



Full wwPDB EM Validation Report ⓘ

Jun 10, 2025 – 02:45 pm BST

PDB ID : 9G33 / pdb_00009g33
EMDB ID : EMD-50991
Title : Stalled 90S - Utp23-Krr1-deltaC3
Authors : Thoms, M.; Berninghausen, O.; Beckmann, R.
Deposited on : 2024-07-11
Resolution : 3.05 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

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>.

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

EMDB validation analysis : 0.0.1.dev118
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.43.1

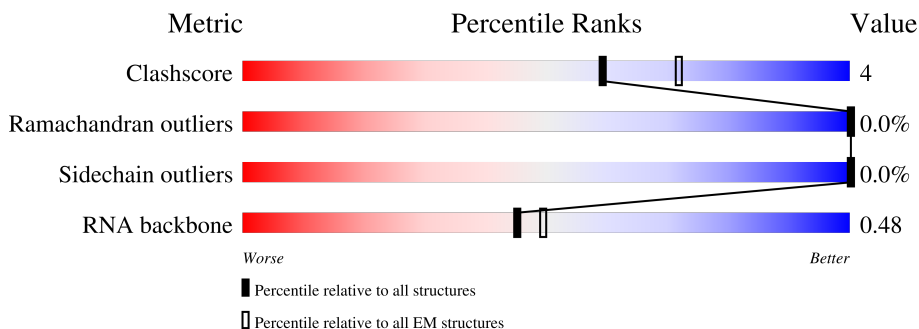
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.05 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 ≥ 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	D3	1808	
2	D2	700	
3	D4	333	
4	CJ	290	
5	CK	593	
6	CL	1183	
7	DY	135	



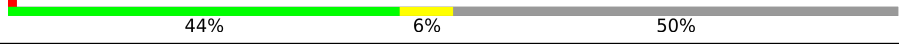


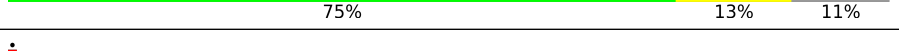
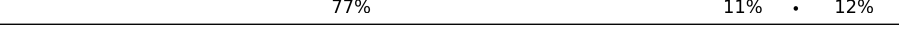
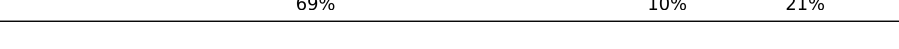
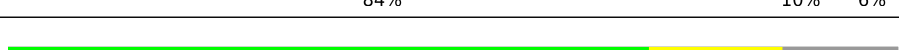

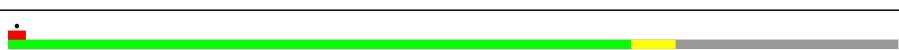

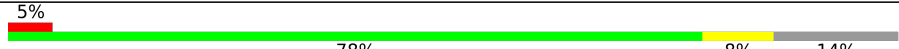
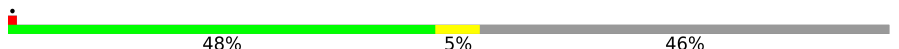



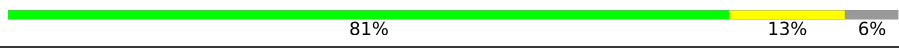
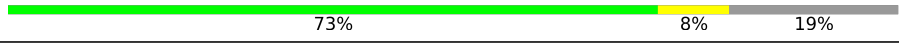


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Mol	Chain	Length	Quality of chain
8	UX	189	
9	JF	252	
9	JG	252	
10	CA	327	
10	CB	327	
11	UB	810	
12	UC	610	
13	UE	643	
14	UH	713	
15	UK	250	
16	UL	943	
17	UM	817	
18	UO	513	
19	UP	214	
20	US	552	
21	CF	126	
21	CG	126	
22	CI	183	
23	JE	357	
24	JH	483	
25	JJ	274	
26	JK	534	
27	JM	217	
28	JQ	206	
29	DF	225	








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Mol	Chain	Length	Quality of chain
30	DI	200	
31	DJ	197	
32	DS	146	
33	JC	707	
34	DE	261	
35	DX	145	
36	DW	130	
37	DG	236	
38	DL	156	
39	CH	573	
40	Dc	67	
41	DQ	143	
42	CE	511	
43	CD	504	
44	UN	899	
45	UF	440	
46	UG	554	
47	JN	346	
48	JO	316	
49	CM	367	
50	UZ	274	
51	JP	489	
52	UR	594	
53	UU	939	
54	UD	776	

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Mol	Chain	Length	Quality of chain
55	UQ	896	
56	UA	923	
57	UI	575	
58	UJ	1769	
59	DH	190	
60	UT	2493	
61	JA	1056	
61	JB	1056	

2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 203584 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 RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D3	886	Total	C	N	O	P	0	0
			18883	8442	3361	6194	886		

- Molecule 2 is a RNA chain called 5' ETS.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D2	519	Total	C	N	O	P	0	0
			11078	4950	1970	3639	519		

- Molecule 3 is a RNA chain called U3 snoRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D4	176	Total	C	N	O	P	0	0
			3731	1670	650	1235	176		

- Molecule 4 is a protein called U3 small nucleolar ribonucleoprotein protein IMP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	CJ	282	Total	C	N	O	S	0	0
			2281	1432	426	416	7		

- Molecule 5 is a protein called U3 small nucleolar RNA-associated protein MPP10.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	CK	199	Total	C	N	O	S	0	0
			1584	984	280	316	4		

- Molecule 6 is a protein called Ribosome biogenesis protein BMS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	CL	818	Total	C	N	O	S	0	0
			6472	4155	1141	1147	29		

- Molecule 7 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	DY	96	Total	C	N	O	0	0
			761	487	137	137		

- Molecule 8 is a protein called rRNA-processing protein FCF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	UX	174	Total	C	N	O	S	0	0
			1396	890	255	241	10		

- Molecule 9 is a protein called Ribosomal RNA small subunit methyltransferase NEP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	JG	231	Total	C	N	O	S	0	0
			1789	1137	308	334	10		
9	JF	217	Total	C	N	O	S	0	0
			1647	1047	281	308	11		

- Molecule 10 is a protein called rRNA 2'-O-methyltransferase fibrillarin.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	CA	241	Total	C	N	O	S	0	0
			1868	1185	334	339	10		
10	CB	227	Total	C	N	O	S	0	0
			1778	1129	319	320	10		

- Molecule 11 is a protein called Nucleolar complex protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	UB	491	Total	C	N	O	S	0	0
			3660	2331	643	675	11		

- Molecule 12 is a protein called Something about silencing protein 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	UC	128	Total	C	N	O	0	0
			1027	633	204	190		

- Molecule 13 is a protein called U3 small nucleolar RNA-associated protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	UE	478	Total	C	N	O	S	0	0
			3773	2401	647	712	13		

- Molecule 14 is a protein called U3 small nucleolar RNA-associated protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	UH	581	Total	C	N	O	S	0	0
			3518	2204	633	678	3		

- Molecule 15 is a protein called U3 small nucleolar RNA-associated protein 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	UK	240	Total	C	N	O	S	0	0
			1985	1233	384	361	7		

- Molecule 16 is a protein called U3 small nucleolar RNA-associated protein 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	UL	849	Total	C	N	O	S	0	0
			6393	4104	1080	1185	24		

- Molecule 17 is a protein called U3 small nucleolar RNA-associated protein 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	UM	160	Total	C	N	O	S	0	0
			1269	800	224	236	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	UO	494	Total	C	N	O	S	0	0
			3905	2459	700	734	12		

- Molecule 19 is a protein called U3 small nucleolar RNA-associated protein 16.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	UP	60	Total	C	N	O	0	0
			419	259	81	79		

- Molecule 20 is a protein called Nucleolar complex protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	US	542	Total	C	N	O	S	0	0
			3967	2581	663	711	12		

- Molecule 21 is a protein called 13 kDa ribonucleoprotein-associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	CF	123	Total	C	N	O	S	0	0
			932	594	160	174	4		
21	CG	121	Total	C	N	O	S	0	0
			916	583	158	171	4		

- Molecule 22 is a protein called U3 small nucleolar ribonucleoprotein protein IMP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	CI	182	Total	C	N	O	S	0	0
			1531	967	287	270	7		

- Molecule 23 is a protein called U3 small nucleolar ribonucleoprotein protein LCP5.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	JE	136	Total	C	N	O	S	0	0
			959	580	180	197	2		

- Molecule 24 is a protein called Essential nuclear protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	JH	257	Total	C	N	O		0	0
			1276	762	257	257			

- Molecule 25 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	JJ	96	Total	C	N	O		0	0
			500	300	101	99			

- Molecule 26 is a protein called Protein BFR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	JK	42	Total	C	N	O		0	0
			330	210	53	67			

- Molecule 27 is a protein called rRNA-processing protein FCF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	JM	135	Total	C	N	O	S	0	0
			1100	697	200	199	4		

- Molecule 28 is a protein called Regulator of rDNA transcription protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	JQ	157	Total	C	N	O		0	0
			860	525	164	171			

- Molecule 29 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	DF	209	Total	C	N	O	S	0	0
			1638	1029	296	310	3		

- Molecule 30 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	DI	175	Total	C	N	O	S	0	0
			1350	836	264	248	2		

- Molecule 31 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	DJ	177	Total	C	N	O	S	0	0
			1406	889	270	246	1		

- Molecule 32 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	DS	104	Total	C	N	O		0	0
			526	315	105	106			

- Molecule 33 is a protein called Ribosome biogenesis protein ENP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	JC	352	Total	C	N	O	S	0	0
			2695	1704	465	517	9		

- Molecule 34 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	DE	236	Total	C	N	O	S	0	0
			1836	1178	339	316	3		

- Molecule 35 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	DX	103	Total	C	N	O	S	0	0
			774	494	141	137	2		

- Molecule 36 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	DW	127	Total	C	N	O	S	0	0
			954	612	167	172	3		

- Molecule 37 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	DG	209	Total	C	N	O	S	0	0
			1577	999	304	272	2		

- Molecule 38 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	DL	138	Total	C	N	O	S	0	0
			1052	673	195	181	3		

- Molecule 39 is a protein called Ribosomal RNA-processing protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	CH	452	Total	C	N	O	S	0	0
			3531	2248	616	658	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Dc	63	Total	C	N	O	S	0	0
			498	306	99	92	1		

- Molecule 41 is a protein called 40S ribosomal protein S16-A.

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

- Molecule 42 is a protein called Nucleolar protein 58.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	CE	436	Total	C	N	O	S		
			3038	1912	541	578	7	0	0

- Molecule 43 is a protein called Nucleolar protein 56.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	CD	380	Total	C	N	O	S		
			2802	1771	489	535	7	0	0

- Molecule 44 is a protein called U3 small nucleolar RNA-associated protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	UN	188	Total	C	N	O	S		
			1441	894	272	273	2	0	0

- Molecule 45 is a protein called U3 small nucleolar RNA-associated protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	UF	379	Total	C	N	O	S		
			2795	1791	500	493	11	0	0

- Molecule 46 is a protein called U3 small nucleolar RNA-associated protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	UG	515	Total	C	N	O	S		
			3917	2462	706	738	11	0	0

- Molecule 47 is a protein called Protein FAF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	JN	186	Total	C	N	O	S		
			1363	844	266	250	3	0	0

- Molecule 48 is a protein called KRR1 small subunit processome component.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	JO	190	Total	C	N	O	S	0	0
			1483	955	260	258	10		

- Molecule 49 is a protein called RNA 3'-terminal phosphate cyclase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	CM	363	Total	C	N	O	S	0	0
			2768	1776	469	512	11		

- Molecule 50 is a protein called Ribosome biogenesis protein UTP30.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	UZ	254	Total	C	N	O	S	0	0
			1963	1256	351	349	7		

- Molecule 51 is a protein called Protein SOF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	JP	460	Total	C	N	O	S	0	0
			3718	2330	674	698	16		

- Molecule 52 is a protein called U3 small nucleolar RNA-associated protein 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	UR	480	Total	C	N	O	S	0	0
			3751	2379	662	700	10		

- Molecule 53 is a protein called U3 small nucleolar RNA-associated protein 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	UU	846	Total	C	N	O	S	0	0
			6606	4197	1139	1249	21		

- Molecule 54 is a protein called U3 small nucleolar RNA-associated protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	UD	680	Total	C	N	O	S	0	0
			5176	3286	901	968	21		

- Molecule 55 is a protein called NET1-associated nuclear protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	UQ	837	Total	C	N	O	S	0	0
			6559	4181	1110	1249	19		

- Molecule 56 is a protein called Periodic tryptophan protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	UA	834	Total	C	N	O	S	0	0
			6602	4203	1135	1246	18		

- Molecule 57 is a protein called U3 small nucleolar RNA-associated protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	UI	134	Total	C	N	O	S	0	0
			959	614	171	172	2		

- Molecule 58 is a protein called U3 small nucleolar RNA-associated protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	UJ	1701	Total	C	N	O	S	0	0
			10158	6323	1863	1958	14		

- Molecule 59 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
59	DH	170	Total	C	N	O	0	0
			1207	776	210	221		

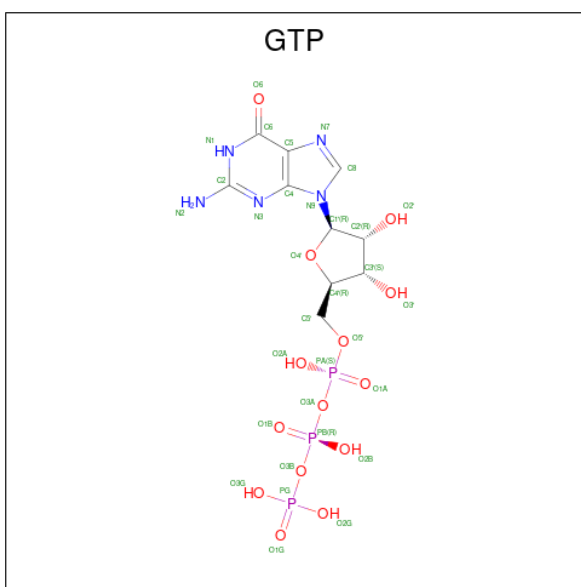
- Molecule 60 is a protein called U3 small nucleolar RNA-associated protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	UT	2345	Total	C	N	O	S	0	0
			13871	8770	2561	2529	11		

- Molecule 61 is a protein called RNA cytidine acetyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	JA	891	Total	C	N	O	S	0	0
			6631	4260	1157	1190	24		
61	JB	856	Total	C	N	O	S	0	0
			6345	4083	1094	1145	23		

- Molecule 62 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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

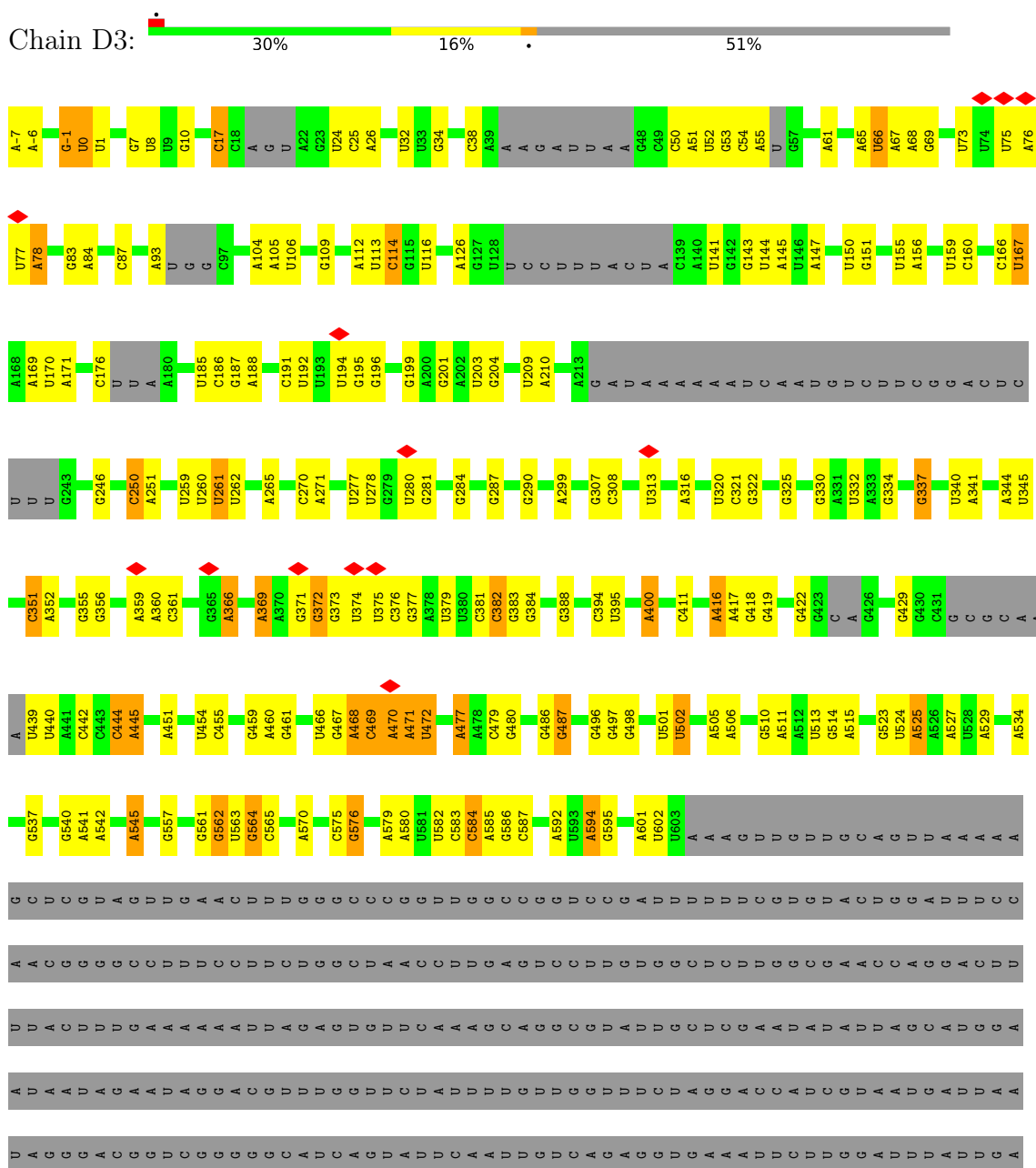
- Molecule 63 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
63	UX	1	Total Zn 1 1	0

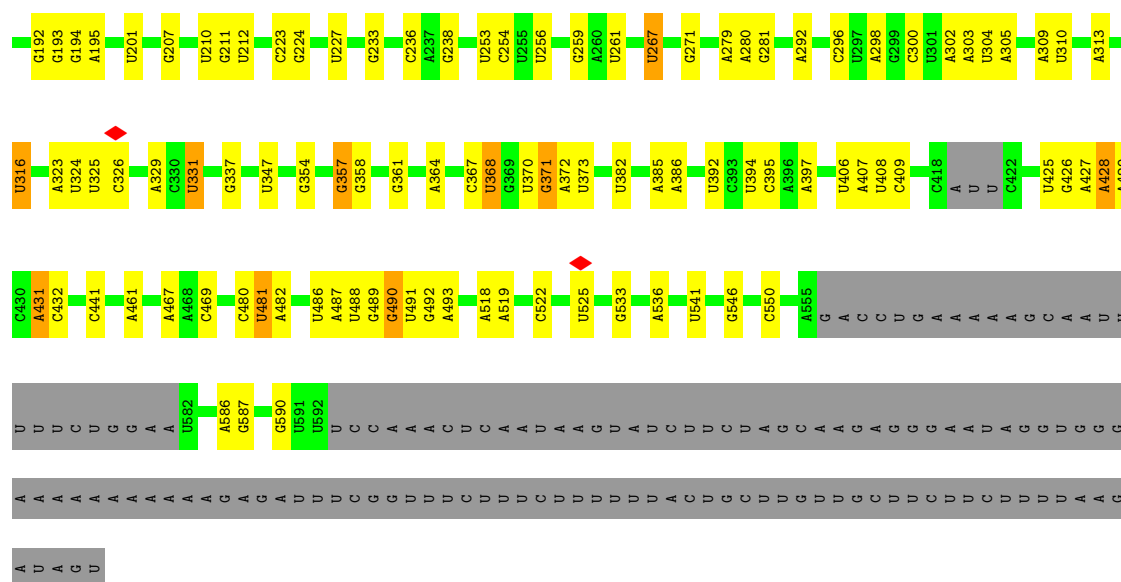
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

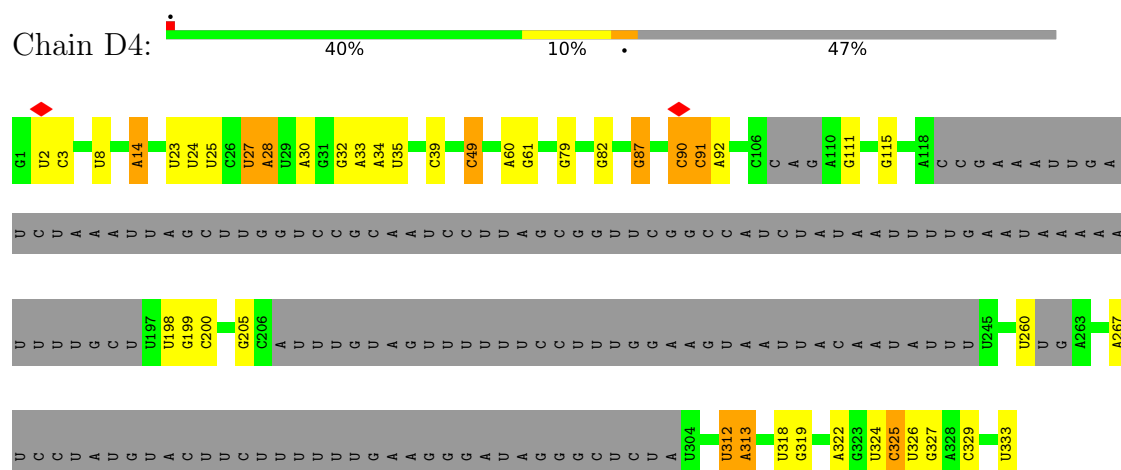
• Molecule 1: 18S rRNA



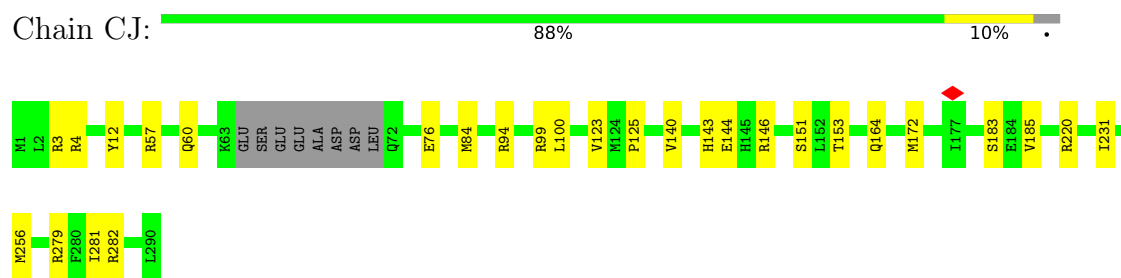




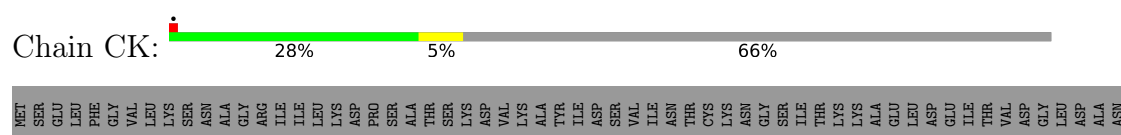
- Molecule 3: U3 snoRNA

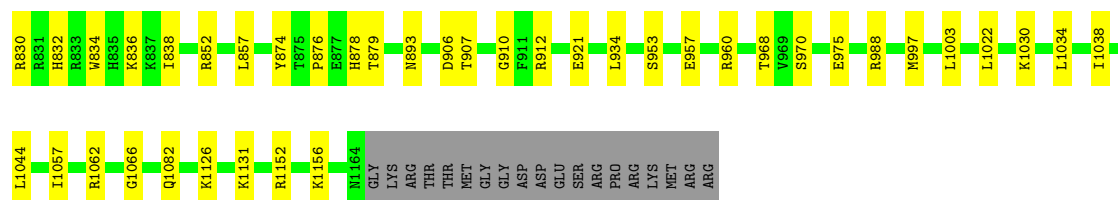


- Molecule 4: U3 small nucleolar ribonucleoprotein protein IMP4

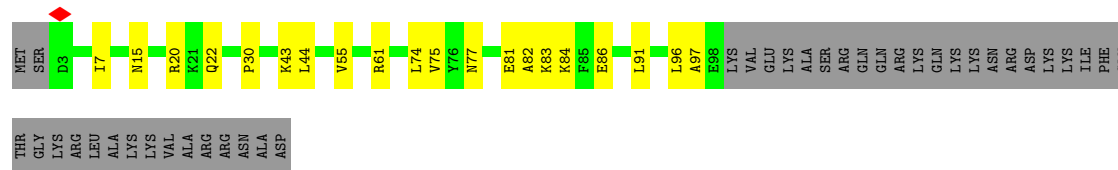


- Molecule 5: U3 small nucleolar RNA-associated protein MPP10

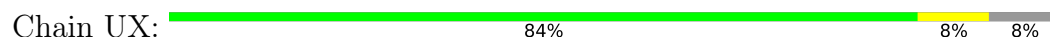




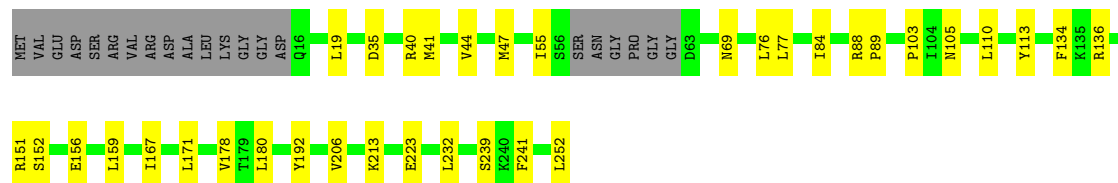
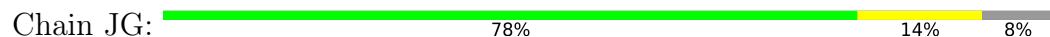
• Molecule 7: 40S ribosomal protein S24-A



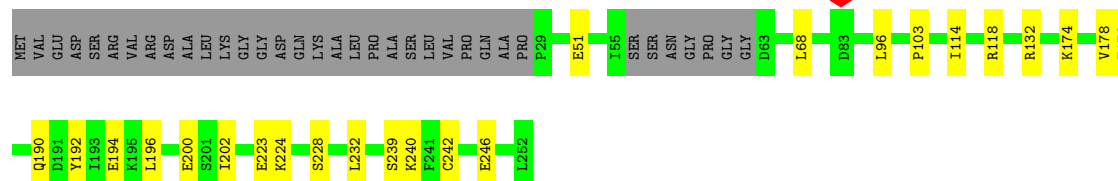
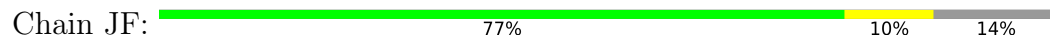
• Molecule 8: rRNA-processing protein FCF1



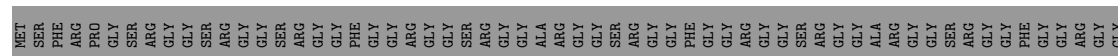
• Molecule 9: Ribosomal RNA small subunit methyltransferase NEP1



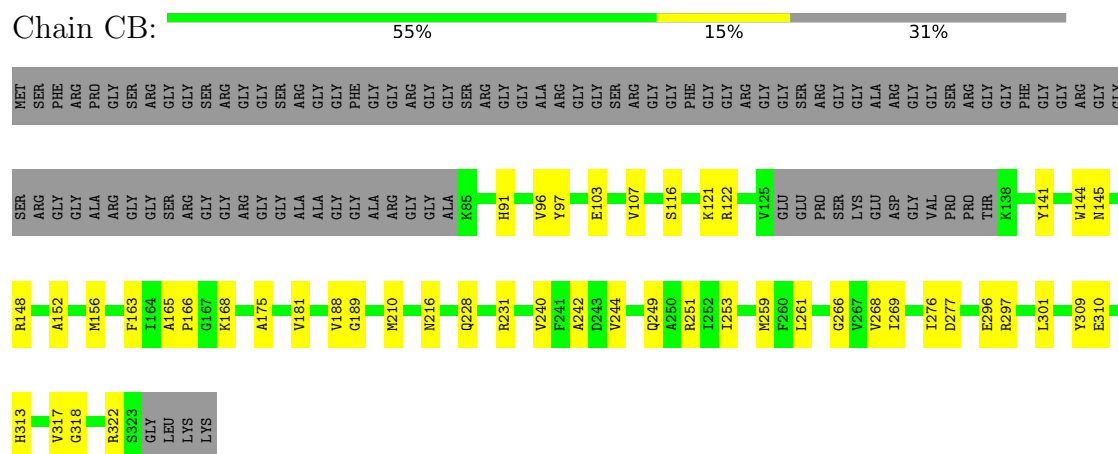
• Molecule 9: Ribosomal RNA small subunit methyltransferase NEP1



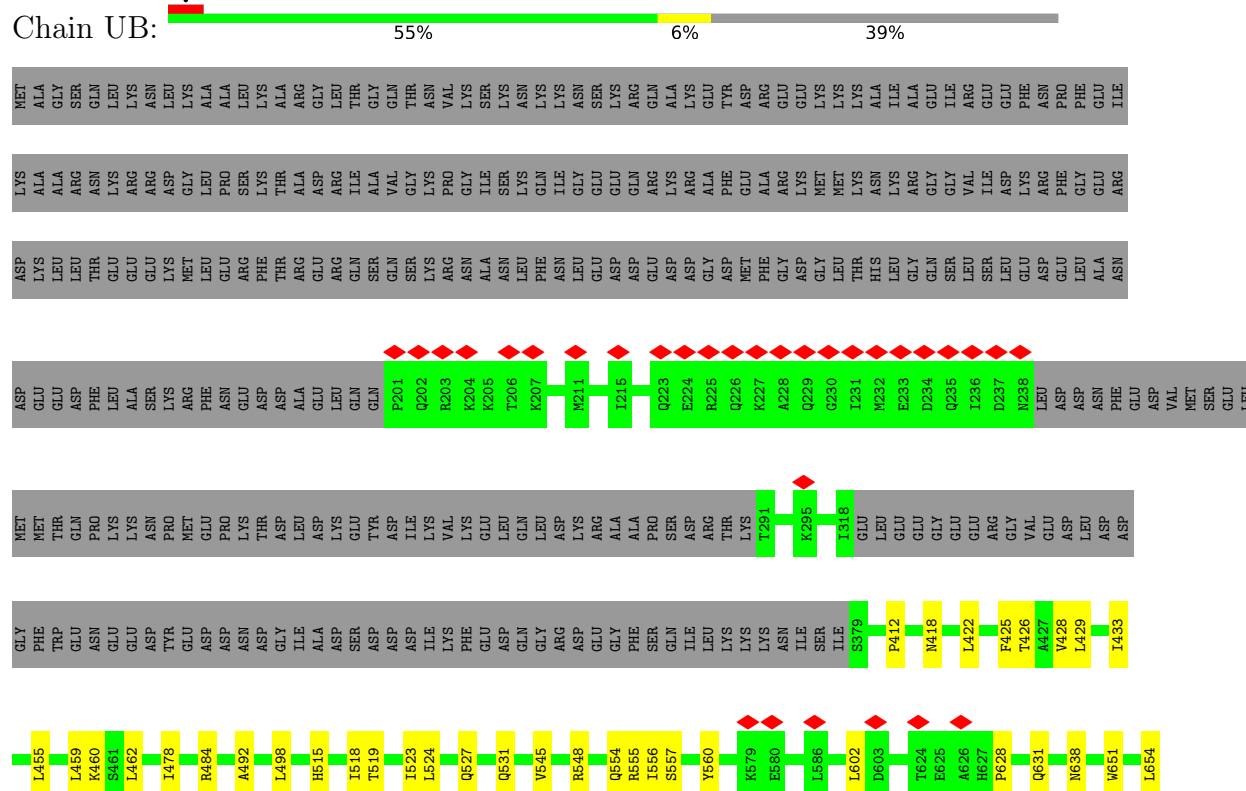
• Molecule 10: rRNA 2'-O-methyltransferase fibrillar

