 29:CE:5:LEU:HG    | 29:CE:88:ILE:O     | 2.21                     | 0.40              |
| 29:CE:126:GLU:C   | 29:CE:129:PRO:HD2  | 2.42                     | 0.40              |
| 32:CI:75:GLU:OE1  | 32:CI:94:ILE:HG21  | 2.21                     | 0.40              |
| 33:CJ:279:ARG:O   | 33:CJ:279:ARG:HG2  | 2.21                     | 0.40              |
| 39:JF:102:SER:O   | 39:JF:105:ASN:HB2  | 2.20                     | 0.40              |
| 39:JF:104:ILE:HB  | 39:JF:246:GLU:CG   | 2.51                     | 0.40              |
| 39:JG:22:SER:OG   | 39:JG:24:VAL:HG22  | 2.21                     | 0.40              |
| 39:JG:52:THR:OG1  | 39:JG:142:VAL:HG23 | 2.21                     | 0.40              |
| 42:JJ:155:GLY:O   | 42:JJ:158:PHE:HB3  | 2.21                     | 0.40              |
| 44:JM:206:TYR:HH  | 66:D3:1490:C:H5    | 1.65                     | 0.40              |
| 47:JP:69:GLY:HA2  | 47:JP:368:ASP:O    | 2.21                     | 0.40              |
| 52:DH:141:ARG:HB2 | 60:DW:51:GLU:OE1   | 2.21                     | 0.40              |
| 58:DQ:45:ARG:HH11 | 58:DQ:45:ARG:HD2   | 1.77                     | 0.40              |
| 62:DY:29:HIS:O    | 62:DY:29:HIS:CG    | 2.74                     | 0.40              |
| 66:D3:163:G:H2'   | 66:D3:164:A:H8     | 1.86                     | 0.40              |
| 66:D3:884:A:H2'   | 66:D3:885:G:C8     | 2.56                     | 0.40              |
| 66:D3:925:G:C2    | 66:D3:926:A:C4     | 3.08                     | 0.40              |
| 66:D3:1156:C:N4   | 66:D3:1622:G:H1    | 2.19                     | 0.40              |
| 66:D3:1176:G:H2'  | 66:D3:1177:C:H6    | 1.86                     | 0.40              |
| 66:D3:1633:A:N3   | 66:D3:1633:A:H2'   | 2.37                     | 0.40              |
| 66:D3:1739:C:C2   | 66:D3:1740:A:C8    | 3.09                     | 0.40              |
| 67:D4:11:U:H2'    | 67:D4:12:U:H6      | 1.83                     | 0.40              |
| 67:D4:78:G:H2'    | 67:D4:79:G:C8      | 2.51                     | 0.40              |
| 79:EN:889:LEU:O   | 79:EN:893:GLY:N    | 2.54                     | 0.40              |
| 2:DA:36:SER:HB3   | 2:DA:41:ARG:HH22   | 1.85                     | 0.40              |
| 2:DA:144:ARG:HH12 | 2:DA:146:GLN:HA    | 1.85                     | 0.40              |
| 3:JA:70:ARG:HA    | 3:JA:73:ARG:CD     | 2.50                     | 0.40              |
| 3:JA:70:ARG:HA    | 3:JA:73:ARG:HG3    | 2.04                     | 0.40              |
| 3:JA:160:GLN:HG3  | 3:JA:164:MET:CE    | 2.51                     | 0.40              |
| 3:JA:533:PHE:CE1  | 3:JA:579:ILE:HG13  | 2.55                     | 0.40              |
| 3:JA:743:VAL:O    | 3:JA:762:MET:HG2   | 2.20                     | 0.40              |
| 3:JA:748:ARG:HH22 | 3:JA:752:ASN:HD22  | 1.69                     | 0.40              |
| 4:UA:415:ASP:O    | 4:UA:416:LEU:HD22  | 2.22                     | 0.40              |
| 1:CB:117:VAL:HB   | 1:CB:210:MET:SD    | 2.61                     | 0.40              |
| 5:UB:575:PHE:CD2  | 5:UB:636:LEU:HD12  | 2.56                     | 0.40              |
| 7:UD:30:ARG:HD2   | 11:UH:720:TYR:HE1  | 1.86                     | 0.40              |
| 7:UD:127:ASP:O    | 7:UD:131:GLY:N     | 2.47                     | 0.40              |
| 7:UD:427:ASN:HB2  | 7:UD:444:ARG:NE    | 2.36                     | 0.40              |
| 7:UD:466:ASP:OD1  | 7:UD:467:ASN:N     | 2.54                     | 0.40              |
| 7:UD:495:VAL:O    | 7:UD:510:GLU:HG2   | 2.21                     | 0.40              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 8:UE:453:LEU:HA     | 8:UE:456:VAL:HG22   | 2.04                     | 0.40              |
| 9:UF:273:ILE:HD13   | 17:UN:341:LYS:HZ3   | 1.86                     | 0.40              |
| 10:UG:373:PHE:CZ    | 10:UG:392:VAL:HG21  | 2.54                     | 0.40              |
| 10:UG:553:PHE:HE1   | 25:UV:791:LYS:O     | 2.04                     | 0.40              |
| 13:UJ:23:LYS:HE3    | 13:UJ:23:LYS:HB3    | 1.89                     | 0.40              |
| 13:UJ:160:LEU:HA    | 29:CE:412:VAL:HG22  | 2.03                     | 0.40              |
| 13:UJ:1597:LEU:O    | 13:UJ:1601:VAL:HG22 | 2.21                     | 0.40              |
| 14:UK:244:TRP:CD1   | 30:CF:31:ARG:NH2    | 2.89                     | 0.40              |
| 15:UL:560:LEU:HD23  | 15:UL:560:LEU:HA    | 1.92                     | 0.40              |
| 16:UM:74:GLN:NE2    | 16:UM:75:TYR:CD2    | 2.89                     | 0.40              |
| 16:UM:618:ASN:ND2   | 16:UM:637:ALA:HB3   | 2.37                     | 0.40              |
| 20:UQ:172:ARG:HG2   | 20:UQ:192:GLU:CD    | 2.42                     | 0.40              |
| 21:UR:244:SER:HB3   | 21:UR:282:ASN:O     | 2.20                     | 0.40              |
| 21:UR:448:LYS:HG2   | 21:UR:449:ASP:O     | 2.22                     | 0.40              |
| 22:US:445:PRO:HG2   | 22:US:460:ASP:HB2   | 2.03                     | 0.40              |
| 23:UT:498:ILE:HD12  | 23:UT:501:LEU:HB2   | 2.03                     | 0.40              |
| 23:UT:649:PHE:CE2   | 23:UT:691:LYS:HD2   | 2.56                     | 0.40              |
| 23:UT:974:TYR:HA    | 23:UT:1028:TYR:CD2  | 2.57                     | 0.40              |
| 23:UT:997:MET:HB3   | 23:UT:1054:LEU:HD11 | 2.02                     | 0.40              |
| 23:UT:1224:LEU:HD23 | 23:UT:1224:LEU:HA   | 1.92                     | 0.40              |
| 23:UT:1285:THR:HG21 | 23:UT:1308:LEU:HB3  | 2.02                     | 0.40              |
| 23:UT:1715:SER:HB3  | 23:UT:1719:LYS:NZ   | 2.36                     | 0.40              |
| 23:UT:1811:ILE:HD12 | 23:UT:1811:ILE:HA   | 1.86                     | 0.40              |
| 24:UU:263:HIS:NE2   | 24:UU:284:ILE:HD11  | 2.36                     | 0.40              |
| 24:UU:833:LEU:O     | 24:UU:836:THR:OG1   | 2.33                     | 0.40              |
| 24:UU:848:GLU:HA    | 24:UU:851:SER:OG    | 2.21                     | 0.40              |
| 25:UV:218:ASP:O     | 25:UV:223:ARG:HB2   | 2.20                     | 0.40              |
| 25:UV:671:THR:OG1   | 25:UV:718:LYS:O     | 2.27                     | 0.40              |
| 25:UV:902:ILE:O     | 25:UV:905:SER:HB3   | 2.21                     | 0.40              |
| 25:UV:909:TYR:O     | 25:UV:913:VAL:HG12  | 2.21                     | 0.40              |
| 28:CD:371:ASN:O     | 28:CD:375:ILE:HG12  | 2.22                     | 0.40              |
| 29:CE:37:LYS:HD2    | 29:CE:38:VAL:N      | 2.36                     | 0.40              |
| 29:CE:116:ILE:HD12  | 29:CE:116:ILE:H     | 1.85                     | 0.40              |
| 29:CE:185:LYS:HA    | 29:CE:205:TYR:OH    | 2.21                     | 0.40              |
| 31:CH:369:LEU:O     | 31:CH:373:MET:HG2   | 2.21                     | 0.40              |
| 31:CH:457:GLU:OE2   | 31:CH:461:LYS:HE3   | 2.22                     | 0.40              |
| 31:CH:487:PHE:HZ    | 31:CH:508:PHE:CD2   | 2.39                     | 0.40              |
| 34:CK:341:LEU:HD21  | 35:CL:957:GLU:HA    | 2.03                     | 0.40              |
| 35:CL:565:ARG:HA    | 35:CL:568:ARG:CD    | 2.52                     | 0.40              |
| 38:JC:99:ALA:O      | 38:JC:118:GLN:NE2   | 2.54                     | 0.40              |
| 38:JC:288:LYS:HE3   | 38:JC:300:TRP:CE3   | 2.56                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:JC:355:PHE:CE2  | 51:DG:68:LEU:HD12  | 2.55                     | 0.40              |
| 39:JF:132:ARG:HD2  | 39:JG:88:ARG:NH1   | 2.36                     | 0.40              |
| 39:JG:125:ASN:HA   | 39:JG:126:PRO:HD3  | 1.93                     | 0.40              |
| 44:JM:175:GLU:HG2  | 44:JM:175:GLU:H    | 1.73                     | 0.40              |
| 45:JN:234:VAL:O    | 45:JN:239:ARG:NH1  | 2.55                     | 0.40              |
| 47:JP:314:SER:O    | 47:JP:317:GLY:N    | 2.54                     | 0.40              |
| 49:DE:185:GLY:H    | 49:DE:224:ASN:HB3  | 1.86                     | 0.40              |
| 50:DF:160:VAL:HG22 | 50:DF:161:ASP:H    | 1.87                     | 0.40              |
| 57:DO:78:ALA:HA    | 57:DO:111:ARG:O    | 2.21                     | 0.40              |
| 58:DQ:44:LEU:HA    | 58:DQ:44:LEU:HD23  | 1.83                     | 0.40              |
| 60:DW:31:SER:HG    | 60:DW:34:ILE:H     | 1.58                     | 0.40              |
| 65:D2:438:U:H2'    | 65:D2:439:A:C8     | 2.56                     | 0.40              |
| 66:D3:67:A:C6      | 66:D3:84:A:C8      | 3.09                     | 0.40              |
| 66:D3:411:C:H3'    | 66:D3:412:A:H8     | 1.86                     | 0.40              |
| 66:D3:1050:G:C4    | 66:D3:1069:A:N1    | 2.89                     | 0.40              |
| 66:D3:1605:G:C5    | 66:D3:1606:C:C5    | 3.09                     | 0.40              |
| 67:D4:23:U:C2      | 67:D4:26:C:C4      | 3.09                     | 0.40              |
| 67:D4:94:A:C2      | 67:D4:95:A:C4      | 3.10                     | 0.40              |
| 1:CA:218:ILE:HD13  | 1:CA:218:ILE:HG21  | 1.90                     | 0.40              |
| 2:DA:241:GLY:O     | 2:DA:242:LYS:HD3   | 2.22                     | 0.40              |
| 3:JA:771:SER:CB    | 3:JA:774:LEU:HG    | 2.50                     | 0.40              |
| 4:UA:633:LYS:HG3   | 65:D2:293:U:H5     | 1.86                     | 0.40              |
| 4:UA:649:GLU:OE2   | 4:UA:649:GLU:HA    | 2.21                     | 0.40              |
| 4:UA:754:VAL:O     | 4:UA:758:ILE:HG12  | 2.20                     | 0.40              |
| 1:CB:93:HIS:NE2    | 1:CB:159:LEU:O     | 2.52                     | 0.40              |
| 5:UB:644:ASP:HB2   | 5:UB:684:ILE:HD11  | 2.04                     | 0.40              |
| 7:UD:497:ILE:O     | 7:UD:509:GLN:HB2   | 2.21                     | 0.40              |
| 7:UD:639:ASP:HB3   | 7:UD:642:ASN:O     | 2.22                     | 0.40              |
| 9:UF:152:LYS:HE2   | 9:UF:152:LYS:HB3   | 1.90                     | 0.40              |
| 12:UI:423:LYS:O    | 12:UI:426:THR:HB   | 2.21                     | 0.40              |
| 15:UL:14:PHE:HE2   | 15:UL:422:HIS:HB3  | 1.86                     | 0.40              |
| 15:UL:57:GLY:HA3   | 15:UL:385:ILE:HD12 | 2.02                     | 0.40              |
| 15:UL:398:ASP:OD2  | 15:UL:438:PHE:N    | 2.54                     | 0.40              |
| 15:UL:604:PHE:CD1  | 36:CM:241:TRP:HZ3  | 2.40                     | 0.40              |
| 15:UL:673:VAL:HG12 | 15:UL:683:ILE:HD12 | 2.03                     | 0.40              |
| 15:UL:794:LEU:HD21 | 15:UL:801:PRO:HD3  | 2.03                     | 0.40              |
| 16:UM:62:GLN:HB2   | 16:UM:80:SER:HB2   | 2.03                     | 0.40              |
| 16:UM:224:ASP:N    | 16:UM:234:LEU:HG   | 2.37                     | 0.40              |
| 16:UM:281:THR:OG1  | 16:UM:282:ASN:N    | 2.54                     | 0.40              |
| 16:UM:362:LEU:HG   | 16:UM:384:TYR:HB2  | 2.03                     | 0.40              |
| 18:UO:241:SER:O    | 18:UO:243:LYS:HG2  | 2.21                     | 0.40              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 18:UO:244:LYS:HB3  | 18:UO:244:LYS:HE3   | 1.81                     | 0.40              |
| 18:UO:282:LYS:HD3  | 18:UO:294:PHE:O     | 2.22                     | 0.40              |
| 18:UO:398:SER:HB2  | 18:UO:434:ARG:NH2   | 2.28                     | 0.40              |
| 20:UQ:143:ASN:OD1  | 20:UQ:145:PHE:HD1   | 2.05                     | 0.40              |
| 20:UQ:156:THR:HG23 | 20:UQ:169:GLN:HB3   | 2.03                     | 0.40              |
| 20:UQ:317:TRP:NE1  | 20:UQ:403:ILE:O     | 2.45                     | 0.40              |
| 20:UQ:397:LYS:O    | 20:UQ:398:HIS:ND1   | 2.55                     | 0.40              |
| 21:UR:233:LEU:HD11 | 21:UR:552:PHE:CD2   | 2.57                     | 0.40              |
| 21:UR:459:GLN:O    | 21:UR:482:LEU:HD12  | 2.22                     | 0.40              |
| 22:US:363:ASP:HA   | 22:US:401:PHE:HE1   | 1.87                     | 0.40              |
| 23:UT:406:GLU:H    | 23:UT:406:GLU:CD    | 2.24                     | 0.40              |
| 23:UT:838:PHE:CD2  | 23:UT:841:ILE:HD13  | 2.55                     | 0.40              |
| 23:UT:855:MET:O    | 23:UT:927:ARG:HG2   | 2.21                     | 0.40              |
| 23:UT:897:PHE:O    | 23:UT:900:GLU:HG3   | 2.22                     | 0.40              |
| 23:UT:1541:MET:O   | 23:UT:1545:VAL:HG22 | 2.22                     | 0.40              |
| 24:UU:605:LEU:C    | 24:UU:607:SER:H     | 2.24                     | 0.40              |
| 24:UU:881:TYR:HD1  | 24:UU:884:PHE:HD2   | 1.68                     | 0.40              |
| 25:UV:684:PHE:O    | 25:UV:688:LYS:HG2   | 2.21                     | 0.40              |
| 26:UX:61:PRO:HG3   | 26:UX:63:TYR:CZ     | 2.57                     | 0.40              |
| 31:CH:150:THR:CG2  | 31:CH:207:ARG:HD3   | 2.51                     | 0.40              |
| 31:CH:196:LEU:HG   | 31:CH:268:LEU:HD11  | 2.03                     | 0.40              |
| 31:CH:331:LEU:HD23 | 31:CH:483:TYR:CZ    | 2.56                     | 0.40              |
| 31:CH:351:ILE:O    | 31:CH:354:GLU:N     | 2.50                     | 0.40              |
| 31:CH:365:PRO:HG2  | 31:CH:366:GLN:OE1   | 2.21                     | 0.40              |
| 34:CK:527:ARG:HA   | 34:CK:530:ARG:HD2   | 2.02                     | 0.40              |
| 35:CL:40:ALA:O     | 35:CL:44:GLN:OE1    | 2.39                     | 0.40              |
| 35:CL:143:ASP:HB3  | 35:CL:146:PHE:O     | 2.22                     | 0.40              |
| 35:CL:1007:TYR:CG  | 35:CL:1008:PRO:HD2  | 2.56                     | 0.40              |
| 36:CM:138:MET:HB2  | 36:CM:139:PRO:HD3   | 2.03                     | 0.40              |
| 37:CN:23:HIS:CD2   | 37:CN:25:ALA:HB3    | 2.57                     | 0.40              |
| 37:CN:180:LEU:HA   | 37:CN:180:LEU:HD12  | 1.81                     | 0.40              |
| 37:CN:196:ALA:O    | 37:CN:200:GLU:HG2   | 2.21                     | 0.40              |
| 38:JC:59:SER:HB2   | 38:JC:332:ALA:HB1   | 2.03                     | 0.40              |
| 38:JC:205:GLU:HG2  | 38:JC:214:ARG:HD3   | 2.02                     | 0.40              |
| 42:JJ:271:LYS:HE3  | 42:JJ:271:LYS:HB2   | 1.88                     | 0.40              |
| 45:JN:157:GLN:CD   | 45:JN:214:ARG:HE    | 2.24                     | 0.40              |
| 49:DE:37:LYS:HD2   | 66:D3:297:U:H5"     | 2.03                     | 0.40              |
| 49:DE:188:ASN:HB3  | 49:DE:191:ARG:NE    | 2.36                     | 0.40              |
| 50:DF:25:LEU:CD1   | 58:DQ:57:LEU:HD12   | 2.51                     | 0.40              |
| 52:DH:129:LEU:HG   | 52:DH:169:PHE:CD1   | 2.56                     | 0.40              |
| 55:DL:67:ARG:O     | 55:DL:127:GLN:HB3   | 2.22                     | 0.40              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 56:DN:109:LYS:NZ   | 66:D3:976:G:P       | 2.94                     | 0.40              |
| 61:DX:69:ARG:O     | 61:DX:93:LEU:HD22   | 2.20                     | 0.40              |
| 61:DX:90:ASP:OD1   | 61:DX:91:GLY:N      | 2.55                     | 0.40              |
| 62:DY:55:VAL:HA    | 62:DY:75:VAL:HA     | 2.03                     | 0.40              |
| 62:DY:60:PHE:CD1   | 62:DY:71:GLY:HA3    | 2.56                     | 0.40              |
| 65:D2:3:G:C5       | 65:D2:4:C:C4        | 3.09                     | 0.40              |
| 65:D2:17:A:H2'     | 65:D2:18:G:H8       | 1.86                     | 0.40              |
| 65:D2:417:C:H2'    | 65:D2:418:C:C6      | 2.57                     | 0.40              |
| 65:D2:427:A:C8     | 65:D2:428:A:H1'     | 2.57                     | 0.40              |
| 66:D3:123:G:C6     | 66:D3:124:A:C6      | 3.10                     | 0.40              |
| 66:D3:172:C:H2'    | 66:D3:173:A:O4'     | 2.22                     | 0.40              |
| 66:D3:966:A:O2'    | 66:D3:967:A:H5'     | 2.21                     | 0.40              |
| 66:D3:1169:G:N2    | 66:D3:1577:A:H61    | 2.20                     | 0.40              |
| 66:D3:1713:G:H2'   | 66:D3:1714:A:C8     | 2.56                     | 0.40              |
| 67:D4:83:A:C5      | 67:D4:84:U:C5       | 3.09                     | 0.40              |
| 1:CA:89:GLU:OE1    | 44:JM:144:PRO:HG3   | 2.20                     | 0.40              |
| 1:CA:204:GLY:O     | 1:CA:208:ILE:HG12   | 2.22                     | 0.40              |
| 3:JA:86:ARG:NH1    | 3:JA:90:GLU:O       | 2.38                     | 0.40              |
| 4:UA:296:GLN:HG3   | 24:UU:752:LYS:HZ1   | 1.86                     | 0.40              |
| 4:UA:617:VAL:HG11  | 4:UA:681:VAL:CG2    | 2.51                     | 0.40              |
| 5:UB:514:TYR:OH    | 5:UB:516:LEU:HD13   | 2.21                     | 0.40              |
| 7:UD:34:HIS:NE2    | 7:UD:751:GLU:OE1    | 2.44                     | 0.40              |
| 7:UD:155:LYS:HZ1   | 7:UD:217:LYS:HE3    | 1.85                     | 0.40              |
| 7:UD:376:GLU:HA    | 7:UD:377:PRO:HD3    | 1.91                     | 0.40              |
| 7:UD:387:GLU:C     | 7:UD:389:ARG:H      | 2.24                     | 0.40              |
| 7:UD:452:HIS:HB2   | 7:UD:465:LEU:HD11   | 2.04                     | 0.40              |
| 8:UE:107:ILE:HD13  | 8:UE:107:ILE:HA     | 1.94                     | 0.40              |
| 9:UF:163:SER:O     | 9:UF:167:ILE:HG12   | 2.21                     | 0.40              |
| 10:UG:334:ARG:NH2  | 10:UG:337:HIS:CG    | 2.90                     | 0.40              |
| 10:UG:465:ASP:O    | 10:UG:469:THR:HG23  | 2.22                     | 0.40              |
| 11:UH:597:GLN:HA   | 11:UH:600:LYS:HZ1   | 1.85                     | 0.40              |
| 11:UH:666:VAL:O    | 11:UH:670:GLU:OE1   | 2.38                     | 0.40              |
| 12:UI:486:LEU:O    | 12:UI:490:GLU:OE1   | 2.39                     | 0.40              |
| 13:UJ:572:ARG:NH1  | 13:UJ:669:VAL:HB    | 2.37                     | 0.40              |
| 13:UJ:585:ILE:HA   | 13:UJ:585:ILE:HD13  | 1.96                     | 0.40              |
| 13:UJ:1404:PHE:CE2 | 13:UJ:1425:VAL:HG21 | 2.57                     | 0.40              |
| 14:UK:200:GLN:HA   | 14:UK:203:GLN:HE22  | 1.86                     | 0.40              |
| 15:UL:180:THR:HG22 | 15:UL:186:ILE:CD1   | 2.51                     | 0.40              |
| 15:UL:285:ARG:O    | 15:UL:327:HIS:HB3   | 2.22                     | 0.40              |
| 15:UL:392:THR:HG23 | 15:UL:409:ALA:HB1   | 2.04                     | 0.40              |
| 15:UL:414:LEU:HD11 | 15:UL:445:VAL:HG21  | 2.03                     | 0.40              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 15:UL:569:LEU:HD23  | 15:UL:600:TRP:CD2   | 2.56                     | 0.40              |
| 16:UM:126:ILE:O     | 16:UM:126:ILE:HG13  | 2.21                     | 0.40              |
| 16:UM:185:THR:C     | 16:UM:186:LEU:HD22  | 2.42                     | 0.40              |
| 18:UO:123:SER:HB3   | 18:UO:150:ARG:CZ    | 2.52                     | 0.40              |
| 18:UO:360:MET:CE    | 65:D2:234:A:C4      | 3.05                     | 0.40              |
| 20:UQ:89:VAL:HG12   | 20:UQ:110:PHE:O     | 2.21                     | 0.40              |
| 20:UQ:492:ASP:CG    | 20:UQ:493:PRO:HD2   | 2.41                     | 0.40              |
| 20:UQ:501:THR:CG2   | 20:UQ:506:TRP:HB2   | 2.51                     | 0.40              |
| 20:UQ:598:LYS:HZ3   | 20:UQ:636:ASP:HA    | 1.86                     | 0.40              |
| 20:UQ:664:LEU:H     | 20:UQ:664:LEU:HD23  | 1.86                     | 0.40              |
| 20:UQ:865:LYS:HE3   | 20:UQ:895:LEU:O     | 2.20                     | 0.40              |
| 21:UR:255:SER:O     | 21:UR:263:LEU:HD12  | 2.22                     | 0.40              |
| 21:UR:257:HIS:HD1   | 21:UR:260:LYS:N     | 2.19                     | 0.40              |
| 23:UT:99:ASP:C      | 23:UT:103:LEU:HG    | 2.41                     | 0.40              |
| 23:UT:181:LEU:O     | 23:UT:189:SER:OG    | 2.27                     | 0.40              |
| 23:UT:412:ASN:O     | 23:UT:415:LYS:HG2   | 2.21                     | 0.40              |
| 23:UT:434:LEU:HD13  | 23:UT:757:ILE:HG13  | 2.02                     | 0.40              |
| 23:UT:476:LEU:HA    | 23:UT:479:ILE:HG12  | 2.03                     | 0.40              |
| 23:UT:1097:GLU:HG2  | 66:D3:198:A:N3      | 2.36                     | 0.40              |
| 23:UT:1591:TYR:OH   | 23:UT:1616:LEU:HD21 | 2.20                     | 0.40              |
| 23:UT:1710:LEU:HD13 | 23:UT:1760:ASN:ND2  | 2.36                     | 0.40              |
| 23:UT:1877:ARG:O    | 23:UT:1880:ILE:HG22 | 2.21                     | 0.40              |
| 24:UU:843:ALA:O     | 24:UU:847:LEU:HB2   | 2.21                     | 0.40              |
| 25:UV:214:PHE:HE2   | 25:UV:299:PRO:HD2   | 1.85                     | 0.40              |
| 25:UV:337:LEU:HG    | 25:UV:474:VAL:HG12  | 2.03                     | 0.40              |
| 25:UV:400:LEU:HD12  | 25:UV:403:GLY:O     | 2.21                     | 0.40              |
| 26:UX:136:TYR:HD2   | 26:UX:139:ASP:OD1   | 2.04                     | 0.40              |
| 27:UZ:75:ILE:HA     | 27:UZ:101:ILE:O     | 2.22                     | 0.40              |
| 27:UZ:135:LEU:O     | 27:UZ:138:VAL:HG22  | 2.22                     | 0.40              |
| 27:UZ:231:GLN:OE1   | 48:JQ:189:PRO:HA    | 2.21                     | 0.40              |
| 28:CD:119:ILE:HD11  | 47:JP:155:TYR:CD1   | 2.46                     | 0.40              |
| 28:CD:181:LEU:HD12  | 28:CD:292:LEU:HD13  | 2.03                     | 0.40              |
| 29:CE:36:ASP:CG     | 29:CE:40:LYS:HZ3    | 2.24                     | 0.40              |
| 31:CH:467:LYS:HD3   | 31:CH:470:LEU:HD23  | 2.04                     | 0.40              |
| 32:CI:9:GLU:O       | 32:CI:13:LEU:HG     | 2.21                     | 0.40              |
| 33:CJ:21:GLN:HA     | 33:CJ:21:GLN:OE1    | 2.21                     | 0.40              |
| 34:CK:470:GLU:HB2   | 34:CK:488:SER:OG    | 2.21                     | 0.40              |
| 35:CL:58:MET:HE1    | 66:D3:434:G:H22     | 1.86                     | 0.40              |
| 35:CL:78:PRO:HA     | 35:CL:82:LYS:HE3    | 2.03                     | 0.40              |
| 35:CL:557:ASN:OD1   | 35:CL:557:ASN:N     | 2.52                     | 0.40              |
| 36:CM:285:LYS:HE3   | 36:CM:291:ARG:HD3   | 2.02                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:CN:15:VAL:HA    | 37:CN:37:MET:O     | 2.21                     | 0.40              |
| 37:CN:51:ASP:O     | 37:CN:127:LYS:HD3  | 2.21                     | 0.40              |
| 38:JC:276:LYS:HD3  | 38:JC:276:LYS:HA   | 1.85                     | 0.40              |
| 42:JJ:204:ARG:NH1  | 42:JJ:253:GLY:HA2  | 2.36                     | 0.40              |
| 45:JN:290:SER:OG   | 45:JN:291:ILE:N    | 2.54                     | 0.40              |
| 47:JP:75:LYS:HD3   | 47:JP:356:TYR:O    | 2.21                     | 0.40              |
| 47:JP:390:GLU:OE2  | 67:D4:36:C:C4      | 2.74                     | 0.40              |
| 49:DE:77:ARG:HD3   | 49:DE:77:ARG:HA    | 1.85                     | 0.40              |
| 49:DE:160:VAL:HG23 | 49:DE:172:PHE:HB3  | 2.02                     | 0.40              |
| 51:DG:12:SER:OG    | 51:DG:124:LEU:HD12 | 2.20                     | 0.40              |
| 51:DG:51:LYS:N     | 51:DG:112:VAL:O    | 2.50                     | 0.40              |
| 51:DG:87:ARG:HA    | 51:DG:87:ARG:NE    | 2.36                     | 0.40              |
| 51:DG:122:GLU:HA   | 51:DG:126:ASP:OD2  | 2.22                     | 0.40              |
| 51:DG:215:ARG:HG3  | 51:DG:216:LEU:N    | 2.37                     | 0.40              |
| 56:DN:16:ILE:HG22  | 56:DN:17:PRO:O     | 2.20                     | 0.40              |
| 57:DO:32:ASP:OD1   | 57:DO:37:GLU:HB2   | 2.21                     | 0.40              |
| 66:D3:86:A:H2'     | 66:D3:87:C:C6      | 2.56                     | 0.40              |
| 66:D3:397:A:C4     | 66:D3:398:G:C8     | 3.10                     | 0.40              |
| 66:D3:457:G:N3     | 66:D3:458:G:C8     | 2.90                     | 0.40              |
| 66:D3:529:A:H2'    | 66:D3:530:C:C6     | 2.56                     | 0.40              |
| 66:D3:839:U:H2'    | 66:D3:840:U:C6     | 2.57                     | 0.40              |
| 66:D3:1048:G:H2'   | 66:D3:1049:U:H6    | 1.86                     | 0.40              |
| 66:D3:1069:A:C5    | 66:D3:1070:C:C4    | 3.09                     | 0.40              |
| 66:D3:1132:A:O2'   | 66:D3:1133:A:O5'   | 2.37                     | 0.40              |
| 66:D3:1532:U:H2'   | 66:D3:1533:C:H6    | 1.86                     | 0.40              |
| 66:D3:1665:U:O2'   | 66:D3:1666:U:H5'   | 2.21                     | 0.40              |
| 1:CA:115:GLU:N     | 1:CA:115:GLU:OE2   | 2.55                     | 0.40              |
| 1:CA:153:ALA:HB1   | 1:CA:309:TYR:HD1   | 1.87                     | 0.40              |
| 3:JA:480:ASP:OD2   | 3:JA:483:GLU:N     | 2.52                     | 0.40              |
| 3:JA:825:LEU:HB3   | 3:JA:870:LYS:HB3   | 2.04                     | 0.40              |
| 4:UA:254:HIS:HB3   | 4:UA:292:PHE:CE2   | 2.56                     | 0.40              |
| 4:UA:726:THR:HG21  | 4:UA:750:LEU:HD21  | 2.03                     | 0.40              |
| 7:UD:164:THR:OG1   | 7:UD:165:VAL:N     | 2.54                     | 0.40              |
| 7:UD:773:LYS:HZ3   | 65:D2:83:U:H3      | 1.67                     | 0.40              |
| 7:UD:773:LYS:O     | 7:UD:775:VAL:HG13  | 2.22                     | 0.40              |
| 10:UG:302:ASP:HB2  | 10:UG:309:LEU:HG   | 2.03                     | 0.40              |
| 10:UG:538:ILE:HG22 | 10:UG:542:HIS:CG   | 2.57                     | 0.40              |
| 11:UH:531:LEU:HD23 | 11:UH:531:LEU:H    | 1.87                     | 0.40              |
| 12:UI:487:ARG:NE   | 12:UI:487:ARG:HA   | 2.37                     | 0.40              |
| 13:UJ:611:ILE:HB   | 13:UJ:660:LEU:HD23 | 2.03                     | 0.40              |
| 13:UJ:680:TYR:CD2  | 13:UJ:681:ALA:N    | 2.90                     | 0.40              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 13:UJ:694:HIS:HA   | 13:UJ:697:GLU:OE1   | 2.22                     | 0.40              |
| 13:UJ:720:LEU:HA   | 13:UJ:723:LEU:HG    | 2.03                     | 0.40              |
| 13:UJ:1459:ARG:O   | 13:UJ:1463:THR:HG23 | 2.22                     | 0.40              |
| 13:UJ:1615:ASN:HB3 | 13:UJ:1618:LEU:HB3  | 2.04                     | 0.40              |
| 14:UK:98:LEU:O     | 14:UK:102:GLN:HG3   | 2.21                     | 0.40              |
| 15:UL:536:CYS:SG   | 15:UL:537:VAL:N     | 2.94                     | 0.40              |
| 15:UL:632:SER:HG   | 15:UL:640:LYS:HB2   | 1.86                     | 0.40              |
| 16:UM:170:GLY:HA2  | 16:UM:189:HIS:HB2   | 2.02                     | 0.40              |
| 16:UM:385:GLU:OE1  | 16:UM:385:GLU:N     | 2.54                     | 0.40              |
| 16:UM:513:LYS:HZ2  | 16:UM:532:HIS:C     | 2.24                     | 0.40              |
| 16:UM:619:ARG:O    | 16:UM:620:LEU:HD22  | 2.21                     | 0.40              |
| 16:UM:702:LEU:O    | 16:UM:706:ARG:HG2   | 2.22                     | 0.40              |
| 18:UO:257:CYS:O    | 18:UO:274:ALA:HA    | 2.22                     | 0.40              |
| 18:UO:279:GLY:CA   | 18:UO:298:PHE:H     | 2.34                     | 0.40              |
| 18:UO:471:GLY:O    | 18:UO:475:GLU:HG2   | 2.21                     | 0.40              |
| 20:UQ:48:PHE:HE2   | 20:UQ:53:LYS:NZ     | 2.19                     | 0.40              |
| 20:UQ:697:PHE:CD1  | 20:UQ:723:VAL:HG21  | 2.55                     | 0.40              |
| 20:UQ:719:ASN:O    | 20:UQ:746:PHE:N     | 2.44                     | 0.40              |
| 21:UR:26:VAL:HG13  | 21:UR:27:PHE:CD1    | 2.56                     | 0.40              |
| 21:UR:382:GLY:C    | 21:UR:399:LYS:HA    | 2.39                     | 0.40              |
| 22:US:350:MET:CA   | 22:US:355:ARG:NH1   | 2.84                     | 0.40              |
| 23:UT:562:VAL:HA   | 23:UT:565:LEU:HG    | 2.03                     | 0.40              |
| 23:UT:695:LEU:O    | 23:UT:698:LYS:HG2   | 2.22                     | 0.40              |
| 24:UU:342:TYR:CZ   | 24:UU:343:LEU:O     | 2.75                     | 0.40              |
| 25:UV:820:THR:HG22 | 25:UV:845:PRO:HG3   | 2.02                     | 0.40              |
| 25:UV:936:LEU:O    | 25:UV:939:ILE:HG22  | 2.22                     | 0.40              |
| 25:UV:955:GLU:OE2  | 25:UV:959:LEU:HD12  | 2.22                     | 0.40              |
| 25:UV:1190:PHE:HA  | 25:UV:1194:HIS:HE1  | 1.85                     | 0.40              |
| 28:CD:385:MET:CE   | 30:CG:63:ILE:HB     | 2.51                     | 0.40              |
| 28:CD:406:LYS:HG3  | 28:CD:410:GLN:OE1   | 2.21                     | 0.40              |
| 32:CI:11:LYS:HB2   | 47:JP:53:MET:HE1    | 2.02                     | 0.40              |
| 32:CI:22:LYS:HZ1   | 65:D2:388:C:P       | 2.43                     | 0.40              |
| 34:CK:327:LYS:HG2  | 34:CK:328:GLY:H     | 1.87                     | 0.40              |
| 34:CK:470:GLU:CA   | 34:CK:490:LEU:HD23  | 2.51                     | 0.40              |
| 35:CL:242:PRO:HB3  | 35:CL:278:THR:O     | 2.20                     | 0.40              |
| 35:CL:826:LYS:HD3  | 35:CL:926:ILE:HG21  | 2.02                     | 0.40              |
| 35:CL:1039:ARG:NE  | 35:CL:1046:THR:HG22 | 2.37                     | 0.40              |
| 36:CM:335:THR:CG2  | 36:CM:354:ILE:HD11  | 2.51                     | 0.40              |
| 37:CN:7:SER:HB2    | 37:CN:149:ALA:HB2   | 2.03                     | 0.40              |
| 37:CN:85:GLU:N     | 37:CN:127:LYS:O     | 2.35                     | 0.40              |
| 38:JC:200:GLU:CG   | 38:JC:230:GLN:HG3   | 2.51                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:JC:241:LEU:O    | 38:JC:257:LEU:HD13 | 2.22                     | 0.40              |
| 42:JJ:226:LEU:HD23 | 42:JJ:226:LEU:H    | 1.86                     | 0.40              |
| 45:JN:292:LYS:HB3  | 45:JN:292:LYS:HE2  | 1.80                     | 0.40              |
| 52:DH:33:GLU:HG3   | 52:DH:37:GLU:HG2   | 2.02                     | 0.40              |
| 52:DH:62:VAL:HG21  | 52:DH:70:PHE:CE2   | 2.56                     | 0.40              |
| 52:DH:72:LYS:HB3   | 52:DH:73:VAL:HG13  | 2.03                     | 0.40              |
| 53:DI:74:LYS:HD2   | 53:DI:74:LYS:HA    | 1.81                     | 0.40              |
| 55:DL:125:VAL:HG12 | 55:DL:139:VAL:HA   | 2.03                     | 0.40              |
| 56:DN:106:ARG:O    | 56:DN:107:LYS:HE2  | 2.21                     | 0.40              |
| 56:DN:117:LEU:HA   | 56:DN:117:LEU:HD23 | 1.89                     | 0.40              |
| 57:DO:83:ILE:HG22  | 57:DO:116:GLU:O    | 2.22                     | 0.40              |
| 58:DQ:4:VAL:HA     | 58:DQ:5:PRO:HD2    | 1.95                     | 0.40              |
| 65:D2:145:A:C2     | 65:D2:146:G:C4     | 3.10                     | 0.40              |
| 65:D2:148:G:C2     | 65:D2:149:U:C2     | 3.09                     | 0.40              |
| 65:D2:149:U:H5''   | 65:D2:150:G:H5''   | 2.04                     | 0.40              |
| 65:D2:263:C:H2'    | 65:D2:264:C:C6     | 2.56                     | 0.40              |
| 65:D2:405:A:C2     | 65:D2:452:A:C4     | 3.10                     | 0.40              |
| 66:D3:778:G:H5''   | 66:D3:780:A:N7     | 2.36                     | 0.40              |
| 66:D3:871:G:N2     | 66:D3:872:G:C2     | 2.89                     | 0.40              |
| 66:D3:873:U:C4     | 66:D3:874:C:N4     | 2.89                     | 0.40              |
| 66:D3:972:G:C6     | 66:D3:973:A:C6     | 3.10                     | 0.40              |
| 66:D3:1165:G:C6    | 66:D3:1166:A:C6    | 3.10                     | 0.40              |
| 66:D3:1495:C:C2    | 66:D3:1513:G:N2    | 2.90                     | 0.40              |
| 78:EK:626:VAL:HA   | 78:EK:640:ASN:O    | 2.21                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 1   | CA    | 238/327 (73%) | 207 (87%) | 31 (13%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | CB    | 224/327 (68%)   | 201 (90%)  | 23 (10%) | 0        | 100         | 100 |
| 2   | DA    | 236/255 (92%)   | 212 (90%)  | 24 (10%) | 0        | 100         | 100 |
| 3   | JA    | 802/1056 (76%)  | 734 (92%)  | 68 (8%)  | 0        | 100         | 100 |
| 3   | JB    | 827/1056 (78%)  | 770 (93%)  | 57 (7%)  | 0        | 100         | 100 |
| 4   | UA    | 830/923 (90%)   | 733 (88%)  | 97 (12%) | 0        | 100         | 100 |
| 5   | UB    | 495/810 (61%)   | 465 (94%)  | 30 (6%)  | 0        | 100         | 100 |
| 6   | UC    | 124/610 (20%)   | 112 (90%)  | 12 (10%) | 0        | 100         | 100 |
| 7   | UD    | 663/776 (85%)   | 575 (87%)  | 88 (13%) | 0        | 100         | 100 |
| 8   | UE    | 465/643 (72%)   | 419 (90%)  | 46 (10%) | 0        | 100         | 100 |
| 9   | UF    | 283/440 (64%)   | 273 (96%)  | 10 (4%)  | 0        | 100         | 100 |
| 10  | UG    | 529/554 (96%)   | 461 (87%)  | 68 (13%) | 0        | 100         | 100 |
| 11  | UH    | 426/713 (60%)   | 375 (88%)  | 46 (11%) | 5 (1%)   | 11          | 44  |
| 12  | UI    | 100/575 (17%)   | 98 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 13  | UJ    | 1092/1769 (62%) | 1031 (94%) | 61 (6%)  | 0        | 100         | 100 |
| 14  | UK    | 238/250 (95%)   | 214 (90%)  | 24 (10%) | 0        | 100         | 100 |
| 15  | UL    | 828/943 (88%)   | 733 (88%)  | 95 (12%) | 0        | 100         | 100 |
| 16  | UM    | 750/817 (92%)   | 662 (88%)  | 87 (12%) | 1 (0%)   | 48          | 83  |
| 17  | UN    | 143/899 (16%)   | 124 (87%)  | 19 (13%) | 0        | 100         | 100 |
| 18  | UO    | 489/513 (95%)   | 432 (88%)  | 57 (12%) | 0        | 100         | 100 |
| 19  | UP    | 58/214 (27%)    | 54 (93%)   | 4 (7%)   | 0        | 100         | 100 |
| 20  | UQ    | 820/896 (92%)   | 735 (90%)  | 85 (10%) | 0        | 100         | 100 |
| 21  | UR    | 474/594 (80%)   | 424 (90%)  | 50 (10%) | 0        | 100         | 100 |
| 22  | US    | 488/552 (88%)   | 440 (90%)  | 48 (10%) | 0        | 100         | 100 |
| 23  | UT    | 2213/2493 (89%) | 2072 (94%) | 141 (6%) | 0        | 100         | 100 |
| 24  | UU    | 842/939 (90%)   | 755 (90%)  | 87 (10%) | 0        | 100         | 100 |
| 25  | UV    | 1069/1237 (86%) | 1018 (95%) | 51 (5%)  | 0        | 100         | 100 |
| 26  | UX    | 170/189 (90%)   | 150 (88%)  | 20 (12%) | 0        | 100         | 100 |
| 27  | UZ    | 245/274 (89%)   | 225 (92%)  | 20 (8%)  | 0        | 100         | 100 |
| 28  | CD    | 376/504 (75%)   | 344 (92%)  | 32 (8%)  | 0        | 100         | 100 |
| 29  | CE    | 431/511 (84%)   | 393 (91%)  | 38 (9%)  | 0        | 100         | 100 |
| 30  | CF    | 121/126 (96%)   | 109 (90%)  | 12 (10%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|----------|----------|-------------|-----|
| 30  | CG    | 121/126 (96%)  | 112 (93%) | 9 (7%)   | 0        | 100         | 100 |
| 31  | CH    | 459/573 (80%)  | 401 (87%) | 57 (12%) | 1 (0%)   | 44          | 78  |
| 32  | CI    | 180/183 (98%)  | 157 (87%) | 23 (13%) | 0        | 100         | 100 |
| 33  | CJ    | 278/290 (96%)  | 242 (87%) | 36 (13%) | 0        | 100         | 100 |
| 34  | CK    | 203/593 (34%)  | 184 (91%) | 18 (9%)  | 1 (0%)   | 25          | 64  |
| 35  | CL    | 771/1183 (65%) | 716 (93%) | 54 (7%)  | 1 (0%)   | 48          | 83  |
| 36  | CM    | 358/367 (98%)  | 335 (94%) | 23 (6%)  | 0        | 100         | 100 |
| 37  | CN    | 224/297 (75%)  | 211 (94%) | 13 (6%)  | 0        | 100         | 100 |
| 38  | JC    | 350/707 (50%)  | 316 (90%) | 34 (10%) | 0        | 100         | 100 |
| 39  | JF    | 212/252 (84%)  | 203 (96%) | 9 (4%)   | 0        | 100         | 100 |
| 39  | JG    | 226/252 (90%)  | 217 (96%) | 9 (4%)   | 0        | 100         | 100 |
| 40  | JH    | 257/483 (53%)  | 243 (95%) | 14 (5%)  | 0        | 100         | 100 |
| 41  | JI    | 263/1729 (15%) | 257 (98%) | 6 (2%)   | 0        | 100         | 100 |
| 42  | JJ    | 180/274 (66%)  | 172 (96%) | 8 (4%)   | 0        | 100         | 100 |
| 43  | JK    | 40/534 (8%)    | 31 (78%)  | 9 (22%)  | 0        | 100         | 100 |
| 44  | JM    | 129/217 (59%)  | 121 (94%) | 8 (6%)   | 0        | 100         | 100 |
| 45  | JN    | 178/346 (51%)  | 160 (90%) | 18 (10%) | 0        | 100         | 100 |
| 46  | JO    | 226/316 (72%)  | 214 (95%) | 12 (5%)  | 0        | 100         | 100 |
| 47  | JP    | 457/489 (94%)  | 392 (86%) | 65 (14%) | 0        | 100         | 100 |
| 48  | JQ    | 59/206 (29%)   | 53 (90%)  | 6 (10%)  | 0        | 100         | 100 |
| 49  | DE    | 243/261 (93%)  | 218 (90%) | 25 (10%) | 0        | 100         | 100 |
| 50  | DF    | 211/225 (94%)  | 189 (90%) | 22 (10%) | 0        | 100         | 100 |
| 51  | DG    | 216/236 (92%)  | 203 (94%) | 13 (6%)  | 0        | 100         | 100 |
| 52  | DH    | 182/190 (96%)  | 165 (91%) | 17 (9%)  | 0        | 100         | 100 |
| 53  | DI    | 173/200 (86%)  | 160 (92%) | 13 (8%)  | 0        | 100         | 100 |
| 54  | DJ    | 183/197 (93%)  | 154 (84%) | 29 (16%) | 0        | 100         | 100 |
| 55  | DL    | 138/156 (88%)  | 124 (90%) | 14 (10%) | 0        | 100         | 100 |
| 56  | DN    | 148/151 (98%)  | 140 (95%) | 8 (5%)   | 0        | 100         | 100 |
| 57  | DO    | 118/137 (86%)  | 107 (91%) | 11 (9%)  | 0        | 100         | 100 |
| 58  | DQ    | 123/143 (86%)  | 109 (89%) | 14 (11%) | 0        | 100         | 100 |
| 59  | DS    | 98/146 (67%)   | 91 (93%)  | 7 (7%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed   | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|-----------|----------|-------------|-----|
| 60  | DW    | 127/130 (98%)     | 110 (87%)   | 17 (13%)  | 0        | 100         | 100 |
| 61  | DX    | 101/145 (70%)     | 79 (78%)    | 21 (21%)  | 1 (1%)   | 13          | 48  |
| 62  | DY    | 132/135 (98%)     | 121 (92%)   | 11 (8%)   | 0        | 100         | 100 |
| 63  | Db    | 79/82 (96%)       | 67 (85%)    | 12 (15%)  | 0        | 100         | 100 |
| 64  | Dc    | 61/67 (91%)       | 53 (87%)    | 8 (13%)   | 0        | 100         | 100 |
| 69  | EB    | 297/305 (97%)     | 274 (92%)   | 21 (7%)   | 2 (1%)   | 19          | 56  |
| 70  | EC    | 242/246 (98%)     | 225 (93%)   | 17 (7%)   | 0        | 100         | 100 |
| 71  | ED    | 308/394 (78%)     | 283 (92%)   | 24 (8%)   | 1 (0%)   | 37          | 72  |
| 72  | EE    | 222/223 (100%)    | 209 (94%)   | 13 (6%)   | 0        | 100         | 100 |
| 73  | EF    | 266/267 (100%)    | 252 (95%)   | 14 (5%)   | 0        | 100         | 100 |
| 74  | EG    | 209/250 (84%)     | 192 (92%)   | 17 (8%)   | 0        | 100         | 100 |
| 75  | EH    | 235/240 (98%)     | 216 (92%)   | 19 (8%)   | 0        | 100         | 100 |
| 76  | EI    | 287/359 (80%)     | 263 (92%)   | 24 (8%)   | 0        | 100         | 100 |
| 77  | EJ    | 214/292 (73%)     | 198 (92%)   | 16 (8%)   | 0        | 100         | 100 |
| 78  | EK    | 965/1001 (96%)    | 939 (97%)   | 25 (3%)   | 1 (0%)   | 48          | 83  |
| 79  | EN    | 960/1073 (90%)    | 890 (93%)   | 66 (7%)   | 4 (0%)   | 30          | 68  |
| All | All   | 28798/39453 (73%) | 26318 (91%) | 2462 (8%) | 18 (0%)  | 50          | 83  |