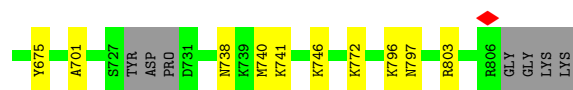


- Molecule 10: rRNA 2'-O-methyltransferase fibrillar



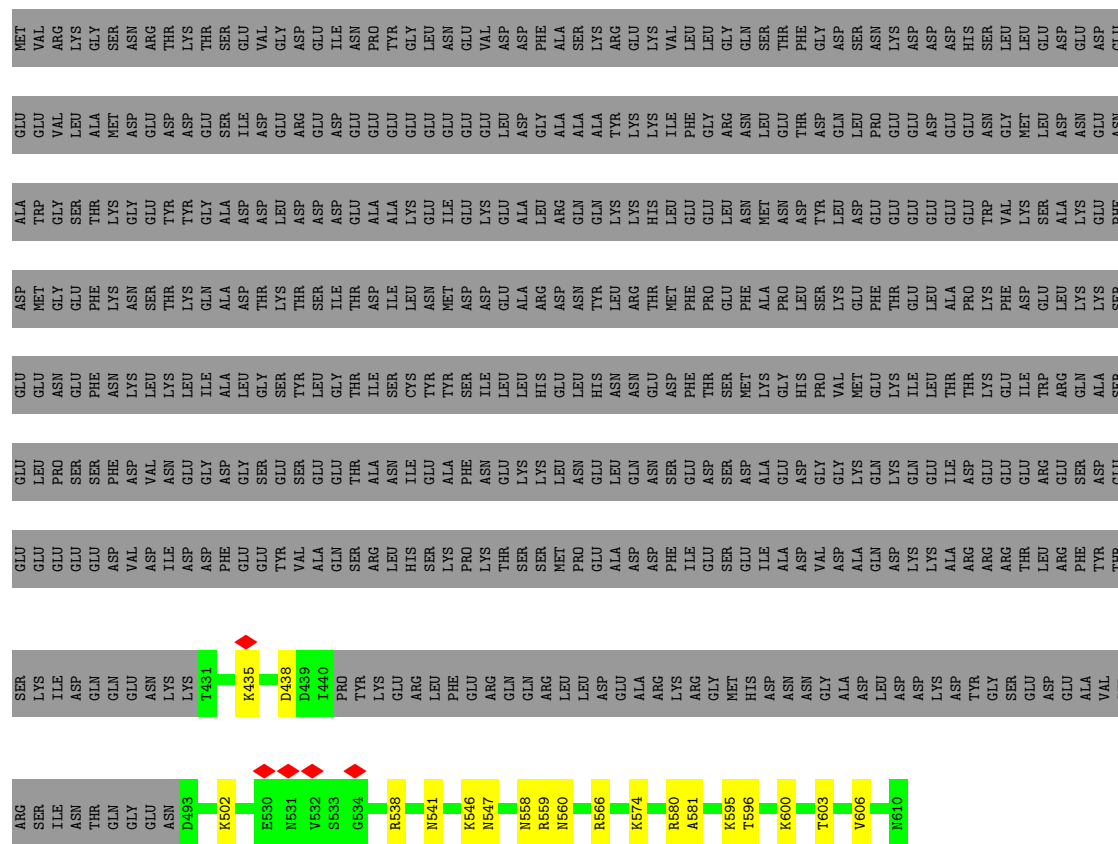
- Molecule 11: Nucleolar complex protein 14





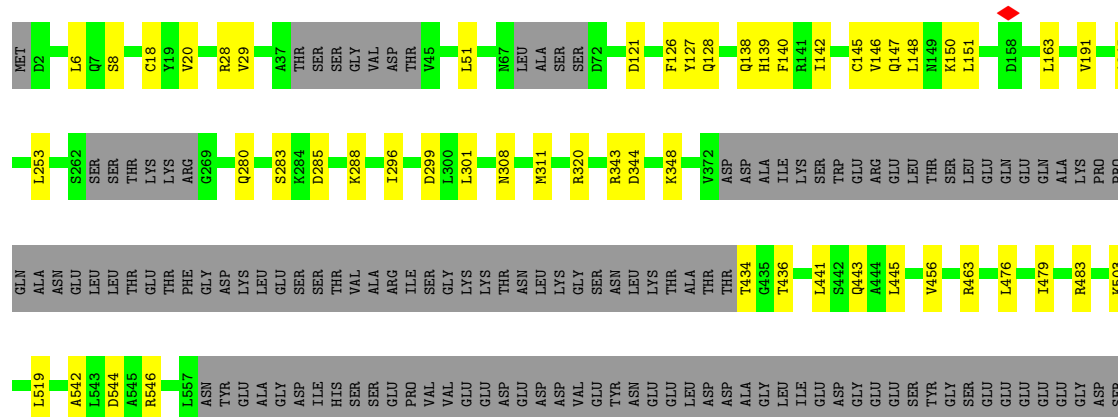
- Molecule 12: Something about silencing protein 10

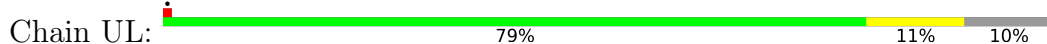
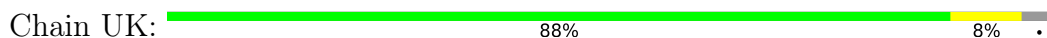
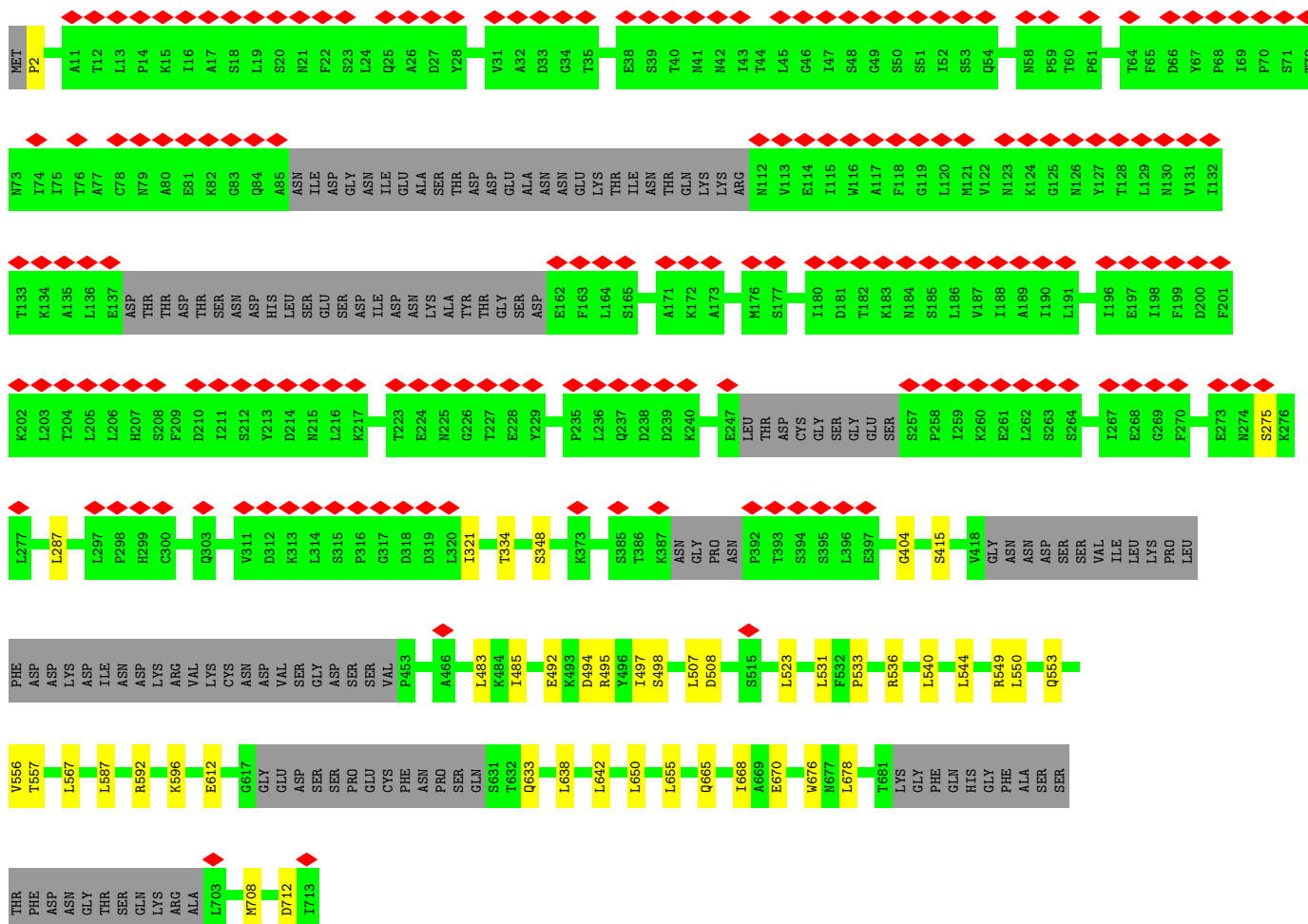
Chain UC: 18% 79%



- Molecule 13: U3 small nucleolar RNA-associated protein 5


Chain UE: 66% 8% 26%

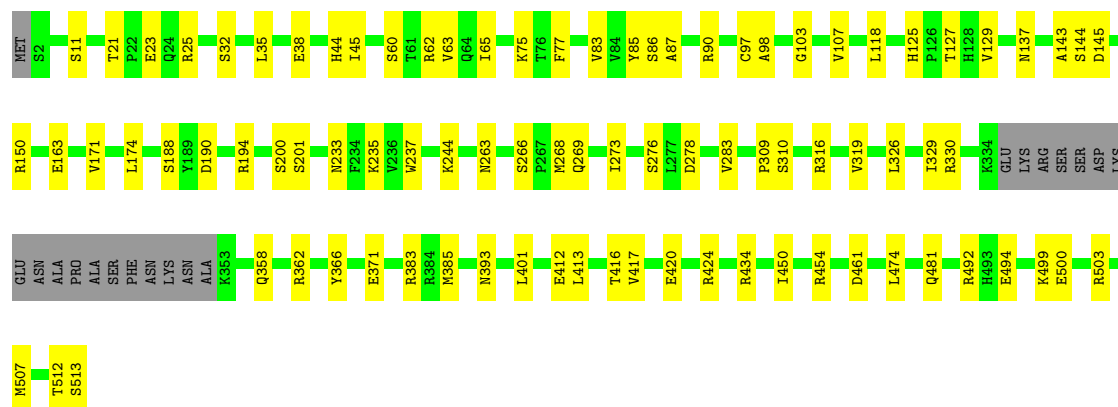






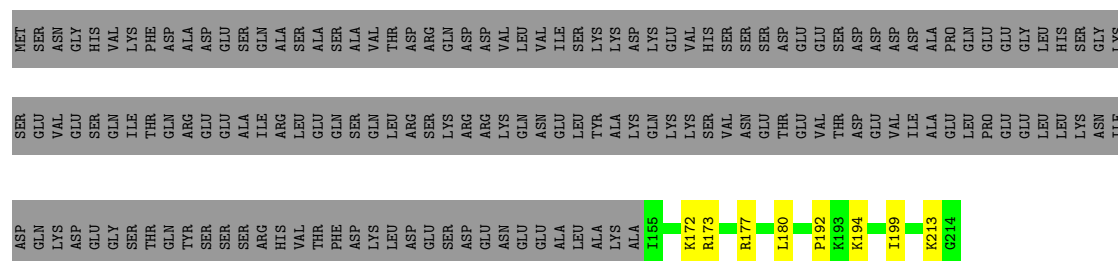
- Molecule 18: U3 small nucleolar RNA-associated protein 15

Chain UO:  79% 17%




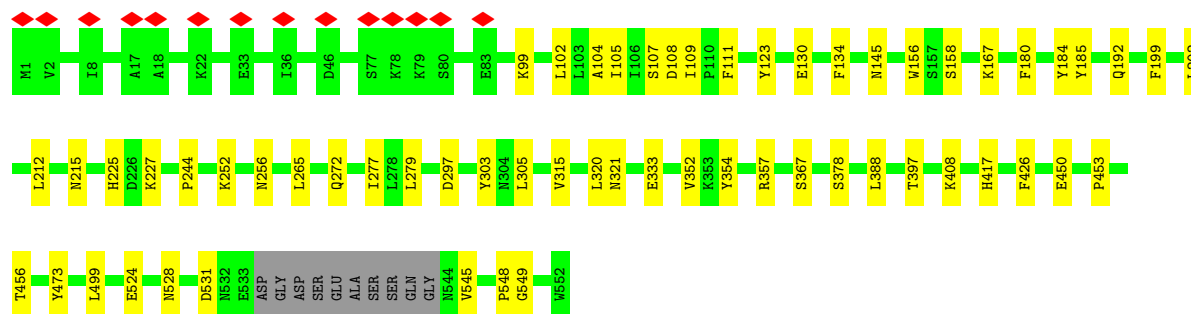
- Molecule 19: U3 small nucleolar RNA-associated protein 16

Chain UP:  24% 72%



- Molecule 20: Nucleolar complex protein 4

Chain US:  87% 11%




- Molecule 21: 13 kDa ribonucleoprotein-associated protein

Chain CF:  91% 6%



- Molecule 21: 13 kDa ribonucleoprotein-associated protein

MTT	SER	ALA	PRO	N5	P6	K7	A8	L33	K34	E39	K42	R46	M54	P60	I61	E62	I63	L64	Y78	R84	V85	P96	V97	I98	A99	A100	L125	I1E
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- Chain CI:  86% 14%

MET	V2	K22	Q23	D24	Q25	D29	K33	I50	L57	K60	L61	S62	L63	L64	P65	P66	Tl02	R108	Q125	V128	K129	E132	N153	R154	E155	D162	Y173	R174	N175	D179	S183
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- Chain JE:  35% 5% 60%

[illegible][illegible]

D324 S330 L334 T338 L357

- Chain JH: 

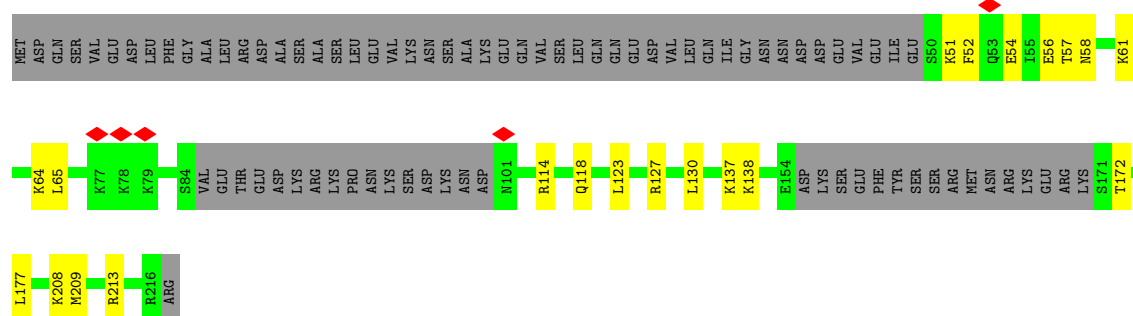
[illegible]

GLY	ASP	TYR	LYS	GLU	GLU	GLU	GLU	ILE	VAL	GLU	ILE	ASP	GLU	GLU	ASP	ALA	ALA	MET	PHE	GLU	GLN	TYR	PHE	LYS	LYS	SER	SER	ASP	ASP	PHE	ASN	SER	SER	LEU	LEU	ALA	ALA	ASP	LYS	ILE	MET	MET	ALA	ALA	SER	SER	ILE	ARG	GLU	GLU	ASP	MET	GLN	GLN	ASP	SER
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----


GLU	PRO	LEU	ALA	ASN	GLU	GLN	ASN	THR	SER	ARG	GLY	ASN	ILE	SER	SER	GLY	LEU	LYS	SER	GLY	GLU	GLY	VAL																																			
S255			A262		S268	N269		A272		I279		E282	T293		H297	S298		L311	Y312		E327	T328		V332	R333	E334	A335	T336		S340		A349		F364		D377		A381	L382		F397	R398	I399	L400	ASP	GLY	SER	ASN	G406	E407	D408	A409	T410	R411	V412	L413		T424

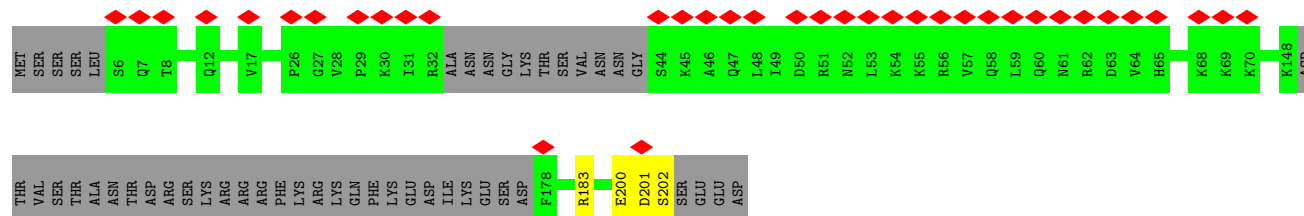
- Molecule 27: rRNA-processing protein FCF2

Chain JM:  53% 10% 38%




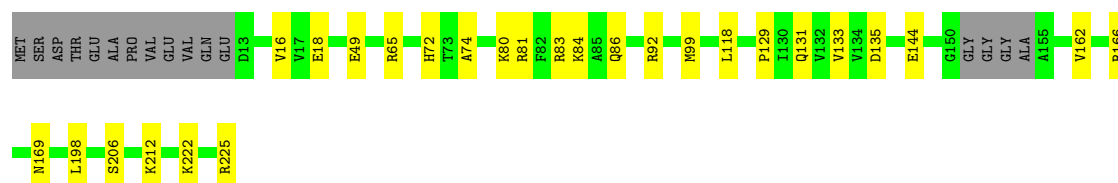
- Molecule 28: Regulator of rDNA transcription protein 14

Chain JQ:  18% 74% 24%



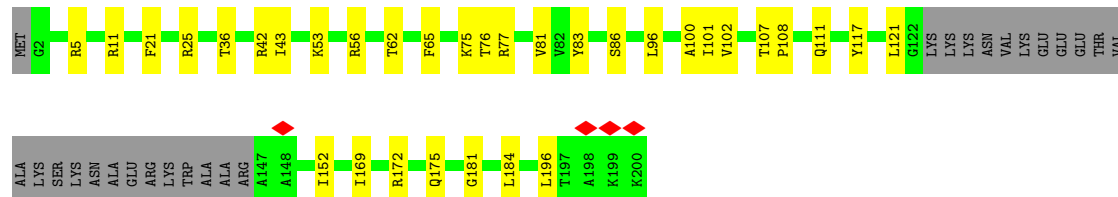
- Molecule 29: 40S ribosomal protein S5

Chain DF:  81% 12% 7%




- Molecule 30: 40S ribosomal protein S8-A

Chain DI:  71% 16% 12%

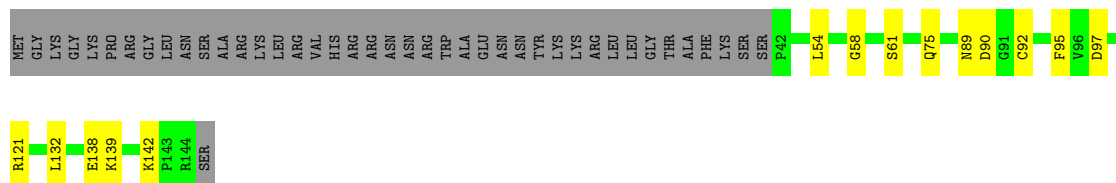


- Molecule 31: 40S ribosomal protein S9-A

Chain DJ:  82% 8% 10%

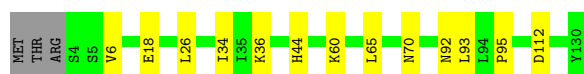
- Molecule 35: 40S ribosomal protein S23-A

Chain DX:  61% 10% 29%




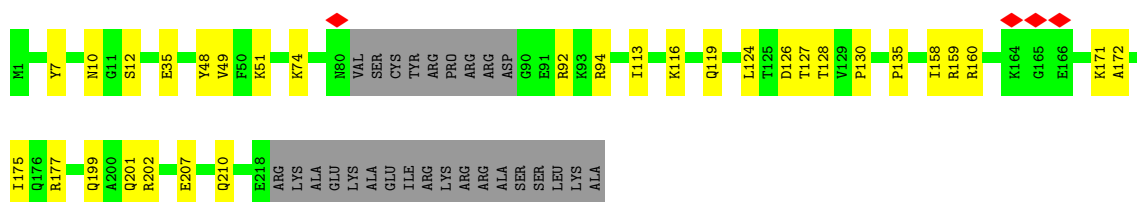
- Molecule 36: 40S ribosomal protein S22-A

Chain DW:  88% 10% .




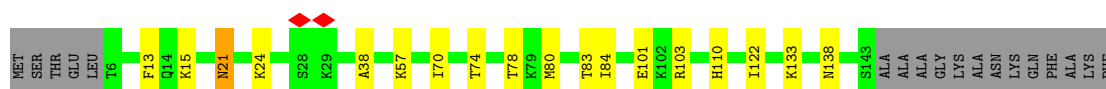
- Molecule 37: 40S ribosomal protein S6-A

Chain DG:  75% 13% 11%



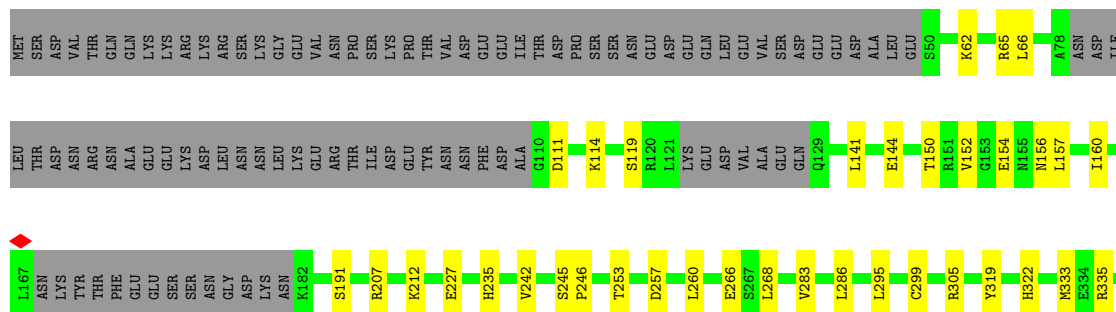
- Molecule 38: 40S ribosomal protein S11-A

Chain DL:  77% 11% . 12%



- Molecule 39: Ribosomal RNA-processing protein 9

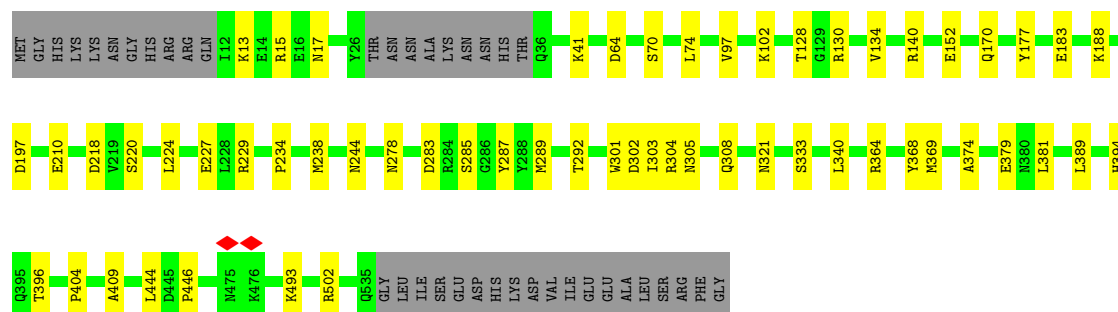
Chain CH:  69% 10% 21%





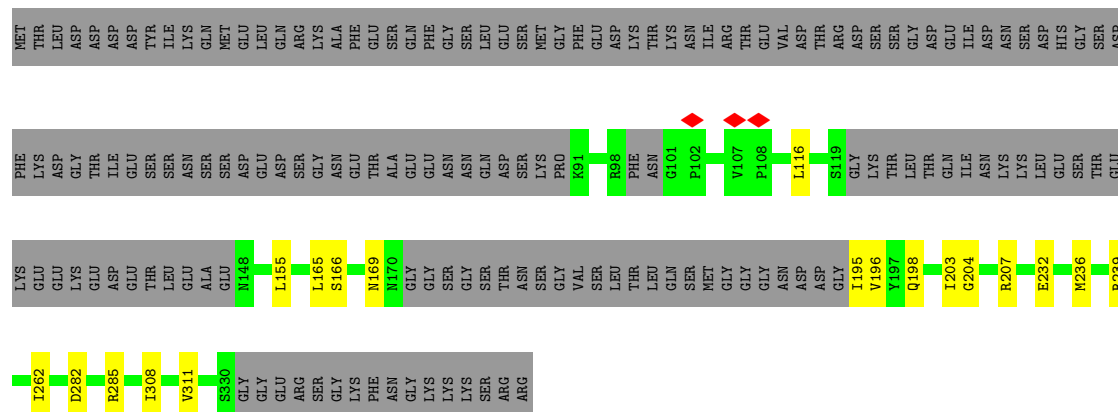
- Molecule 46: U3 small nucleolar RNA-associated protein 7

Chain UG: 82% 10% 7%



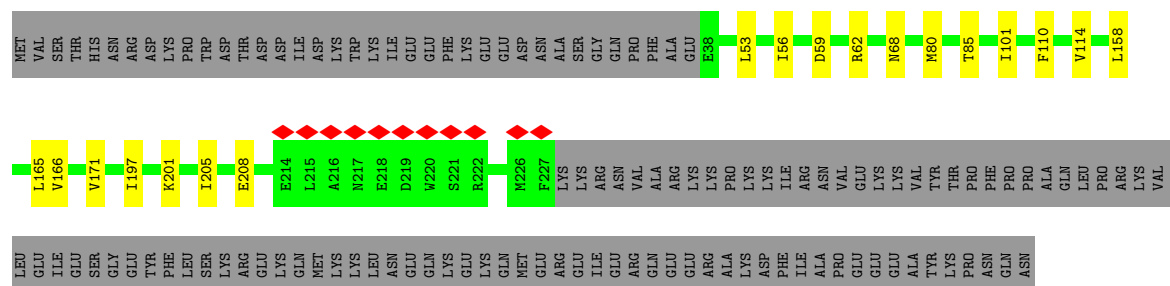
- Molecule 47: Protein FAF1

Chain JN:




- Molecule 48: KRR1 small subunit processome component

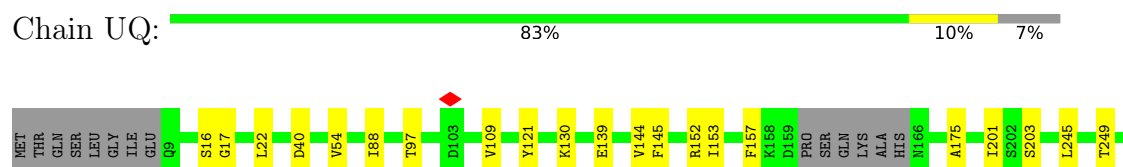
Chain JO: 

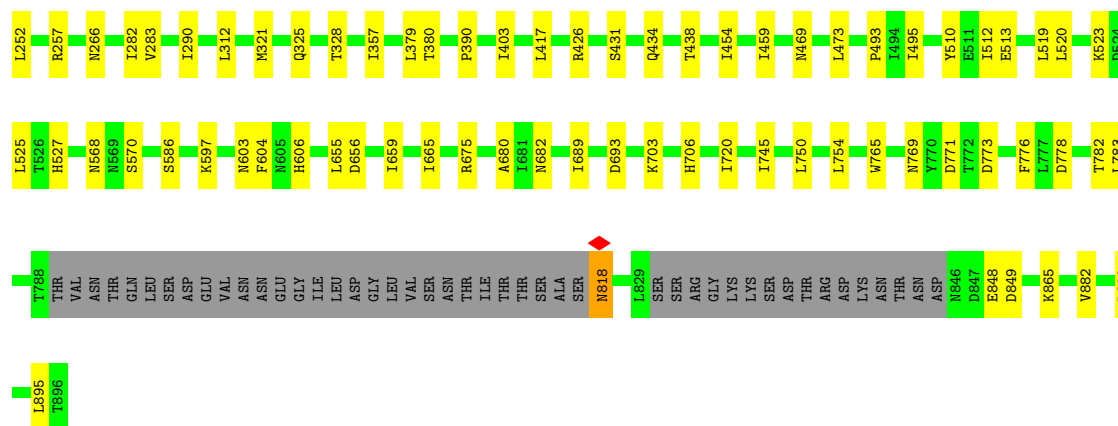


- Molecule 49: RNA 3'-terminal phosphate cyclase-like protein

Chain CM:  82% 17%

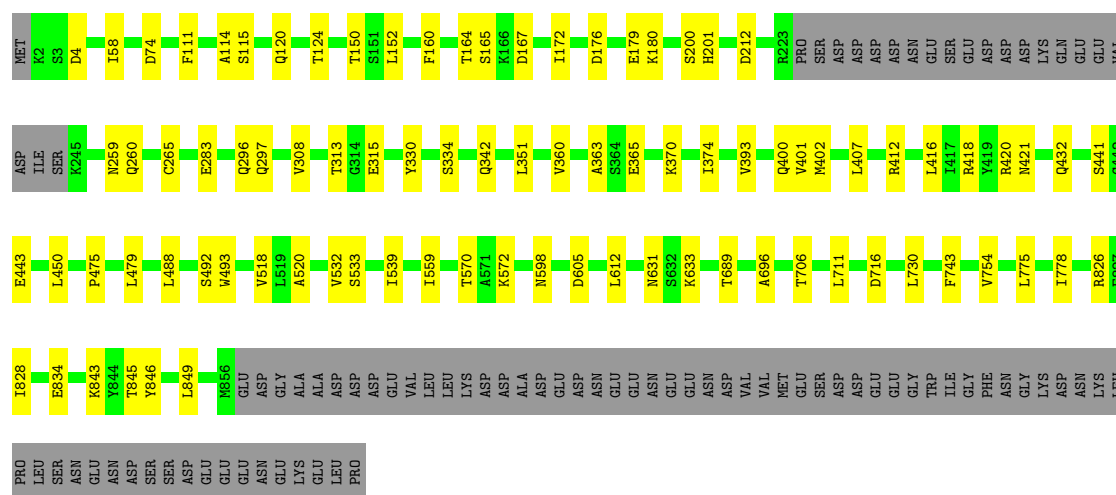






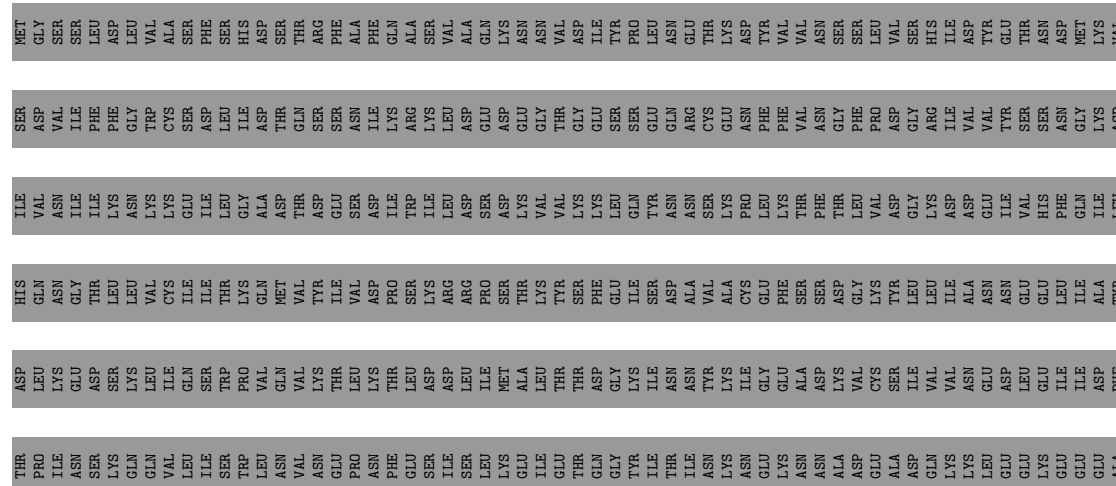
• Molecule 56: Periodic tryptophan protein 2

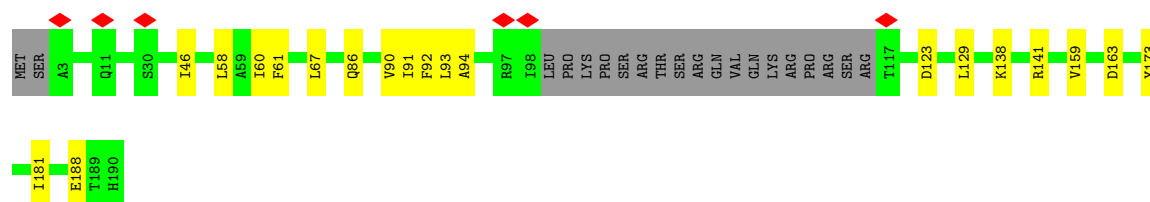
Chain UA: 81% 10% 10%



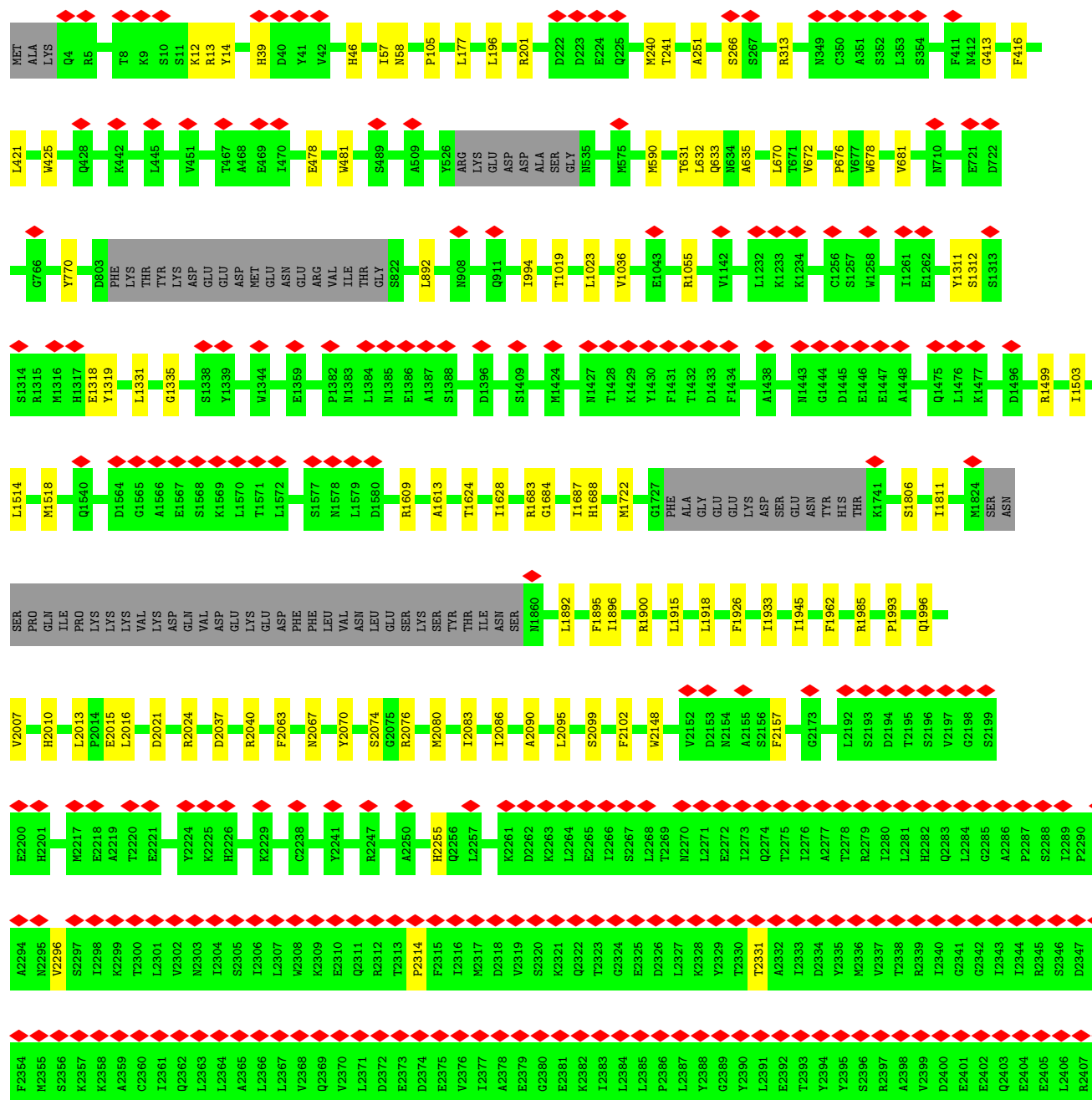
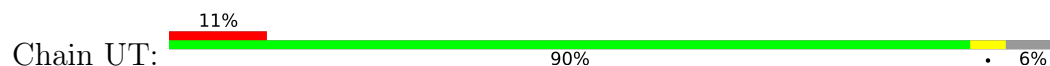
• Molecule 57: U3 small nucleolar RNA-associated protein 9

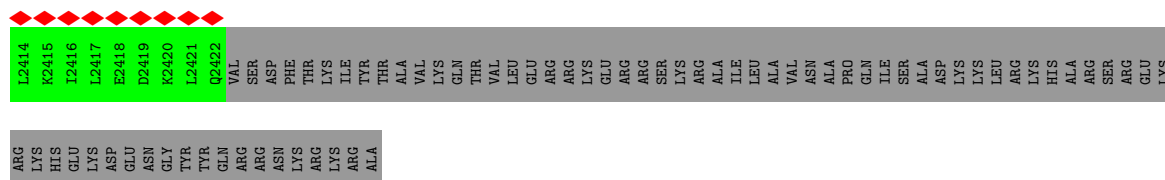
Chain UI: 22% 77%



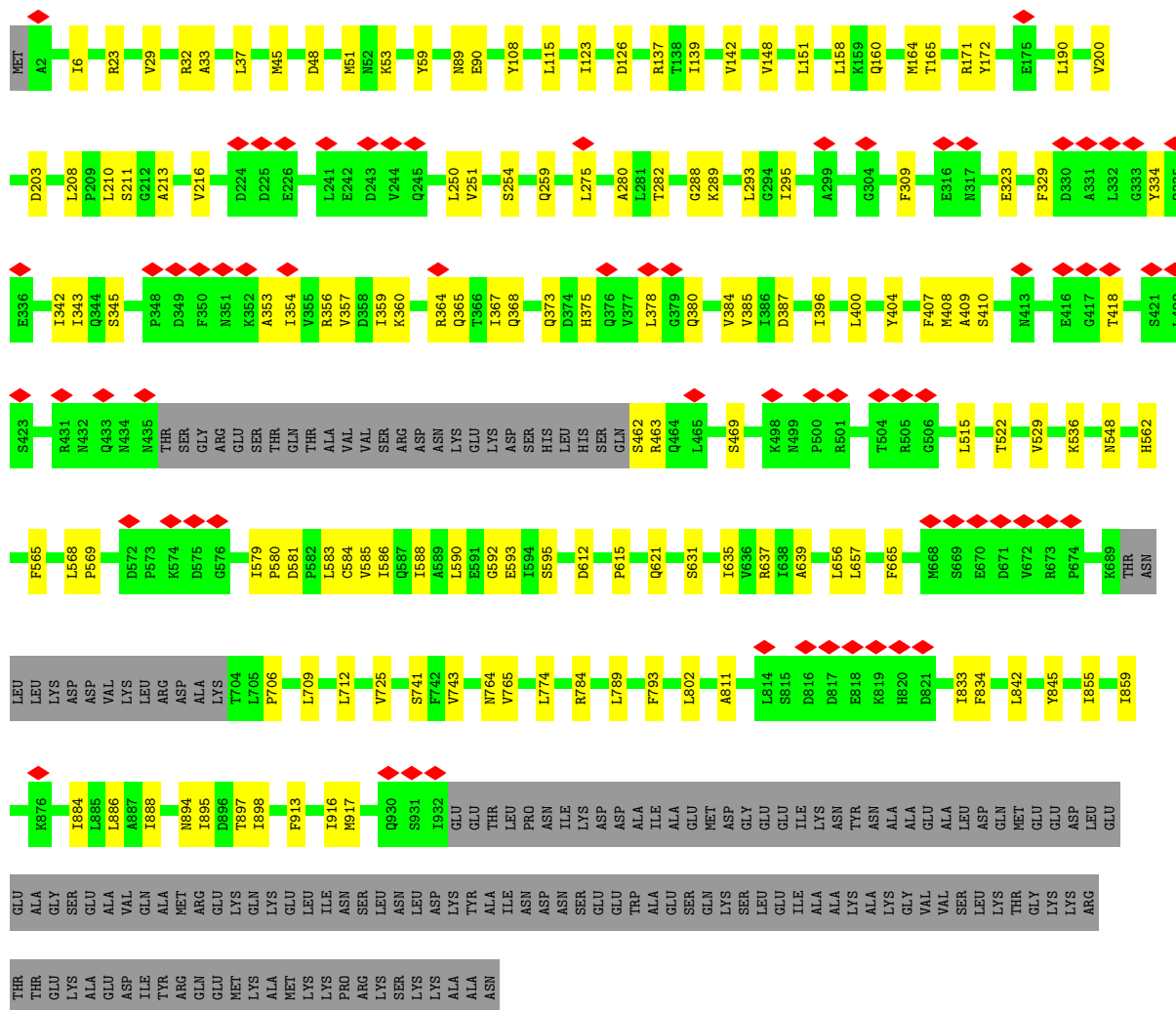


- Molecule 60: U3 small nucleolar RNA-associated protein 20





• Molecule 61: RNA cytidine acetyltransferase



• Molecule 61: RNA cytidine acetyltransferase



ASN	ASN	ASN	SER	GLU	ALA	TRP	ALA	ALA	ALA	GLU	GLN	SER	GLY	GLU	GLU	GLU	ILE	LYS	ALA	ALA	LYS	ASN	TYR	ALA	ALA	ALA	ALA	ALA	GLY	GLN	LEU	LYS	GLY	GLU	ASP	VAL	LYS																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
LEU	ARG	ASP	ALA	LYS	T704	P706	L705	T704	L705	W725	S726	Y727	G811	D612	P615	W616	I635	R636	R637	I638	A639	L656	E662	G663	K664	F665	T666	D667	M668	S669	E670	D671	V672	R673	P674	K675	D676	Y677	S678	I679	R680	V681	V682	S683	D684	K685	E686	L687	A688	K689	THR	ASN	ASN	LEU	LEU	LYS	ASP	ASP	VAL	LYS																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
L486	N487	K488	L489	L490	C491	L492	D493	T495	L496	L497	K498	N499	P500	R501	F502	A503	G506	V518	N519	T522	E531	M537	M538	A539	L540	Y541	V542	S543	H544	H545	K547	N548	L555	A559	K574	D581	C584	V585	T594	S595	K596	E597	S598	V599	R600	N601	E483																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	32278	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	46.4	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	5.585	Depositor
Minimum map value	0.000	Depositor
Average map value	0.022	Depositor
Map value standard deviation	0.132	Depositor
Recommended contour level	0.45	Depositor
Map size (Å)	522.5, 522.5, 522.5	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.045, 1.045, 1.045	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	D3	0.21	0/21102	0.31	0/32834
2	D2	0.25	0/12389	0.27	0/19297
3	D4	0.26	0/4163	0.28	0/6467
4	CJ	0.27	0/2322	0.49	0/3128
5	CK	0.24	0/1601	0.53	2/2150 (0.1%)
6	CL	0.27	0/6612	0.48	0/8919
7	DY	0.25	0/774	0.56	2/1041 (0.2%)
8	UX	0.30	0/1419	0.48	0/1906
9	JF	0.22	0/1673	0.52	0/2268
9	JG	0.26	0/1818	0.50	0/2460
10	CA	0.30	0/1904	0.48	0/2570
10	CB	0.28	0/1811	0.56	2/2443 (0.1%)
11	UB	0.21	0/3722	0.40	0/5048
12	UC	0.26	0/1035	0.54	0/1365
13	UE	0.28	0/3841	0.50	0/5213
14	UH	0.18	0/3555	0.48	2/4897 (0.0%)
15	UK	0.27	0/2010	0.46	0/2662
16	UL	0.31	0/6526	0.55	0/8873
17	UM	0.27	0/1287	0.55	0/1739
18	UO	0.30	0/3987	0.56	0/5405
19	UP	0.26	0/423	0.45	0/571
20	US	0.23	0/4074	0.47	0/5581
21	CF	0.32	0/945	0.48	0/1284
21	CG	0.25	0/928	0.48	0/1262
22	CI	0.31	0/1560	0.51	0/2097
23	JE	0.22	0/971	0.59	2/1314 (0.2%)
24	JH	0.13	0/1274	0.32	0/1775
25	JJ	0.14	0/502	0.42	0/692
26	JK	0.25	0/338	0.53	0/458
27	JM	0.24	0/1119	0.49	0/1494
28	JQ	0.18	0/867	0.41	0/1203
29	DF	0.28	0/1658	0.55	0/2242

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	DI	0.28	0/1372	0.52	0/1839
31	DJ	0.25	0/1428	0.50	0/1916
32	DS	0.14	0/523	0.38	0/724
33	JC	0.27	0/2753	0.49	0/3742
34	DE	0.23	0/1876	0.51	0/2536
35	DX	0.28	0/786	0.52	0/1053
36	DW	0.26	0/970	0.52	0/1312
37	DG	0.24	0/1598	0.52	0/2151
38	DL	0.22	0/1077	0.43	0/1466
39	CH	0.24	0/3601	0.55	0/4862
40	Dc	0.29	0/500	0.54	0/670
41	DQ	0.32	0/990	0.55	0/1335
42	CE	0.23	0/3075	0.46	0/4186
43	CD	0.25	0/2847	0.47	0/3860
44	UN	0.26	0/1468	0.50	0/1993
45	UF	0.24	0/2852	0.46	0/3871
46	UG	0.32	0/3997	0.51	0/5413
47	JN	0.25	0/1370	0.56	0/1830
48	JO	0.23	0/1510	0.49	0/2043
49	CM	0.24	0/2820	0.49	0/3814
50	UZ	0.23	0/1998	0.52	0/2704
51	JP	0.35	1/3797 (0.0%)	0.56	0/5116
52	UR	0.34	0/3835	0.52	0/5201
53	UU	0.31	0/6743	0.54	1/9126 (0.0%)
54	UD	0.30	0/5275	0.54	0/7180
55	UQ	0.32	0/6692	0.52	0/9087
56	UA	0.33	0/6747	0.54	0/9136
57	UI	0.23	0/974	0.54	0/1329
58	UJ	0.21	0/10267	0.46	1/14176 (0.0%)
59	DH	0.22	0/1229	0.50	0/1676
60	UT	0.17	0/14115	0.40	0/19566
61	JA	0.21	0/6767	0.49	1/9207 (0.0%)
61	JB	0.18	0/6479	0.46	0/8830
All	All	0.25	1/210541 (0.0%)	0.46	13/293608 (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
9	JG	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
29	DF	0	1
50	UZ	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	JP	198	GLY	C-O	5.92	1.27	1.24

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	CK	426	LEU	CA-C-N	6.11	133.22	121.54
5	CK	426	LEU	C-N-CA	6.11	133.22	121.54
10	CB	296	GLU	CA-C-N	5.88	132.77	121.54
10	CB	296	GLU	C-N-CA	5.88	132.77	121.54
53	UU	930	MET	CB-CG-SD	-5.78	95.36	112.70
23	JE	253	SER	CA-C-N	5.61	134.81	124.82
23	JE	253	SER	C-N-CA	5.61	134.81	124.82
7	DY	30	PRO	CA-C-N	5.43	131.92	121.54
7	DY	30	PRO	C-N-CA	5.43	131.92	121.54
14	UH	612	GLU	CA-CB-CG	5.40	124.89	114.10
58	UJ	405	GLU	N-CA-CB	5.24	118.40	110.28
14	UH	612	GLU	N-CA-CB	5.16	118.28	110.28
61	JA	323	GLU	N-CA-CB	5.11	118.16	110.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
29	DF	49	GLU	Peptide
9	JG	213	LYS	Peptide
50	UZ	78	ASP	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	D3	18883	0	9534	126	0
2	D2	11078	0	5570	60	0
3	D4	3731	0	1892	16	0
4	CJ	2281	0	2297	22	0
5	CK	1584	0	1589	25	0
6	CL	6472	0	6530	72	0
7	DY	761	0	782	15	0
8	UX	1396	0	1473	12	0
9	JF	1647	0	1643	16	0
9	JG	1789	0	1841	26	0
10	CA	1868	0	1909	27	0
10	CB	1778	0	1823	30	0
11	UB	3660	0	3404	34	0
12	UC	1027	0	1080	21	0
13	UE	3773	0	3787	33	0
14	UH	3518	0	2497	34	0
15	UK	1985	0	2051	18	0
16	UL	6393	0	6116	66	0
17	UM	1269	0	1247	13	0
18	UO	3905	0	3894	52	0
19	UP	419	0	380	6	0
20	US	3967	0	3505	39	0
21	CF	932	0	983	6	0
21	CG	916	0	964	11	0
22	CI	1531	0	1572	21	0
23	JE	959	0	787	12	0
24	JH	1276	0	561	1	0
25	JJ	500	0	275	2	0
26	JK	330	0	302	6	0
27	JM	1100	0	1099	14	0
28	JQ	860	0	469	4	0
29	DF	1638	0	1683	17	0
30	DI	1350	0	1343	25	0
31	DJ	1406	0	1465	14	0
32	DS	526	0	247	2	0
33	JC	2695	0	2512	25	0
34	DE	1836	0	1867	27	0
35	DX	774	0	810	10	0
36	DW	954	0	945	9	0
37	DG	1577	0	1597	22	0
38	DL	1052	0	1035	16	0
39	CH	3531	0	3473	37	0
40	Dc	498	0	535	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	DQ	973	0	1029	15	0
42	CE	3038	0	2817	33	0
43	CD	2802	0	2625	21	0
44	UN	1441	0	1330	13	0
45	UF	2795	0	2461	27	0
46	UG	3917	0	3777	42	0
47	JN	1363	0	1295	18	0
48	JO	1483	0	1522	12	0
49	CM	2768	0	2844	42	0
50	UZ	1963	0	1971	20	0
51	JP	3718	0	3645	40	0
52	UR	3751	0	3706	34	0
53	UU	6606	0	6523	69	0
54	UD	5176	0	4984	49	0
55	UQ	6559	0	6385	59	0
56	UA	6602	0	6461	56	0
57	UI	959	0	881	7	0
58	UJ	10158	0	7084	41	0
59	DH	1207	0	1092	12	0
60	UT	13871	0	8948	60	0
61	JA	6631	0	6373	85	0
61	JB	6345	0	6043	93	0
62	CL	32	0	12	0	0
63	UX	1	0	0	0	0
All	All	203584	0	173176	1597	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 4.