All (18) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | UH    | 258 | PRO  |
| 31  | CH    | 438 | ILE  |
| 34  | CK    | 454 | VAL  |
| 79  | EN    | 615 | VAL  |
| 79  | EN    | 617 | SER  |
| 11  | UH    | 235 | PRO  |
| 61  | DX    | 90  | ASP  |
| 11  | UH    | 309 | PRO  |
| 11  | UH    | 533 | PRO  |
| 35  | CL    | 208 | SER  |
| 11  | UH    | 257 | SER  |
| 69  | EB    | 181 | GLU  |
| 69  | EB    | 182 | ARG  |
| 79  | EN    | 873 | SER  |
| 16  | UM    | 420 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 71  | ED    | 337 | GLU  |
| 78  | EK    | 68  | PRO  |
| 79  | EN    | 616 | ILE  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 1   | CA    | 202/240 (84%)   | 202 (100%) | 0        | 100         | 100 |
| 1   | CB    | 192/240 (80%)   | 189 (98%)  | 3 (2%)   | 58          | 74  |
| 2   | DA    | 212/224 (95%)   | 212 (100%) | 0        | 100         | 100 |
| 3   | JA    | 555/934 (59%)   | 553 (100%) | 2 (0%)   | 89          | 90  |
| 4   | UA    | 730/812 (90%)   | 728 (100%) | 2 (0%)   | 91          | 91  |
| 5   | UB    | 344/732 (47%)   | 343 (100%) | 1 (0%)   | 91          | 91  |
| 6   | UC    | 107/538 (20%)   | 107 (100%) | 0        | 100         | 100 |
| 7   | UD    | 615/713 (86%)   | 612 (100%) | 3 (0%)   | 86          | 89  |
| 8   | UE    | 428/574 (75%)   | 428 (100%) | 0        | 100         | 100 |
| 9   | UF    | 277/414 (67%)   | 275 (99%)  | 2 (1%)   | 81          | 87  |
| 10  | UG    | 462/480 (96%)   | 461 (100%) | 1 (0%)   | 92          | 93  |
| 11  | UH    | 152/657 (23%)   | 151 (99%)  | 1 (1%)   | 81          | 87  |
| 12  | UI    | 99/533 (19%)    | 98 (99%)   | 1 (1%)   | 73          | 81  |
| 13  | UJ    | 1031/1633 (63%) | 1025 (99%) | 6 (1%)   | 84          | 88  |
| 14  | UK    | 226/234 (97%)   | 225 (100%) | 1 (0%)   | 89          | 90  |
| 15  | UL    | 747/832 (90%)   | 746 (100%) | 1 (0%)   | 92          | 94  |
| 16  | UM    | 668/719 (93%)   | 665 (100%) | 3 (0%)   | 89          | 90  |
| 17  | UN    | 137/808 (17%)   | 137 (100%) | 0        | 100         | 100 |
| 18  | UO    | 437/454 (96%)   | 437 (100%) | 0        | 100         | 100 |
| 19  | UP    | 57/196 (29%)    | 56 (98%)   | 1 (2%)   | 54          | 71  |
| 20  | UQ    | 769/826 (93%)   | 766 (100%) | 3 (0%)   | 89          | 90  |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 21  | UR    | 425/529 (80%)   | 424 (100%)  | 1 (0%)   | 92          | 93  |
| 22  | US    | 332/506 (66%)   | 332 (100%)  | 0        | 100         | 100 |
| 23  | UT    | 1787/2307 (78%) | 1780 (100%) | 7 (0%)   | 89          | 90  |
| 24  | UU    | 743/819 (91%)   | 743 (100%)  | 0        | 100         | 100 |
| 25  | UV    | 986/1125 (88%)  | 982 (100%)  | 4 (0%)   | 89          | 90  |
| 26  | UX    | 156/169 (92%)   | 156 (100%)  | 0        | 100         | 100 |
| 27  | UZ    | 230/256 (90%)   | 230 (100%)  | 0        | 100         | 100 |
| 28  | CD    | 326/435 (75%)   | 326 (100%)  | 0        | 100         | 100 |
| 29  | CE    | 353/433 (82%)   | 350 (99%)   | 3 (1%)   | 79          | 84  |
| 30  | CF    | 102/104 (98%)   | 102 (100%)  | 0        | 100         | 100 |
| 30  | CG    | 101/104 (97%)   | 100 (99%)   | 1 (1%)   | 73          | 81  |
| 31  | CH    | 406/503 (81%)   | 405 (100%)  | 1 (0%)   | 92          | 93  |
| 32  | CI    | 171/172 (99%)   | 171 (100%)  | 0        | 100         | 100 |
| 33  | CJ    | 251/258 (97%)   | 250 (100%)  | 1 (0%)   | 89          | 90  |
| 34  | CK    | 187/535 (35%)   | 186 (100%)  | 1 (0%)   | 86          | 89  |
| 35  | CL    | 690/1039 (66%)  | 679 (98%)   | 11 (2%)  | 58          | 74  |
| 36  | CM    | 307/312 (98%)   | 306 (100%)  | 1 (0%)   | 91          | 91  |
| 37  | CN    | 212/274 (77%)   | 212 (100%)  | 0        | 100         | 100 |
| 38  | JC    | 318/636 (50%)   | 316 (99%)   | 2 (1%)   | 84          | 88  |
| 39  | JF    | 195/222 (88%)   | 194 (100%)  | 1 (0%)   | 86          | 89  |
| 39  | JG    | 206/222 (93%)   | 206 (100%)  | 0        | 100         | 100 |
| 42  | JJ    | 158/238 (66%)   | 157 (99%)   | 1 (1%)   | 84          | 88  |
| 43  | JK    | 35/482 (7%)     | 35 (100%)   | 0        | 100         | 100 |
| 44  | JM    | 124/200 (62%)   | 123 (99%)   | 1 (1%)   | 79          | 84  |
| 45  | JN    | 141/304 (46%)   | 141 (100%)  | 0        | 100         | 100 |
| 46  | JO    | 210/289 (73%)   | 210 (100%)  | 0        | 100         | 100 |
| 47  | JP    | 416/443 (94%)   | 415 (100%)  | 1 (0%)   | 92          | 93  |
| 48  | JQ    | 22/192 (12%)    | 22 (100%)   | 0        | 100         | 100 |
| 49  | DE    | 209/222 (94%)   | 206 (99%)   | 3 (1%)   | 62          | 75  |
| 50  | DF    | 180/191 (94%)   | 180 (100%)  | 0        | 100         | 100 |
| 51  | DG    | 187/201 (93%)   | 183 (98%)   | 4 (2%)   | 48          | 67  |