All (1597) 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)
20:US:130:GLU:O	20:US:134:PHE:HB2	1.75	0.86
54:UD:614:TRP:NE1	54:UD:618:ASN:HD22	1.75	0.85
61:JA:309:PHE:HB2	61:JA:384:VAL:HG22	1.63	0.81
55:UQ:818:ASN:N	55:UQ:818:ASN:HD22	1.78	0.80
55:UQ:16:SER:O	55:UQ:783:LEU:HB2	1.83	0.78
52:UR:307:GLN:NE2	52:UR:471:LEU:O	2.20	0.75
61:JA:343:ILE:HB	61:JA:356:ARG:HB2	1.68	0.75
23:JE:263:GLY:HA3	31:DJ:138:LYS:H	1.53	0.73
50:UZ:243:PHE:HB3	50:UZ:251:SER:HB2	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:JM:114:ARG:O	27:JM:118:GLN:HB3	1.90	0.72
4:CJ:123:VAL:HG12	4:CJ:125:PRO:HD2	1.71	0.72
22:CI:65:PRO:HD3	47:JN:203:ILE:HG22	1.72	0.71
16:UL:538:ARG:NH1	16:UL:580:ASP:OD1	2.23	0.70
58:UJ:151:ILE:O	58:UJ:155:ILE:HB	1.92	0.69
36:DW:93:LEU:HD13	47:JN:311:VAL:HG21	1.74	0.69
23:JE:251:GLU:OE2	31:DJ:78:ARG:NH1	2.25	0.69
55:UQ:459:ILE:HD12	55:UQ:469:ASN:HB3	1.75	0.69
55:UQ:882:VAL:HG11	55:UQ:890:ARG:HH22	1.58	0.68
33:JC:101:ASN:HD21	33:JC:104:PHE:HB3	1.57	0.68
54:UD:426:GLN:O	54:UD:444:ARG:NH1	2.27	0.68
10:CA:218:ILE:HD11	43:CD:152:LEU:HD22	1.75	0.67
49:CM:176:GLN:HE21	49:CM:305:LYS:HE2	1.59	0.67
1:D3:259:U:OP1	30:DI:75:LYS:NZ	2.28	0.67
49:CM:196:TYR:HA	49:CM:228:ASP:O	1.94	0.67
49:CM:289:VAL:O	49:CM:317:GLN:NE2	2.27	0.67
16:UL:387:LEU:O	16:UL:415:LYS:NZ	2.27	0.67
2:D2:125:G:OP1	20:US:145:ASN:ND2	2.28	0.67
30:DI:172:ARG:HE	30:DI:175:GLN:HG3	1.58	0.67
23:JE:256:PRO:HB2	39:CH:357:LEU:HD22	1.76	0.66
16:UL:137:ILE:HG12	16:UL:147:VAL:HG22	1.76	0.66
61:JA:165:THR:HG21	61:JA:210:LEU:HD22	1.76	0.66
61:JA:359:ILE:HB	61:JA:365:GLN:HB2	1.77	0.66
1:D3:1606:C:OP2	4:CJ:94:ARG:NH2	2.29	0.66
1:D3:1514:U:OP2	50:UZ:142:ARG:NH2	2.29	0.66
47:JN:166:SER:HB2	48:JO:158:LEU:HD11	1.77	0.66
14:UH:556:VAL:HG23	14:UH:557:THR:HG23	1.78	0.66
61:JA:375:HIS:HA	61:JA:378:LEU:HD23	1.77	0.65
2:D2:358:G:H1	2:D2:367:C:H42	1.42	0.65
46:UG:224:LEU:HD21	46:UG:227:GLU:HG3	1.76	0.65
54:UD:549:VAL:HG22	54:UD:565:ARG:HD2	1.79	0.65
23:JE:334:LEU:HD12	31:DJ:68:LYS:HA	1.78	0.65
10:CB:242:ALA:HB2	10:CB:253:ILE:HD11	1.78	0.65
6:CL:832:HIS:HD2	6:CL:834:TRP:H	1.45	0.65
29:DF:74:ALA:O	41:DQ:122:ARG:NH2	2.30	0.64
1:D3:469:C:H5'	1:D3:471:A:H62	1.62	0.64
20:US:102:LEU:HA	20:US:105:ILE:HD12	1.80	0.64
41:DQ:94:GLN:HB3	41:DQ:102:LYS:HG3	1.78	0.64
20:US:352:VAL:HG12	20:US:354:TYR:H	1.63	0.64
41:DQ:98:ASP:OD1	53:UU:495:ARG:NH2	2.31	0.64
51:JP:83:LEU:HB2	51:JP:97:MET:HE2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:UR:450:GLN:O	52:UR:492:ASN:ND2	2.31	0.64
61:JA:360:LYS:O	61:JA:364:ARG:NH2	2.31	0.64
10:CA:186:ASP:OD1	10:CA:214:ARG:NH1	2.31	0.64
34:DE:203:GLY:HA2	38:DL:70:ILE:H	1.63	0.64
42:CE:207:ARG:HH12	42:CE:226:ILE:HA	1.62	0.63
42:CE:264:GLU:HB3	43:CD:277:ARG:HH22	1.64	0.63
53:UU:835:ALA:O	53:UU:839:ASN:ND2	2.31	0.63
13:UE:280:GLN:HB3	13:UE:288:LYS:HE2	1.80	0.63
20:US:279:LEU:HA	20:US:357:ARG:HH12	1.64	0.63
4:CJ:143:HIS:HB2	4:CJ:151:SER:HB3	1.80	0.63
56:UA:570:THR:HG22	56:UA:572:LYS:H	1.64	0.63
1:D3:332:U:OP1	30:DI:56:ARG:NH2	2.32	0.63
51:JP:273:GLU:OE1	51:JP:276:ASN:ND2	2.30	0.63
52:UR:344:ARG:HH12	55:UQ:379:LEU:HB2	1.63	0.63
11:UB:527:GLN:O	11:UB:531:GLN:HB2	1.99	0.63
38:DL:57:LYS:O	38:DL:138:ASN:ND2	2.32	0.62
47:JN:232:GLU:O	47:JN:239:ARG:NH2	2.32	0.62
16:UL:549:SER:HA	16:UL:555:VAL:HG12	1.82	0.62
56:UA:58:ILE:HA	56:UA:74:ASP:HA	1.80	0.62
2:D2:316:U:OP1	46:UG:364:ARG:NH2	2.31	0.62
6:CL:1152:ARG:HE	6:CL:1156:LYS:HZ1	1.47	0.62
31:DJ:57:ARG:NH1	31:DJ:61:THR:OG1	2.32	0.62
14:UH:498:SER:HB3	14:UH:531:LEU:HD12	1.82	0.62
55:UQ:390:PRO:HB2	55:UQ:438:THR:HG21	1.81	0.62
61:JB:160:GLN:HG3	61:JB:172:TYR:HB3	1.82	0.62
7:DY:15:ASN:ND2	34:DE:54:TYR:O	2.33	0.62
16:UL:220:THR:HG23	16:UL:259:ILE:HD11	1.81	0.62
42:CE:161:VAL:O	42:CE:165:GLN:NE2	2.32	0.62
42:CE:65:GLU:O	42:CE:93:LYS:NZ	2.33	0.62
10:CA:100:ARG:NH1	10:CA:104:ASP:OD2	2.31	0.61
13:UE:245:ALA:HB1	13:UE:253:LEU:HD11	1.81	0.61
53:UU:724:SER:O	53:UU:728:ARG:NH2	2.34	0.61
61:JB:187:ARG:NH2	61:JB:488:LYS:O	2.33	0.61
1:D3:1599:C:H3'	6:CL:988:ARG:HH12	1.64	0.61
21:CG:8:ALA:HB2	21:CG:61:ILE:HD11	1.83	0.61
61:JB:548:ASN:OD1	61:JB:637:ARG:NH1	2.33	0.61
14:UH:596:LYS:HE2	18:UO:513:SER:HB2	1.81	0.61
52:UR:140:THR:HG1	52:UR:143:THR:HG1	1.43	0.61
1:D3:584:C:H5''	15:UK:12:GLN:HG2	1.83	0.61
46:UG:74:LEU:HD22	46:UG:369:MET:HE2	1.81	0.61
61:JA:23:ARG:NH1	61:JA:139:ILE:O	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:UF:16:ASP:OD2	46:UG:15:ARG:NH2	2.32	0.61
61:JB:187:ARG:NH2	61:JB:491:CYS:SG	2.72	0.61
51:JP:311:VAL:HG22	51:JP:322:THR:HG22	1.83	0.60
2:D2:68:U:H5'	55:UQ:426:ARG:HH22	1.65	0.60
10:CB:116:SER:HB3	10:CB:122:ARG:HD2	1.83	0.60
33:JC:147:ASN:ND2	33:JC:150:ASN:OD1	2.34	0.60
61:JA:548:ASN:OD1	61:JA:637:ARG:NH1	2.28	0.60
6:CL:828:ARG:NH1	35:DX:97:ASP:OD1	2.35	0.60
8:UX:161:LYS:HG2	8:UX:172:LEU:HD21	1.83	0.60
10:CA:228:GLN:O	10:CA:231:ARG:NH1	2.34	0.60
56:UA:492:SER:OG	56:UA:493:TRP:N	2.34	0.60
4:CJ:185:VAL:O	4:CJ:220:ARG:NH1	2.32	0.60
46:UG:369:MET:HE1	46:UG:404:PRO:HD2	1.84	0.60
49:CM:228:ASP:OD2	49:CM:230:TRP:NE1	2.34	0.60
2:D2:316:U:H5'	46:UG:364:ARG:HH22	1.66	0.60
8:UX:9:LYS:HE3	8:UX:10:PHE:H	1.66	0.60
53:UU:897:HIS:O	53:UU:900:ASN:ND2	2.34	0.60
61:JA:380:GLN:NE2	61:JB:366:THR:OG1	2.35	0.60
1:D3:545:A:H3'	12:UC:559:ARG:HH21	1.66	0.60
11:UB:796:LYS:HB2	35:DX:121:ARG:HD3	1.84	0.60
14:UH:650:LEU:HD23	14:UH:655:LEU:HD12	1.84	0.60
37:DG:199:GLN:OE1	37:DG:202:ARG:NH1	2.35	0.60
61:JB:23:ARG:NH1	61:JB:139:ILE:O	2.34	0.60
61:JA:565:PHE:HB2	61:JA:586:ILE:HB	1.82	0.60
6:CL:91:ARG:NE	61:JA:89:ASN:O	2.32	0.60
10:CB:240:VAL:HG23	10:CB:261:LEU:HD13	1.83	0.60
14:UH:321:ILE:HA	14:UH:334:THR:O	2.02	0.60
39:CH:348:LEU:HD23	39:CH:357:LEU:HD12	1.82	0.60
42:CE:408:THR:O	58:UJ:166:ASN:ND2	2.34	0.60
51:JP:345:THR:HG22	51:JP:347:ARG:H	1.66	0.60
54:UD:338:ALA:HB1	54:UD:361:LEU:HD11	1.83	0.60
56:UA:402:MET:HG2	56:UA:416:LEU:HD11	1.84	0.60
56:UA:407:LEU:HD22	56:UA:432:GLN:HB3	1.84	0.60
61:JA:833:ILE:HG13	61:JA:834:PHE:HD1	1.66	0.60
1:D3:592:A:H62	12:UC:558:ASN:HD22	1.50	0.59
4:CJ:183:SER:HB2	4:CJ:220:ARG:HD2	1.83	0.59
5:CK:449:ASP:O	5:CK:453:SER:HB3	2.02	0.59
61:JA:522:THR:HB	61:JA:706:PRO:HG2	1.83	0.59
6:CL:830:ARG:HH21	6:CL:878:HIS:HA	1.66	0.59
6:CL:997:MET:O	15:UK:22:ARG:NH2	2.36	0.59
16:UL:356:THR:HG22	16:UL:362:ILE:HG12	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:CH:414:ILE:HD11	39:CH:480:ALA:HB2	1.82	0.59
49:CM:267:ILE:HB	49:CM:270:GLU:HG3	1.84	0.59
60:UT:2086:ILE:O	60:UT:2090:ALA:HB2	2.02	0.59
52:UR:446:ARG:NH2	54:UD:269:PHE:O	2.33	0.59
53:UU:569:VAL:HB	53:UU:579:ARG:HB2	1.84	0.59
10:CA:299:LYS:HB2	10:CA:325:LEU:HD22	1.82	0.59
10:CB:166:PRO:HA	10:CB:188:VAL:HA	1.84	0.59
11:UB:548:ARG:NH2	11:UB:638:ASN:OD1	2.35	0.59
14:UH:494:ASP:HB2	14:UH:497:ILE:HD13	1.85	0.59
61:JA:309:PHE:O	61:JA:384:VAL:HA	2.03	0.59
16:UL:633:CYS:HB2	16:UL:663:LEU:HD22	1.85	0.59
52:UR:165:ARG:NH2	53:UU:219:ASP:OD1	2.36	0.59
2:D2:12:G:H21	2:D2:70:A:H8	1.49	0.59
13:UE:434:THR:O	13:UE:463:ARG:NH1	2.35	0.59
44:UN:879:ILE:HA	51:JP:399:LYS:HG3	1.85	0.59
51:JP:48:THR:HG21	51:JP:410:ILE:HG23	1.85	0.59
1:D3:17:C:O2	3:D4:14:A:N6	2.35	0.59
1:D3:334:G:O6	30:DI:5:ARG:NH2	2.35	0.59
1:D3:1654:G:H1	1:D3:1746:A:H62	1.51	0.59
53:UU:605:LEU:HD23	53:UU:628:VAL:HG11	1.85	0.59
18:UO:60:SER:HA	18:UO:83:VAL:HG23	1.83	0.59
29:DF:222:LYS:HA	29:DF:225:ARG:HE	1.68	0.59
61:JA:515:LEU:HB3	61:JA:712:LEU:HD11	1.84	0.59
61:JB:491:CYS:HB3	61:JB:538:MET:HE2	1.84	0.59
10:CB:253:ILE:HG13	10:CB:269:ILE:HD12	1.84	0.58
53:UU:500:LEU:HD11	53:UU:539:LYS:HD3	1.84	0.58
5:CK:436:GLU:OE2	22:CI:60:LYS:NZ	2.36	0.58
42:CE:161:VAL:HA	42:CE:164:ILE:HG12	1.85	0.58
53:UU:463:VAL:HG13	53:UU:477:ILE:HG23	1.85	0.58
61:JB:112:GLU:OE2	61:JB:137:ARG:NH1	2.36	0.58
61:JB:124:LEU:HD11	61:JB:150:ILE:HG23	1.84	0.58
1:D3:477:A:H5'	12:UC:560:ASN:HD22	1.68	0.58
2:D2:347:U:OP1	48:JO:62:ARG:NH2	2.35	0.58
61:JA:32:ARG:HB2	61:JA:203:ASP:HB2	1.84	0.58
6:CL:968:THR:HG22	6:CL:970:SER:H	1.68	0.58
9:JF:174:LYS:HE2	9:JF:200:GLU:HB2	1.85	0.58
10:CB:144:TRP:CE2	10:CB:152:ALA:HB3	2.38	0.58
34:DE:55:ALA:HB1	34:DE:60:GLU:HG3	1.86	0.58
53:UU:326:PRO:O	53:UU:338:GLN:NE2	2.36	0.58
54:UD:498:VAL:HG12	54:UD:500:LEU:H	1.68	0.58
34:DE:100:ARG:HB2	34:DE:114:ILE:HD13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:DE:195:ILE:HA	34:DE:210:ILE:HA	1.84	0.58
55:UQ:568:ASN:ND2	55:UQ:586:SER:OG	2.36	0.58
6:CL:87:ARG:NH2	6:CL:213:GLY:O	2.36	0.58
38:DL:80:MET:HG3	38:DL:83:THR:HB	1.86	0.58
61:JB:385:VAL:HG22	61:JB:407:PHE:HB2	1.86	0.58
61:JB:889:GLY:O	61:JB:892:ARG:NH1	2.36	0.58
2:D2:162:U:OP1	52:UR:318:ARG:NH1	2.37	0.58
21:CG:6:PRO:HG2	39:CH:465:GLN:HG3	1.84	0.58
34:DE:195:ILE:HG22	34:DE:210:ILE:HG12	1.83	0.58
53:UU:596:GLU:HB2	56:UA:711:LEU:HA	1.86	0.58
60:UT:58:ASN:HD22	60:UT:105:PRO:HG2	1.68	0.58
1:D3:372:G:OP2	23:JE:243:GLN:NE2	2.37	0.58
2:D2:102:A:OP2	2:D2:103:G:N2	2.33	0.58
15:UK:248:ARG:NH1	21:CF:94:SER:OG	2.37	0.58
19:UP:213:LYS:O	54:UD:767:LYS:NZ	2.34	0.58
58:UJ:235:VAL:HG22	58:UJ:264:PHE:HZ	1.69	0.58
61:JB:26:PHE:HA	61:JB:199:LEU:O	2.04	0.58
1:D3:561:G:OP2	4:CJ:282:ARG:NH2	2.35	0.57
10:CA:122:ARG:NE	10:CA:140:GLU:OE2	2.33	0.57
18:UO:11:SER:H	18:UO:416:THR:HG22	1.69	0.57
52:UR:315:ALA:HB2	52:UR:321:MET:HG3	1.86	0.57
4:CJ:3:ARG:NH2	22:CI:155:GLU:O	2.36	0.57
6:CL:907:THR:HG22	6:CL:912:ARG:HD3	1.85	0.57
51:JP:324:SER:OG	51:JP:325:TYR:N	2.37	0.57
53:UU:733:THR:O	53:UU:737:LEU:HB2	2.04	0.57
41:DQ:32:ASN:OD1	41:DQ:68:ARG:NH1	2.38	0.57
55:UQ:283:VAL:HG22	55:UQ:290:ILE:HG22	1.87	0.57
1:D3:1545:A:H61	1:D3:1566:U:H3	1.50	0.57
10:CA:240:VAL:HG23	10:CA:261:LEU:HD13	1.87	0.57
13:UE:145:CYS:HB3	13:UE:148:LEU:HD11	1.86	0.57
29:DF:16:VAL:HG21	53:UU:534:SER:HB3	1.85	0.57
39:CH:260:LEU:HD21	39:CH:283:VAL:HG11	1.86	0.57
55:UQ:769:ASN:HB3	55:UQ:773:ASP:HB2	1.86	0.57
60:UT:201:ARG:NH2	60:UT:241:THR:O	2.38	0.57
1:D3:497:G:O6	6:CL:1131:LYS:NZ	2.37	0.57
18:UO:358:GLN:O	18:UO:362:ARG:HB3	2.05	0.57
52:UR:365:ASN:ND2	52:UR:370:SER:OG	2.37	0.57
42:CE:238:ALA:O	42:CE:242:SER:HB2	2.04	0.57
48:JO:53:LEU:HA	48:JO:56:ILE:HG12	1.86	0.57
52:UR:513:GLN:HG3	52:UR:551:VAL:HG21	1.87	0.57
54:UD:618:ASN:HD21	54:UD:662:ASP:HA	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:UJ:153:SER:O	58:UJ:169:ARG:NH1	2.38	0.57
61:JB:343:ILE:HD12	61:JB:356:ARG:HB3	1.86	0.57
61:JB:555:LEU:O	61:JB:559:ALA:HB2	2.04	0.57
14:UH:540:LEU:HD12	14:UH:544:LEU:HD13	1.87	0.57
1:D3:487:G:OP1	6:CL:1126:LYS:NZ	2.37	0.57
16:UL:227:LYS:NZ	16:UL:244:GLU:OE2	2.32	0.57
18:UO:90:ARG:HH21	18:UO:137:ASN:HB3	1.69	0.57
61:JB:395:PRO:HA	61:JB:398:LYS:HD2	1.85	0.57
2:D2:489:G:O6	45:UF:120:ARG:NH1	2.37	0.56
11:UB:701:ALA:HA	20:US:417:HIS:HA	1.87	0.56
21:CF:54:MET:HB3	21:CF:64:LEU:HD13	1.86	0.56
39:CH:212:LYS:HG3	39:CH:268:LEU:HD22	1.86	0.56
49:CM:66:GLU:HB2	49:CM:75:ILE:HB	1.86	0.56
51:JP:89:ASP:O	51:JP:107:LYS:NZ	2.37	0.56
29:DF:118:LEU:HD22	29:DF:129:PRO:HB2	1.86	0.56
31:DJ:136:VAL:HG22	31:DJ:156:ILE:HG12	1.87	0.56
39:CH:150:THR:HG22	39:CH:207:ARG:HD3	1.86	0.56
45:UF:11:CYS:SG	45:UF:91:ARG:NH1	2.78	0.56
61:JB:319:LYS:HA	61:JB:322:PHE:HD2	1.70	0.56
1:D3:515:A:N6	1:D3:537:G:O2'	2.39	0.56
2:D2:480:C:O2	45:UF:46:ARG:NH1	2.39	0.56
5:CK:489:SER:O	56:UA:420:ARG:NH2	2.38	0.56
9:JG:151:ARG:NH1	9:JG:156:GLU:O	2.37	0.56
10:CB:268:VAL:HG12	10:CB:317:VAL:HG22	1.87	0.56
16:UL:217:LEU:HB3	16:UL:229:TRP:HB2	1.87	0.56
52:UR:280:LYS:HG3	52:UR:281:THR:HG23	1.86	0.56
54:UD:33:VAL:HG22	54:UD:752:LEU:HB3	1.87	0.56
54:UD:61:THR:HG21	54:UD:681:ILE:HD12	1.87	0.56
4:CJ:4:ARG:NH2	22:CI:153:ASN:OD1	2.27	0.56
8:UX:114:ARG:NH1	36:DW:70:ASN:OD1	2.38	0.56
10:CA:231:ARG:NH2	43:CD:10:GLU:OE1	2.32	0.56
43:CD:166:SER:HB3	43:CD:169:LYS:HB2	1.88	0.56
6:CL:553:ILE:HG12	49:CM:323:ILE:HD12	1.86	0.56
14:UH:587:LEU:HD12	14:UH:633:GLN:HG3	1.88	0.56
39:CH:235:HIS:ND1	39:CH:257:ASP:OD2	2.35	0.56
46:UG:130:ARG:NH2	46:UG:379:GLU:OE2	2.39	0.56
10:CA:236:MET:HG3	43:CD:133:LEU:HA	1.87	0.56
27:JM:54:GLU:HA	27:JM:57:THR:HG22	1.87	0.56
34:DE:196:VAL:N	34:DE:209:HIS:O	2.38	0.56
20:US:367:SER:OG	20:US:408:LYS:NZ	2.37	0.56
61:JA:593:GLU:HG2	61:JA:631:SER:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:JB:420:ARG:NH1	61:JB:494:VAL:O	2.39	0.56
1:D3:334:G:N7	30:DI:5:ARG:NH1	2.48	0.56
33:JC:194:LEU:HD21	33:JC:206:PHE:HD2	1.71	0.56
37:DG:7:TYR:HB2	37:DG:113:ILE:HD12	1.88	0.56
56:UA:114:ALA:HB2	56:UA:152:LEU:HD23	1.88	0.56
1:D3:1204:A:H5'	1:D3:1209:C:H4'	1.86	0.56
2:D2:6:A:N6	2:D2:8:A:N3	2.54	0.56
7:DY:82:ALA:O	7:DY:86:GLU:HB2	2.06	0.56
61:JA:259:GLN:HE21	61:JA:288:GLY:HA3	1.71	0.56
13:UE:308:ASN:HB2	13:UE:311:MET:HG3	1.88	0.56
16:UL:913:ASN:O	16:UL:917:ASN:HB2	2.06	0.56
17:UM:665:GLN:HB3	17:UM:688:LEU:HD21	1.88	0.56
35:DX:92:CYS:HA	35:DX:95:PHE:HD2	1.71	0.56
41:DQ:97:VAL:HG12	41:DQ:98:ASP:H	1.71	0.56
42:CE:380:ARG:NH1	42:CE:382:ASP:OD1	2.38	0.56
46:UG:283:ASP:OD1	46:UG:285:SER:OG	2.24	0.56
49:CM:137:LEU:HD22	49:CM:296:LEU:HD22	1.88	0.56
18:UO:276:SER:OG	18:UO:278:ASP:OD1	2.22	0.55
44:UN:857:TYR:O	44:UN:860:SER:OG	2.21	0.55
54:UD:573:VAL:HG22	54:UD:584:VAL:HG22	1.88	0.55
3:D4:325:C:N4	42:CE:318:GLN:OE1	2.40	0.55
18:UO:309:PRO:O	18:UO:316:ARG:NH1	2.39	0.55
56:UA:450:LEU:HA	56:UA:475:PRO:HB3	1.88	0.55
11:UB:484:ARG:NH1	11:UB:492:ALA:O	2.40	0.55
46:UG:409:ALA:O	51:JP:8:ARG:NH2	2.39	0.55
54:UD:301:ASP:O	54:UD:771:GLN:NE2	2.39	0.55
55:UQ:17:GLY:HA3	55:UQ:782:THR:HA	1.87	0.55
1:D3:1217:A:O2'	1:D3:1218:G:N2	2.39	0.55
6:CL:553:ILE:HD13	49:CM:326:LEU:HD12	1.89	0.55
54:UD:106:ASN:O	54:UD:153:GLN:NE2	2.40	0.55
5:CK:480:GLN:NE2	5:CK:482:LEU:O	2.40	0.55
20:US:252:LYS:O	20:US:256:ASN:ND2	2.40	0.55
6:CL:819:GLU:O	6:CL:852:ARG:NH2	2.38	0.55
34:DE:106:LYS:HD3	34:DE:108:ARG:HH22	1.71	0.55
61:JB:518:VAL:HG21	61:JB:537:MET:HE1	1.88	0.55
49:CM:310:ARG:HG2	49:CM:353:THR:HG22	1.88	0.55
9:JF:192:TYR:OH	9:JF:223:GLU:OE2	2.25	0.55
20:US:305:LEU:HD23	20:US:315:VAL:HG21	1.87	0.55
51:JP:267:ILE:HG12	51:JP:279:THR:HG22	1.88	0.55
52:UR:136:PRO:HG3	52:UR:154:LYS:HE2	1.88	0.55
55:UQ:818:ASN:N	55:UQ:818:ASN:ND2	2.50	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:DH:91:ILE:HG21	59:DH:129:LEU:HD23	1.89	0.55
2:D2:90:G:O2'	2:D2:91:U:O4'	2.24	0.55
16:UL:592:SER:OG	16:UL:593:ALA:N	2.40	0.55
21:CG:84:ARG:HG3	21:CG:96:PRO:HB3	1.89	0.55
30:DI:42:ARG:HH21	33:JC:335:SER:HA	1.71	0.55
5:CK:305:ILE:HD13	5:CK:308:ARG:HH21	1.71	0.55
7:DY:7:ILE:HD13	7:DY:43:LYS:HG2	1.89	0.55
46:UG:140:ARG:HD2	58:UJ:20:LEU:HD22	1.89	0.55
46:UG:152:GLU:OE1	46:UG:170:GLN:NE2	2.41	0.55
60:UT:994:ILE:HD11	60:UT:1036:VAL:HG21	1.88	0.55
61:JA:275:LEU:O	61:JA:463:ARG:NH1	2.40	0.55
61:JB:744:PRO:HD3	61:JB:762:MET:HE3	1.88	0.55
26:JK:497:LEU:HD23	26:JK:498:LEU:HG	1.89	0.54
20:US:528:ASN:HB2	20:US:545:VAL:HG12	1.89	0.54
55:UQ:145:PHE:HE1	55:UQ:201:ILE:HD13	1.72	0.54
61:JA:282:THR:HG22	61:JA:410:SER:HB3	1.88	0.54
1:D3:8:U:C4	47:JN:236:MET:HG3	2.42	0.54
3:D4:92:A:O2'	42:CE:323:GLU:OE1	2.25	0.54
6:CL:410:LYS:NZ	61:JA:165:THR:O	2.35	0.54
55:UQ:54:VAL:HG21	55:UQ:121:TYR:HB2	1.88	0.54
55:UQ:403:ILE:HD11	55:UQ:417:LEU:HD22	1.89	0.54
56:UA:775:LEU:HA	56:UA:778:ILE:HG22	1.89	0.54
2:D2:126:A:H5''	20:US:244:PRO:HB3	1.89	0.54
6:CL:157:ASN:O	6:CL:161:HIS:ND1	2.41	0.54
14:UH:592:ARG:H	55:UQ:603:ASN:HB3	1.72	0.54
51:JP:73:ILE:HG12	51:JP:85:THR:HG22	1.89	0.54
58:UJ:675:ASN:HA	58:UJ:681:ALA:HB2	1.88	0.54
61:JA:357:VAL:HB	61:JA:367:ILE:HB	1.90	0.54
3:D4:198:U:O2	3:D4:200:C:N4	2.40	0.54
4:CJ:231:ILE:HB	4:CJ:256:MET:HG2	1.89	0.54
29:DF:65:ARG:NH2	29:DF:86:GLN:OE1	2.38	0.54
36:DW:18:GLU:HG2	36:DW:65:LEU:HD13	1.88	0.54
43:CD:382:LYS:HD2	43:CD:404:LEU:HD22	1.89	0.54
11:UB:459:LEU:HD12	11:UB:462:LEU:HD11	1.89	0.54
49:CM:192:THR:HA	49:CM:224:ASN:O	2.08	0.54
56:UA:115:SER:OG	56:UA:120:GLN:NE2	2.37	0.54
59:DH:58:LEU:HB2	59:DH:90:VAL:HG12	1.90	0.54
60:UT:2070:TYR:O	60:UT:2076:ARG:NH1	2.41	0.54
61:JB:201:VAL:HG12	61:JB:207:VAL:HA	1.90	0.54
1:D3:147:A:H62	1:D3:167:U:H3	1.56	0.54
5:CK:456:PHE:HB3	56:UA:365:GLU:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:UX:25:LEU:O	8:UX:29:GLN:HB2	2.07	0.54
49:CM:22:VAL:HG11	49:CM:105:TYR:HD1	1.71	0.54
59:DH:67:LEU:HD22	59:DH:94:ALA:HB2	1.89	0.54
61:JA:387:ASP:HA	61:JA:409:ALA:HB3	1.88	0.54
1:D3:1207:C:O2	1:D3:1209:C:N4	2.41	0.54
5:CK:515:MET:HE2	5:CK:520:LEU:HD21	1.88	0.54
8:UX:79:LYS:NZ	36:DW:92:ASN:O	2.39	0.54
12:UC:580:ARG:NH1	12:UC:581:ALA:O	2.41	0.54
17:UM:669:LEU:HD22	17:UM:693:ARG:HH11	1.73	0.54
20:US:185:TYR:O	20:US:192:GLN:NE2	2.40	0.54
49:CM:365:LYS:HE2	49:CM:367:ALA:HB2	1.90	0.54
54:UD:774:LEU:HD23	54:UD:776:PHE:HE1	1.72	0.54
53:UU:632:VAL:HG22	53:UU:643:THR:HG22	1.90	0.54
53:UU:897:HIS:HB2	56:UA:849:LEU:HD22	1.89	0.54
55:UQ:778:ASP:OD2	55:UQ:782:THR:OG1	2.25	0.54
61:JA:171:ARG:HH12	61:JA:190:LEU:HD11	1.73	0.54
1:D3:1490:C:OP1	6:CL:1062:ARG:NH2	2.41	0.54
20:US:109:ILE:HG22	20:US:111:PHE:H	1.73	0.54
34:DE:176:ASP:HB3	34:DE:179:LYS:HE3	1.88	0.54
54:UD:326:ARG:NH1	54:UD:364:PHE:O	2.39	0.54
60:UT:2314:PRO:HA	60:UT:2331:THR:HA	1.90	0.54
2:D2:185:A:H61	2:D2:212:U:H3	1.55	0.53
15:UK:248:ARG:NH2	52:UR:514:LEU:O	2.41	0.53
18:UO:200:SER:OG	18:UO:201:SER:N	2.37	0.53
51:JP:435:SER:HB3	51:JP:439:ARG:HH12	1.73	0.53
47:JN:282:ASP:OD2	47:JN:285:ARG:NH1	2.42	0.53
51:JP:140:SER:OG	51:JP:141:ASP:N	2.41	0.53
1:D3:61:A:OP2	60:UT:12:LYS:NZ	2.42	0.53
14:UH:348:SER:HA	14:UH:415:SER:HA	1.89	0.53
29:DF:80:LYS:HB3	29:DF:83:ARG:HB2	1.90	0.53
29:DF:92:ARG:NH2	29:DF:169:ASN:OD1	2.42	0.53
51:JP:80:LEU:HD11	51:JP:359:ASP:HB2	1.90	0.53
1:D3:1597:A:H5'	4:CJ:279:ARG:HG3	1.90	0.53
7:DY:20:ARG:NH2	7:DY:22:GLN:OE1	2.38	0.53
16:UL:479:LEU:HG	16:UL:488:LEU:HD11	1.89	0.53
39:CH:299:CYS:SG	39:CH:305:ARG:NH1	2.81	0.53
61:JB:308:ILE:HG12	61:JB:383:LEU:HD23	1.89	0.53
1:D3:246:G:N2	38:DL:38:ALA:O	2.40	0.53
2:D2:168:G:H22	2:D2:227:U:H3	1.56	0.53
52:UR:321:MET:HB2	52:UR:355:PHE:HD2	1.74	0.53
54:UD:614:TRP:NE1	54:UD:618:ASN:ND2	2.53	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:UA:342:GLN:O	56:UA:370:LYS:NZ	2.42	0.53
58:UJ:637:ILE:O	58:UJ:641:LEU:HB2	2.08	0.53
60:UT:421:LEU:O	60:UT:425:TRP:HB3	2.08	0.53
61:JB:29:VAL:HG13	61:JB:152:LEU:HB2	1.91	0.53
1:D3:469:C:OP1	1:D3:471:A:N6	2.42	0.53
6:CL:826:LYS:HD3	6:CL:921:GLU:HB3	1.90	0.53
11:UB:560:TYR:OH	20:US:388:LEU:O	2.26	0.53
33:JC:74:THR:HG21	33:JC:101:ASN:HD22	1.73	0.53
46:UG:244:ASN:HB3	46:UG:446:PRO:HG3	1.91	0.53
56:UA:313:THR:OG1	56:UA:315:GLU:OE1	2.23	0.53
1:D3:524:U:N3	1:D3:527:A:OP2	2.37	0.53
18:UO:500:GLU:OE2	18:UO:503:ARG:NH1	2.39	0.53
43:CD:182:ASP:OD2	43:CD:314:ARG:NH1	2.40	0.53
54:UD:105:SER:HB3	54:UD:113:ARG:HB2	1.91	0.53
58:UJ:1659:GLU:O	58:UJ:1663:GLY:N	2.42	0.53
61:JB:98:ILE:HG23	61:JB:103:ILE:HG21	1.91	0.53
61:JB:308:ILE:O	61:JB:367:ILE:HA	2.09	0.53
2:D2:267:U:O4	41:DQ:66:ARG:NH2	2.42	0.53
3:D4:91:C:OP1	42:CE:324:LYS:NZ	2.35	0.53
18:UO:263:ASN:OD1	18:UO:269:GLN:NE2	2.41	0.53
56:UA:160:PHE:HB3	56:UA:172:ILE:HD11	1.91	0.53
56:UA:559:ILE:HG23	56:UA:598:ASN:HD22	1.74	0.53
61:JB:398:LYS:HE3	61:JB:429:GLN:HE22	1.74	0.53
1:D3:1745:G:OP2	1:D3:1745:G:N2	2.36	0.53
12:UC:502:LYS:HZ2	50:UZ:250:THR:HG1	1.53	0.53
26:JK:496:GLY:HA3	61:JB:506:GLY:HA3	1.91	0.53
59:DH:173:TYR:HE2	59:DH:181:ILE:HD12	1.74	0.53
61:JA:33:ALA:HB1	61:JA:151:LEU:HD22	1.90	0.53
61:JB:283:ALA:HB3	61:JB:289:LYS:HD3	1.91	0.53
4:CJ:57:ARG:HG2	47:JN:207:ARG:HH12	1.74	0.53
11:UB:555:ARG:HG3	11:UB:556:ILE:HG12	1.90	0.53
52:UR:278:ASP:OD1	52:UR:281:THR:OG1	2.26	0.53
61:JA:329:PHE:HB3	61:JA:334:TYR:HB2	1.91	0.53
1:D3:24:U:O4	1:D3:601:A:N6	2.42	0.52
2:D2:148:G:N7	18:UO:383:ARG:NH2	2.57	0.52
2:D2:394:U:OP1	22:CI:108:ARG:NH2	2.38	0.52
13:UE:6:LEU:HD21	52:UR:280:LYS:HE2	1.91	0.52
39:CH:333:MET:HG3	39:CH:335:ARG:HG2	1.91	0.52
42:CE:414:ARG:NH2	58:UJ:187:ASP:OD2	2.42	0.52
60:UT:1900:ARG:HD3	60:UT:1933:ILE:HG23	1.90	0.52
1:D3:442:C:O2'	1:D3:525:A:N1	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:US:130:GLU:O	20:US:134:PHE:CB	2.55	0.52
1:D3:1499:G:N2	50:UZ:194:ASP:OD2	2.42	0.52
14:UH:670:GLU:OE2	18:UO:499:LYS:NZ	2.41	0.52
18:UO:474:LEU:O	18:UO:481:GLN:NE2	2.42	0.52
45:UF:120:ARG:HG3	45:UF:124:THR:HG23	1.91	0.52
60:UT:635:ALA:HB1	60:UT:676:PRO:HG3	1.91	0.52
9:JF:196:LEU:HD11	9:JF:202:ILE:HD13	1.91	0.52
10:CB:103:GLU:OE2	10:CB:121:LYS:NZ	2.42	0.52
18:UO:129:VAL:HB	18:UO:143:ALA:HB3	1.91	0.52
42:CE:290:LEU:O	42:CE:391:ARG:NH1	2.42	0.52
56:UA:259:ASN:OD1	56:UA:260:GLN:N	2.41	0.52
61:JB:276:ASN:HA	61:JB:463:ARG:HD2	1.90	0.52
11:UB:426:THR:HG22	11:UB:462:LEU:HD13	1.91	0.52
38:DL:101:GLU:OE2	38:DL:103:ARG:NH2	2.42	0.52
44:UN:295:VAL:HG21	51:JP:291:MET:HE1	1.92	0.52
45:UF:15:MET:HE3	45:UF:36:ARG:HH12	1.73	0.52
51:JP:149:SER:HB3	51:JP:173:ILE:HD11	1.90	0.52
61:JA:142:VAL:HG21	61:JA:148:VAL:HG22	1.91	0.52
10:CB:228:GLN:HA	10:CB:259:MET:HE1	1.92	0.52
16:UL:367:ILE:HG12	16:UL:379:PRO:HB3	1.90	0.52
16:UL:877:LYS:NZ	17:UM:814:ASP:OD1	2.37	0.52
27:JM:127:ARG:HA	27:JM:130:LEU:HD13	1.92	0.52
43:CD:195:VAL:HG22	43:CD:274:PHE:HB3	1.91	0.52
49:CM:342:VAL:HG12	49:CM:344:GLU:H	1.74	0.52
1:D3:53:G:N2	1:D3:439:U:O2	2.42	0.52
6:CL:88:SER:HB3	6:CL:220:ILE:HG13	1.91	0.52
18:UO:233:ASN:OD1	18:UO:235:LYS:NZ	2.42	0.52
2:D2:102:A:OP1	18:UO:454:ARG:NH2	2.42	0.52
6:CL:118:LEU:HD21	6:CL:809:PRO:HB3	1.91	0.52
10:CB:228:GLN:O	10:CB:231:ARG:NH1	2.43	0.52
13:UE:544:ASP:OD2	18:UO:492:ARG:NH1	2.41	0.52
27:JM:123:LEU:HD13	27:JM:177:LEU:HD12	1.91	0.52
51:JP:330:ARG:NH1	51:JP:339:SER:OG	2.43	0.52
1:D3:1210:C:H42	1:D3:1453:G:H1	1.58	0.52
1:D3:1510:U:OP1	50:UZ:50:ARG:NH1	2.43	0.52
53:UU:335:VAL:HG11	58:UJ:194:SER:HB3	1.91	0.52
23:JE:257:ASP:OD2	23:JE:257:ASP:N	2.41	0.52
42:CE:11:GLY:HA3	42:CE:49:LYS:HA	1.92	0.52
61:JB:32:ARG:HE	61:JB:203:ASP:HB2	1.74	0.52
61:JB:104:ARG:NH1	61:JB:105:TYR:O	2.43	0.52
1:D3:1221:A:N6	1:D3:1261:G:O6	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:UA:150:THR:N	56:UA:164:THR:O	2.41	0.51
61:JA:585:VAL:HB	61:JA:639:ALA:HB3	1.92	0.51
14:UH:508:ASP:OD1	14:UH:536:ARG:NH1	2.43	0.51
34:DE:141:THR:OG1	34:DE:143:ASP:OD1	2.27	0.51
54:UD:80:ASN:O	54:UD:85:TRP:HA	2.09	0.51
59:DH:123:ASP:OD1	59:DH:138:LYS:NZ	2.43	0.51
13:UE:441:LEU:HD13	13:UE:456:VAL:HG11	1.92	0.51
16:UL:332:ILE:HG12	16:UL:379:PRO:HG3	1.92	0.51
60:UT:631:THR:O	60:UT:635:ALA:N	2.44	0.51
5:CK:491:ALA:HA	56:UA:418:ARG:HH12	1.75	0.51
28:JQ:201:ASP:OD2	28:JQ:202:SER:N	2.44	0.51
46:UG:17:ASN:ND2	46:UG:64:ASP:OD2	2.42	0.51
4:CJ:100:LEU:HD13	4:CJ:144:GLU:HB3	1.91	0.51
18:UO:310:SER:O	18:UO:316:ARG:NH2	2.41	0.51
34:DE:118:GLU:OE1	34:DE:237:SER:N	2.42	0.51
42:CE:430:ASP:HA	53:UU:125:GLY:HA2	1.92	0.51
44:UN:894:LEU:HD22	51:JP:272:MET:HA	1.91	0.51
61:JA:200:VAL:HG12	61:JA:208:LEU:HD12	1.92	0.51
61:JB:132:PRO:HB3	61:JB:490:LEU:HD22	1.91	0.51
61:JB:164:MET:HE1	61:JB:186:GLU:HA	1.92	0.51
61:JB:391:ALA:HA	61:JB:422:LEU:HD13	1.93	0.51
9:JG:178:VAL:HA	9:JG:223:GLU:O	2.11	0.51
10:CB:165:ALA:HB3	10:CB:168:LYS:HG2	1.93	0.51
21:CF:62:GLU:HG3	21:CF:65:LEU:HD12	1.93	0.51
35:DX:54:LEU:HD11	35:DX:75:GLN:HB2	1.93	0.51
53:UU:576:ARG:NH2	56:UA:716:ASP:OD1	2.39	0.51
15:UK:185:MET:HG2	15:UK:190:LEU:HB2	1.92	0.51
16:UL:589:ILE:HG21	16:UL:621:VAL:HG11	1.92	0.51
45:UF:66:LEU:HD11	45:UF:70:ARG:HH21	1.75	0.51
51:JP:220:ASP:OD1	59:DH:141:ARG:NH2	2.38	0.51
58:UJ:579:ARG:NH1	58:UJ:632:THR:O	2.44	0.51
11:UB:554:GLN:OE1	11:UB:557:SER:OG	2.29	0.51
21:CG:54:MET:HE1	21:CG:78:TYR:HB2	1.93	0.51
53:UU:430:ILE:HB	53:UU:443:TRP:HB2	1.93	0.51
55:UQ:745:ILE:O	55:UQ:754:LEU:N	2.44	0.51
58:UJ:363:LEU:HD13	58:UJ:366:ILE:HD12	1.92	0.51
1:D3:564:G:O6	15:UK:42:HIS:NE2	2.43	0.51
1:D3:1559:A:H62	1:D3:1563:C:H41	1.57	0.51
2:D2:490:G:O2'	45:UF:86:TRP:NE1	2.40	0.51
4:CJ:60:GLN:OE1	47:JN:207:ARG:NH2	2.43	0.51
16:UL:606:ASP:OD1	16:UL:606:ASP:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:CD:29:SER:O	43:CD:35:GLN:NE2	2.44	0.51
45:UF:67:ARG:NH2	45:UF:84:SER:OG	2.38	0.51
61:JB:408:MET:HE1	61:JB:426:LEU:HD21	1.93	0.51
2:D2:12:G:HO2'	2:D2:70:A:H62	1.55	0.51
10:CB:144:TRP:NE1	10:CB:152:ALA:HB3	2.26	0.51
11:UB:460:LYS:NZ	20:US:524:GLU:O	2.43	0.51
13:UE:436:THR:OG1	20:US:297:ASP:OD2	2.29	0.51
16:UL:433:ALA:HB1	16:UL:447:LEU:HD11	1.93	0.51
55:UQ:665:ILE:HD11	55:UQ:720:ILE:HD11	1.93	0.51
56:UA:689:THR:HG21	56:UA:826:ARG:HH11	1.75	0.51
61:JA:48:ASP:HB3	61:JA:51:MET:HB2	1.92	0.51
61:JB:425:LYS:NZ	61:JB:543:SER:O	2.44	0.51
5:CK:516:SER:HB3	5:CK:519:GLU:HG2	1.93	0.50
16:UL:177:LEU:HB3	16:UL:189:TRP:HB2	1.93	0.50
18:UO:38:GLU:OE1	18:UO:62:ARG:NH2	2.45	0.50
26:JK:493:PHE:O	26:JK:497:LEU:HB2	2.11	0.50
51:JP:50:LEU:HA	51:JP:53:MET:HE3	1.92	0.50
53:UU:32:ASN:HA	53:UU:317:ASN:HD21	1.75	0.50
53:UU:909:LEU:HB3	56:UA:846:TYR:HE1	1.75	0.50
60:UT:2095:LEU:O	60:UT:2099:SER:N	2.44	0.50
61:JB:55:VAL:HG22	61:JB:121:MET:HB2	1.93	0.50
61:JB:359:ILE:HB	61:JB:365:GLN:HB2	1.93	0.50
61:JB:540:LEU:HD23	61:JB:585:VAL:HG23	1.93	0.50
1:D3:199:G:H5'	60:UT:1055:ARG:HH12	1.76	0.50
1:D3:1610:G:OP1	29:DF:72:HIS:NE2	2.39	0.50
6:CL:364:VAL:HG12	6:CL:373:ILE:HG12	1.91	0.50
9:JG:77:LEU:HD13	9:JG:84:ILE:HA	1.92	0.50
46:UG:197:ASP:HB2	46:UG:238:MET:HE3	1.93	0.50
47:JN:155:LEU:HD21	48:JO:197:ILE:HG12	1.93	0.50
61:JA:741:SER:O	61:JA:764:ASN:ND2	2.44	0.50
16:UL:23:CYS:HB2	16:UL:41:LEU:HD11	1.93	0.50
47:JN:195:ILE:HG13	47:JN:196:VAL:H	1.77	0.50
53:UU:27:PHE:HB2	53:UU:655:THR:HG23	1.94	0.50
60:UT:1683:ARG:O	60:UT:1687:ILE:N	2.43	0.50
1:D3:-7:A:N3	44:UN:303:GLN:NE2	2.60	0.50
6:CL:166:ARG:HB3	6:CL:230:MET:HE1	1.93	0.50
16:UL:643:ASP:HB2	16:UL:650:ILE:HD11	1.92	0.50
33:JC:19:THR:H	33:JC:339:HIS:CE1	2.29	0.50
46:UG:289:MET:HB2	46:UG:303:ILE:HD11	1.92	0.50
49:CM:140:VAL:HB	49:CM:296:LEU:HD23	1.94	0.50
53:UU:21:SER:HB2	53:UU:623:ILE:HG12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:UU:731:MET:HE1	56:UA:834:GLU:HB3	1.92	0.50
56:UA:165:SER:OG	56:UA:167:ASP:OD1	2.30	0.50
1:D3:381:C:H2'	1:D3:382:C:H4'	1.93	0.50
33:JC:13:VAL:HG22	33:JC:343:ILE:HG12	1.93	0.50
61:JA:621:GLN:OE1	61:JA:784:ARG:NH1	2.44	0.50
61:JB:895:ILE:HD13	61:JB:910:ILE:HG12	1.93	0.50
1:D3:337:G:N2	1:D3:340:U:OP2	2.45	0.50
2:D2:481:U:O2'	45:UF:102:LYS:NZ	2.44	0.50
11:UB:740:MET:HE1	32:DS:102:ALA:HB3	1.94	0.50
14:UH:483:LEU:HD12	14:UH:485:ILE:H	1.76	0.50