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| Mol | Chain | Analysed          | Rotameric    | Outliers | Percentiles |     |
|-----|-------|-------------------|--------------|----------|-------------|-----|
| 52  | DH    | 165/170 (97%)     | 165 (100%)   | 0        | 100         | 100 |
| 53  | DI    | 142/161 (88%)     | 139 (98%)    | 3 (2%)   | 48          | 67  |
| 54  | DJ    | 158/166 (95%)     | 158 (100%)   | 0        | 100         | 100 |
| 55  | DL    | 125/137 (91%)     | 124 (99%)    | 1 (1%)   | 79          | 84  |
| 56  | DN    | 127/128 (99%)     | 126 (99%)    | 1 (1%)   | 79          | 84  |
| 57  | DO    | 91/105 (87%)      | 90 (99%)     | 1 (1%)   | 70          | 80  |
| 58  | DQ    | 105/119 (88%)     | 105 (100%)   | 0        | 100         | 100 |
| 60  | DW    | 110/111 (99%)     | 110 (100%)   | 0        | 100         | 100 |
| 61  | DX    | 85/120 (71%)      | 85 (100%)    | 0        | 100         | 100 |
| 62  | DY    | 112/113 (99%)     | 111 (99%)    | 1 (1%)   | 75          | 83  |
| 63  | Db    | 70/71 (99%)       | 69 (99%)     | 1 (1%)   | 62          | 75  |
| 64  | Dc    | 56/60 (93%)       | 56 (100%)    | 0        | 100         | 100 |
| All | All   | 19959/27976 (71%) | 19876 (100%) | 83 (0%)  | 88          | 90  |