39:CH:286:LEU:HD22	39:CH:295:LEU:HD21	1.94	0.50
42:CE:214:ILE:HG22	42:CE:216:SER:H	1.75	0.50
2:D2:192:G:H2'	2:D2:193:G:H8	1.76	0.50
6:CL:953:SER:OG	6:CL:957:GLU:OE1	2.25	0.50
15:UK:6:HIS:HB2	15:UK:9:GLN:HG3	1.93	0.50
18:UO:45:ILE:HD13	18:UO:319:VAL:HG12	1.94	0.50
18:UO:127:THR:HG22	18:UO:144:SER:HB3	1.93	0.50
30:DI:43:ILE:HA	30:DI:56:ARG:O	2.12	0.50
46:UG:70:SER:OG	51:JP:4:LYS:NZ	2.44	0.50
55:UQ:655:LEU:HD12	55:UQ:659:ILE:HD11	1.93	0.50
59:DH:61:PHE:HA	59:DH:93:LEU:O	2.12	0.50
1:D3:50:C:H42	1:D3:429:G:H1	1.60	0.50
6:CL:293:VAL:HG13	6:CL:1022:LEU:HD21	1.94	0.50
14:UH:523:LEU:HD21	14:UH:544:LEU:HD21	1.94	0.50
17:UM:768:ASN:HB3	17:UM:771:LYS:HG2	1.93	0.50
33:JC:153:LEU:HB2	33:JC:167:LEU:HD11	1.94	0.50
54:UD:340:GLN:HG3	54:UD:361:LEU:HD12	1.94	0.50
55:UQ:139:GLU:HG2	55:UQ:157:PHE:HB3	1.93	0.50
61:JA:280:ALA:HB1	61:JA:408:MET:HE3	1.94	0.50
2:D2:357:G:H1	2:D2:368:U:H3	1.60	0.50
9:JF:179:THR:HB	9:JF:224:LYS:HG2	1.94	0.50
10:CB:251:ARG:NH1	54:UD:178:GLU:OE1	2.44	0.50
18:UO:87:ALA:HA	18:UO:97:CYS:O	2.12	0.50
56:UA:351:LEU:HD23	56:UA:696:ALA:HB2	1.93	0.50
58:UJ:29:HIS:O	58:UJ:123:ARG:NH2	2.36	0.50
61:JA:108:TYR:OH	61:JA:126:ASP:O	2.27	0.50
4:CJ:99:ARG:HG2	4:CJ:172:MET:HE1	1.94	0.49
7:DY:55:VAL:HG22	7:DY:75:VAL:HG22	1.93	0.49
9:JG:103:PRO:HG3	9:JF:232:LEU:HD21	1.93	0.49
22:CI:125:GLN:HG2	22:CI:129:LYS:HE3	1.94	0.49
29:DF:84:LYS:HD3	29:DF:92:ARG:HH12	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:CB:322:ARG:HH22	42:CE:114:LEU:HD23	1.77	0.49
16:UL:159:LEU:HD23	16:UL:189:TRP:CD2	2.46	0.49
16:UL:185:MET:HE3	16:UL:187:LYS:HE2	1.93	0.49
34:DE:128:LYS:HB2	34:DE:140:VAL:HB	1.93	0.49
1:D3:1273:G:H1	1:D3:1437:U:H3	1.61	0.49
20:US:378:SER:OG	20:US:453:PRO:O	2.29	0.49
35:DX:58:GLY:O	35:DX:61:SER:OG	2.27	0.49
39:CH:405:VAL:HG23	39:CH:415:THR:HG22	1.93	0.49
46:UG:128:THR:HG23	46:UG:134:VAL:HG22	1.94	0.49
54:UD:232:ASP:OD2	54:UD:263:LYS:NZ	2.42	0.49
56:UA:520:ALA:HB3	56:UA:533:SER:HB3	1.95	0.49
58:UJ:362:LYS:HB3	58:UJ:365:ILE:HB	1.94	0.49
61:JB:281:LEU:HD11	61:JB:470:LEU:HG	1.95	0.49
33:JC:15:GLN:NE2	33:JC:20:ASN:OD1	2.46	0.49
61:JB:134:LEU:HA	61:JB:137:ARG:HD2	1.93	0.49
61:JB:182:ALA:HB1	61:JB:185:ASN:HB2	1.94	0.49
61:JB:913:PHE:HA	61:JB:916:ILE:HD12	1.95	0.49
3:D4:8:U:OP1	11:UB:797:ASN:ND2	2.41	0.49
11:UB:425:PHE:HA	11:UB:428:VAL:HG22	1.95	0.49
14:UH:665:GLN:HA	14:UH:668:ILE:HG22	1.95	0.49
16:UL:903:GLN:NE2	56:UA:845:THR:OG1	2.45	0.49
29:DF:18:GLU:HG2	53:UU:496:LYS:HG2	1.94	0.49
42:CE:366:LYS:HB3	42:CE:390:SER:HB2	1.95	0.49
53:UU:840:PHE:HE2	53:UU:848:GLU:HG3	1.77	0.49
54:UD:458:ASN:OD1	54:UD:459:LYS:N	2.45	0.49
58:UJ:48:ILE:HD13	58:UJ:123:ARG:HD3	1.93	0.49
61:JB:255:LYS:HD2	61:JB:474:ILE:HD12	1.95	0.49
7:DY:91:LEU:HD22	7:DY:96:LEU:HD22	1.93	0.49
9:JG:152:SER:HB2	9:JG:159:LEU:HD11	1.94	0.49
13:UE:253:LEU:HD21	13:UE:301:LEU:HD11	1.95	0.49
20:US:450:GLU:HB3	20:US:456:THR:HG22	1.94	0.49
21:CG:34:LYS:HB3	21:CG:39:GLU:HG2	1.93	0.49
22:CI:23:GLN:NE2	22:CI:24:ASP:OD1	2.46	0.49
56:UA:363:ALA:HB2	56:UA:393:VAL:HG23	1.94	0.49
56:UA:400:GLN:HG3	56:UA:401:VAL:HG23	1.94	0.49
61:JB:187:ARG:NH1	61:JB:531:GLU:OE1	2.45	0.49
5:CK:449:ASP:O	5:CK:453:SER:CB	2.61	0.49
7:DY:81:GLU:HA	7:DY:84:LYS:HG2	1.94	0.49
26:JK:460:LYS:O	33:JC:121:ARG:NH2	2.42	0.49
51:JP:145:VAL:HB	51:JP:176:PHE:HB2	1.93	0.49
61:JA:356:ARG:HH21	61:JA:368:GLN:HB2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D3:451:A:N6	1:D3:455:C:OP2	2.46	0.49
2:D2:426:G:C2	2:D2:428:A:H5''	2.46	0.49
17:UM:673:MET:HE1	17:UM:693:ARG:HB3	1.95	0.49
20:US:199:PHE:HE1	20:US:212:LEU:HD22	1.77	0.49
50:UZ:83:TYR:OH	50:UZ:169:GLU:OE2	2.30	0.49
56:UA:518:VAL:HG13	56:UA:532:VAL:HG13	1.92	0.49
8:UX:16:THR:HG22	46:UG:183:GLU:HB3	1.95	0.49
9:JG:55:ILE:HG12	9:JG:76:LEU:HD21	1.94	0.49
16:UL:676:SER:OG	16:UL:677:HIS:N	2.44	0.49
58:UJ:398:SER:HA	58:UJ:401:VAL:HG12	1.95	0.49
18:UO:86:SER:O	18:UO:98:ALA:HA	2.12	0.49
54:UD:310:ASN:OD1	54:UD:310:ASN:N	2.46	0.49
54:UD:473:THR:HG21	54:UD:496:PHE:HZ	1.78	0.49
61:JB:743:VAL:HG21	61:JB:811:ALA:HB2	1.94	0.49
5:CK:350:THR:HG21	6:CL:975:GLU:HB2	1.95	0.48
10:CB:309:TYR:OH	15:UK:127:PHE:O	2.27	0.48
18:UO:63:VAL:HB	18:UO:77:PHE:HB2	1.95	0.48
22:CI:29:ASP:O	22:CI:33:MET:HG3	2.12	0.48
54:UD:44:ALA:HB3	54:UD:71:ARG:HB3	1.95	0.48
54:UD:631:GLU:HG2	54:UD:651:ALA:HB3	1.95	0.48
1:D3:444:C:N4	1:D3:459:G:OP2	2.37	0.48
5:CK:299:SER:HA	5:CK:302:LYS:HE2	1.94	0.48
6:CL:830:ARG:NH2	35:DX:138:GLU:OE1	2.46	0.48
10:CA:236:MET:HE2	43:CD:133:LEU:HB2	1.95	0.48
45:UF:144:VAL:HG21	45:UF:178:VAL:HG11	1.94	0.48
50:UZ:72:ILE:HD13	50:UZ:180:LEU:HD21	1.95	0.48
53:UU:416:ALA:HB3	53:UU:433:ALA:HB3	1.94	0.48
60:UT:2086:ILE:O	60:UT:2090:ALA:CB	2.61	0.48
61:JB:123:ILE:HG23	61:JB:149:VAL:HG23	1.95	0.48
1:D3:366:A:H2	1:D3:379:U:H3	1.60	0.48
4:CJ:140:VAL:HA	4:CJ:153:THR:O	2.13	0.48
13:UE:146:VAL:HG23	13:UE:147:GLN:HG3	1.95	0.48
20:US:107:SER:HA	20:US:158:SER:HB3	1.95	0.48
41:DQ:37:THR:O	41:DQ:45:ARG:NH1	2.45	0.48
42:CE:113:THR:HA	42:CE:116:ILE:HD13	1.95	0.48
49:CM:214:LYS:HA	49:CM:217:LYS:HE3	1.95	0.48
60:UT:1331:LEU:HA	60:UT:1335:GLY:HA3	1.93	0.48
61:JB:32:ARG:HA	61:JB:35:ASN:HB2	1.95	0.48
11:UB:478:ILE:HG23	11:UB:524:LEU:HD22	1.95	0.48
15:UK:72:THR:O	22:CI:175:ASN:ND2	2.47	0.48
4:CJ:57:ARG:HD2	22:CI:62:SER:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:UH:495:ARG:NH2	55:UQ:693:ASP:OD2	2.41	0.48
34:DE:207:LEU:HD22	34:DE:219:VAL:HG12	1.94	0.48
44:UN:277:ARG:NH2	59:DH:163:ASP:OD2	2.46	0.48
49:CM:291:ARG:HG2	49:CM:317:GLN:HG2	1.95	0.48
54:UD:324:SER:OG	54:UD:325:ASN:N	2.47	0.48
61:JB:418:THR:HB	61:JB:548:ASN:H	1.78	0.48
1:D3:261:U:H4'	1:D3:262:U:H5'	1.94	0.48
9:JG:252:LEU:OXT	9:JF:228:SER:OG	2.26	0.48
39:CH:212:LYS:NZ	39:CH:266:GLU:O	2.45	0.48
48:JO:166:VAL:HG13	48:JO:171:VAL:HG22	1.95	0.48
50:UZ:110:PHE:HA	50:UZ:114:LYS:HD2	1.94	0.48
52:UR:321:MET:HB2	52:UR:355:PHE:CD2	2.49	0.48
60:UT:1019:THR:HA	60:UT:1023:LEU:HB3	1.96	0.48
61:JA:160:GLN:HG2	61:JA:172:TYR:HB3	1.94	0.48
61:JB:200:VAL:HG12	61:JB:208:LEU:HD12	1.95	0.48
16:UL:386:GLU:O	16:UL:391:ARG:NH1	2.41	0.48
33:JC:290:VAL:HG22	33:JC:299:ILE:HG12	1.95	0.48
39:CH:150:THR:HG22	39:CH:207:ARG:HH11	1.79	0.48
48:JO:68:ASN:O	48:JO:85:THR:OG1	2.28	0.48
52:UR:475:LYS:NZ	55:UQ:849:ASP:OD2	2.42	0.48
60:UT:1684:GLY:O	60:UT:1688:HIS:ND1	2.45	0.48
2:D2:467:A:H61	3:D4:49:C:H42	1.62	0.48
31:DJ:148:VAL:HG11	31:DJ:156:ILE:HD11	1.96	0.48
34:DE:202:ASP:N	34:DE:202:ASP:OD1	2.45	0.48
35:DX:92:CYS:HB3	35:DX:132:LEU:HD22	1.95	0.48
49:CM:124:SER:OG	49:CM:125:HIS:N	2.46	0.48
58:UJ:22:ARG:O	58:UJ:26:GLN:HG2	2.13	0.48
58:UJ:401:VAL:HG23	58:UJ:433:LEU:HD13	1.96	0.48
59:DH:86:GLN:HE22	60:UT:2074:SER:H	1.62	0.48
10:CB:156:MET:HE3	10:CB:156:MET:HB3	1.71	0.48
17:UM:747:ASN:HD21	17:UM:789:THR:HG23	1.78	0.48
53:UU:641:LEU:HB3	53:UU:654:TRP:HB2	1.96	0.48
60:UT:177:LEU:HD12	60:UT:196:LEU:HD13	1.96	0.48
1:D3:513:U:O2'	1:D3:514:G:O4'	2.25	0.48
1:D3:1588:G:H1	1:D3:1608:U:H3	1.61	0.48
6:CL:124:ASP:OD1	6:CL:127:ALA:N	2.42	0.48
9:JF:51:GLU:OE2	9:JF:118:ARG:NH1	2.44	0.48
9:JF:96:LEU:HD21	9:JF:114:ILE:HD11	1.96	0.48
37:DG:12:SER:OG	37:DG:124:LEU:O	2.32	0.48
45:UF:15:MET:HG3	45:UF:33:MET:HE2	1.94	0.48
58:UJ:136:LEU:O	58:UJ:140:LEU:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:DH:46:ILE:HD11	59:DH:58:LEU:HD23	1.96	0.48
60:UT:2007:VAL:O	60:UT:2010:HIS:ND1	2.47	0.48
6:CL:244:MET:HB2	6:CL:275:LEU:HD23	1.95	0.47
6:CL:373:ILE:HD12	61:JA:6:ILE:HG21	1.95	0.47
18:UO:412:GLU:O	18:UO:416:THR:HG23	2.14	0.47
38:DL:101:GLU:OE1	38:DL:103:ARG:NE	2.46	0.47
43:CD:33:GLU:HB3	51:JP:384:ASN:HB3	1.96	0.47
47:JN:165:LEU:O	47:JN:169:ASN:HB2	2.14	0.47
60:UT:2099:SER:HA	60:UT:2102:PHE:HB2	1.96	0.47
37:DG:74:LYS:HB3	37:DG:94:ARG:HD2	1.95	0.47
46:UG:321:ASN:ND2	46:UG:333:SER:OG	2.44	0.47
2:D2:12:G:O2'	2:D2:70:A:N6	2.43	0.47
10:CB:210:MET:HE2	10:CB:210:MET:HB3	1.77	0.47
13:UE:20:VAL:HG22	13:UE:29:VAL:HG22	1.95	0.47
13:UE:296:ILE:HD12	13:UE:301:LEU:HD12	1.97	0.47
17:UM:747:ASN:HD22	17:UM:785:ILE:HG23	1.78	0.47
21:CG:42:LYS:O	21:CG:46:ARG:HG2	2.14	0.47
42:CE:288:THR:HG23	42:CE:293:GLU:HG3	1.96	0.47
53:UU:242:ARG:NH1	53:UU:278:LEU:O	2.46	0.47
54:UD:487:VAL:HG22	54:UD:497:ILE:HG12	1.96	0.47
61:JB:9:ARG:NE	61:JB:214:LYS:O	2.47	0.47
61:JB:289:LYS:HD2	61:JB:409:ALA:HB1	1.95	0.47
5:CK:534:ARG:HE	5:CK:534:ARG:HB2	1.51	0.47
34:DE:31:PRO:HG3	34:DE:43:PRO:HG3	1.95	0.47
55:UQ:682:ASN:HB2	55:UQ:689:ILE:HD11	1.95	0.47
61:JB:378:LEU:HD22	61:JB:400:LEU:HD22	1.95	0.47
1:D3:-6:A:H1'	46:UG:41:LYS:HG2	1.96	0.47
1:D3:68:A:OP1	37:DG:171:LYS:NZ	2.47	0.47
1:D3:523:G:H4'	7:DY:61:ARG:HH12	1.79	0.47
2:D2:371:G:N7	46:UG:502:ARG:NH2	2.62	0.47
6:CL:246:ALA:HB3	6:CL:810:ILE:HB	1.96	0.47
10:CA:290:VAL:HG13	10:CA:300:PRO:HG3	1.97	0.47
12:UC:435:LYS:HA	12:UC:435:LYS:HD3	1.64	0.47
34:DE:192:ILE:HD13	34:DE:238:LEU:HD13	1.97	0.47
52:UR:352:GLN:NE2	52:UR:354:SER:O	2.47	0.47
1:D3:1165:G:H5''	29:DF:99:MET:HE1	1.97	0.47
2:D2:97:G:O2'	2:D2:154:A:N3	2.45	0.47
3:D4:312:U:H2'	3:D4:313:A:H8	1.79	0.47
10:CA:249:GLN:HE22	10:CA:271:ILE:HG12	1.80	0.47
14:UH:275:SER:HA	14:UH:287:LEU:O	2.14	0.47
51:JP:333:LYS:HD3	51:JP:340:ARG:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D3:66:U:O2	37:DG:160:ARG:NE	2.48	0.47
1:D3:67:A:N6	1:D3:83:G:O2'	2.47	0.47
1:D3:106:U:O4	1:D3:308:C:N4	2.48	0.47
6:CL:1057:ILE:HD12	15:UK:15:GLU:HB3	1.96	0.47
10:CB:261:LEU:O	42:CE:118:ARG:NH1	2.43	0.47
12:UC:502:LYS:NZ	50:UZ:251:SER:OG	2.46	0.47
15:UK:75:LYS:HB2	15:UK:75:LYS:HE2	1.71	0.47
20:US:167:LYS:O	20:US:272:GLN:NE2	2.46	0.47
33:JC:55:PHE:HE1	33:JC:80:GLN:HG3	1.79	0.47
37:DG:10:ASN:HA	37:DG:128:THR:HG23	1.96	0.47
39:CH:504:ASN:HD22	39:CH:506:ARG:HH21	1.62	0.47
45:UF:73:ARG:NH1	52:UR:19:GLU:OE2	2.48	0.47
52:UR:415:SER:OG	52:UR:416:ARG:N	2.46	0.47
60:UT:240:MET:HA	60:UT:251:ALA:HB1	1.97	0.47
61:JA:612:ASP:HB2	61:JA:615:PRO:HD2	1.97	0.47
61:JA:845:TYR:HD2	61:JA:917:MET:HE3	1.79	0.47
61:JB:203:ASP:N	61:JB:203:ASP:OD1	2.46	0.47
61:JB:422:LEU:HA	61:JB:425:LYS:HE2	1.96	0.47
1:D3:602:U:OP2	11:UB:803:ARG:NH2	2.46	0.47
16:UL:549:SER:HB3	16:UL:579:ILE:HD11	1.97	0.47
18:UO:319:VAL:HG22	18:UO:329:ILE:HG23	1.96	0.47
18:UO:385:MET:SD	18:UO:393:ASN:ND2	2.88	0.47
30:DI:62:THR:HG22	30:DI:77:ARG:HG2	1.97	0.47
38:DL:21:ASN:O	38:DL:21:ASN:ND2	2.46	0.47
52:UR:142:LYS:HG3	52:UR:143:THR:HG23	1.96	0.47
55:UQ:656:ASP:OD1	55:UQ:656:ASP:N	2.44	0.47
56:UA:631:ASN:ND2	56:UA:633:LYS:HB2	2.29	0.47
58:UJ:168:VAL:HG12	58:UJ:169:ARG:HG2	1.96	0.47
58:UJ:328:ASP:O	58:UJ:331:SER:OG	2.26	0.47
58:UJ:559:ASN:ND2	58:UJ:597:HIS:O	2.48	0.47
60:UT:2013:LEU:HB2	60:UT:2016:LEU:HG	1.96	0.47
1:D3:78:A:H1'	37:DG:175:ILE:HG12	1.96	0.47
2:D2:169:A:H4'	2:D2:170:U:H3'	1.96	0.47
10:CA:273:ALA:HA	10:CA:285:VAL:HG11	1.97	0.47
10:CB:253:ILE:HD13	10:CB:253:ILE:HA	1.74	0.47
33:JC:315:VAL:HG21	33:JC:335:SER:HB3	1.97	0.47
44:UN:867:GLN:O	51:JP:26:ARG:NH2	2.48	0.47
61:JA:37:LEU:HD13	61:JA:123:ILE:HD13	1.97	0.47
5:CK:297:LEU:HD12	5:CK:301:GLU:HG2	1.96	0.47
11:UB:555:ARG:NH2	20:US:524:GLU:OE1	2.37	0.47
54:UD:207:ASP:O	54:UD:233:LYS:NZ	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:UQ:520:LEU:O	55:UQ:523:LYS:NZ	2.47	0.47
60:UT:1311:TYR:HA	60:UT:1319:TYR:HA	1.97	0.47
61:JA:293:LEU:HD11	61:JA:409:ALA:HB2	1.96	0.47
61:JB:29:VAL:HG22	61:JB:152:LEU:HD12	1.96	0.47
2:D2:99:U:O4	18:UO:25:ARG:NH1	2.49	0.46
15:UK:143:MET:HE1	19:UP:180:LEU:HB2	1.96	0.46
18:UO:366:TYR:OH	18:UO:371:GLU:OE2	2.25	0.46
37:DG:48:TYR:OH	37:DG:119:GLN:O	2.27	0.46
39:CH:141:LEU:HD13	39:CH:144:GLU:HB2	1.95	0.46
45:UF:33:MET:O	45:UF:37:THR:OG1	2.30	0.46
50:UZ:39:ILE:HB	50:UZ:243:PHE:HB2	1.97	0.46
53:UU:894:ASP:OD1	53:UU:895:VAL:N	2.49	0.46
54:UD:211:ARG:HB3	54:UD:225:LEU:HD11	1.96	0.46
55:UQ:771:ASP:N	55:UQ:771:ASP:OD1	2.45	0.46
56:UA:730:LEU:HD13	56:UA:754:VAL:HG22	1.98	0.46
1:D3:38:C:O2'	1:D3:470:A:N1	2.37	0.46
10:CA:128:PRO:HA	10:CA:136:PRO:HA	1.97	0.46
34:DE:155:LYS:HD3	34:DE:155:LYS:HA	1.75	0.46
44:UN:837:LYS:HA	44:UN:840:LEU:HD13	1.97	0.46
45:UF:274:PHE:O	45:UF:278:MET:HG2	2.14	0.46
61:JA:200:VAL:N	61:JA:211:SER:OG	2.48	0.46
61:JA:203:ASP:OD1	61:JA:203:ASP:N	2.47	0.46
61:JB:420:ARG:NH1	61:JB:492:LEU:O	2.48	0.46
9:JF:178:VAL:HA	9:JF:223:GLU:O	2.15	0.46
16:UL:181:SER:OG	16:UL:182:LYS:N	2.48	0.46
16:UL:209:GLY:O	16:UL:219:THR:HA	2.16	0.46
27:JM:52:PHE:O	27:JM:56:GLU:HG2	2.14	0.46
27:JM:64:LYS:NZ	45:UF:156:GLU:OE1	2.48	0.46
35:DX:97:ASP:OD2	35:DX:142:LYS:NZ	2.43	0.46
45:UF:335:ILE:HA	45:UF:338:VAL:HG12	1.98	0.46
53:UU:821:LEU:HA	53:UU:833:LEU:HD22	1.98	0.46
61:JA:536:LYS:NZ	61:JA:581:ASP:OD1	2.43	0.46
61:JA:802:LEU:HD12	61:JA:886:LEU:HD13	1.98	0.46
2:D2:358:G:O6	46:UG:493:LYS:NZ	2.37	0.46
5:CK:494:GLU:OE2	56:UA:420:ARG:NH1	2.49	0.46
6:CL:906:ASP:OD2	6:CL:1030:LYS:NZ	2.49	0.46
14:UH:678:LEU:HD11	57:UI:457:LYS:HG3	1.97	0.46
18:UO:44:HIS:ND1	18:UO:85:TYR:O	2.48	0.46
38:DL:21:ASN:HD22	38:DL:21:ASN:C	2.21	0.46
42:CE:161:VAL:HB	42:CE:165:GLN:HE22	1.80	0.46
47:JN:262:ILE:HD13	48:JO:165:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:UU:179:LYS:HA	53:UU:191:PHE:O	2.15	0.46
6:CL:547:TRP:HB3	6:CL:552:LEU:HD11	1.97	0.46
9:JG:88:ARG:HH22	9:JF:132:ARG:HD2	1.80	0.46
10:CA:92:ARG:NE	12:UC:600:LYS:O	2.44	0.46
11:UB:484:ARG:HB3	11:UB:492:ALA:HB1	1.98	0.46
11:UB:515:HIS:HB3	11:UB:518:ILE:HB	1.96	0.46
29:DF:133:VAL:HG22	29:DF:198:LEU:HD13	1.98	0.46
49:CM:95:PRO:HG3	49:CM:124:SER:HB3	1.96	0.46
49:CM:204:LEU:HD22	49:CM:268:PRO:HG2	1.97	0.46
54:UD:166:VAL:HG22	54:UD:182:ILE:HG12	1.98	0.46
55:UQ:88:ILE:HG23	55:UQ:109:VAL:HG13	1.97	0.46
60:UT:2255:HIS:NE2	60:UT:2296:VAL:O	2.48	0.46
1:D3:1525:A:N3	1:D3:1589:C:O2'	2.45	0.46
1:D3:1602:C:H5'	4:CJ:146:ARG:HD2	1.97	0.46
9:JG:192:TYR:OH	9:JG:223:GLU:OE2	2.24	0.46
16:UL:7:ARG:HH12	16:UL:71:ALA:HA	1.80	0.46
33:JC:3:LEU:HB2	33:JC:359:ILE:HG22	1.97	0.46
33:JC:74:THR:HG22	33:JC:81:ILE:HG23	1.97	0.46
34:DE:181:VAL:HG12	34:DE:227:VAL:HG22	1.98	0.46
46:UG:394:HIS:HD1	46:UG:396:THR:H	1.62	0.46
56:UA:111:PHE:HD1	56:UA:124:THR:HG22	1.81	0.46
60:UT:1892:LEU:HA	60:UT:1895:PHE:HD2	1.80	0.46
61:JA:115:LEU:HD21	61:JA:137:ARG:HG2	1.96	0.46
61:JB:792:ASP:O	61:JB:795:LYS:NZ	2.49	0.46
1:D3:1482:C:O2'	41:DQ:72:GLY:O	2.26	0.46
6:CL:91:ARG:HH21	61:JA:90:GLU:HB3	1.80	0.46
6:CL:415:GLY:HA2	6:CL:426:HIS:HA	1.97	0.46
10:CA:103:GLU:HG2	12:UC:595:LYS:HA	1.97	0.46
14:UH:533:PRO:HB2	14:UH:536:ARG:HG2	1.96	0.46
20:US:531:ASP:HA	20:US:545:VAL:HG11	1.98	0.46
37:DG:159:ARG:HE	37:DG:172:ALA:HB2	1.81	0.46
43:CD:29:SER:HA	43:CD:34:VAL:HG11	1.98	0.46
49:CM:185:ARG:HG3	49:CM:312:ARG:HH11	1.80	0.46
51:JP:402:GLU:O	51:JP:405:ARG:NH1	2.48	0.46
61:JA:289:LYS:NZ	61:JA:387:ASP:OD1	2.49	0.46
2:D2:292:A:H4'	53:UU:385:GLN:HA	1.97	0.46
5:CK:520:LEU:HD22	5:CK:524:ASP:HB3	1.97	0.46
6:CL:876:PRO:HB2	6:CL:879:THR:HB	1.96	0.46
11:UB:548:ARG:HH12	20:US:549:GLY:HA3	1.81	0.46
23:JE:319:VAL:HG22	23:JE:324:ASP:HB3	1.97	0.46
45:UF:317:LEU:HA	45:UF:320:ILE:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:UU:595:PRO:HD3	53:UU:634:PHE:CD2	2.50	0.46
55:UQ:144:VAL:HG22	55:UQ:153:ILE:HG22	1.96	0.46
55:UQ:512:ILE:HG21	55:UQ:525:LEU:HD23	1.97	0.46
61:JA:592:GLY:HA3	61:JA:631:SER:HA	1.98	0.46
61:JB:124:LEU:HD13	61:JB:130:LEU:HD11	1.97	0.46
6:CL:300:GLN:HB2	6:CL:792:VAL:HB	1.98	0.46
12:UC:546:LYS:HA	12:UC:546:LYS:HD3	1.74	0.46
23:JE:324:ASP:O	31:DJ:79:ARG:NH1	2.47	0.46
30:DI:100:ALA:HB3	30:DI:169:ILE:HD12	1.98	0.46
49:CM:339:LEU:HB3	49:CM:350:MET:HE2	1.97	0.46
54:UD:148:SER:OG	54:UD:157:SER:OG	2.34	0.46
11:UB:602:LEU:HA	11:UB:675:TYR:HE1	1.81	0.46
30:DI:36:THR:O	30:DI:96:LEU:N	2.39	0.46
53:UU:503:ARG:HG3	53:UU:523:ASP:HB3	1.97	0.46
6:CL:910:GLY:O	12:UC:538:ARG:NH2	2.49	0.45
7:DY:84:LYS:O	60:UT:14:TYR:OH	2.32	0.45
10:CB:107:VAL:HB	10:CB:141:TYR:HB3	1.98	0.45
15:UK:105:ASN:HB3	42:CE:330:LEU:HD22	1.98	0.45
42:CE:61:ASN:HA	42:CE:64:ILE:HB	1.98	0.45
42:CE:359:ILE:HG13	42:CE:398:LEU:HD13	1.97	0.45
46:UG:210:GLU:HA	46:UG:234:PRO:HB3	1.98	0.45
46:UG:301:TRP:HA	46:UG:308:GLN:HA	1.98	0.45
54:UD:66:ARG:NE	54:UD:88:GLU:OE2	2.49	0.45
55:UQ:604:PHE:HB3	55:UQ:606:HIS:H	1.80	0.45
60:UT:478:GLU:HA	60:UT:481:TRP:CD1	2.51	0.45
61:JB:139:ILE:HD12	61:JB:486:LEU:HD13	1.98	0.45
1:D3:1641:C:H5	5:CK:534:ARG:HH11	1.65	0.45
11:UB:515:HIS:O	11:UB:519:THR:OG1	2.32	0.45
17:UM:686:MET:HE3	17:UM:686:MET:HB3	1.84	0.45
39:CH:488:ILE:HG12	39:CH:498:VAL:HG22	1.98	0.45
42:CE:183:ARG:HG2	43:CD:180:LEU:HD13	1.98	0.45
50:UZ:92:HIS:HB3	50:UZ:177:ARG:HH11	1.80	0.45
51:JP:41:TYR:HE1	51:JP:407:MET:HG3	1.81	0.45
53:UU:115:ASP:OD2	53:UU:115:ASP:N	2.48	0.45
55:UQ:245:LEU:HD13	55:UQ:257:ARG:HG2	1.98	0.45
61:JA:164:MET:HE2	61:JA:171:ARG:HH11	1.81	0.45
1:D3:1133:A:H4'	49:CM:199:ARG:HD3	1.99	0.45
10:CB:244:VAL:HG23	10:CB:249:GLN:HG2	1.97	0.45
11:UB:523:ILE:HG22	20:US:473:TYR:HE1	1.81	0.45
20:US:180:PHE:O	20:US:184:TYR:HB2	2.16	0.45
22:CI:63:LEU:HB3	47:JN:204:GLY:HA2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:DJ:59:LEU:HD22	31:DJ:69:ARG:HA	1.98	0.45
1:D3:113:U:H5''	1:D3:114:C:H5'	1.98	0.45
2:D2:68:U:H2'	2:D2:70:A:H2	1.81	0.45
5:CK:515:MET:SD	5:CK:528:LEU:HD21	2.56	0.45
6:CL:84:THR:HG22	6:CL:87:ARG:HH21	1.82	0.45
6:CL:1044:LEU:HD23	6:CL:1044:LEU:HA	1.82	0.45
8:UX:88:ASP:OD2	31:DJ:57:ARG:NE	2.42	0.45
10:CA:103:GLU:OE2	12:UC:595:LYS:NZ	2.49	0.45
16:UL:393:ASP:N	16:UL:393:ASP:OD1	2.47	0.45
20:US:225:HIS:HD2	20:US:227:LYS:HB2	1.82	0.45
54:UD:420:LEU:HD11	54:UD:462:VAL:HG21	1.99	0.45
55:UQ:473:LEU:HB2	55:UQ:495:ILE:HD11	1.99	0.45
61:JB:285:ARG:HB2	61:JB:414:GLY:HA2	1.97	0.45
6:CL:69:PRO:HD3	6:CL:114:ARG:HH21	1.82	0.45
9:JG:47:MET:HE3	9:JG:47:MET:HB3	1.86	0.45
10:CB:145:ASN:HB3	10:CB:148:ARG:HB2	1.98	0.45
11:UB:651:TRP:HA	11:UB:654:LEU:HD12	1.98	0.45
16:UL:658:SER:OG	16:UL:659:GLU:OE1	2.35	0.45
26:JK:459:SER:OG	26:JK:460:LYS:N	2.48	0.45
33:JC:283:VAL:HG21	33:JC:346:LEU:HB3	1.99	0.45
37:DG:135:PRO:HD2	37:DG:158:ILE:HD13	1.98	0.45
39:CH:160:ILE:HG22	39:CH:523:LYS:HB3	1.99	0.45
48:JO:80:MET:HE2	48:JO:101:ILE:HB	1.99	0.45
54:UD:382:VAL:HG11	54:UD:755:ILE:HG13	1.97	0.45
56:UA:605:ASP:HB2	56:UA:612:LEU:HD21	1.99	0.45
58:UJ:960:VAL:O	58:UJ:964:PHE:N	2.43	0.45
61:JA:282:THR:O	61:JA:469:SER:HA	2.16	0.45
1:D3:1511:U:OP1	50:UZ:147:SER:OG	2.33	0.45
13:UE:151:LEU:HD11	13:UE:163:LEU:HD13	1.99	0.45
13:UE:519:LEU:HB3	18:UO:512:THR:HG22	1.98	0.45
16:UL:673:VAL:HG22	16:UL:683:ILE:HG12	1.99	0.45
22:CI:25:GLN:OE1	46:UG:188:LYS:NZ	2.50	0.45
22:CI:179:ASP:HB2	41:DQ:7:VAL:HG13	1.99	0.45
34:DE:106:LYS:HE3	34:DE:108:ARG:HH12	1.81	0.45
46:UG:244:ASN:ND2	46:UG:444:LEU:O	2.45	0.45
52:UR:512:ASP:OD1	52:UR:512:ASP:N	2.48	0.45
53:UU:455:PHE:HB3	53:UU:477:ILE:HD11	1.99	0.45
55:UQ:431:SER:O	55:UQ:434:GLN:NE2	2.50	0.45
1:D3:53:G:H5'	6:CL:221:LEU:HD11	1.98	0.45
13:UE:121:ASP:HB2	13:UE:127:TYR:HE1	1.82	0.45
16:UL:634:SER:OG	16:UL:635:LYS:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:JC:52:ASP:OD2	37:DG:92:ARG:NH1	2.50	0.45
49:CM:279:LEU:O	49:CM:283:ILE:HG12	2.16	0.45
51:JP:35:PHE:O	51:JP:39:ARG:HB2	2.16	0.45
61:JA:584:CYS:HA	61:JA:639:ALA:O	2.17	0.45
1:D3:337:G:H3'	38:DL:133:LYS:HB2	1.99	0.45
1:D3:562:G:N7	4:CJ:281:ILE:HG23	2.31	0.45
13:UE:343:ARG:HH22	55:UQ:380:THR:HG21	1.82	0.45
20:US:202:LEU:HB3	20:US:212:LEU:HD11	1.99	0.45
39:CH:156:ASN:HA	39:CH:544:ALA:HB1	1.99	0.45
41:DQ:40:GLU:OE1	41:DQ:45:ARG:NH2	2.49	0.45
53:UU:212:ALA:HA	53:UU:222:ALA:O	2.17	0.45
61:JB:635:ILE:HB	61:JB:725:VAL:HG12	1.98	0.45
61:JB:656:LEU:HD22	61:JB:665:PHE:HZ	1.81	0.45
6:CL:49:VAL:HA	6:CL:52:ARG:HD3	1.98	0.45
6:CL:236:LYS:HB3	6:CL:236:LYS:HE3	1.79	0.45
9:JG:69:ASN:HD21	9:JG:134:PHE:HE2	1.63	0.45
9:JG:136:ARG:NH2	12:UC:438:ASP:O	2.41	0.45
16:UL:261:PHE:HE2	16:UL:286:ILE:HD11	1.81	0.45
16:UL:631:PHE:HB3	16:UL:663:LEU:HD21	1.99	0.45
18:UO:32:SER:O	18:UO:330:ARG:HA	2.16	0.45
18:UO:65:ILE:HB	18:UO:75:LYS:HB2	1.98	0.45
49:CM:263:ASP:OD1	49:CM:264:ALA:N	2.46	0.45
54:UD:183:LEU:HD22	54:UD:223:GLY:HA2	1.99	0.45
55:UQ:510:TYR:HE1	55:UQ:527:HIS:HB3	1.81	0.45
61:JA:656:LEU:HD22	61:JA:665:PHE:HZ	1.82	0.45
61:JA:894:ASN:O	61:JA:897:THR:OG1	2.33	0.45
61:JB:124:LEU:HG	61:JB:150:ILE:HA	1.99	0.45
1:D3:472:U:H4'	23:JE:316:ARG:HH22	1.82	0.45
14:UH:553:GLN:O	14:UH:557:THR:OG1	2.31	0.45
16:UL:107:ASP:OD1	16:UL:107:ASP:N	2.49	0.45
46:UG:170:GLN:OE1	46:UG:177:TYR:OH	2.31	0.45
55:UQ:203:SER:HB2	55:UQ:266:ASN:HD21	1.82	0.45
55:UQ:848:GLU:OE1	58:UJ:381:ARG:NH1	2.50	0.45
60:UT:1892:LEU:HB2	60:UT:1926:PHE:HZ	1.82	0.45
6:CL:768:GLU:HG3	49:CM:308:ILE:HG21	1.99	0.44
10:CA:111:MET:HE1	10:CA:190:PRO:HG3	1.99	0.44
15:UK:70:ARG:HD3	15:UK:78:LEU:HD11	1.99	0.44
18:UO:107:VAL:HB	18:UO:118:LEU:HB3	1.99	0.44
30:DI:101:ILE:HD12	30:DI:184:LEU:HD11	1.97	0.44
53:UU:352:PRO:HA	53:UU:353:PRO:HD3	1.88	0.44
61:JA:568:LEU:HD11	61:JA:709:LEU:HD22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D3:1206:U:O2'	1:D3:1208:A:N7	2.49	0.44
3:D4:39:C:O2'	51:JP:18:SER:O	2.31	0.44
6:CL:934:LEU:HD12	6:CL:1003:LEU:HD23	2.00	0.44
10:CB:91:HIS:HB3	10:CB:96:VAL:O	2.17	0.44
14:UH:655:LEU:HD11	57:UI:506:LEU:HB3	1.99	0.44
54:UD:392:VAL:HG22	54:UD:401:ILE:HG12	1.99	0.44
60:UT:2063:PHE:O	60:UT:2067:ASN:ND2	2.50	0.44
5:CK:341:LEU:O	6:CL:960:ARG:NH1	2.50	0.44
6:CL:555:MET:O	49:CM:327:ARG:NH2	2.50	0.44
9:JG:41:MET:HE3	9:JG:241:PHE:HD1	1.83	0.44
39:CH:475:ILE:HG21	39:CH:478:LEU:HD12	1.99	0.44
40:Dc:12:VAL:HA	40:Dc:30:VAL:HG12	1.99	0.44
51:JP:217:TRP:HE3	51:JP:254:PRO:HB2	1.82	0.44
54:UD:402:TRP:HA	54:UD:415:LYS:O	2.18	0.44
58:UJ:1510:PHE:O	58:UJ:1514:SER:CB	2.65	0.44
1:D3:-1:G:H4'	1:D3:0:U:H3'	1.99	0.44
1:D3:498:G:N7	27:JM:138:LYS:NZ	2.61	0.44
5:CK:480:GLN:O	53:UU:743:ARG:NH2	2.51	0.44
7:DY:77:ASN:ND2	60:UT:57:ILE:HG12	2.32	0.44
40:Dc:64:ARG:HD3	40:Dc:64:ARG:HA	1.72	0.44
58:UJ:1038:PRO:O	58:UJ:1042:LEU:CB	2.66	0.44
61:JA:590:LEU:O	61:JA:595:SER:OG	2.36	0.44
1:D3:259:U:O2'	1:D3:261:U:OP2	2.33	0.44
1:D3:369:A:O2'	1:D3:377:G:N2	2.50	0.44
2:D2:192:G:H2'	2:D2:193:G:C8	2.52	0.44
2:D2:427:A:N6	2:D2:428:A:N3	2.66	0.44
8:UX:186:PRO:HA	31:DJ:23:ARG:HH21	1.83	0.44
13:UE:299:ASP:OD1	13:UE:320:ARG:NE	2.39	0.44
18:UO:237:TRP:HA	18:UO:244:LYS:HA	1.99	0.44
21:CG:85:VAL:HG13	39:CH:552:TRP:HB3	1.99	0.44
34:DE:48:LEU:HD11	34:DE:70:VAL:HG21	1.99	0.44
49:CM:23:LEU:HD22	49:CM:333:PHE:HE2	1.83	0.44
60:UT:1624:THR:O	60:UT:1628:ILE:N	2.42	0.44
61:JB:160:GLN:HG2	61:JB:164:MET:HE3	1.99	0.44
1:D3:105:A:H62	1:D3:308:C:H42	1.65	0.44
1:D3:337:G:H1	26:JK:460:LYS:NZ	2.16	0.44
6:CL:549:ILE:HG21	49:CM:350:MET:HE1	2.00	0.44
24:JH:222:LYS:HA	24:JH:255:SER:H	1.83	0.44
51:JP:280:ALA:HB2	51:JP:311:VAL:HG23	2.00	0.44
56:UA:296:GLN:OE1	56:UA:330:TYR:OH	2.23	0.44
60:UT:1609:ARG:O	60:UT:1613:ALA:N	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:JA:579:ILE:HD12	61:JA:580:PRO:HD2	2.00	0.44
1:D3:7:G:N7	3:D4:28:A:O2'	2.45	0.44
1:D3:209:U:H2'	1:D3:210:A:C8	2.53	0.44
1:D3:411:C:H42	1:D3:422:G:H1	1.66	0.44
8:UX:70:ASN:HD21	8:UX:157:ASP:HB2	1.82	0.44
9:JG:180:LEU:HD12	9:JG:206:VAL:HG22	1.99	0.44
9:JG:252:LEU:HB2	20:US:426:PHE:HE2	1.83	0.44
10:CB:189:GLY:O	10:CB:216:ASN:ND2	2.51	0.44
13:UE:126:PHE:O	13:UE:139:HIS:HA	2.18	0.44
15:UK:183:SER:OG	15:UK:184:ILE:N	2.51	0.44
15:UK:183:SER:O	15:UK:185:MET:N	2.51	0.44
16:UL:388:GLN:HE22	16:UL:423:LYS:HB2	1.82	0.44
18:UO:450:ILE:HG22	18:UO:494:GLU:HG3	1.98	0.44
36:DW:95:PRO:HB3	47:JN:308:ILE:HD11	1.99	0.44
39:CH:157:LEU:HD23	39:CH:191:SER:HB3	1.99	0.44
46:UG:287:TYR:HD1	46:UG:304:ARG:HD2	1.82	0.44
50:UZ:229:ARG:HE	50:UZ:233:GLY:HA3	1.82	0.44
53:UU:309:ILE:HG12	53:UU:323:VAL:HG23	1.99	0.44
56:UA:200:SER:OG	56:UA:201:HIS:N	2.49	0.44
58:UJ:218:ILE:HG23	58:UJ:263:VAL:HG11	2.00	0.44
59:DH:60:ILE:HB	59:DH:92:PHE:HD1	1.82	0.44
60:UT:670:LEU:HG	60:UT:681:VAL:HG11	2.00	0.44
61:JA:251:VAL:O	61:JA:254:SER:OG	2.33	0.44
1:D3:351:C:O2	38:DL:103:ARG:NH2	2.50	0.44
1:D3:1491:U:OP2	27:JM:213:ARG:NH1	2.51	0.44
1:D3:1642:G:OP2	5:CK:530:ARG:NH2	2.37	0.44
9:JG:105:ASN:HB2	9:JG:110:LEU:HD23	1.99	0.44
16:UL:140:SER:OG	16:UL:141:LYS:N	2.50	0.44
17:UM:808:TYR:HB2	53:UU:932:VAL:HG22	2.00	0.44
18:UO:125:HIS:HB3	18:UO:145:ASP:HB2	2.00	0.44
37:DG:116:LYS:HE3	37:DG:116:LYS:HB2	1.90	0.44
39:CH:322:HIS:HB2	39:CH:343:ASP:HB3	1.99	0.44
60:UT:2080:MET:HA	60:UT:2083:ILE:HG22	1.99	0.44
61:JA:342:ILE:HG23	61:JA:354:ILE:HG23	1.99	0.44
2:D2:5:G:H2'	2:D2:6:A:H5''	1.99	0.44
4:CJ:153:THR:HG23	4:CJ:164:GLN:HG2	2.00	0.44
10:CA:219:PRO:O	43:CD:159:SER:OG	2.25	0.44
14:UH:655:LEU:HD21	57:UI:507:ARG:HG2	2.00	0.44
15:UK:18:GLN:HB2	15:UK:28:LEU:HB2	2.00	0.44
16:UL:836:ILE:O	16:UL:840:MET:HG2	2.18	0.44
16:UL:843:LYS:HD3	16:UL:843:LYS:HA	1.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:UO:21:THR:HG22	18:UO:23:GLU:H	1.83	0.44
33:JC:254:ILE:O	33:JC:263:SER:N	2.47	0.44
46:UG:278:ASN:N	46:UG:292:THR:O	2.50	0.44
48:JO:110:PHE:O	48:JO:114:VAL:HG23	2.18	0.44
53:UU:546:ILE:HG21	53:UU:560:LEU:HD22	2.00	0.44
58:UJ:1281:ALA:O	58:UJ:1285:VAL:N	2.42	0.44
61:JB:584:CYS:HA	61:JB:639:ALA:O	2.18	0.44
2:D2:329:A:OP1	46:UG:229:ARG:NH2	2.51	0.43
7:DY:7:ILE:HG21	7:DY:44:LEU:HD21	1.99	0.43
14:UH:492:GLU:OE1	55:UQ:675:ARG:NH1	2.43	0.43
14:UH:549:ARG:NH1	14:UH:549:ARG:HA	2.33	0.43
16:UL:753:MET:HG2	16:UL:824:MET:HG2	1.99	0.43
18:UO:420:GLU:O	18:UO:424:ARG:HG2	2.18	0.43
31:DJ:166:GLY:HA2	39:CH:227:GLU:HB3	2.00	0.43
42:CE:173:LEU:HD22	42:CE:269:ARG:HD3	2.00	0.43
53:UU:587:ARG:HB3	53:UU:605:LEU:HD12	2.00	0.43
55:UQ:152:ARG:HD3	55:UQ:175:ALA:HA	2.00	0.43
60:UT:1918:LEU:HB3	60:UT:1962:PHE:HE1	1.83	0.43
1:D3:445:A:H1'	1:D3:525:A:H5''	1.99	0.43
19:UP:172:LYS:HA	19:UP:177:ARG:HA	1.98	0.43
29:DF:144:GLU:OE1	29:DF:225:ARG:NH2	2.51	0.43
34:DE:174:LYS:HE3	34:DE:174:LYS:HB2	1.84	0.43
52:UR:20:GLN:O	52:UR:24:LYS:HG2	2.18	0.43
53:UU:173:LEU:HD11	53:UU:235:MET:HG3	2.00	0.43
53:UU:464:LYS:HA	53:UU:464:LYS:HD2	1.84	0.43
56:UA:441:SER:O	56:UA:443:GLU:N	2.51	0.43
60:UT:1514:LEU:O	60:UT:1518:MET:N	2.50	0.43
61:JA:250:LEU:HB3	61:JA:295:ILE:HG23	2.00	0.43
61:JB:421:SER:HB3	61:JB:542:VAL:HG12	1.98	0.43
6:CL:416:LEU:HD23	61:JA:529:VAL:HB	2.01	0.43
11:UB:422:LEU:O	11:UB:426:THR:HG23	2.18	0.43
14:UH:712:ASP:OD1	14:UH:712:ASP:N	2.45	0.43
16:UL:884:LYS:HB3	16:UL:884:LYS:HE3	1.70	0.43
18:UO:190:ASP:OD2	18:UO:194:ARG:NH2	2.38	0.43