All (83) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | JA    | 60   | LYS  |
| 3   | JA    | 823  | LYS  |
| 4   | UA    | 273  | ARG  |
| 4   | UA    | 430  | ARG  |
| 1   | CB    | 225  | ARG  |
| 1   | CB    | 231  | ARG  |
| 1   | CB    | 303  | GLN  |
| 5   | UB    | 680  | LYS  |
| 7   | UD    | 370  | ARG  |
| 7   | UD    | 389  | ARG  |
| 7   | UD    | 689  | ASN  |
| 9   | UF    | 191  | ASN  |
| 9   | UF    | 288  | LYS  |
| 10  | UG    | 334  | ARG  |
| 11  | UH    | 604  | LYS  |
| 12  | UI    | 513  | ARG  |
| 13  | UJ    | 51   | ASN  |
| 13  | UJ    | 251  | LYS  |
| 13  | UJ    | 289  | LYS  |
| 13  | UJ    | 699  | ARG  |
| 13  | UJ    | 1542 | LYS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 13  | UJ    | 1587 | ARG  |
| 14  | UK    | 187  | LYS  |
| 15  | UL    | 297  | LYS  |
| 16  | UM    | 159  | LYS  |
| 16  | UM    | 230  | LYS  |
| 16  | UM    | 256  | ARG  |
| 19  | UP    | 158  | LYS  |
| 20  | UQ    | 336  | ARG  |
| 20  | UQ    | 675  | ARG  |
| 20  | UQ    | 704  | ASN  |
| 21  | UR    | 420  | ARG  |
| 23  | UT    | 5    | ARG  |
| 23  | UT    | 13   | ARG  |
| 23  | UT    | 328  | ARG  |
| 23  | UT    | 449  | ARG  |
| 23  | UT    | 482  | ARG  |
| 23  | UT    | 1477 | LYS  |
| 23  | UT    | 1716 | MET  |
| 25  | UV    | 99   | LYS  |
| 25  | UV    | 307  | LYS  |
| 25  | UV    | 347  | LYS  |
| 25  | UV    | 598  | LYS  |
| 29  | CE    | 37   | LYS  |
| 29  | CE    | 80   | LYS  |
| 29  | CE    | 215  | ARG  |
| 30  | CG    | 35   | LYS  |
| 31  | CH    | 146  | LYS  |
| 33  | CJ    | 118  | ASN  |
| 34  | CK    | 538  | LYS  |
| 35  | CL    | 82   | LYS  |
| 35  | CL    | 92   | ARG  |
| 35  | CL    | 119  | GLU  |
| 35  | CL    | 173  | HIS  |
| 35  | CL    | 175  | ASP  |
| 35  | CL    | 208  | SER  |
| 35  | CL    | 215  | TYR  |
| 35  | CL    | 366  | MET  |
| 35  | CL    | 568  | ARG  |
| 35  | CL    | 624  | LYS  |
| 35  | CL    | 1049 | ASN  |
| 36  | CM    | 340  | LYS  |
| 38  | JC    | 142  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38  | JC    | 266 | LYS  |
| 39  | JF    | 188 | ARG  |
| 42  | JJ    | 144 | LYS  |
| 44  | JM    | 216 | ARG  |
| 47  | JP    | 440 | ARG  |
| 49  | DE    | 108 | ARG  |
| 49  | DE    | 191 | ARG  |
| 49  | DE    | 211 | LYS  |
| 51  | DG    | 31  | ARG  |
| 51  | DG    | 58  | LYS  |
| 51  | DG    | 95  | LYS  |
| 51  | DG    | 149 | LYS  |
| 53  | DI    | 22  | ARG  |
| 53  | DI    | 47  | ARG  |
| 53  | DI    | 151 | LYS  |
| 55  | DL    | 67  | ARG  |
| 56  | DN    | 64  | ARG  |
| 57  | DO    | 24  | ASN  |
| 62  | DY    | 128 | LYS  |
| 63  | Db    | 80  | ARG  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (161) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | CA    | 93  | HIS  |
| 1   | CA    | 183 | HIS  |
| 2   | DA    | 146 | GLN  |
| 2   | DA    | 149 | GLN  |
| 2   | DA    | 211 | HIS  |
| 3   | JA    | 16  | ASN  |
| 3   | JA    | 39  | ASN  |
| 3   | JA    | 75  | ASN  |
| 3   | JA    | 89  | ASN  |
| 3   | JA    | 487 | ASN  |
| 3   | JA    | 587 | GLN  |
| 3   | JA    | 734 | HIS  |
| 4   | UA    | 88  | ASN  |
| 4   | UA    | 303 | ASN  |
| 4   | UA    | 342 | GLN  |
| 4   | UA    | 434 | ASN  |
| 5   | UB    | 446 | GLN  |
| 5   | UB    | 658 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 5   | UB    | 666  | GLN  |
| 5   | UB    | 705  | HIS  |
| 7   | UD    | 53   | HIS  |
| 7   | UD    | 306  | GLN  |
| 7   | UD    | 312  | ASN  |
| 7   | UD    | 315  | GLN  |
| 7   | UD    | 574  | HIS  |
| 7   | UD    | 632  | ASN  |
| 8   | UE    | 103  | ASN  |
| 8   | UE    | 293  | ASN  |
| 9   | UF    | 169  | GLN  |
| 9   | UF    | 289  | HIS  |
| 10  | UG    | 115  | HIS  |
| 10  | UG    | 170  | GLN  |
| 10  | UG    | 337  | HIS  |
| 10  | UG    | 410  | ASN  |
| 10  | UG    | 531  | HIS  |
| 13  | UJ    | 84   | ASN  |
| 13  | UJ    | 209  | GLN  |
| 13  | UJ    | 304  | GLN  |
| 13  | UJ    | 715  | HIS  |
| 13  | UJ    | 747  | GLN  |
| 13  | UJ    | 1580 | ASN  |
| 14  | UK    | 65   | HIS  |
| 14  | UK    | 200  | GLN  |
| 14  | UK    | 204  | HIS  |
| 15  | UL    | 88   | HIS  |
| 15  | UL    | 330  | GLN  |
| 15  | UL    | 403  | ASN  |
| 15  | UL    | 629  | ASN  |
| 15  | UL    | 901  | ASN  |
| 15  | UL    | 916  | HIS  |
| 16  | UM    | 89   | HIS  |
| 16  | UM    | 241  | GLN  |
| 16  | UM    | 268  | GLN  |
| 16  | UM    | 387  | HIS  |
| 16  | UM    | 418  | ASN  |
| 16  | UM    | 532  | HIS  |
| 16  | UM    | 585  | ASN  |
| 16  | UM    | 732  | ASN  |
| 17  | UN    | 299  | ASN  |
| 18  | UO    | 233  | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 18  | UO    | 280  | HIS  |
| 18  | UO    | 391  | ASN  |
| 18  | UO    | 394  | GLN  |
| 18  | UO    | 403  | ASN  |
| 18  | UO    | 444  | ASN  |
| 20  | UQ    | 50   | ASN  |
| 20  | UQ    | 51   | GLN  |
| 20  | UQ    | 115  | HIS  |
| 20  | UQ    | 200  | ASN  |
| 20  | UQ    | 248  | GLN  |
| 20  | UQ    | 329  | ASN  |
| 20  | UQ    | 366  | ASN  |
| 20  | UQ    | 412  | ASN  |
| 20  | UQ    | 434  | GLN  |
| 20  | UQ    | 471  | GLN  |
| 20  | UQ    | 491  | GLN  |
| 20  | UQ    | 579  | ASN  |
| 20  | UQ    | 606  | HIS  |
| 20  | UQ    | 609  | ASN  |
| 20  | UQ    | 690  | ASN  |
| 20  | UQ    | 868  | ASN  |
| 21  | UR    | 242  | ASN  |
| 21  | UR    | 307  | GLN  |
| 21  | UR    | 365  | ASN  |
| 21  | UR    | 388  | HIS  |
| 21  | UR    | 472  | GLN  |
| 22  | US    | 268  | GLN  |
| 22  | US    | 288  | HIS  |
| 22  | US    | 472  | HIS  |
| 23  | UT    | 227  | ASN  |
| 23  | UT    | 248  | HIS  |
| 23  | UT    | 300  | GLN  |
| 23  | UT    | 492  | GLN  |
| 23  | UT    | 890  | ASN  |
| 23  | UT    | 1366 | ASN  |
| 23  | UT    | 1401 | ASN  |
| 23  | UT    | 1618 | ASN  |
| 23  | UT    | 1760 | ASN  |
| 23  | UT    | 1996 | GLN  |
| 24  | UU    | 208  | GLN  |
| 24  | UU    | 263  | HIS  |
| 24  | UU    | 338  | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | UU    | 364  | HIS  |
| 24  | UU    | 387  | GLN  |
| 24  | UU    | 552  | HIS  |
| 24  | UU    | 575  | GLN  |
| 25  | UV    | 177  | ASN  |
| 25  | UV    | 414  | HIS  |
| 25  | UV    | 441  | GLN  |
| 25  | UV    | 506  | GLN  |
| 25  | UV    | 1026 | ASN  |
| 25  | UV    | 1221 | HIS  |
| 26  | UX    | 147  | GLN  |
| 28  | CD    | 85   | ASN  |
| 28  | CD    | 173  | HIS  |
| 28  | CD    | 287  | GLN  |
| 29  | CE    | 165  | GLN  |
| 29  | CE    | 254  | ASN  |
| 30  | CG    | 18   | GLN  |
| 31  | CH    | 164  | GLN  |
| 31  | CH    | 195  | GLN  |
| 31  | CH    | 419  | ASN  |
| 31  | CH    | 463  | GLN  |
| 31  | CH    | 465  | GLN  |
| 33  | CJ    | 18   | GLN  |
| 33  | CJ    | 102  | GLN  |
| 33  | CJ    | 226  | ASN  |
| 34  | CK    | 480  | GLN  |
| 35  | CL    | 765  | ASN  |
| 35  | CL    | 776  | GLN  |
| 35  | CL    | 835  | HIS  |
| 35  | CL    | 1114 | GLN  |
| 36  | CM    | 220  | GLN  |
| 36  | CM    | 248  | GLN  |
| 38  | JC    | 126  | GLN  |
| 38  | JC    | 333  | ASN  |
| 38  | JC    | 339  | HIS  |
| 39  | JF    | 115  | GLN  |
| 39  | JF    | 143  | GLN  |
| 39  | JF    | 215  | ASN  |
| 44  | JM    | 135  | HIS  |
| 46  | JO    | 58   | ASN  |
| 47  | JP    | 284  | HIS  |
| 50  | DF    | 103  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50  | DF    | 169 | ASN  |
| 50  | DF    | 200 | ASN  |
| 51  | DG    | 56  | ASN  |
| 51  | DG    | 197 | ASN  |
| 52  | DH    | 5   | GLN  |
| 52  | DH    | 147 | ASN  |
| 53  | DI    | 87  | ASN  |
| 54  | DJ    | 131 | GLN  |
| 55  | DL    | 98  | ASN  |
| 56  | DN    | 5   | HIS  |
| 56  | DN    | 105 | ASN  |
| 60  | DW    | 15  | ASN  |
| 60  | DW    | 42  | GLN  |
| 60  | DW    | 80  | ASN  |
| 62  | DY    | 77  | ASN  |
| 63  | Db    | 19  | HIS  |
| 63  | Db    | 42  | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 65  | D2    | 443/700 (63%)   | 140 (31%)         | 4 (0%)          |
| 66  | D3    | 1303/1808 (72%) | 498 (38%)         | 26 (1%)         |
| 67  | D4    | 223/333 (66%)   | 72 (32%)          | 4 (1%)          |
| 68  | EA    | 21/22 (95%)     | 15 (71%)          | 0               |
| All | All   | 1990/2863 (69%) | 725 (36%)         | 34 (1%)         |

All (725) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 65  | D2    | 6   | A    |
| 65  | D2    | 8   | A    |
| 65  | D2    | 14  | U    |
| 65  | D2    | 15  | G    |
| 65  | D2    | 17  | A    |
| 65  | D2    | 58  | U    |
| 65  | D2    | 63  | G    |
| 65  | D2    | 64  | U    |
| 65  | D2    | 66  | C    |
| 65  | D2    | 68  | U    |
| 65  | D2    | 70  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 65  | D2    | 82  | A    |
| 65  | D2    | 83  | U    |
| 65  | D2    | 84  | G    |
| 65  | D2    | 86  | C    |
| 65  | D2    | 90  | G    |
| 65  | D2    | 98  | G    |
| 65  | D2    | 102 | A    |
| 65  | D2    | 103 | G    |
| 65  | D2    | 104 | A    |
| 65  | D2    | 108 | U    |
| 65  | D2    | 109 | C    |
| 65  | D2    | 110 | G    |
| 65  | D2    | 122 | U    |
| 65  | D2    | 124 | A    |
| 65  | D2    | 125 | G    |
| 65  | D2    | 129 | U    |
| 65  | D2    | 130 | G    |
| 65  | D2    | 141 | A    |
| 65  | D2    | 142 | U    |
| 65  | D2    | 144 | C    |
| 65  | D2    | 147 | C    |
| 65  | D2    | 149 | U    |
| 65  | D2    | 150 | G    |
| 65  | D2    | 152 | U    |
| 65  | D2    | 153 | U    |
| 65  | D2    | 154 | A    |
| 65  | D2    | 155 | A    |
| 65  | D2    | 156 | U    |
| 65  | D2    | 161 | A    |
| 65  | D2    | 162 | U    |
| 65  | D2    | 163 | G    |
| 65  | D2    | 169 | A    |
| 65  | D2    | 171 | G    |
| 65  | D2    | 177 | U    |
| 65  | D2    | 181 | A    |
| 65  | D2    | 191 | U    |
| 65  | D2    | 193 | G    |
| 65  | D2    | 197 | G    |
| 65  | D2    | 198 | A    |
| 65  | D2    | 200 | A    |
| 65  | D2    | 207 | G    |
| 65  | D2    | 221 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 65  | D2    | 226 | U    |
| 65  | D2    | 227 | U    |
| 65  | D2    | 232 | U    |
| 65  | D2    | 233 | G    |
| 65  | D2    | 234 | A    |
| 65  | D2    | 235 | A    |
| 65  | D2    | 236 | C    |
| 65  | D2    | 238 | G    |
| 65  | D2    | 239 | U    |
| 65  | D2    | 240 | C    |
| 65  | D2    | 252 | A    |
| 65  | D2    | 253 | U    |
| 65  | D2    | 254 | C    |
| 65  | D2    | 256 | U    |
| 65  | D2    | 257 | G    |
| 65  | D2    | 259 | G    |
| 65  | D2    | 261 | U    |
| 65  | D2    | 267 | U    |
| 65  | D2    | 268 | G    |
| 65  | D2    | 271 | G    |
| 65  | D2    | 277 | C    |
| 65  | D2    | 278 | G    |
| 65  | D2    | 279 | A    |
| 65  | D2    | 280 | A    |
| 65  | D2    | 281 | G    |
| 65  | D2    | 286 | U    |
| 65  | D2    | 291 | G    |
| 65  | D2    | 296 | C    |
| 65  | D2    | 297 | U    |
| 65  | D2    | 304 | U    |
| 65  | D2    | 305 | A    |
| 65  | D2    | 306 | G    |
| 65  | D2    | 310 | U    |
| 65  | D2    | 311 | C    |
| 65  | D2    | 312 | U    |
| 65  | D2    | 313 | A    |
| 65  | D2    | 314 | U    |
| 65  | D2    | 315 | U    |
| 65  | D2    | 316 | U    |
| 65  | D2    | 323 | A    |
| 65  | D2    | 324 | U    |
| 65  | D2    | 325 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 65  | D2    | 326 | C    |
| 65  | D2    | 327 | A    |
| 65  | D2    | 330 | C    |
| 65  | D2    | 333 | G    |
| 65  | D2    | 337 | G    |
| 65  | D2    | 338 | A    |
| 65  | D2    | 339 | A    |
| 65  | D2    | 340 | U    |
| 65  | D2    | 349 | G    |
| 65  | D2    | 354 | G    |
| 65  | D2    | 356 | C    |
| 65  | D2    | 365 | G    |
| 65  | D2    | 369 | G    |
| 65  | D2    | 370 | U    |
| 65  | D2    | 371 | G    |
| 65  | D2    | 372 | A    |
| 65  | D2    | 373 | U    |
| 65  | D2    | 378 | C    |
| 65  | D2    | 379 | A    |
| 65  | D2    | 381 | G    |
| 65  | D2    | 385 | A    |
| 65  | D2    | 386 | A    |
| 65  | D2    | 395 | C    |
| 65  | D2    | 396 | A    |
| 65  | D2    | 399 | U    |
| 65  | D2    | 404 | G    |
| 65  | D2    | 405 | A    |
| 65  | D2    | 406 | U    |
| 65  | D2    | 407 | A    |
| 65  | D2    | 422 | C    |
| 65  | D2    | 428 | A    |
| 65  | D2    | 430 | C    |
| 65  | D2    | 431 | A    |
| 65  | D2    | 432 | C    |
| 65  | D2    | 433 | C    |
| 65  | D2    | 451 | G    |
| 65  | D2    | 456 | U    |
| 65  | D2    | 458 | A    |
| 65  | D2    | 461 | A    |
| 65  | D2    | 464 | G    |
| 65  | D2    | 481 | U    |
| 65  | D2    | 482 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 65  | D2    | 485 | G    |
| 65  | D2    | 486 | U    |
| 65  | D2    | 487 | A    |
| 66  | D3    | -6  | A    |
| 66  | D3    | -5  | G    |
| 66  | D3    | -2  | A    |
| 66  | D3    | -1  | G    |
| 66  | D3    | 1   | U    |
| 66  | D3    | 2   | A    |
| 66  | D3    | 3   | U    |
| 66  | D3    | 4   | C    |
| 66  | D3    | 5   | U    |
| 66  | D3    | 7   | G    |
| 66  | D3    | 9   | U    |
| 66  | D3    | 16  | G    |
| 66  | D3    | 17  | C    |
| 66  | D3    | 18  | C    |
| 66  | D3    | 25  | C    |
| 66  | D3    | 26  | A    |
| 66  | D3    | 32  | U    |
| 66  | D3    | 33  | U    |
| 66  | D3    | 34  | G    |
| 66  | D3    | 35  | U    |
| 66  | D3    | 36  | C    |
| 66  | D3    | 37  | U    |
| 66  | D3    | 38  | C    |
| 66  | D3    | 39  | A    |
| 66  | D3    | 42  | G    |
| 66  | D3    | 43  | A    |
| 66  | D3    | 45  | U    |
| 66  | D3    | 46  | A    |
| 66  | D3    | 57  | G    |
| 66  | D3    | 59  | C    |
| 66  | D3    | 60  | U    |
| 66  | D3    | 65  | A    |
| 66  | D3    | 68  | A    |
| 66  | D3    | 69  | G    |
| 66  | D3    | 71  | A    |
| 66  | D3    | 72  | A    |
| 66  | D3    | 73  | U    |
| 66  | D3    | 74  | U    |
| 66  | D3    | 75  | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 66  | D3    | 76  | A    |
| 66  | D3    | 77  | U    |
| 66  | D3    | 78  | A    |
| 66  | D3    | 81  | G    |
| 66  | D3    | 100 | A    |
| 66  | D3    | 103 | A    |
| 66  | D3    | 104 | A    |
| 66  | D3    | 108 | A    |
| 66  | D3    | 114 | C    |
| 66  | D3    | 118 | U    |
| 66  | D3    | 126 | A    |
| 66  | D3    | 140 | A    |
| 66  | D3    | 141 | U    |
| 66  | D3    | 145 | A    |
| 66  | D3    | 146 | U    |
| 66  | D3    | 156 | A    |
| 66  | D3    | 158 | U    |
| 66  | D3    | 159 | U    |
| 66  | D3    | 160 | C    |
| 66  | D3    | 162 | A    |
| 66  | D3    | 171 | A    |
| 66  | D3    | 176 | C    |
| 66  | D3    | 177 | U    |
| 66  | D3    | 184 | C    |
| 66  | D3    | 186 | C    |
| 66  | D3    | 187 | G    |
| 66  | D3    | 188 | A    |
| 66  | D3    | 190 | C    |
| 66  | D3    | 191 | C    |
| 66  | D3    | 193 | U    |
| 66  | D3    | 194 | U    |
| 66  | D3    | 195 | G    |
| 66  | D3    | 197 | A    |
| 66  | D3    | 198 | A    |
| 66  | D3    | 199 | G    |
| 66  | D3    | 203 | U    |
| 66  | D3    | 211 | U    |
| 66  | D3    | 215 | A    |
| 66  | D3    | 216 | U    |
| 66  | D3    | 232 | U    |
| 66  | D3    | 233 | C    |
| 66  | D3    | 234 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 66  | D3    | 237 | C    |
| 66  | D3    | 238 | U    |
| 66  | D3    | 239 | C    |
| 66  | D3    | 240 | U    |
| 66  | D3    | 243 | G    |
| 66  | D3    | 244 | A    |
| 66  | D3    | 246 | G    |
| 66  | D3    | 247 | A    |
| 66  | D3    | 249 | U    |
| 66  | D3    | 250 | C    |
| 66  | D3    | 253 | A    |
| 66  | D3    | 257 | A    |
| 66  | D3    | 263 | C    |
| 66  | D3    | 266 | A    |
| 66  | D3    | 267 | U    |
| 66  | D3    | 271 | A    |
| 66  | D3    | 273 | G    |
| 66  | D3    | 274 | G    |
| 66  | D3    | 275 | C    |
| 66  | D3    | 277 | U    |
| 66  | D3    | 278 | U    |
| 66  | D3    | 279 | G    |
| 66  | D3    | 280 | U    |
| 66  | D3    | 281 | G    |
| 66  | D3    | 282 | C    |
| 66  | D3    | 288 | A    |
| 66  | D3    | 299 | A    |
| 66  | D3    | 302 | U    |
| 66  | D3    | 303 | U    |
| 66  | D3    | 305 | C    |
| 66  | D3    | 312 | A    |
| 66  | D3    | 313 | U    |
| 66  | D3    | 314 | C    |
| 66  | D3    | 315 | A    |
| 66  | D3    | 316 | A    |
| 66  | D3    | 317 | C    |
| 66  | D3    | 318 | U    |
| 66  | D3    | 320 | U    |
| 66  | D3    | 321 | C    |
| 66  | D3    | 322 | G    |
| 66  | D3    | 323 | A    |
| 66  | D3    | 324 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 66  | D3    | 330 | G    |
| 66  | D3    | 333 | A    |
| 66  | D3    | 335 | U    |
| 66  | D3    | 336 | G    |
| 66  | D3    | 337 | G    |
| 66  | D3    | 338 | C    |
| 66  | D3    | 342 | C    |
| 66  | D3    | 344 | A    |
| 66  | D3    | 345 | U    |
| 66  | D3    | 346 | G    |
| 66  | D3    | 347 | G    |
| 66  | D3    | 350 | U    |
| 66  | D3    | 351 | C    |
| 66  | D3    | 352 | A    |
| 66  | D3    | 355 | G    |
| 66  | D3    | 359 | A    |
| 66  | D3    | 360 | A    |
| 66  | D3    | 361 | C    |
| 66  | D3    | 365 | G    |
| 66  | D3    | 366 | A    |
| 66  | D3    | 369 | A    |
| 66  | D3    | 371 | G    |
| 66  | D3    | 373 | G    |
| 66  | D3    | 378 | A    |
| 66  | D3    | 379 | U    |
| 66  | D3    | 380 | U    |
| 66  | D3    | 387 | A    |
| 66  | D3    | 388 | G    |
| 66  | D3    | 389 | G    |
| 66  | D3    | 399 | A    |
| 66  | D3    | 400 | A    |
| 66  | D3    | 401 | A    |
| 66  | D3    | 402 | C    |
| 66  | D3    | 404 | G    |
| 66  | D3    | 407 | A    |
| 66  | D3    | 408 | C    |
| 66  | D3    | 413 | U    |
| 66  | D3    | 416 | A    |
| 66  | D3    | 417 | A    |
| 66  | D3    | 418 | G    |
| 66  | D3    | 419 | G    |
| 66  | D3    | 423 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 66  | D3    | 424 | C    |
| 66  | D3    | 425 | A    |
| 66  | D3    | 426 | G    |
| 66  | D3    | 428 | A    |
| 66  | D3    | 430 | G    |
| 66  | D3    | 436 | A    |
| 66  | D3    | 437 | A    |
| 66  | D3    | 438 | A    |
| 66  | D3    | 439 | U    |
| 66  | D3    | 440 | U    |
| 66  | D3    | 441 | A    |
| 66  | D3    | 444 | C    |
| 66  | D3    | 445 | A    |
| 66  | D3    | 448 | C    |
| 66  | D3    | 457 | G    |
| 66  | D3    | 459 | G    |
| 66  | D3    | 460 | A    |
| 66  | D3    | 464 | A    |
| 66  | D3    | 467 | G    |
| 66  | D3    | 468 | A    |
| 66  | D3    | 473 | A    |
| 66  | D3    | 475 | A    |
| 66  | D3    | 477 | A    |
| 66  | D3    | 480 | G    |
| 66  | D3    | 482 | U    |
| 66  | D3    | 487 | G    |
| 66  | D3    | 488 | G    |
| 66  | D3    | 491 | C    |
| 66  | D3    | 493 | U    |
| 66  | D3    | 494 | U    |
| 66  | D3    | 496 | G    |
| 66  | D3    | 500 | C    |
| 66  | D3    | 501 | U    |
| 66  | D3    | 505 | A    |
| 66  | D3    | 506 | A    |
| 66  | D3    | 507 | U    |
| 66  | D3    | 510 | G    |
| 66  | D3    | 511 | A    |
| 66  | D3    | 520 | A    |
| 66  | D3    | 525 | A    |
| 66  | D3    | 532 | U    |
| 66  | D3    | 536 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 66  | D3    | 539 | G    |
| 66  | D3    | 540 | G    |
| 66  | D3    | 541 | A    |
| 66  | D3    | 542 | A    |
| 66  | D3    | 545 | A    |
| 66  | D3    | 546 | U    |
| 66  | D3    | 548 | G    |
| 66  | D3    | 551 | G    |
| 66  | D3    | 557 | G    |
| 66  | D3    | 561 | G    |
| 66  | D3    | 563 | U    |
| 66  | D3    | 564 | G    |
| 66  | D3    | 565 | C    |
| 66  | D3    | 566 | C    |
| 66  | D3    | 570 | A    |
| 66  | D3    | 572 | C    |
| 66  | D3    | 573 | C    |
| 66  | D3    | 574 | G    |
| 66  | D3    | 576 | G    |
| 66  | D3    | 577 | G    |
| 66  | D3    | 578 | U    |
| 66  | D3    | 579 | A    |
| 66  | D3    | 580 | A    |
| 66  | D3    | 583 | C    |
| 66  | D3    | 584 | C    |
| 66  | D3    | 585 | A    |
| 66  | D3    | 586 | G    |
| 66  | D3    | 587 | C    |
| 66  | D3    | 594 | A    |
| 66  | D3    | 595 | G    |
| 66  | D3    | 597 | G    |
| 66  | D3    | 628 | G    |
| 66  | D3    | 633 | U    |
| 66  | D3    | 634 | G    |
| 66  | D3    | 635 | A    |
| 66  | D3    | 639 | U    |
| 66  | D3    | 640 | U    |
| 66  | D3    | 642 | G    |
| 66  | D3    | 648 | G    |
| 66  | D3    | 650 | U    |
| 66  | D3    | 654 | C    |
| 66  | D3    | 655 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 66  | D3    | 656 | G    |
| 66  | D3    | 657 | U    |
| 66  | D3    | 658 | C    |
| 66  | D3    | 677 | G    |
| 66  | D3    | 678 | A    |
| 66  | D3    | 679 | U    |
| 66  | D3    | 680 | U    |
| 66  | D3    | 681 | U    |
| 66  | D3    | 682 | C    |
| 66  | D3    | 684 | A    |
| 66  | D3    | 685 | A    |
| 66  | D3    | 688 | G    |
| 66  | D3    | 692 | C    |
| 66  | D3    | 693 | U    |
| 66  | D3    | 695 | U    |
| 66  | D3    | 748 | U    |
| 66  | D3    | 751 | G    |
| 66  | D3    | 755 | A    |
| 66  | D3    | 757 | A    |
| 66  | D3    | 758 | U    |
| 66  | D3    | 761 | G    |
| 66  | D3    | 762 | A    |
| 66  | D3    | 763 | G    |
| 66  | D3    | 764 | U    |
| 66  | D3    | 765 | G    |
| 66  | D3    | 766 | U    |
| 66  | D3    | 767 | U    |
| 66  | D3    | 768 | C    |
| 66  | D3    | 769 | A    |
| 66  | D3    | 771 | A    |
| 66  | D3    | 773 | C    |
| 66  | D3    | 774 | A    |
| 66  | D3    | 775 | G    |
| 66  | D3    | 776 | G    |
| 66  | D3    | 777 | C    |
| 66  | D3    | 778 | G    |
| 66  | D3    | 779 | U    |
| 66  | D3    | 780 | A    |
| 66  | D3    | 781 | U    |
| 66  | D3    | 782 | U    |
| 66  | D3    | 783 | G    |
| 66  | D3    | 786 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 66  | D3    | 787 | G    |
| 66  | D3    | 788 | A    |
| 66  | D3    | 792 | U    |
| 66  | D3    | 793 | A    |
| 66  | D3    | 794 | U    |
| 66  | D3    | 795 | U    |
| 66  | D3    | 796 | A    |
| 66  | D3    | 802 | G    |
| 66  | D3    | 803 | A    |
| 66  | D3    | 808 | U    |
| 66  | D3    | 810 | G    |
| 66  | D3    | 819 | G    |
| 66  | D3    | 820 | U    |
| 66  | D3    | 821 | U    |
| 66  | D3    | 822 | U    |
| 66  | D3    | 826 | U    |
| 66  | D3    | 830 | U    |
| 66  | D3    | 831 | U    |
| 66  | D3    | 832 | U    |
| 66  | D3    | 834 | G    |
| 66  | D3    | 835 | U    |
| 66  | D3    | 839 | U    |
| 66  | D3    | 840 | U    |
| 66  | D3    | 841 | U    |
| 66  | D3    | 847 | A    |
| 66  | D3    | 851 | U    |
| 66  | D3    | 852 | C    |
| 66  | D3    | 853 | G    |
| 66  | D3    | 860 | U    |
| 66  | D3    | 862 | A    |
| 66  | D3    | 863 | A    |
| 66  | D3    | 865 | A    |
| 66  | D3    | 873 | U    |
| 66  | D3    | 875 | G    |
| 66  | D3    | 878 | G    |
| 66  | D3    | 886 | U    |
| 66  | D3    | 898 | A    |
| 66  | D3    | 899 | G    |
| 66  | D3    | 906 | A    |
| 66  | D3    | 912 | U    |
| 66  | D3    | 913 | G    |
| 66  | D3    | 914 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 66  | D3    | 915  | A    |
| 66  | D3    | 926  | A    |
| 66  | D3    | 931  | C    |
| 66  | D3    | 933  | A    |
| 66  | D3    | 934  | C    |
| 66  | D3    | 935  | U    |
| 66  | D3    | 937  | C    |
| 66  | D3    | 942  | G    |
| 66  | D3    | 944  | A    |
| 66  | D3    | 948  | G    |
| 66  | D3    | 956  | C    |
| 66  | D3    | 958  | U    |
| 66  | D3    | 960  | U    |
| 66  | D3    | 963  | A    |
| 66  | D3    | 964  | U    |
| 66  | D3    | 970  | A    |
| 66  | D3    | 1029 | U    |
| 66  | D3    | 1031 | U    |
| 66  | D3    | 1033 | C    |
| 66  | D3    | 1034 | C    |
| 66  | D3    | 1035 | G    |
| 66  | D3    | 1037 | C    |
| 66  | D3    | 1038 | U    |
| 66  | D3    | 1039 | A    |
| 66  | D3    | 1040 | G    |
| 66  | D3    | 1042 | G    |
| 66  | D3    | 1044 | U    |
| 66  | D3    | 1047 | G    |
| 66  | D3    | 1053 | G    |
| 66  | D3    | 1058 | U    |
| 66  | D3    | 1060 | U    |
| 66  | D3    | 1061 | A    |
| 66  | D3    | 1062 | A    |
| 66  | D3    | 1063 | U    |
| 66  | D3    | 1064 | G    |
| 66  | D3    | 1072 | C    |
| 66  | D3    | 1074 | G    |
| 66  | D3    | 1076 | A    |
| 66  | D3    | 1080 | U    |
| 66  | D3    | 1081 | A    |
| 66  | D3    | 1084 | A    |
| 66  | D3    | 1113 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 66  | D3    | 1117 | U    |
| 66  | D3    | 1118 | G    |
| 66  | D3    | 1119 | G    |
| 66  | D3    | 1122 | G    |
| 66  | D3    | 1127 | G    |
| 66  | D3    | 1128 | C    |
| 66  | D3    | 1130 | G    |
| 66  | D3    | 1133 | A    |
| 66  | D3    | 1136 | U    |
| 66  | D3    | 1143 | A    |
| 66  | D3    | 1144 | U    |
| 66  | D3    | 1145 | U    |
| 66  | D3    | 1146 | G    |
| 66  | D3    | 1157 | A    |
| 66  | D3    | 1158 | C    |
| 66  | D3    | 1159 | C    |
| 66  | D3    | 1160 | A    |
| 66  | D3    | 1175 | U    |
| 66  | D3    | 1203 | A    |
| 66  | D3    | 1204 | A    |
| 66  | D3    | 1205 | C    |
| 66  | D3    | 1207 | C    |
| 66  | D3    | 1208 | A    |
| 66  | D3    | 1214 | U    |
| 66  | D3    | 1217 | A    |
| 66  | D3    | 1218 | G    |
| 66  | D3    | 1219 | A    |
| 66  | D3    | 1267 | G    |
| 66  | D3    | 1268 | G    |
| 66  | D3    | 1269 | U    |
| 66  | D3    | 1270 | G    |
| 66  | D3    | 1434 | U    |
| 66  | D3    | 1436 | A    |
| 66  | D3    | 1437 | U    |
| 66  | D3    | 1438 | G    |
| 66  | D3    | 1439 | C    |
| 66  | D3    | 1442 | U    |
| 66  | D3    | 1443 | U    |
| 66  | D3    | 1470 | C    |
| 66  | D3    | 1472 | C    |
| 66  | D3    | 1473 | U    |
| 66  | D3    | 1474 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 66  | D3    | 1479 | A    |
| 66  | D3    | 1482 | C    |
| 66  | D3    | 1485 | C    |
| 66  | D3    | 1486 | G    |
| 66  | D3    | 1488 | G    |
| 66  | D3    | 1489 | U    |
| 66  | D3    | 1490 | C    |
| 66  | D3    | 1491 | U    |
| 66  | D3    | 1492 | A    |
| 66  | D3    | 1493 | A    |
| 66  | D3    | 1495 | C    |
| 66  | D3    | 1498 | G    |
| 66  | D3    | 1506 | G    |
| 66  | D3    | 1514 | U    |
| 66  | D3    | 1516 | A    |
| 66  | D3    | 1525 | A    |
| 66  | D3    | 1571 | C    |
| 66  | D3    | 1573 | A    |
| 66  | D3    | 1574 | G    |
| 66  | D3    | 1575 | G    |
| 66  | D3    | 1577 | A    |
| 66  | D3    | 1584 | G    |
| 66  | D3    | 1589 | C    |
| 66  | D3    | 1590 | G    |
| 66  | D3    | 1595 | U    |
| 66  | D3    | 1596 | C    |
| 66  | D3    | 1600 | A    |
| 66  | D3    | 1602 | C    |
| 66  | D3    | 1607 | G    |
| 66  | D3    | 1616 | G    |
| 66  | D3    | 1617 | U    |
| 66  | D3    | 1618 | C    |
| 66  | D3    | 1619 | C    |
| 66  | D3    | 1621 | U    |
| 66  | D3    | 1622 | G    |
| 66  | D3    | 1623 | C    |
| 66  | D3    | 1628 | U    |
| 66  | D3    | 1629 | G    |
| 66  | D3    | 1630 | U    |
| 66  | D3    | 1631 | A    |
| 66  | D3    | 1635 | A    |
| 66  | D3    | 1636 | C    |