18:UO:401:LEU:HB3	18:UO:434:ARG:HH22	1.83	0.43
34:DE:113:ARG:NH2	39:CH:119:SER:OG	2.48	0.43
35:DX:89:ASN:OD1	35:DX:90:ASP:N	2.52	0.43
41:DQ:48:VAL:HG23	41:DQ:78:VAL:HG13	2.00	0.43
45:UF:123:GLN:N	45:UF:123:GLN:OE1	2.51	0.43
46:UG:218:ASP:OD1	46:UG:220:SER:OG	2.28	0.43
53:UU:235:MET:HE3	53:UU:235:MET:HB3	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:UU:828:LYS:HA	53:UU:828:LYS:HD3	1.82	0.43
54:UD:736:ASP:OD1	54:UD:736:ASP:N	2.51	0.43
61:JA:635:ILE:HB	61:JA:725:VAL:HG12	2.00	0.43
1:D3:372:G:N3	23:JE:330:SER:OG	2.51	0.43
12:UC:547:ASN:O	35:DX:139:LYS:NZ	2.52	0.43
16:UL:444:LEU:HD23	16:UL:456:LEU:HD11	2.00	0.43
16:UL:800:THR:HG23	16:UL:803:GLN:H	1.83	0.43
40:Dc:58:GLU:CD	40:Dc:61:ARG:HE	2.26	0.43
42:CE:248:THR:HG22	42:CE:250:THR:H	1.82	0.43
48:JO:59:ASP:OD2	48:JO:62:ARG:NH1	2.52	0.43
60:UT:590:MET:O	60:UT:770:TYR:OH	2.34	0.43
2:D2:392:U:H5''	22:CI:102:THR:HG22	1.99	0.43
6:CL:53:LYS:HD2	6:CL:53:LYS:HA	1.77	0.43
6:CL:94:THR:HG21	6:CL:354:ILE:HB	2.01	0.43
6:CL:250:THR:HG23	6:CL:270:ALA:HB3	2.01	0.43
22:CI:128:VAL:O	22:CI:132:GLU:HG3	2.19	0.43
43:CD:399:VAL:O	43:CD:402:SER:OG	2.35	0.43
55:UQ:586:SER:HB3	55:UQ:597:LYS:HG3	2.01	0.43
60:UT:2037:ASP:OD1	60:UT:2040:ARG:NH1	2.47	0.43
61:JB:9:ARG:HD2	61:JB:216:VAL:H	1.83	0.43
61:JB:107:TYR:HD2	61:JB:109:LYS:HG2	1.84	0.43
1:D3:523:G:H1'	1:D3:529:A:H61	1.83	0.43
1:D3:1272:U:H2'	1:D3:1273:G:H8	1.83	0.43
5:CK:483:TYR:CE1	53:UU:732:ASN:HB3	2.53	0.43
27:JM:58:ASN:HA	27:JM:61:LYS:HG2	2.00	0.43
36:DW:6:VAL:HG12	36:DW:34:ILE:HD11	2.00	0.43
39:CH:152:VAL:HG12	39:CH:154:GLU:H	1.83	0.43
39:CH:547:HIS:HB2	39:CH:553:ILE:HD13	1.99	0.43
42:CE:229:GLU:O	42:CE:233:GLU:N	2.50	0.43
46:UG:13:LYS:HE3	46:UG:13:LYS:HB2	1.76	0.43
55:UQ:145:PHE:CE1	55:UQ:201:ILE:HD13	2.54	0.43
60:UT:1499:ARG:O	60:UT:1503:ILE:HG12	2.19	0.43
60:UT:1945:ILE:O	60:UT:1985:ARG:NH1	2.51	0.43
1:D3:250:C:H2'	1:D3:251:A:H8	1.84	0.43
1:D3:1743:U:H2'	1:D3:1744:A:C8	2.54	0.43
10:CA:303:GLN:HB3	12:UC:606:VAL:HG13	2.01	0.43
16:UL:888:ARG:NH2	17:UM:807:ASP:OD2	2.44	0.43
18:UO:461:ASP:HB3	55:UQ:519:LEU:HD22	2.00	0.43
38:DL:74:THR:HG22	38:DL:122:ILE:HG13	1.99	0.43
43:CD:100:ILE:HG22	43:CD:102:ASP:H	1.83	0.43
45:UF:50:ILE:HD12	45:UF:50:ILE:HA	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:UG:102:LYS:HB3	46:UG:389:LEU:HD11	2.00	0.43
46:UG:287:TYR:HD1	46:UG:304:ARG:HH11	1.66	0.43
47:JN:116:LEU:O	49:CM:134:LYS:NZ	2.40	0.43
52:UR:165:ARG:HH21	53:UU:236:ARG:HH21	1.66	0.43
53:UU:354:SER:H	53:UU:370:SER:HA	1.84	0.43
53:UU:370:SER:OG	53:UU:371:LYS:N	2.51	0.43
54:UD:568:ASN:HD22	54:UD:588:ASP:HB2	1.83	0.43
56:UA:360:VAL:HG23	56:UA:374:ILE:HD11	2.01	0.43
61:JA:765:VAL:HG23	61:JA:774:LEU:HD22	2.01	0.43
10:CA:163:PHE:CG	10:CA:266:GLY:HA3	2.53	0.43
16:UL:646:LYS:HE3	16:UL:646:LYS:HB2	1.92	0.43
19:UP:173:ARG:HA	19:UP:173:ARG:HD3	1.80	0.43
28:JQ:183:ARG:HD3	50:UZ:161:LYS:HE3	1.99	0.43
54:UD:179:HIS:HE1	54:UD:182:ILE:HG13	1.83	0.43
54:UD:552:ILE:O	54:UD:560:SER:HA	2.18	0.43
56:UA:532:VAL:O	56:UA:539:ILE:HA	2.18	0.43
60:UT:413:GLY:HA2	60:UT:416:PHE:HD2	1.84	0.43
3:D4:326:U:OP1	21:CF:46:ARG:NH2	2.42	0.43
9:JG:44:VAL:HG22	9:JG:113:TYR:HB2	2.00	0.43
10:CB:97:TYR:HB2	10:CB:107:VAL:HG23	2.00	0.43
13:UE:140:PHE:HE2	13:UE:142:ILE:HD11	1.83	0.43
14:UH:494:ASP:OD1	14:UH:494:ASP:N	2.52	0.43
14:UH:523:LEU:HD23	14:UH:550:LEU:HD13	2.01	0.43
14:UH:638:LEU:HD22	57:UI:499:ILE:HD13	2.01	0.43
27:JM:65:LEU:HD23	45:UF:187:LYS:HD2	2.00	0.43
30:DI:107:THR:O	30:DI:111:GLN:HG3	2.19	0.43
49:CM:122:THR:HG21	49:CM:156:ARG:HA	1.99	0.43
61:JB:418:THR:OG1	61:JB:546:TYR:O	2.34	0.43
1:D3:330:G:OP2	30:DI:172:ARG:NH1	2.52	0.43
1:D3:1461:C:OP2	11:UB:746:LYS:NZ	2.43	0.43
7:DY:86:GLU:O	60:UT:13:ARG:NH2	2.48	0.43
13:UE:8:SER:HA	13:UE:18:CYS:O	2.18	0.43
16:UL:631:PHE:CE2	16:UL:672:VAL:HG21	2.54	0.43
16:UL:635:LYS:HA	16:UL:659:GLU:HB2	2.01	0.43
20:US:303:TYR:CZ	20:US:320:LEU:HD13	2.54	0.43
52:UR:406:ASP:HB3	52:UR:458:ILE:HG22	2.01	0.43
53:UU:544:ALA:HB1	53:UU:563:ASP:HB2	2.01	0.43
55:UQ:493:PRO:HG3	55:UQ:513:GLU:HG3	2.00	0.43
1:D3:479:C:OP1	12:UC:566:ARG:NH2	2.46	0.42
2:D2:12:G:HO2'	2:D2:70:A:N6	2.16	0.42
2:D2:300:C:H4'	46:UG:374:ALA:HB1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:CL:609:GLU:OE2	49:CM:17:PHE:N	2.50	0.42
8:UX:47:VAL:HB	12:UC:580:ARG:HB3	2.01	0.42
9:JG:35:ASP:O	9:JG:40:ARG:NH2	2.49	0.42
16:UL:822:MET:SD	40:Dc:14:LYS:HE2	2.59	0.42
20:US:321:ASN:HB3	20:US:357:ARG:HH21	1.84	0.42
29:DF:131:GLN:NE2	29:DF:135:ASP:OD1	2.52	0.42
34:DE:182:TYR:O	34:DE:226:PHE:N	2.52	0.42
43:CD:26:ASP:HA	43:CD:29:SER:HB3	2.01	0.42
44:UN:231:SER:O	44:UN:240:GLY:N	2.52	0.42
45:UF:5:ARG:HD2	45:UF:5:ARG:HA	1.83	0.42
52:UR:228:LEU:HD12	52:UR:229:PRO:HD2	2.00	0.42
55:UQ:325:GLN:OE1	55:UQ:328:THR:OG1	2.34	0.42
61:JB:789:LEU:HA	61:JB:793:PHE:HB2	2.00	0.42
61:JB:793:PHE:O	61:JB:796:PHE:HB2	2.19	0.42
1:D3:562:G:C5	4:CJ:281:ILE:HG23	2.54	0.42
1:D3:1743:U:H2'	1:D3:1744:A:H8	1.84	0.42
2:D2:428:A:H2'	2:D2:429:A:H8	1.84	0.42
6:CL:310:THR:HG23	6:CL:313:TYR:H	1.84	0.42
16:UL:589:ILE:HG12	16:UL:599:ILE:HG12	2.00	0.42
23:JE:319:VAL:HA	23:JE:324:ASP:HA	2.01	0.42
25:JJ:273:ARG:HB2	56:UA:315:GLU:HG2	2.01	0.42
34:DE:37:LYS:HD3	34:DE:39:ARG:HH21	1.84	0.42
42:CE:319:ILE:HD12	42:CE:326:LEU:HD22	2.00	0.42
60:UT:892:LEU:HD23	60:UT:892:LEU:HA	1.88	0.42
1:D3:17:C:O2'	3:D4:14:A:N6	2.52	0.42
1:D3:87:C:O2'	1:D3:169:A:N1	2.44	0.42
6:CL:1034:LEU:O	6:CL:1038:ILE:HG13	2.19	0.42
10:CB:301:LEU:HG	10:CB:318:GLY:HA2	2.00	0.42
18:UO:35:LEU:HD23	18:UO:326:LEU:HD13	2.01	0.42
21:CG:7:LYS:NZ	21:CG:62:GLU:OE1	2.52	0.42
30:DI:117:TYR:OH	38:DL:24:LYS:NZ	2.51	0.42
38:DL:78:THR:HG22	38:DL:84:ILE:HG22	2.02	0.42
42:CE:190:TRP:HE1	43:CD:172:ASN:HD22	1.66	0.42
50:UZ:75:ILE:HG21	50:UZ:135:LEU:HD21	2.00	0.42
54:UD:88:GLU:OE2	54:UD:527:TYR:OH	2.32	0.42
55:UQ:570:SER:O	55:UQ:570:SER:OG	2.27	0.42
61:JA:373:GLN:HG3	61:JA:396:ILE:HD13	2.01	0.42
61:JA:586:ILE:HG21	61:JA:657:LEU:HD22	2.00	0.42
61:JB:858:MET:HE3	61:JB:858:MET:HB3	1.78	0.42
1:D3:1452:U:H2'	1:D3:1453:G:C8	2.54	0.42
2:D2:361:G:N2	2:D2:364:A:OP2	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D2:428:A:H2'	2:D2:429:A:C8	2.54	0.42
7:DY:22:GLN:HG2	7:DY:74:LEU:HD22	2.01	0.42
18:UO:273:ILE:HD13	18:UO:283:VAL:HG22	2.01	0.42
58:UJ:387:LEU:HD12	58:UJ:407:PHE:HE2	1.84	0.42
61:JA:345:SER:N	61:JA:353:ALA:O	2.52	0.42
61:JB:352:LYS:HB2	61:JB:352:LYS:HE3	1.83	0.42
61:JB:555:LEU:O	61:JB:559:ALA:CB	2.68	0.42
1:D3:341:A:O2'	30:DI:86:SER:O	2.38	0.42
1:D3:400:A:H5''	30:DI:25:ARG:HA	2.01	0.42
4:CJ:12:TYR:OH	4:CJ:76:GLU:OE2	2.29	0.42
11:UB:429:LEU:HD11	11:UB:455:LEU:HD22	2.01	0.42
14:UH:507:LEU:HD13	14:UH:536:ARG:HG3	2.02	0.42
14:UH:708:MET:HG2	54:UD:32:ILE:HD11	2.02	0.42
19:UP:192:PRO:HG2	54:UD:122:VAL:HG21	2.00	0.42
20:US:397:THR:HG23	20:US:499:LEU:HD23	2.01	0.42
33:JC:323:VAL:HA	33:JC:324:PRO:HD3	1.93	0.42
39:CH:335:ARG:HD3	39:CH:348:LEU:HD11	2.00	0.42
42:CE:60:ALA:HB1	42:CE:147:ILE:HD11	2.02	0.42
49:CM:143:LYS:HD2	49:CM:143:LYS:HA	1.94	0.42
52:UR:298:CYS:HA	52:UR:313:PHE:O	2.18	0.42
53:UU:232:MET:HG3	53:UU:242:ARG:HB3	2.02	0.42
56:UA:265:CYS:SG	56:UA:308:VAL:HG23	2.59	0.42
56:UA:283:GLU:OE2	56:UA:297:GLN:NE2	2.53	0.42
61:JB:871:MET:HE1	61:JB:920:MET:HE1	2.01	0.42
9:JG:89:PRO:HG2	9:JG:134:PHE:HZ	1.84	0.42
18:UO:103:GLY:HA2	18:UO:127:THR:HG23	2.01	0.42
32:DS:27:LYS:HA	32:DS:57:ARG:HA	2.00	0.42
36:DW:44:HIS:NE2	36:DW:112:ASP:OD2	2.39	0.42
49:CM:138:MET:HE1	49:CM:151:LEU:HB2	2.02	0.42
51:JP:210:LYS:HD3	51:JP:210:LYS:HA	1.95	0.42
55:UQ:379:LEU:HD23	55:UQ:379:LEU:HA	1.90	0.42
58:UJ:209:GLN:O	58:UJ:213:THR:HG23	2.20	0.42
61:JA:418:THR:HB	61:JA:548:ASN:H	1.85	0.42
61:JA:895:ILE:HA	61:JA:898:ILE:HD12	2.01	0.42
61:JB:727:TYR:OH	61:JB:762:MET:SD	2.71	0.42
1:D3:1592:A:H2'	1:D3:1593:A:C8	2.54	0.42
1:D3:1663:G:H1	1:D3:1738:U:H3	1.66	0.42
2:D2:20:C:H2'	2:D2:21:A:H8	1.83	0.42
27:JM:51:LYS:HA	27:JM:54:GLU:CD	2.45	0.42
30:DI:53:LYS:HB3	30:DI:53:LYS:HE2	1.74	0.42
39:CH:114:LYS:HB2	39:CH:114:LYS:HE2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:UU:455:PHE:HE1	53:UU:492:GLY:HA2	1.85	0.42
56:UA:180:LYS:HE3	56:UA:180:LYS:HB2	1.84	0.42
56:UA:479:LEU:HD22	56:UA:488:LEU:HD11	2.01	0.42
58:UJ:408:ILE:HD12	58:UJ:412:GLU:HG3	2.02	0.42
61:JA:789:LEU:HA	61:JA:793:PHE:HB2	2.01	0.42
1:D3:1644:C:H2'	1:D3:1645:G:H8	1.85	0.42
2:D2:20:C:H2'	2:D2:21:A:C8	2.54	0.42
10:CB:276:ILE:HG22	10:CB:277:ASP:H	1.85	0.42
13:UE:542:ALA:O	13:UE:546:ARG:HG2	2.19	0.42
16:UL:751:ARG:HA	16:UL:754:GLU:HG2	2.02	0.42
37:DG:35:GLU:OE2	37:DG:49:VAL:HG12	2.19	0.42
51:JP:185:ILE:HG13	51:JP:196:THR:HG22	2.01	0.42
53:UU:353:PRO:HA	53:UU:370:SER:HA	2.02	0.42
60:UT:2148:TRP:HD1	60:UT:2157:PHE:CZ	2.38	0.42
61:JB:293:LEU:O	61:JB:297:ILE:HG12	2.20	0.42
6:CL:89:LEU:HD22	6:CL:93:MET:HE3	2.02	0.42
16:UL:574:LEU:HD23	16:UL:574:LEU:HA	1.87	0.42
18:UO:150:ARG:HG2	18:UO:163:GLU:HG2	2.00	0.42
22:CI:66:PRO:HD3	47:JN:207:ARG:HE	1.85	0.42
41:DQ:39:VAL:HG11	41:DQ:48:VAL:HG21	2.01	0.42
53:UU:876:LYS:HE3	53:UU:876:LYS:HB2	1.87	0.42
55:UQ:680:ALA:HB2	55:UQ:750:LEU:HD12	2.01	0.42
56:UA:4:ASP:O	56:UA:706:THR:OG1	2.37	0.42
61:JB:136:ALA:HB1	61:JB:415:TYR:HB2	2.00	0.42
61:JB:159:LYS:HB3	61:JB:687:LEU:HD13	2.01	0.42
61:JB:165:THR:HG22	61:JB:210:LEU:HB3	2.01	0.42
1:D3:34:G:H21	1:D3:468:A:H1'	1.84	0.42
1:D3:511:A:OP2	31:DJ:176:ASN:ND2	2.34	0.42
6:CL:150:MET:HE1	12:UC:541:ASN:HD22	1.85	0.42
11:UB:738:ASN:OD1	11:UB:741:LYS:NZ	2.49	0.42
19:UP:194:LYS:HD2	19:UP:199:ILE:HD11	2.02	0.42
23:JE:338:THR:HB	39:CH:66:LEU:HD22	2.02	0.42
37:DG:126:ASP:OD1	37:DG:127:THR:N	2.53	0.42
41:DQ:46:PHE:HA	41:DQ:49:TYR:HB2	2.00	0.42
52:UR:251:ILE:O	52:UR:566:THR:OG1	2.34	0.42
54:UD:252:GLN:HA	54:UD:265:TRP:O	2.20	0.42
55:UQ:321:MET:HE2	55:UQ:321:MET:HB3	1.88	0.42
55:UQ:703:LYS:HB2	55:UQ:706:HIS:CD2	2.55	0.42
58:UJ:137:LEU:HD11	58:UJ:191:LEU:HG	2.01	0.42
60:UT:1722:MET:HE2	60:UT:1722:MET:HB2	1.81	0.42
61:JA:400:LEU:O	61:JA:404:TYR:OH	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D3:469:C:H5''	1:D3:470:A:N7	2.35	0.41
1:D3:502:U:H5''	12:UC:574:LYS:HD3	2.01	0.41
2:D2:254:C:H2'	28:JQ:183:ARG:HH11	1.85	0.41
2:D2:329:A:O2'	2:D2:331:U:OP2	2.38	0.41
7:DY:83:LYS:HG2	7:DY:96:LEU:HD21	2.01	0.41
8:UX:121:ARG:NH1	51:JP:66:HIS:O	2.53	0.41
13:UE:445:LEU:HD23	13:UE:445:LEU:HA	1.91	0.41
16:UL:220:THR:HG22	16:UL:226:VAL:HG22	2.02	0.41
16:UL:757:ASP:OD1	16:UL:831:LYS:NZ	2.48	0.41
21:CG:64:LEU:HD23	21:CG:98:ILE:HD12	2.02	0.41
33:JC:329:PHE:HE2	33:JC:343:ILE:HD12	1.85	0.41
39:CH:62:LYS:HA	39:CH:65:ARG:HG2	2.02	0.41
51:JP:122:ARG:NH1	51:JP:191:ASN:O	2.53	0.41
54:UD:141:SER:HB2	54:UD:164:THR:HG21	2.02	0.41
61:JA:842:LEU:HD12	61:JA:917:MET:HE2	2.02	0.41
61:JB:115:LEU:HD11	61:JB:137:ARG:HG2	2.02	0.41
1:D3:384:G:O2'	30:DI:21:PHE:O	2.37	0.41
2:D2:194:G:H2'	2:D2:195:A:H8	1.84	0.41
10:CA:291:GLN:O	10:CA:295:GLU:HG2	2.20	0.41
13:UE:150:LYS:HG3	13:UE:191:VAL:HG12	2.01	0.41
16:UL:89:LYS:HD2	16:UL:89:LYS:HA	1.91	0.41
30:DI:76:THR:HG22	30:DI:108:PRO:HG2	2.02	0.41
33:JC:62:ILE:HD13	33:JC:330:PHE:HB3	2.02	0.41
38:DL:57:LYS:HB2	38:DL:110:HIS:CE1	2.55	0.41
39:CH:111:ASP:HA	39:CH:114:LYS:HE2	2.02	0.41
49:CM:47:ASP:OD1	49:CM:48:TYR:N	2.53	0.41
49:CM:321:ARG:HA	49:CM:324:ILE:HG22	2.01	0.41
53:UU:718:LYS:HA	53:UU:718:LYS:HD2	1.70	0.41
59:DH:159:VAL:HG11	59:DH:188:GLU:HG3	2.02	0.41
60:UT:2021:ASP:O	60:UT:2024:ARG:HG2	2.20	0.41
61:JA:385:VAL:HG22	61:JA:407:PHE:HB2	2.02	0.41
61:JB:57:TRP:HE1	61:JB:59:TYR:HB3	1.85	0.41
61:JB:178:GLY:O	61:JB:601:ASN:ND2	2.47	0.41
1:D3:416:A:N1	61:JA:59:TYR:OH	2.43	0.41
1:D3:1512:G:H2'	1:D3:1513:G:C8	2.54	0.41
9:JF:242:CYS:O	9:JF:246:GLU:HG3	2.20	0.41
10:CA:160:ASP:HB2	12:UC:603:THR:HG21	2.02	0.41
11:UB:412:PRO:HA	11:UB:418:ASN:HB2	2.02	0.41
41:DQ:83:GLN:HE22	41:DQ:119:ALA:HA	1.85	0.41
44:UN:299:ASN:HA	44:UN:302:VAL:HG22	2.02	0.41
45:UF:14:GLU:OE2	45:UF:91:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:UG:333:SER:HB3	46:UG:381:LEU:HD11	2.02	0.41
49:CM:46:LYS:HD3	49:CM:46:LYS:HA	1.74	0.41
49:CM:176:GLN:HE21	49:CM:305:LYS:HB3	1.85	0.41
50:UZ:114:LYS:HA	50:UZ:117:GLN:HG3	2.02	0.41
53:UU:516:LYS:HE2	53:UU:573:VAL:HG12	2.02	0.41
53:UU:557:LEU:HD23	53:UU:571:ASP:HA	2.02	0.41
53:UU:834:LEU:O	53:UU:838:ILE:HG12	2.20	0.41
54:UD:80:ASN:ND2	54:UD:88:GLU:OE1	2.43	0.41
55:UQ:97:THR:OG1	55:UQ:130:LYS:NZ	2.36	0.41
56:UA:475:PRO:HD2	56:UA:493:TRP:HB2	2.01	0.41
60:UT:670:LEU:HD23	60:UT:670:LEU:HA	1.92	0.41
61:JA:380:GLN:NE2	61:JB:307:ASN:OD1	2.54	0.41
2:D2:223:C:H2'	2:D2:224:G:C8	2.56	0.41
6:CL:248:ARG:HD3	6:CL:357:PRO:HB2	2.02	0.41
10:CA:85:LYS:HG3	27:JM:172:THR:HA	2.02	0.41
13:UE:443:GLN:NE2	20:US:333:GLU:O	2.53	0.41
22:CI:162:ASP:OD1	22:CI:162:ASP:N	2.53	0.41
28:JQ:200:GLU:O	50:UZ:181:ARG:NH1	2.42	0.41
42:CE:215:ARG:HB3	42:CE:239:ALA:HB1	2.01	0.41
55:UQ:249:THR:HA	55:UQ:252:LEU:HD12	2.03	0.41
56:UA:843:LYS:HE2	56:UA:843:LYS:HB3	1.90	0.41
57:UI:435:LEU:HD23	57:UI:478:ASN:HD22	1.85	0.41
58:UJ:559:ASN:HB2	58:UJ:598:TYR:HA	2.02	0.41
60:UT:266:SER:O	60:UT:313:ARG:NH1	2.53	0.41
61:JA:855:ILE:O	61:JA:859:ILE:HG13	2.20	0.41
61:JB:308:ILE:HB	61:JB:367:ILE:HG12	2.03	0.41
1:D3:52:U:H2'	1:D3:53:G:C8	2.55	0.41
1:D3:1572:G:O6	9:JG:151:ARG:NH1	2.53	0.41
3:D4:327:G:OP1	15:UK:222:ARG:NH2	2.47	0.41
11:UB:548:ARG:NH1	20:US:548:PRO:O	2.51	0.41
33:JC:257:LEU:HD23	33:JC:257:LEU:HA	1.88	0.41
33:JC:331:THR:OG1	33:JC:339:HIS:HB2	2.19	0.41
34:DE:139:VAL:HG13	34:DE:150:PRO:HG3	2.03	0.41
37:DG:207:GLU:HA	37:DG:210:GLN:HG3	2.01	0.41
43:CD:146:ASP:OD1	43:CD:146:ASP:N	2.51	0.41
61:JA:45:MET:HE2	61:JA:53:LYS:HG2	2.03	0.41
61:JA:913:PHE:HA	61:JA:916:ILE:HD12	2.01	0.41
61:JB:258:ASN:ND2	61:JB:472:GLU:H	2.18	0.41
1:D3:209:U:H2'	1:D3:210:A:H8	1.85	0.41
1:D3:1615:C:C5	29:DF:81:ARG:HA	2.55	0.41
2:D2:425:U:H3	2:D2:431:A:H62	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:CK:314:LEU:HD13	6:CL:857:LEU:HD11	2.03	0.41
9:JG:232:LEU:HD21	9:JF:103:PRO:HG3	2.02	0.41
10:CA:171:LEU:HB2	10:CA:237:VAL:HG11	2.02	0.41
10:CB:175:ALA:HB1	10:CB:181:VAL:HG21	2.03	0.41
13:UE:28:ARG:HA	13:UE:51:LEU:O	2.21	0.41
13:UE:283:SER:OG	13:UE:285:ASP:OD1	2.37	0.41
13:UE:503:LYS:HG2	18:UO:507:MET:HE1	2.02	0.41
16:UL:749:GLY:O	16:UL:753:MET:HG3	2.20	0.41
37:DG:51:LYS:HE2	37:DG:51:LYS:HB3	1.80	0.41
46:UG:287:TYR:CD1	46:UG:304:ARG:HD2	2.55	0.41
52:UR:345:LEU:HD13	52:UR:352:GLN:HB3	2.02	0.41
55:UQ:40:ASP:OD1	55:UQ:40:ASP:N	2.52	0.41
58:UJ:539:LEU:HD13	58:UJ:542:ILE:HD11	2.03	0.41
9:JF:51:GLU:HB2	9:JF:68:LEU:HB2	2.02	0.41
10:CA:227:PRO:HG2	10:CA:255:LEU:HB3	2.02	0.41
10:CB:163:PHE:CG	10:CB:266:GLY:HA3	2.56	0.41
10:CB:310:GLU:HB2	10:CB:313:HIS:HB2	2.03	0.41
11:UB:772:LYS:HB3	11:UB:772:LYS:HE3	1.91	0.41
21:CG:33:LEU:HD11	21:CG:100:ALA:HB1	2.03	0.41
34:DE:188:ASN:HD22	34:DE:218:PHE:HD2	1.69	0.41
45:UF:128:LYS:HE3	45:UF:128:LYS:HB3	1.89	0.41
45:UF:286:ILE:HD13	45:UF:286:ILE:HA	1.91	0.41
49:CM:176:GLN:NE2	49:CM:305:LYS:HB3	2.35	0.41
60:UT:2015:GLU:N	60:UT:2015:GLU:OE2	2.54	0.41
1:D3:1615:C:H5''	1:D3:1616:G:O4'	2.20	0.41
1:D3:1658:G:H1	1:D3:1743:U:H3	1.68	0.41
2:D2:550:C:H42	2:D2:587:G:H1	1.69	0.41
3:D4:79:G:C5	21:CF:95:ARG:HD3	2.56	0.41
3:D4:87:G:H21	3:D4:90:C:N4	2.19	0.41
10:CA:97:TYR:HB2	10:CA:107:VAL:HG23	2.01	0.41
11:UB:498:LEU:HD13	11:UB:545:VAL:HG11	2.03	0.41
11:UB:628:PRO:HG2	11:UB:631:GLN:HB3	2.02	0.41
13:UE:519:LEU:HD12	13:UE:519:LEU:HA	1.85	0.41
16:UL:555:VAL:HG23	16:UL:569:LEU:HB2	2.02	0.41
17:UM:728:ILE:HA	17:UM:731:LEU:HD13	2.02	0.41
30:DI:65:PHE:HA	30:DI:181:GLY:O	2.21	0.41
30:DI:121:LEU:HD11	30:DI:152:ILE:HD11	2.02	0.41
33:JC:273:ASP:OD1	33:JC:273:ASP:N	2.51	0.41
37:DG:130:PRO:HB3	60:UT:633:GLN:HA	2.03	0.41
41:DQ:71:GLY:O	41:DQ:77:GLN:NE2	2.48	0.41
50:UZ:147:SER:HA	50:UZ:150:LEU:HG	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:UZ:161:LYS:NZ	50:UZ:162:LEU:O	2.52	0.41
55:UQ:22:LEU:HD11	55:UQ:357:ILE:HD13	2.02	0.41
55:UQ:282:ILE:HD11	55:UQ:312:LEU:HD22	2.02	0.41
55:UQ:765:TRP:O	55:UQ:776:PHE:HA	2.20	0.41
1:D3:65:A:N6	1:D3:84:A:OP2	2.53	0.41
1:D3:143:G:O6	37:DG:177:ARG:NH2	2.51	0.41
1:D3:1131:A:N6	1:D3:1137:A:OP2	2.52	0.41
2:D2:210:U:H2'	2:D2:211:G:H8	1.85	0.41
2:D2:522:C:O2'	51:JP:125:ASP:O	2.29	0.41
6:CL:288:VAL:HG12	6:CL:814:GLY:HA2	2.02	0.41
6:CL:411:PHE:HZ	61:JA:190:LEU:HD13	1.85	0.41
6:CL:1082:GLN:OE1	22:CI:173:TYR:OH	2.30	0.41
7:DY:91:LEU:HB3	7:DY:97:ALA:HB3	2.02	0.41
9:JG:19:LEU:O	18:UO:125:HIS:NE2	2.39	0.41
9:JG:239:SER:OG	9:JF:239:SER:OG	2.26	0.41
18:UO:129:VAL:HG11	18:UO:174:LEU:HG	2.03	0.41
20:US:156:TRP:HB3	20:US:215:ASN:HD21	1.86	0.41
27:JM:208:LYS:HE3	27:JM:209:MET:HE2	2.02	0.41
34:DE:148:ARG:NH1	37:DG:201:GLN:OE1	2.54	0.41
38:DL:13:PHE:CE2	38:DL:15:LYS:HB3	2.56	0.41
39:CH:66:LEU:HD23	39:CH:66:LEU:HA	1.93	0.41
43:CD:21:LYS:HE2	43:CD:49:GLU:HB2	2.02	0.41
44:UN:315:LEU:HD12	51:JP:272:MET:HE1	2.01	0.41
46:UG:97:VAL:HG21	58:UJ:91:ILE:HD12	2.02	0.41
46:UG:340:LEU:O	46:UG:368:TYR:N	2.54	0.41
48:JO:201:LYS:HE3	48:JO:205:ILE:HD11	2.03	0.41
50:UZ:72:ILE:HG12	50:UZ:124:LEU:HD23	2.03	0.41
51:JP:18:SER:HA	58:UJ:26:GLN:HE22	1.85	0.41
51:JP:154:ASP:OD1	51:JP:154:ASP:N	2.54	0.41
52:UR:396:MET:HE1	52:UR:437:LEU:HB3	2.03	0.41
52:UR:464:THR:HG21	52:UR:476:ILE:HA	2.02	0.41
53:UU:121:LEU:HD22	53:UU:128:LEU:HD11	2.03	0.41
53:UU:611:THR:HB	53:UU:621:ASP:HB3	2.03	0.41
53:UU:830:TYR:HD1	53:UU:833:LEU:HD23	1.85	0.41
56:UA:412:ARG:HD3	56:UA:421:ASN:ND2	2.35	0.41
56:UA:743:PHE:HZ	56:UA:778:ILE:HD13	1.86	0.41
57:UI:463:LYS:HE3	57:UI:466:GLU:OE2	2.21	0.41
60:UT:1806:SER:HA	60:UT:1811:ILE:HG13	2.01	0.41
60:UT:1915:LEU:HA	60:UT:1915:LEU:HD23	1.83	0.41
60:UT:1993:PRO:HA	60:UT:1996:GLN:HG2	2.03	0.41
61:JB:190:LEU:HD23	61:JB:190:LEU:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:JB:612:ASP:HB3	61:JB:615:PRO:HD2	2.03	0.41
61:JB:662:GLU:HG3	61:JB:664:LYS:HE3	2.03	0.41
2:D2:194:G:H2'	2:D2:195:A:C8	2.56	0.41
2:D2:408:U:H2'	2:D2:409:C:C6	2.56	0.41
5:CK:451:LEU:HD11	22:CI:50:ILE:HD13	2.03	0.41
6:CL:836:LYS:HD3	6:CL:836:LYS:HA	1.92	0.41
6:CL:893:ASN:HB2	49:CM:366:ILE:HG13	2.03	0.41
9:JG:41:MET:HE3	9:JG:241:PHE:CD1	2.56	0.41
9:JG:103:PRO:HG2	9:JF:240:LYS:HE3	2.03	0.41
18:UO:266:SER:OG	18:UO:268:MET:O	2.33	0.41
20:US:104:ALA:O	20:US:108:ASP:HB2	2.21	0.41
22:CI:22:LYS:HE3	22:CI:22:LYS:HB2	1.91	0.41
37:DG:159:ARG:NE	37:DG:172:ALA:HB2	2.36	0.41
39:CH:245:SER:HA	39:CH:246:PRO:HD3	1.98	0.41
43:CD:26:ASP:OD1	43:CD:26:ASP:N	2.49	0.41
44:UN:327:PHE:CD2	45:UF:167:ILE:HD11	2.56	0.41
46:UG:140:ARG:HG3	58:UJ:20:LEU:HD13	2.03	0.41
46:UG:302:ASP:OD2	46:UG:305:ASN:ND2	2.46	0.41
53:UU:929:CYS:HB3	56:UA:828:ILE:HD13	2.03	0.41
55:UQ:895:LEU:HD11	58:UJ:263:VAL:HA	2.02	0.41
60:UT:1312:SER:N	60:UT:1318:GLU:O	2.45	0.41
61:JA:562:HIS:HA	61:JA:588:ILE:O	2.21	0.41
61:JB:519:ASN:HB3	61:JB:522:THR:HG22	2.02	0.41
5:CK:440:LEU:HB3	22:CI:57:LEU:HD13	2.02	0.40
6:CL:275:LEU:HD23	6:CL:275:LEU:HA	1.90	0.40
6:CL:295:ASP:OD2	6:CL:852:ARG:NH1	2.54	0.40
8:UX:87:MET:HE3	8:UX:87:MET:HB2	1.85	0.40
9:JF:190:GLN:O	9:JF:194:GLU:HG3	2.21	0.40
12:UC:596:THR:HB	27:JM:137:LYS:HG3	2.03	0.40
13:UE:476:LEU:HD23	13:UE:479:ILE:HD12	2.04	0.40
14:UH:2:PRO:HG3	14:UH:404:GLY:HA3	2.03	0.40
14:UH:676:TRP:CZ3	57:UI:483:LYS:HG3	2.56	0.40
18:UO:413:LEU:O	18:UO:417:VAL:HG23	2.21	0.40
21:CF:35:LYS:HE3	21:CF:35:LYS:HB2	1.95	0.40
30:DI:11:ARG:O	38:DL:133:LYS:NZ	2.40	0.40
30:DI:83:TYR:HB2	30:DI:196:LEU:HD21	2.04	0.40
33:JC:208:ASP:OD1	33:JC:210:ARG:NH1	2.54	0.40
36:DW:36:LYS:HA	36:DW:36:LYS:HD3	1.87	0.40
39:CH:242:VAL:HG23	39:CH:253:THR:HG22	2.03	0.40
39:CH:257:ASP:N	39:CH:257:ASP:OD1	2.49	0.40
53:UU:366:MET:HE2	53:UU:366:MET:HB3	1.78	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:UA:176:ASP:HB2	56:UA:179:GLU:HB2	2.02	0.40
56:UA:631:ASN:HD22	56:UA:633:LYS:HB2	1.86	0.40
60:UT:39:HIS:HB2	60:UT:46:HIS:HB3	2.02	0.40
60:UT:1892:LEU:O	60:UT:1896:ILE:HG13	2.21	0.40
61:JB:677:TYR:HB3	61:JB:706:PRO:HB3	2.02	0.40
1:D3:575:C:HO2'	1:D3:576:G:H8	1.69	0.40
2:D2:163:G:H4'	52:UR:354:SER:HB3	2.03	0.40
2:D2:182:G:H2'	2:D2:183:A:C8	2.56	0.40
6:CL:100:ASP:O	6:CL:359:SER:OG	2.36	0.40
16:UL:888:ARG:HH22	17:UM:807:ASP:CG	2.28	0.40
17:UM:702:LEU:O	17:UM:706:ARG:HG2	2.21	0.40
18:UO:171:VAL:HG22	18:UO:188:SER:HB3	2.02	0.40
20:US:99:LYS:HG2	20:US:123:TYR:CE1	2.56	0.40
31:DJ:132:ARG:HG2	31:DJ:142:ASN:HB3	2.03	0.40
40:Dc:18:ARG:HD3	40:Dc:18:ARG:HA	1.84	0.40
44:UN:311:LEU:HD23	44:UN:315:LEU:HD11	2.03	0.40
58:UJ:256:ALA:O	58:UJ:259:THR:OG1	2.37	0.40
61:JA:462:SER:OG	61:JA:463:ARG:N	2.54	0.40
61:JB:894:ASN:O	61:JB:898:ILE:HG12	2.21	0.40
1:D3:355:G:H2'	1:D3:356:G:H8	1.87	0.40
13:UE:128:GLN:OE1	13:UE:138:GLN:NE2	2.38	0.40
13:UE:344:ASP:OD1	13:UE:348:LYS:N	2.55	0.40
14:UH:642:LEU:HD23	14:UH:642:LEU:HA	1.93	0.40
16:UL:7:ARG:NH2	16:UL:70:GLY:O	2.54	0.40
16:UL:68:PRO:HA	16:UL:69:PRO:HD3	1.96	0.40
21:CG:60:PRO:HG2	21:CG:63:ILE:HG23	2.03	0.40
45:UF:196:LEU:HD23	45:UF:196:LEU:HA	1.96	0.40
49:CM:141:MET:HE2	49:CM:141:MET:HB3	1.94	0.40
53:UU:859:ASP:OD1	53:UU:860:GLU:N	2.55	0.40
55:UQ:865:LYS:HE2	55:UQ:865:LYS:HB3	1.77	0.40
56:UA:212:ASP:OD2	56:UA:212:ASP:N	2.55	0.40
58:UJ:262:VAL:HG13	58:UJ:301:LYS:HG2	2.03	0.40
58:UJ:566:CYS:SG	58:UJ:567:LEU:N	2.95	0.40
3:D4:27:U:N3	47:JN:236:MET:HE2	2.36	0.40
4:CJ:84:MET:HE3	4:CJ:84:MET:HB2	1.94	0.40
6:CL:838:ILE:HD12	6:CL:874:TYR:HB3	2.02	0.40
11:UB:433:ILE:HD12	11:UB:459:LEU:HD22	2.03	0.40
14:UH:567:LEU:HD23	14:UH:567:LEU:HA	1.97	0.40
16:UL:126:LEU:HD13	16:UL:168:GLY:HA2	2.03	0.40
16:UL:255:ARG:NH1	16:UL:257:LEU:HD21	2.36	0.40
16:UL:671:PHE:HA	16:UL:684:TRP:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:UL:836:ILE:HD12	16:UL:853:ILE:HG23	2.03	0.40
20:US:265:LEU:HD21	20:US:277:ILE:HG21	2.02	0.40
25:JJ:271:LYS:HB2	56:UA:334:SER:HB3	2.02	0.40
29:DF:162:VAL:HG23	29:DF:166:ARG:HD3	2.03	0.40
30:DI:172:ARG:HH21	30:DI:175:GLN:HE21	1.69	0.40
37:DG:158:ILE:HG12	60:UT:632:LEU:HD11	2.03	0.40
52:UR:253:SER:OG	52:UR:297:THR:HA	2.22	0.40
53:UU:872:LEU:HD23	53:UU:872:LEU:HA	1.90	0.40
60:UT:672:VAL:O	60:UT:678:TRP:NE1	2.55	0.40
61:JA:29:VAL:HG11	61:JA:158:LEU:HD13	2.03	0.40
61:JA:213:ALA:O	61:JA:216:VAL:HB	2.21	0.40
61:JA:569:PRO:HD3	61:JA:583:LEU:HG	2.04	0.40
61:JA:884:ILE:O	61:JA:888:ILE:HG13	2.21	0.40
1:D3:32:U:O2'	1:D3:594:A:N1	2.44	0.40
2:D2:406:U:H5''	6:CL:1066:GLY:HA3	2.03	0.40
6:CL:217:ASP:OD1	6:CL:218:ARG:N	2.54	0.40
9:JG:167:ILE:HG13	9:JG:171:LEU:HG	2.03	0.40
13:UE:479:ILE:O	13:UE:483:ARG:HG2	2.21	0.40
16:UL:255:ARG:NH1	16:UL:277:ALA:HB2	2.37	0.40
29:DF:206:SER:O	29:DF:212:LYS:NZ	2.52	0.40
30:DI:81:VAL:HA	30:DI:102:VAL:HG12	2.03	0.40
31:DJ:138:LYS:HA	39:CH:319:TYR:HE2	1.87	0.40
36:DW:26:LEU:HD11	36:DW:60:LYS:HE3	2.03	0.40
47:JN:198:GLN:NE2	48:JO:208:GLU:OE2	2.51	0.40
49:CM:22:VAL:HG11	49:CM:105:TYR:CD1	2.55	0.40
51:JP:75:LYS:NZ	51:JP:356:TYR:O	2.42	0.40
53:UU:749:ALA:HA	53:UU:750:PRO:HD3	1.95	0.40
54:UD:127:ASP:HB2	54:UD:134:LEU:HB2	2.03	0.40
55:UQ:22:LEU:HD12	55:UQ:22:LEU:HA	1.87	0.40
61:JA:743:VAL:HG11	61:JA:811:ALA:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	
4	CJ	278/290 (96%)	272 (98%)	6 (2%)	0	100	100
5	CK	193/593 (32%)	192 (100%)	0	1 (0%)	25	54
6	CL	806/1183 (68%)	792 (98%)	14 (2%)	0	100	100
7	DY	94/135 (70%)	91 (97%)	3 (3%)	0	100	100
8	UX	170/189 (90%)	167 (98%)	3 (2%)	0	100	100
9	JF	213/252 (84%)	209 (98%)	4 (2%)	0	100	100
9	JG	227/252 (90%)	223 (98%)	4 (2%)	0	100	100
10	CA	237/327 (72%)	230 (97%)	7 (3%)	0	100	100
10	CB	223/327 (68%)	211 (95%)	11 (5%)	1 (0%)	30	58
11	UB	483/810 (60%)	477 (99%)	6 (1%)	0	100	100
12	UC	124/610 (20%)	124 (100%)	0	0	100	100
13	UE	468/643 (73%)	453 (97%)	15 (3%)	0	100	100
14	UH	565/713 (79%)	550 (97%)	15 (3%)	0	100	100
15	UK	234/250 (94%)	226 (97%)	7 (3%)	1 (0%)	30	58
16	UL	841/943 (89%)	815 (97%)	26 (3%)	0	100	100
17	UM	156/817 (19%)	154 (99%)	2 (1%)	0	100	100
18	UO	490/513 (96%)	478 (98%)	12 (2%)	0	100	100
19	UP	58/214 (27%)	57 (98%)	1 (2%)	0	100	100
20	US	538/552 (98%)	518 (96%)	20 (4%)	0	100	100
21	CF	121/126 (96%)	119 (98%)	2 (2%)	0	100	100
21	CG	119/126 (94%)	118 (99%)	1 (1%)	0	100	100
22	CI	180/183 (98%)	178 (99%)	2 (1%)	0	100	100
23	JE	134/357 (38%)	129 (96%)	5 (4%)	0	100	100
24	JH	253/483 (52%)	249 (98%)	4 (2%)	0	100	100
25	JJ	94/274 (34%)	93 (99%)	1 (1%)	0	100	100
26	JK	40/534 (8%)	39 (98%)	1 (2%)	0	100	100
27	JM	129/217 (59%)	127 (98%)	2 (2%)	0	100	100
28	JQ	151/206 (73%)	148 (98%)	3 (2%)	0	100	100
29	DF	205/225 (91%)	198 (97%)	7 (3%)	0	100	100
30	DI	171/200 (86%)	168 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	DJ	175/197 (89%)	171 (98%)	4 (2%)	0	100	100
32	DS	98/146 (67%)	98 (100%)	0	0	100	100
33	JC	346/707 (49%)	341 (99%)	5 (1%)	0	100	100
34	DE	234/261 (90%)	230 (98%)	4 (2%)	0	100	100
35	DX	101/145 (70%)	99 (98%)	2 (2%)	0	100	100
36	DW	125/130 (96%)	124 (99%)	1 (1%)	0	100	100
37	DG	205/236 (87%)	203 (99%)	2 (1%)	0	100	100
38	DL	136/156 (87%)	132 (97%)	4 (3%)	0	100	100
39	CH	442/573 (77%)	428 (97%)	14 (3%)	0	100	100
40	Dc	61/67 (91%)	60 (98%)	1 (2%)	0	100	100
41	DQ	123/143 (86%)	120 (98%)	3 (2%)	0	100	100
42	CE	434/511 (85%)	427 (98%)	7 (2%)	0	100	100
43	CD	376/504 (75%)	369 (98%)	7 (2%)	0	100	100
44	UN	182/899 (20%)	180 (99%)	2 (1%)	0	100	100
45	UF	373/440 (85%)	370 (99%)	3 (1%)	0	100	100
46	UG	511/554 (92%)	499 (98%)	12 (2%)	0	100	100
47	JN	178/346 (51%)	169 (95%)	9 (5%)	0	100	100
48	JO	188/316 (60%)	187 (100%)	1 (0%)	0	100	100
49	CM	361/367 (98%)	354 (98%)	7 (2%)	0	100	100
50	UZ	252/274 (92%)	245 (97%)	7 (3%)	0	100	100
51	JP	456/489 (93%)	446 (98%)	10 (2%)	0	100	100
52	UR	472/594 (80%)	457 (97%)	15 (3%)	0	100	100
53	UU	840/939 (90%)	818 (97%)	22 (3%)	0	100	100
54	UD	670/776 (86%)	648 (97%)	21 (3%)	1 (0%)	48	77
55	UQ	829/896 (92%)	805 (97%)	23 (3%)	1 (0%)	48	77
56	UA	830/923 (90%)	808 (97%)	22 (3%)	0	100	100
57	UI	132/575 (23%)	130 (98%)	2 (2%)	0	100	100
58	UJ	1693/1769 (96%)	1659 (98%)	33 (2%)	1 (0%)	48	77
59	DH	166/190 (87%)	163 (98%)	3 (2%)	0	100	100
60	UT	2335/2493 (94%)	2313 (99%)	22 (1%)	0	100	100
61	JA	885/1056 (84%)	867 (98%)	18 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
61	JB	848/1056 (80%)	833 (98%)	15 (2%)	0	100	100
All	All	23052/31272 (74%)	22558 (98%)	488 (2%)	6 (0%)	100	100