*Continued on next page...*

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 66  | D3    | 1637 | C    |
| 66  | D3    | 1639 | C    |
| 66  | D3    | 1654 | G    |
| 66  | D3    | 1655 | A    |
| 66  | D3    | 1657 | U    |
| 66  | D3    | 1658 | G    |
| 66  | D3    | 1659 | A    |
| 66  | D3    | 1664 | C    |
| 66  | D3    | 1666 | U    |
| 66  | D3    | 1670 | G    |
| 66  | D3    | 1678 | A    |
| 66  | D3    | 1681 | A    |
| 66  | D3    | 1682 | U    |
| 66  | D3    | 1683 | C    |
| 66  | D3    | 1684 | U    |
| 66  | D3    | 1686 | C    |
| 66  | D3    | 1695 | G    |
| 66  | D3    | 1697 | G    |
| 66  | D3    | 1699 | G    |
| 66  | D3    | 1703 | C    |
| 66  | D3    | 1705 | C    |
| 66  | D3    | 1709 | C    |
| 66  | D3    | 1711 | C    |
| 66  | D3    | 1712 | A    |
| 66  | D3    | 1715 | G    |
| 66  | D3    | 1717 | G    |
| 66  | D3    | 1731 | A    |
| 66  | D3    | 1742 | U    |
| 66  | D3    | 1746 | A    |
| 66  | D3    | 1747 | G    |
| 66  | D3    | 1750 | A    |
| 66  | D3    | 1769 | U    |
| 66  | D3    | 1770 | U    |
| 66  | D3    | 1773 | C    |
| 66  | D3    | 1780 | G    |
| 66  | D3    | 1782 | A    |
| 66  | D3    | 1783 | C    |
| 66  | D3    | 1784 | C    |
| 66  | D3    | 1787 | C    |
| 67  | D4    | 2    | U    |
| 67  | D4    | 3    | C    |
| 67  | D4    | 5    | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 67  | D4    | 14  | A    |
| 67  | D4    | 15  | U    |
| 67  | D4    | 16  | A    |
| 67  | D4    | 18  | G    |
| 67  | D4    | 23  | U    |
| 67  | D4    | 24  | U    |
| 67  | D4    | 25  | U    |
| 67  | D4    | 28  | A    |
| 67  | D4    | 29  | U    |
| 67  | D4    | 30  | A    |
| 67  | D4    | 33  | A    |
| 67  | D4    | 35  | U    |
| 67  | D4    | 36  | C    |
| 67  | D4    | 38  | U    |
| 67  | D4    | 39  | C    |
| 67  | D4    | 46  | U    |
| 67  | D4    | 47  | G    |
| 67  | D4    | 48  | A    |
| 67  | D4    | 49  | C    |
| 67  | D4    | 56  | A    |
| 67  | D4    | 59  | G    |
| 67  | D4    | 61  | G    |
| 67  | D4    | 80  | U    |
| 67  | D4    | 83  | A    |
| 67  | D4    | 88  | U    |
| 67  | D4    | 90  | C    |
| 67  | D4    | 91  | C    |
| 67  | D4    | 92  | A    |
| 67  | D4    | 93  | U    |
| 67  | D4    | 115 | G    |
| 67  | D4    | 118 | A    |
| 67  | D4    | 138 | A    |
| 67  | D4    | 140 | C    |
| 67  | D4    | 143 | G    |
| 67  | D4    | 144 | G    |
| 67  | D4    | 145 | U    |
| 67  | D4    | 149 | C    |
| 67  | D4    | 150 | A    |
| 67  | D4    | 151 | A    |
| 67  | D4    | 152 | U    |
| 67  | D4    | 155 | U    |
| 67  | D4    | 156 | U    |

*Continued on next page...*

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 67  | D4    | 157 | A    |
| 67  | D4    | 158 | G    |
| 67  | D4    | 159 | C    |
| 67  | D4    | 162 | U    |
| 67  | D4    | 176 | A    |
| 67  | D4    | 178 | U    |
| 67  | D4    | 183 | A    |
| 67  | D4    | 185 | A    |
| 67  | D4    | 186 | A    |
| 67  | D4    | 187 | A    |
| 67  | D4    | 188 | A    |
| 67  | D4    | 199 | G    |
| 67  | D4    | 205 | G    |
| 67  | D4    | 247 | U    |
| 67  | D4    | 256 | G    |
| 67  | D4    | 267 | A    |
| 67  | D4    | 305 | G    |
| 67  | D4    | 312 | U    |
| 67  | D4    | 313 | A    |
| 67  | D4    | 319 | G    |
| 67  | D4    | 322 | A    |
| 67  | D4    | 324 | U    |
| 67  | D4    | 325 | C    |
| 67  | D4    | 326 | U    |
| 67  | D4    | 328 | A    |
| 67  | D4    | 329 | C    |
| 67  | D4    | 333 | U    |
| 68  | EA    | 161 | U    |
| 68  | EA    | 162 | U    |
| 68  | EA    | 163 | U    |
| 68  | EA    | 164 | A    |
| 68  | EA    | 165 | A    |
| 68  | EA    | 166 | A    |
| 68  | EA    | 167 | U    |
| 68  | EA    | 169 | U    |
| 68  | EA    | 170 | U    |
| 68  | EA    | 171 | U    |
| 68  | EA    | 172 | U    |
| 68  | EA    | 175 | U    |
| 68  | EA    | 176 | U    |
| 68  | EA    | 177 | U    |
| 68  | EA    | 178 | U    |

All (34) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 65  | D2    | 82   | A    |
| 65  | D2    | 311  | C    |
| 65  | D2    | 314  | U    |
| 65  | D2    | 370  | U    |
| 66  | D3    | -6   | A    |
| 66  | D3    | -2   | A    |
| 66  | D3    | 0    | U    |
| 66  | D3    | 1    | U    |
| 66  | D3    | 72   | A    |
| 66  | D3    | 139  | C    |
| 66  | D3    | 278  | U    |
| 66  | D3    | 417  | A    |
| 66  | D3    | 500  | C    |
| 66  | D3    | 540  | G    |
| 66  | D3    | 547  | U    |
| 66  | D3    | 578  | U    |
| 66  | D3    | 579  | A    |
| 66  | D3    | 586  | G    |
| 66  | D3    | 782  | U    |
| 66  | D3    | 912  | U    |
| 66  | D3    | 925  | G    |
| 66  | D3    | 1057 | U    |
| 66  | D3    | 1063 | U    |
| 66  | D3    | 1158 | C    |
| 66  | D3    | 1491 | U    |
| 66  | D3    | 1573 | A    |
| 66  | D3    | 1594 | G    |
| 66  | D3    | 1620 | C    |
| 66  | D3    | 1638 | G    |
| 66  | D3    | 1657 | U    |
| 67  | D4    | 143  | G    |
| 67  | D4    | 151  | A    |
| 67  | D4    | 157  | A    |
| 67  | D4    | 318  | U    |

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 82  | GTP  | CL    | 2001 | 81   | 26,34,34     | 0.92 | 1 (3%)      | 32,54,54    | 1.49 | 5 (15%)     |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 82  | GTP  | CL    | 2001 | 81   | -       | 7/18/38/38 | 0/3/3/3 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 82  | CL    | 2001 | GTP  | C6-N1 | -2.49 | 1.34        | 1.37     |

All (5) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 82  | CL    | 2001 | GTP  | PB-O3B-PG   | -3.53 | 120.73      | 132.83   |
| 82  | CL    | 2001 | GTP  | PA-O3A-PB   | -3.32 | 121.42      | 132.83   |
| 82  | CL    | 2001 | GTP  | C3'-C2'-C1' | 3.21  | 105.81      | 100.98   |
| 82  | CL    | 2001 | GTP  | C8-N7-C5    | 2.39  | 107.54      | 102.99   |
| 82  | CL    | 2001 | GTP  | C5-C6-N1    | 2.32  | 118.05      | 113.95   |

There are no chirality outliers.

All (7) torsion outliers are listed below:

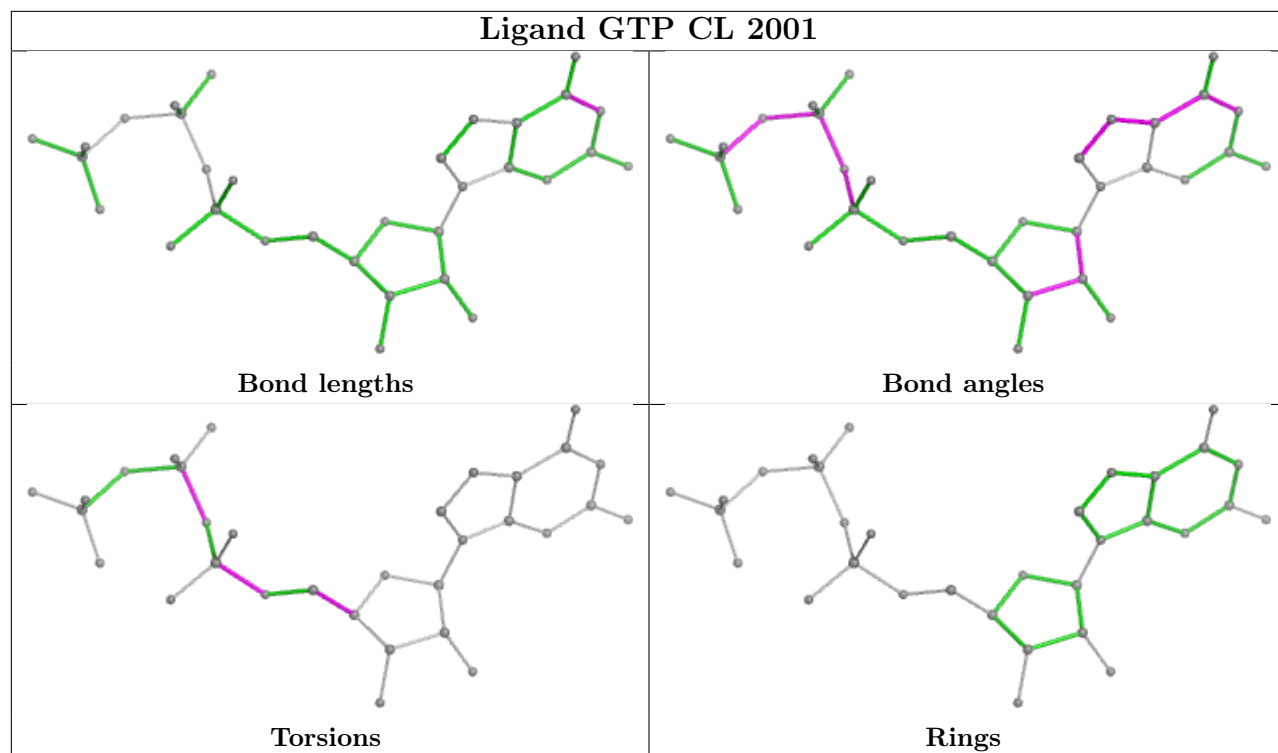
| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 82  | CL    | 2001 | GTP  | C5'-O5'-PA-O1A  |
| 82  | CL    | 2001 | GTP  | C3'-C4'-C5'-O5' |
| 82  | CL    | 2001 | GTP  | O4'-C4'-C5'-O5' |
| 82  | CL    | 2001 | GTP  | C5'-O5'-PA-O3A  |
| 82  | CL    | 2001 | GTP  | C5'-O5'-PA-O2A  |
| 82  | CL    | 2001 | GTP  | PA-O3A-PB-O1B   |
| 82  | CL    | 2001 | GTP  | PA-O3A-PB-O2B   |

There are no ring outliers.

1 monomer is involved in 2 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 82  | CL    | 2001 | GTP  | 2       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

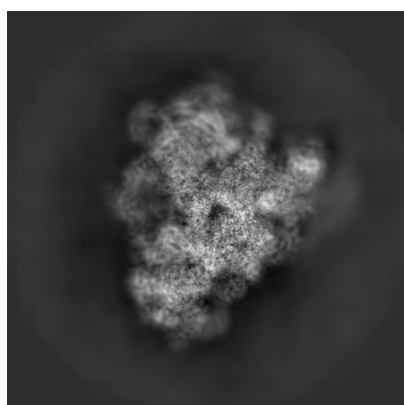
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11807. These allow visual inspection of the internal detail of the map and identification of artifacts.

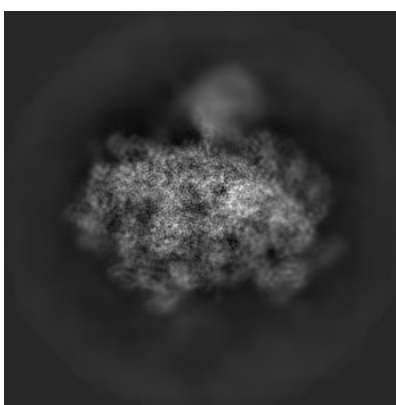
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

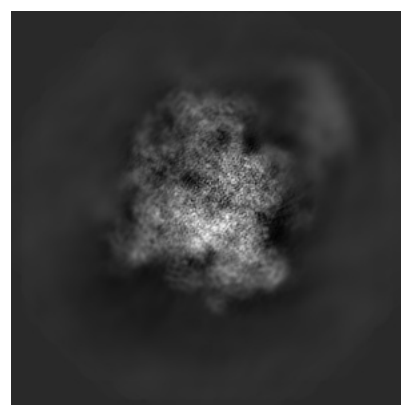
#### 6.1.1 Primary map



X



Y

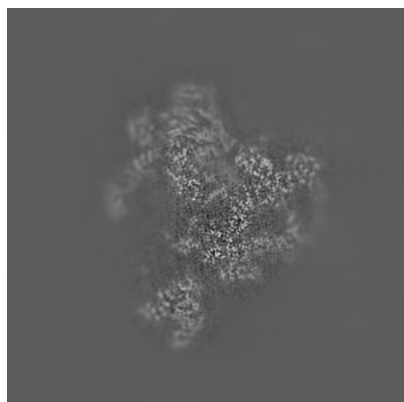


Z

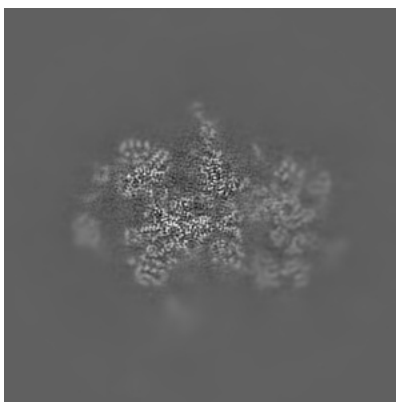
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

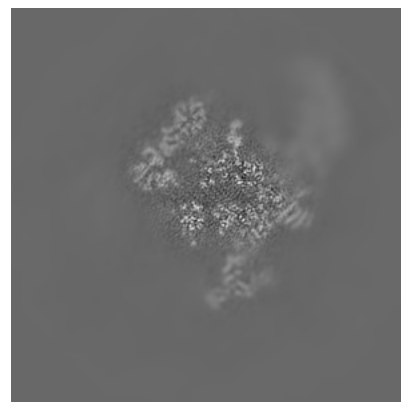
#### 6.2.1 Primary map



X Index: 270



Y Index: 270



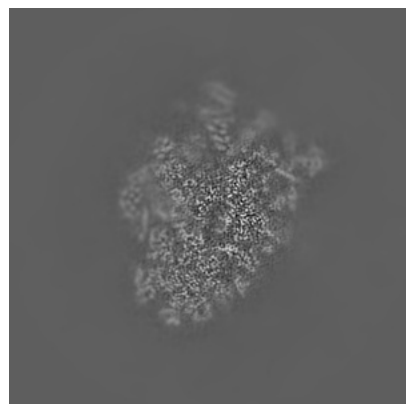
Z Index: 270



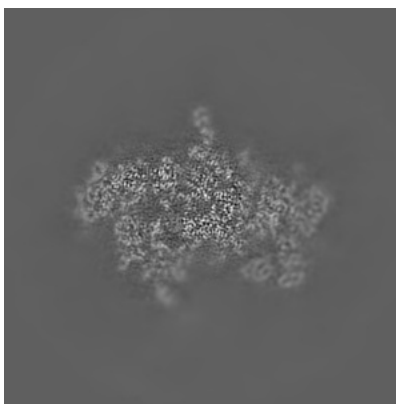
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

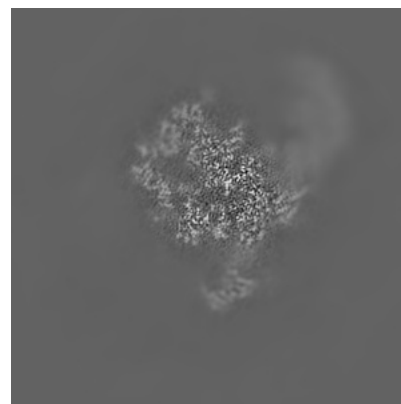
### 6.3.1 Primary map



X Index: 310



Y Index: 252

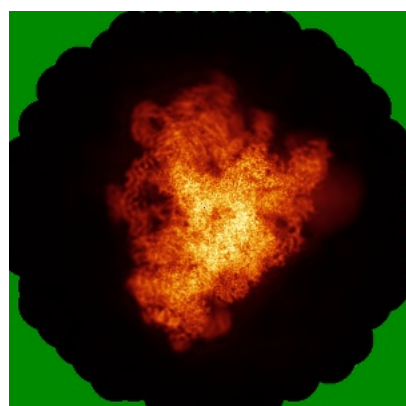


Z Index: 279

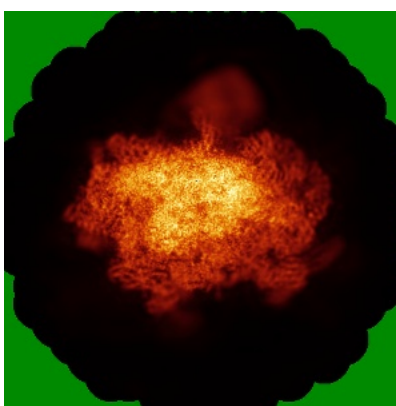
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

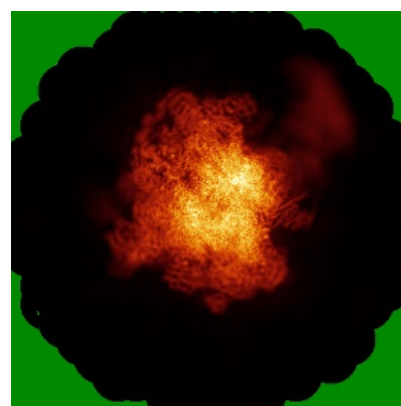
### 6.4.1 Primary map



X



Y

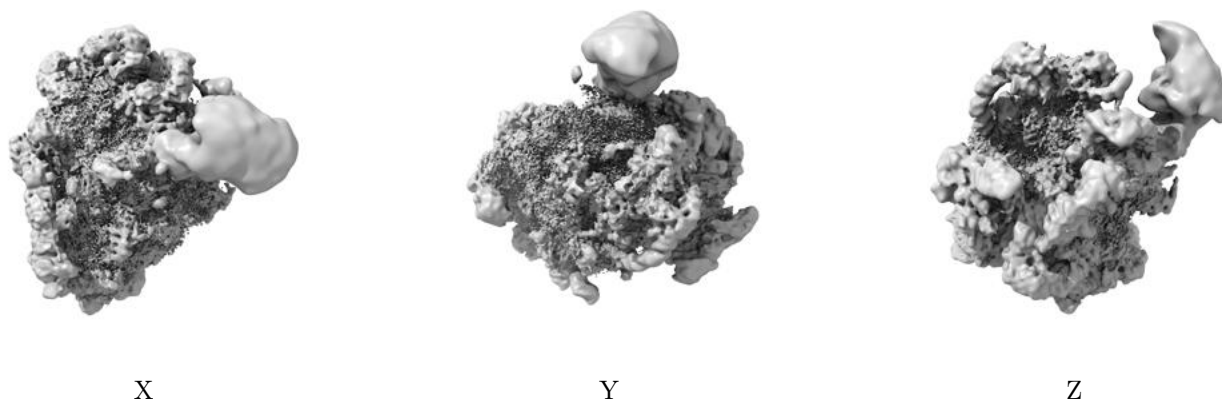


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

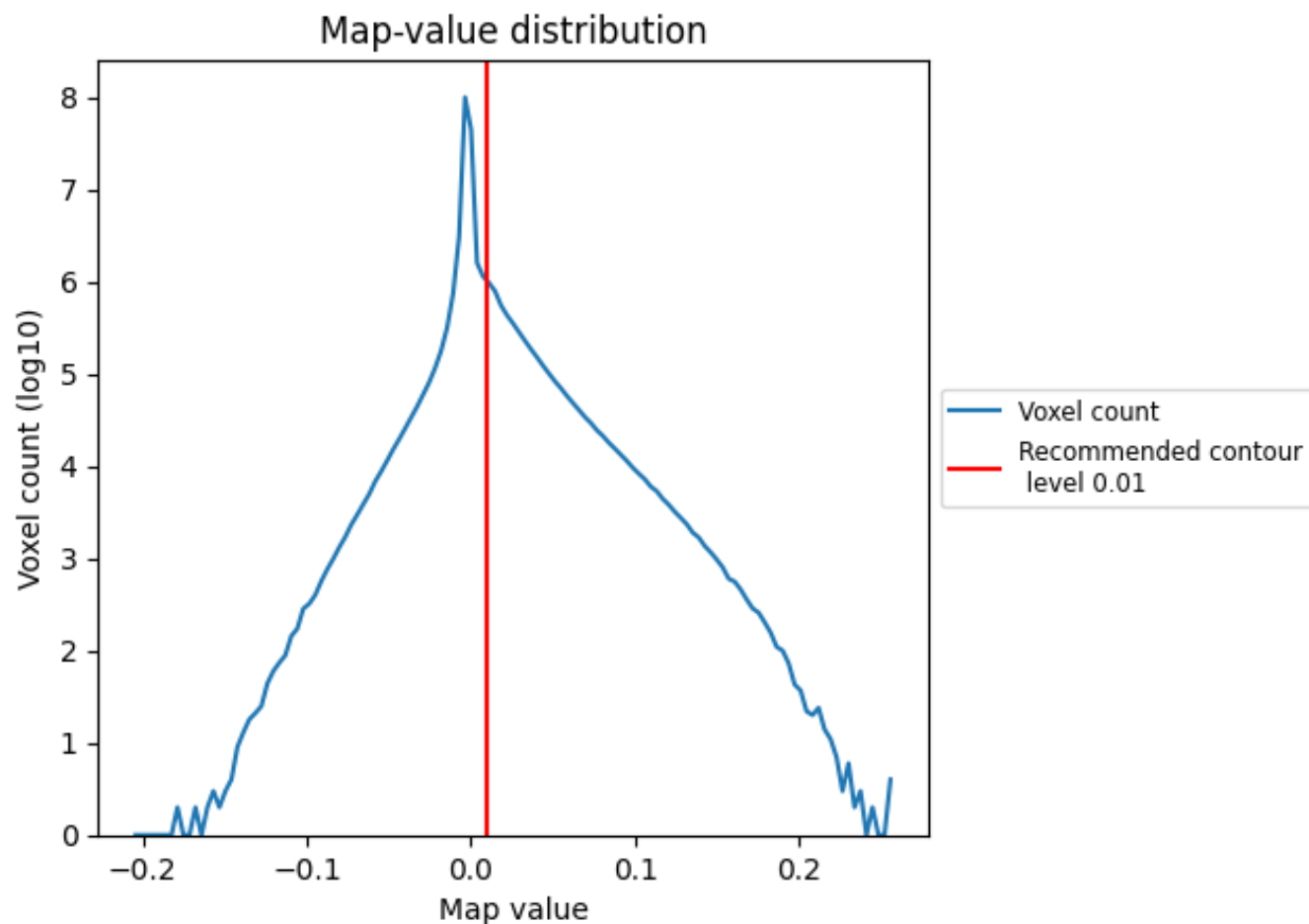
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

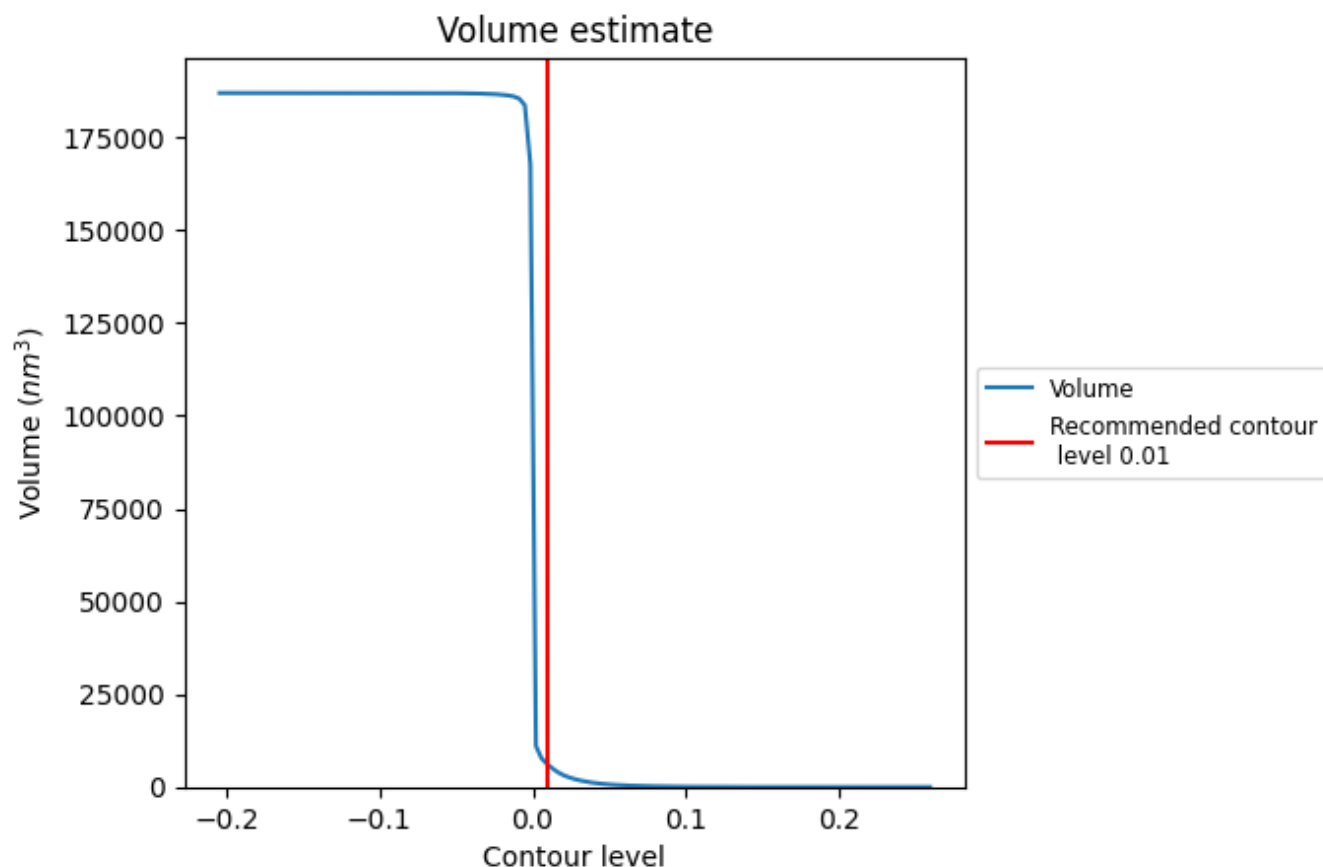
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

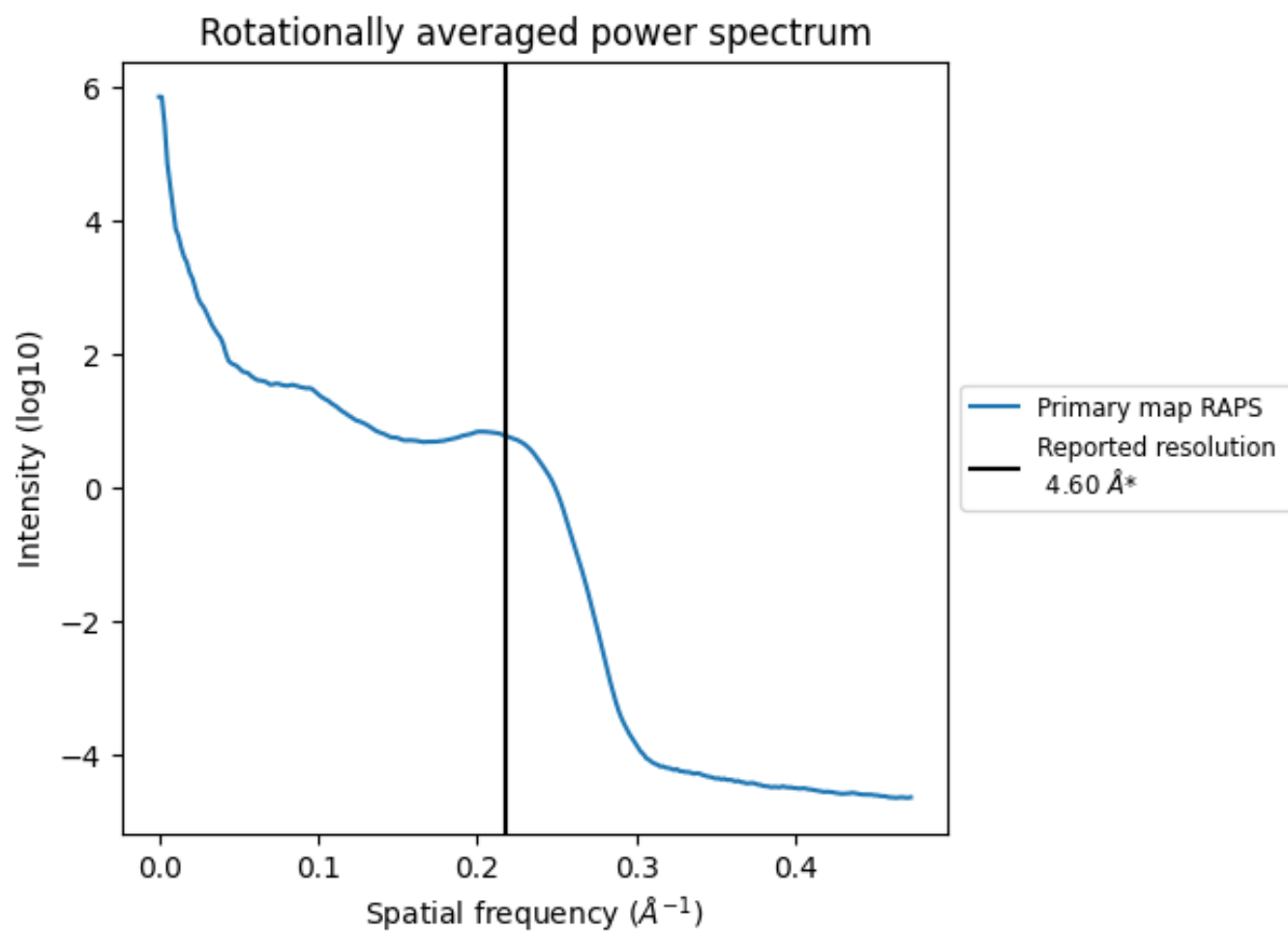
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5975 nm<sup>3</sup>; this corresponds to an approximate mass of 5397 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