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	CK	427	SER
10	CB	297	ARG
55	UQ	454	ILE
58	UJ	1037	ASP
15	UK	184	ILE
54	UD	85	TRP

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	
4	CJ	247/258 (96%)	247 (100%)	0	100	100
5	CK	174/535 (32%)	174 (100%)	0	100	100
6	CL	683/1039 (66%)	683 (100%)	0	100	100
7	DY	80/113 (71%)	80 (100%)	0	100	100
8	UX	156/169 (92%)	156 (100%)	0	100	100
9	JF	179/222 (81%)	179 (100%)	0	100	100
9	JG	202/222 (91%)	202 (100%)	0	100	100
10	CA	200/240 (83%)	200 (100%)	0	100	100
10	CB	192/240 (80%)	192 (100%)	0	100	100
11	UB	348/732 (48%)	348 (100%)	0	100	100
12	UC	107/538 (20%)	107 (100%)	0	100	100
13	UE	425/574 (74%)	425 (100%)	0	100	100
14	UH	193/657 (29%)	193 (100%)	0	100	100
15	UK	219/234 (94%)	219 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	UL	648/832 (78%)	648 (100%)	0	100	100
17	UM	135/719 (19%)	135 (100%)	0	100	100
18	UO	435/454 (96%)	435 (100%)	0	100	100
19	UP	37/196 (19%)	37 (100%)	0	100	100
20	US	357/506 (71%)	357 (100%)	0	100	100
21	CF	102/104 (98%)	102 (100%)	0	100	100
21	CG	100/104 (96%)	100 (100%)	0	100	100
22	CI	171/172 (99%)	171 (100%)	0	100	100
23	JE	80/315 (25%)	80 (100%)	0	100	100
25	JJ	7/238 (3%)	7 (100%)	0	100	100
26	JK	34/482 (7%)	34 (100%)	0	100	100
27	JM	114/200 (57%)	114 (100%)	0	100	100
28	JQ	24/192 (12%)	24 (100%)	0	100	100
29	DF	177/191 (93%)	177 (100%)	0	100	100
30	DI	134/161 (83%)	134 (100%)	0	100	100
31	DJ	146/166 (88%)	146 (100%)	0	100	100
32	DS	4/129 (3%)	4 (100%)	0	100	100
33	JC	280/636 (44%)	279 (100%)	1 (0%)	89	93
34	DE	190/222 (86%)	190 (100%)	0	100	100
35	DX	82/120 (68%)	82 (100%)	0	100	100
36	DW	96/111 (86%)	96 (100%)	0	100	100
37	DG	152/201 (76%)	152 (100%)	0	100	100
38	DL	109/137 (80%)	108 (99%)	1 (1%)	75	86
39	CH	372/503 (74%)	372 (100%)	0	100	100
40	Dc	56/60 (93%)	56 (100%)	0	100	100
41	DQ	105/119 (88%)	105 (100%)	0	100	100
42	CE	258/433 (60%)	258 (100%)	0	100	100
43	CD	267/435 (61%)	267 (100%)	0	100	100
44	UN	143/808 (18%)	142 (99%)	1 (1%)	81	89
45	UF	240/414 (58%)	240 (100%)	0	100	100
46	UG	399/480 (83%)	399 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	JN	124/304 (41%)	124 (100%)	0	100	100
48	JO	158/289 (55%)	158 (100%)	0	100	100
49	CM	300/312 (96%)	300 (100%)	0	100	100
50	UZ	208/256 (81%)	208 (100%)	0	100	100
51	JP	406/443 (92%)	406 (100%)	0	100	100
52	UR	411/529 (78%)	411 (100%)	0	100	100
53	UU	724/819 (88%)	724 (100%)	0	100	100
54	UD	554/713 (78%)	554 (100%)	0	100	100
55	UQ	732/826 (89%)	731 (100%)	1 (0%)	92	96
56	UA	721/812 (89%)	721 (100%)	0	100	100
57	UI	85/533 (16%)	85 (100%)	0	100	100
58	UJ	512/1633 (31%)	512 (100%)	0	100	100
59	DH	105/170 (62%)	105 (100%)	0	100	100
60	UT	571/2307 (25%)	571 (100%)	0	100	100
61	JA	652/934 (70%)	652 (100%)	0	100	100
61	JB	622/934 (67%)	622 (100%)	0	100	100
All	All	15744/27427 (57%)	15740 (100%)	4 (0%)	100	100