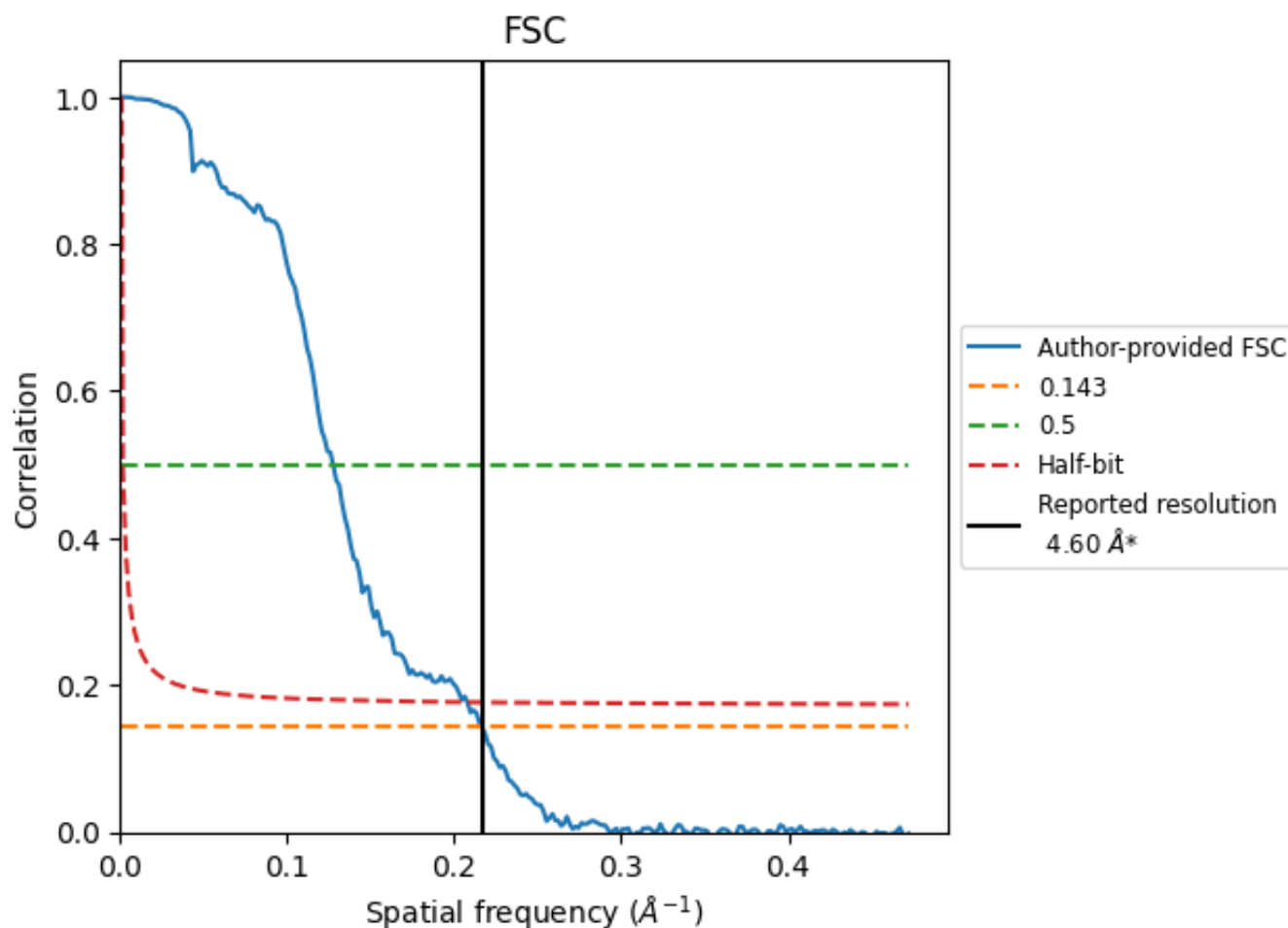


\*Reported resolution corresponds to spatial frequency of 0.217 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.217 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 4.60                               | -    | -        |
| Author-provided FSC curve | 4.62                               | 7.84 | 4.81     |
| Unmasked-calculated*      | -                                  | -    | -        |

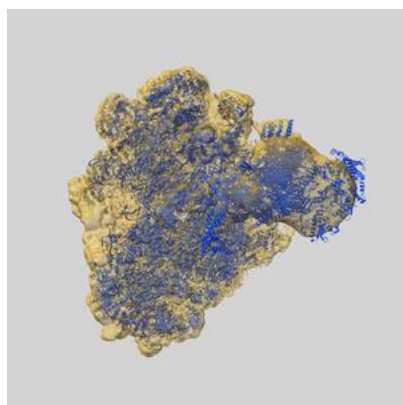
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.



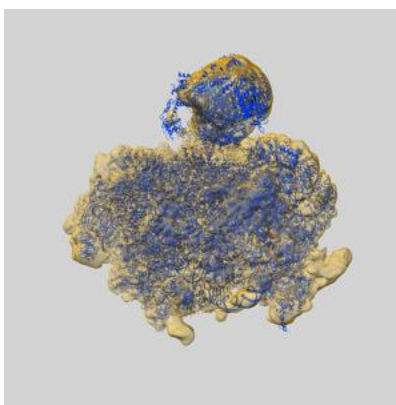
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11807 and PDB model 7AJT. Per-residue inclusion information can be found in [section 3](#) on [page 21](#).

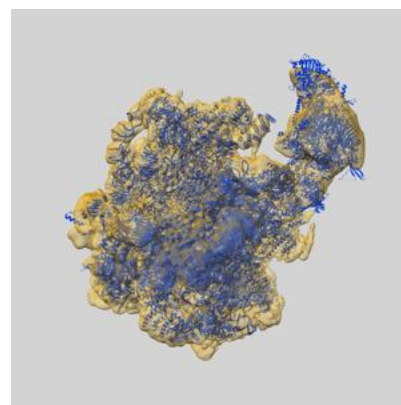
### 9.1 Map-model overlay [i](#)



X



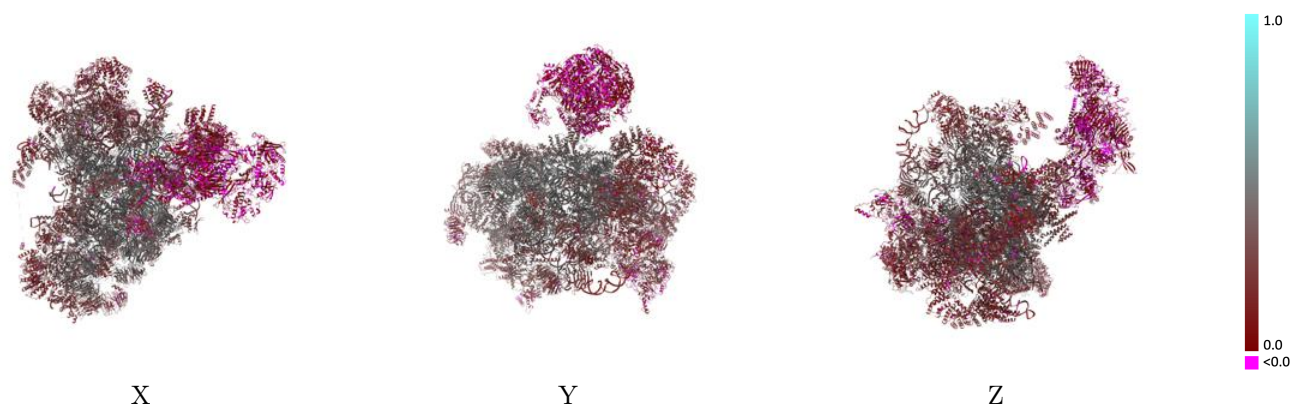
Y



Z

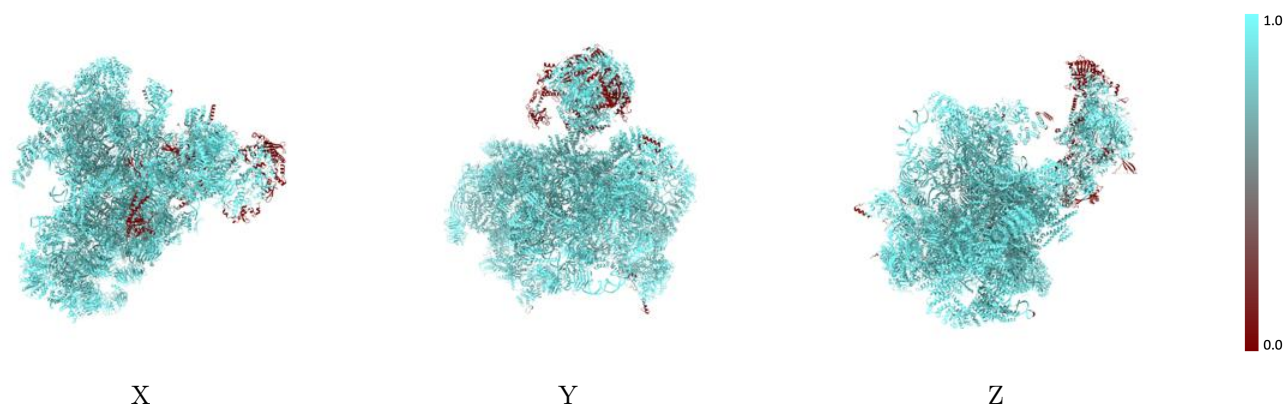
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



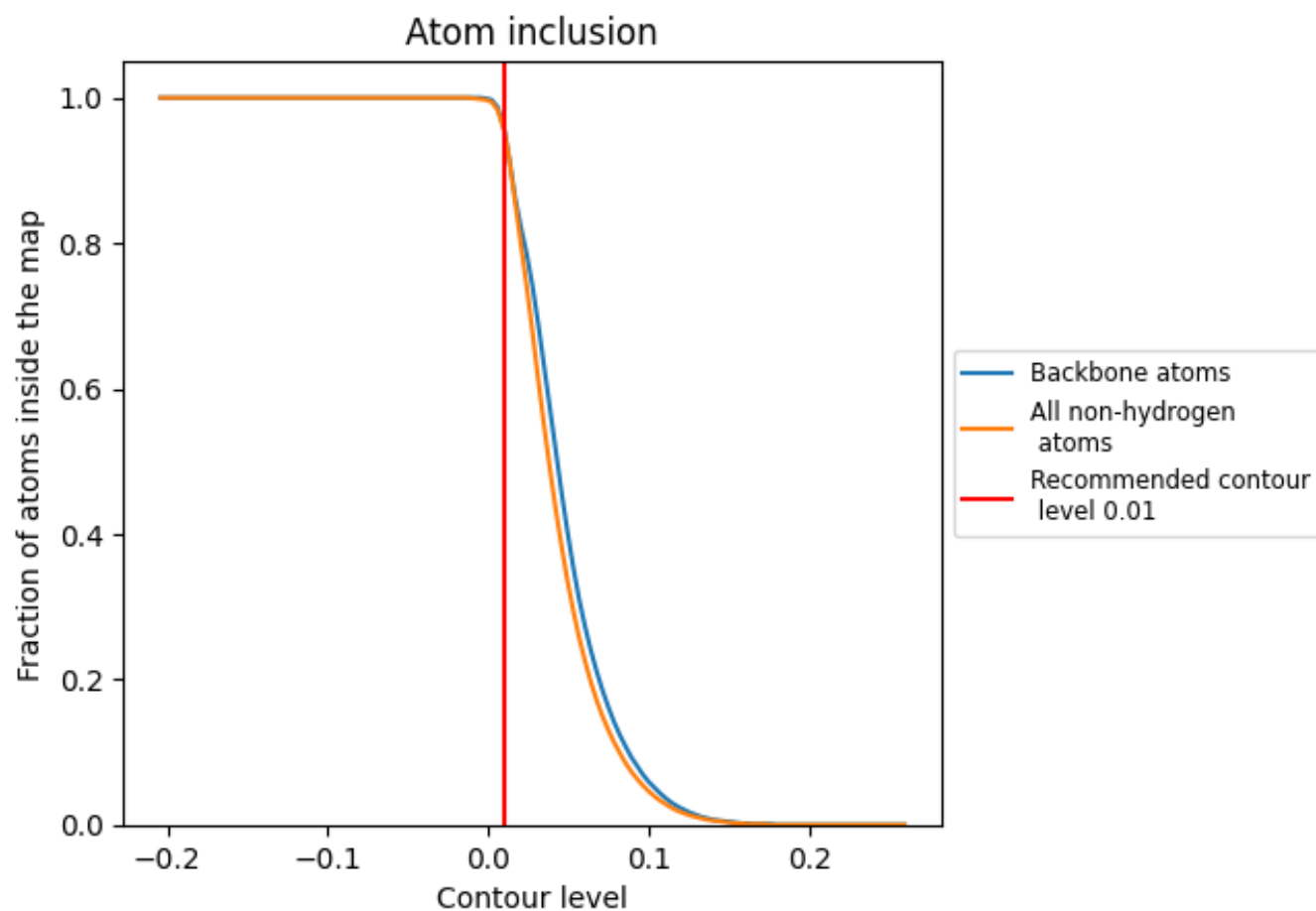
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary





















































































The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.9540   |  0.3080   |
| CA    |  0.9740   |  0.4780   |
| CB    |  0.9640   |  0.3520   |
| CD    |  0.9760   |  0.3780   |
| CE    |  0.9710   |  0.3380   |
| CF    |  0.9680   |  0.4410   |
| CG    |  0.9650   |  0.4290   |
| CH    |  0.9840   |  0.3800   |
| CI    |  0.9820   |  0.5020   |
| CJ    |  0.9740   |  0.4640   |
| CK    |  0.9710   |  0.4120   |
| CL    |  0.9710   |  0.3950   |
| CM    |  0.9760   |  0.3510   |
| CN    |  0.9730   |  0.2290   |
| D2    |  0.9950  |  0.3830  |
| D3    |  0.9840 |  0.3300 |
| D4    |  0.9740 |  0.3570 |
| DA    |  0.9670 |  0.4030 |
| DE    |  0.9630 |  0.3290 |
| DF    |  0.9820 |  0.4290 |
| DG    |  0.9620 |  0.2000 |
| DH    |  0.9530 |  0.3050 |
| DI    |  0.9680 |  0.2110 |
| DJ    |  0.9580 |  0.4480 |
| DL    |  0.9580 |  0.2070 |
| DN    |  0.9630 |  0.3770 |
| DO    |  0.9740 |  0.4170 |
| DQ    |  0.9730 |  0.4730 |
| DS    |  0.9860 |  0.3270 |
| DW    |  0.9700 |  0.4610 |
| DX    |  0.9760 |  0.4450 |
| DY    |  0.9710 |  0.3820 |
| Db    |  0.9850 |  0.4420 |
| Dc    |  0.9750 |  0.4500 |
| EA    |  0.9180 |  0.0410 |

















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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| EB    |  0.8550   |  0.0250   |
| EC    |  0.9640   |  0.0340   |
| ED    |  0.9200   |  0.0480   |
| EE    |  0.8910   |  0.0310   |
| EF    |  0.9320   |  0.0460   |
| EG    |  0.8690   |  0.0230   |
| EH    |  0.6400   |  0.0500   |
| EI    |  0.8720   |  0.0500   |
| EJ    |  0.5890   |  0.0360   |
| EK    |  0.5680   |  0.0340   |
| EN    |  0.6120   |  0.0570   |
| JA    |  0.9600   |  0.1970   |
| JB    |  0.9280   |  0.1730   |
| JC    |  0.9340   |  0.1790   |
| JF    |  0.9800   |  0.2710   |
| JG    |  0.9620   |  0.3670   |
| JH    |  0.9510   |  0.1210   |
| JI    |  0.8140  |  0.1750  |
| JJ    |  0.9710 |  0.2930 |
| JK    |  0.9360 |  0.1590 |
| JM    |  0.9720 |  0.4140 |
| JN    |  0.9730 |  0.4460 |
| JO    |  0.9720 |  0.4170 |
| JP    |  0.9740 |  0.4840 |
| JQ    |  0.9890 |  0.3430 |
| UA    |  0.9810 |  0.4650 |
| UB    |  0.9860 |  0.2670 |
| UC    |  0.9710 |  0.4160 |
| UD    |  0.9820 |  0.3340 |
| UE    |  0.9780 |  0.3730 |
| UF    |  0.9790 |  0.3530 |
| UG    |  0.9810 |  0.4670 |
| UH    |  0.9890 |  0.1870 |
| UI    |  0.9780 |  0.2160 |
| UJ    |  0.9700 |  0.2600 |
| UK    |  0.9740 |  0.4070 |
| UL    |  0.9820 |  0.3270 |
| UM    |  0.9740 |  0.2870 |
| UN    |  0.9590 |  0.4230 |
| UO    |  0.9760 |  0.3790 |
| UP    |  0.9770 |  0.3200 |
| UQ    |  0.9820 |  0.3440 |

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| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| UR    |  0.9830 |  0.4350 |
| US    |  0.9810 |  0.2890 |
| UT    |  0.9750 |  0.2090 |
| UU    |  0.9790 |  0.4300 |
| UV    |  0.9750 |  0.2370 |
| UX    |  0.9730 |  0.4970 |
| UZ    |  0.9820 |  0.3500 |