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
33	JC	76	THR
38	DL	21	ASN
44	UN	299	ASN
55	UQ	818	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (160) such sidechains are listed below:

Mol	Chain	Res	Type
4	CJ	121	ASN
4	CJ	164	GLN
4	CJ	168	HIS
5	CK	316	ASN
6	CL	126	ASN
6	CL	222	ASN

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Mol	Chain	Res	Type
6	CL	289	HIS
6	CL	426	HIS
6	CL	832	HIS
6	CL	1074	GLN
8	UX	43	ASN
9	JG	69	ASN
9	JG	93	HIS
9	JF	73	HIS
9	JF	74	GLN
10	CA	249	GLN
10	CB	183	HIS
10	CB	249	GLN
11	UB	308	GLN
11	UB	418	ASN
11	UB	453	ASN
11	UB	479	ASN
11	UB	658	ASN
11	UB	666	GLN
11	UB	683	ASN
11	UB	697	HIS
12	UC	503	GLN
12	UC	560	ASN
13	UE	35	GLN
13	UE	302	ASN
13	UE	316	ASN
13	UE	336	ASN
13	UE	527	HIS
14	UH	597	GLN
14	UH	633	GLN
15	UK	203	GLN
16	UL	10	GLN
16	UL	553	ASN
16	UL	596	ASN
16	UL	803	GLN
16	UL	879	GLN
16	UL	903	GLN
17	UM	690	HIS
17	UM	726	GLN
17	UM	747	ASN
17	UM	757	GLN
18	UO	137	ASN
18	UO	161	GLN

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Mol	Chain	Res	Type
20	US	225	HIS
20	US	260	ASN
20	US	427	GLN
20	US	441	ASN
21	CF	18	GLN
21	CF	25	GLN
22	CI	8	HIS
22	CI	23	GLN
22	CI	37	HIS
22	CI	45	HIS
22	CI	116	HIS
23	JE	238	ASN
27	JM	112	ASN
27	JM	135	HIS
27	JM	184	ASN
29	DF	116	HIS
29	DF	170	GLN
29	DF	186	ASN
33	JC	15	GLN
33	JC	96	HIS
33	JC	101	ASN
33	JC	230	GLN
33	JC	339	HIS
34	DE	153	ASN
35	DX	65	ASN
37	DG	59	GLN
37	DG	139	ASN
38	DL	14	GLN
38	DL	21	ASN
39	CH	156	ASN
42	CE	61	ASN
42	CE	165	GLN
42	CE	428	ASN
43	CD	65	ASN
43	CD	85	ASN
43	CD	151	GLN
43	CD	183	GLN
43	CD	328	GLN
43	CD	391	ASN
44	UN	335	GLN
44	UN	832	ASN
45	UF	44	ASN

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Mol	Chain	Res	Type
45	UF	191	ASN
45	UF	337	HIS
46	UG	71	ASN
46	UG	240	GLN
46	UG	248	HIS
46	UG	310	HIS
48	JO	167	GLN
49	CM	176	GLN
50	UZ	192	ASN
50	UZ	214	GLN
52	UR	162	ASN
52	UR	217	ASN
52	UR	276	HIS
52	UR	283	HIS
52	UR	310	GLN
52	UR	380	ASN
52	UR	450	GLN
53	UU	387	GLN
53	UU	627	ASN
53	UU	910	GLN
54	UD	75	ASN
54	UD	87	GLN
54	UD	329	HIS
54	UD	426	GLN
54	UD	533	HIS
54	UD	595	ASN
54	UD	618	ASN
55	UQ	469	ASN
55	UQ	489	ASN
55	UQ	491	GLN
55	UQ	542	ASN
55	UQ	660	GLN
55	UQ	679	ASN
55	UQ	682	ASN
55	UQ	699	ASN
55	UQ	868	ASN
56	UA	147	GLN
56	UA	421	ASN
56	UA	552	ASN
56	UA	707	ASN
57	UI	468	ASN
57	UI	474	HIS

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Mol	Chain	Res	Type
58	UJ	10	GLN
58	UJ	96	ASN
58	UJ	131	ASN
58	UJ	144	GLN
58	UJ	209	GLN
58	UJ	293	HIS
59	DH	150	GLN
59	DH	160	GLN
59	DH	190	HIS
60	UT	248	HIS
60	UT	829	ASN
60	UT	1891	HIS
60	UT	1943	ASN
60	UT	2067	ASN
61	JA	19	GLN
61	JA	36	GLN
61	JA	39	ASN
61	JA	307	ASN
61	JA	380	GLN
61	JA	428	GLN
61	JA	432	ASN
61	JA	434	ASN
61	JA	734	HIS
61	JA	847	ASN
61	JB	347	ASN
61	JB	363	HIS
61	JB	641	ASN
61	JB	749	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	D3	866/1808 (47%)	213 (24%)	17 (1%)
2	D2	513/700 (73%)	96 (18%)	3 (0%)
3	D4	170/333 (51%)	34 (20%)	1 (0%)
All	All	1549/2841 (54%)	343 (22%)	21 (1%)

All (343) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	D3	-1	G

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Mol	Chain	Res	Type
1	D3	0	U
1	D3	1	U
1	D3	10	G
1	D3	17	C
1	D3	25	C
1	D3	26	A
1	D3	51	A
1	D3	54	C
1	D3	55	A
1	D3	66	U
1	D3	69	G
1	D3	73	U
1	D3	75	U
1	D3	76	A
1	D3	77	U
1	D3	78	A
1	D3	93	A
1	D3	104	A
1	D3	109	G
1	D3	112	A
1	D3	114	C
1	D3	116	U
1	D3	126	A
1	D3	141	U
1	D3	144	U
1	D3	145	A
1	D3	150	U
1	D3	151	G
1	D3	155	U
1	D3	156	A
1	D3	159	U
1	D3	160	C
1	D3	166	C
1	D3	167	U
1	D3	170	U
1	D3	171	A
1	D3	176	C
1	D3	186	C
1	D3	187	G
1	D3	188	A
1	D3	191	C
1	D3	192	U

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Mol	Chain	Res	Type
1	D3	194	U
1	D3	195	G
1	D3	196	G
1	D3	201	G
1	D3	203	U
1	D3	204	G
1	D3	250	C
1	D3	260	U
1	D3	261	U
1	D3	265	A
1	D3	270	C
1	D3	271	A
1	D3	277	U
1	D3	278	U
1	D3	280	U
1	D3	281	G
1	D3	284	G
1	D3	287	G
1	D3	290	G
1	D3	299	A
1	D3	307	G
1	D3	313	U
1	D3	316	A
1	D3	320	U
1	D3	321	C
1	D3	322	G
1	D3	325	G
1	D3	337	G
1	D3	344	A
1	D3	345	U
1	D3	351	C
1	D3	352	A
1	D3	359	A
1	D3	360	A
1	D3	361	C
1	D3	366	A
1	D3	369	A
1	D3	371	G
1	D3	372	G
1	D3	373	G
1	D3	374	U
1	D3	376	C

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Mol	Chain	Res	Type
1	D3	382	C
1	D3	383	G
1	D3	388	G
1	D3	395	U
1	D3	400	A
1	D3	416	A
1	D3	418	G
1	D3	419	G
1	D3	440	U
1	D3	444	C
1	D3	445	A
1	D3	454	U
1	D3	460	A
1	D3	461	G
1	D3	466	U
1	D3	467	G
1	D3	468	A
1	D3	469	C
1	D3	470	A
1	D3	471	A
1	D3	472	U
1	D3	477	A
1	D3	480	G
1	D3	486	G
1	D3	487	G
1	D3	496	G
1	D3	501	U
1	D3	502	U
1	D3	505	A
1	D3	506	A
1	D3	510	G
1	D3	525	A
1	D3	534	A
1	D3	540	G
1	D3	541	A
1	D3	542	A
1	D3	545	A
1	D3	557	G
1	D3	563	U
1	D3	564	G
1	D3	565	C
1	D3	570	A

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Mol	Chain	Res	Type
1	D3	576	G
1	D3	579	A
1	D3	580	A
1	D3	582	U
1	D3	583	C
1	D3	584	C
1	D3	585	A
1	D3	586	G
1	D3	587	C
1	D3	594	A
1	D3	595	G
1	D3	1118	G
1	D3	1119	G
1	D3	1127	G
1	D3	1128	C
1	D3	1131	A
1	D3	1132	A
1	D3	1134	C
1	D3	1136	U
1	D3	1139	A
1	D3	1140	G
1	D3	1141	G
1	D3	1144	U
1	D3	1145	U
1	D3	1146	G
1	D3	1158	C
1	D3	1159	C
1	D3	1178	G
1	D3	1205	C
1	D3	1207	C
1	D3	1208	A
1	D3	1211	A
1	D3	1212	G
1	D3	1214	U
1	D3	1217	A
1	D3	1223	A
1	D3	1224	A
1	D3	1225	U
1	D3	1260	U
1	D3	1261	G
1	D3	1263	G
1	D3	1267	G

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Mol	Chain	Res	Type
1	D3	1268	G
1	D3	1269	U
1	D3	1270	G
1	D3	1276	U
1	D3	1443	U
1	D3	1449	U
1	D3	1451	C
1	D3	1471	A
1	D3	1474	G
1	D3	1487	A
1	D3	1488	G
1	D3	1491	U
1	D3	1492	A
1	D3	1493	A
1	D3	1495	C
1	D3	1498	G
1	D3	1506	G
1	D3	1512	G
1	D3	1537	C
1	D3	1539	G
1	D3	1541	G
1	D3	1543	A
1	D3	1553	G
1	D3	1554	U
1	D3	1559	A
1	D3	1570	A
1	D3	1573	A
1	D3	1574	G
1	D3	1584	G
1	D3	1585	U
1	D3	1590	G
1	D3	1595	U
1	D3	1596	C
1	D3	1601	G
1	D3	1602	C
1	D3	1607	G
1	D3	1614	A
1	D3	1618	C
1	D3	1621	U
1	D3	1628	U
1	D3	1633	A
1	D3	1656	U

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Mol	Chain	Res	Type
1	D3	1746	A
1	D3	1747	G
2	D2	6	A
2	D2	9	G
2	D2	16	A
2	D2	68	U
2	D2	69	U
2	D2	70	A
2	D2	83	U
2	D2	85	G
2	D2	86	C
2	D2	89	C
2	D2	91	U
2	D2	102	A
2	D2	103	G
2	D2	104	A
2	D2	105	G
2	D2	109	C
2	D2	124	A
2	D2	125	G
2	D2	129	U
2	D2	130	G
2	D2	142	U
2	D2	150	G
2	D2	156	U
2	D2	163	G
2	D2	168	G
2	D2	169	A
2	D2	176	U
2	D2	177	U
2	D2	178	G
2	D2	188	A
2	D2	201	U
2	D2	207	G
2	D2	233	G
2	D2	236	C
2	D2	238	G
2	D2	253	U
2	D2	256	U
2	D2	259	G
2	D2	261	U
2	D2	267	U

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Mol	Chain	Res	Type
2	D2	271	G
2	D2	279	A
2	D2	280	A
2	D2	281	G
2	D2	296	C
2	D2	298	A
2	D2	302	A
2	D2	303	A
2	D2	304	U
2	D2	305	A
2	D2	309	A
2	D2	310	U
2	D2	313	A
2	D2	316	U
2	D2	323	A
2	D2	324	U
2	D2	325	U
2	D2	326	C
2	D2	331	U
2	D2	337	G
2	D2	354	G
2	D2	357	G
2	D2	368	U
2	D2	370	U
2	D2	371	G
2	D2	372	A
2	D2	373	U
2	D2	382	U
2	D2	385	A
2	D2	386	A
2	D2	395	C
2	D2	397	A
2	D2	407	A
2	D2	428	A
2	D2	431	A
2	D2	432	C
2	D2	441	C
2	D2	461	A
2	D2	469	C
2	D2	481	U
2	D2	482	A
2	D2	486	U

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Mol	Chain	Res	Type
2	D2	487	A
2	D2	488	U
2	D2	490	G
2	D2	491	U
2	D2	493	A
2	D2	518	A
2	D2	519	A
2	D2	525	U
2	D2	533	G
2	D2	536	A
2	D2	541	U
2	D2	546	G
2	D2	586	A
2	D2	590	G
3	D4	2	U
3	D4	3	C
3	D4	14	A
3	D4	23	U
3	D4	24	U
3	D4	25	U
3	D4	27	U
3	D4	28	A
3	D4	30	A
3	D4	32	G
3	D4	33	A
3	D4	34	A
3	D4	35	U
3	D4	49	C
3	D4	60	A
3	D4	61	G
3	D4	82	G
3	D4	87	G
3	D4	90	C
3	D4	91	C
3	D4	111	G
3	D4	115	G
3	D4	199	G
3	D4	205	G
3	D4	260	U
3	D4	267	A
3	D4	313	A
3	D4	318	U

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Mol	Chain	Res	Type
3	D4	319	G
3	D4	322	A
3	D4	324	U
3	D4	325	C
3	D4	329	C
3	D4	333	U

All (21) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	D3	0	U
1	D3	144	U
1	D3	185	U
1	D3	195	G
1	D3	375	U
1	D3	394	C
1	D3	417	A
1	D3	540	G
1	D3	562	G
1	D3	579	A
1	D3	1118	G
1	D3	1140	G
1	D3	1267	G
1	D3	1573	A
1	D3	1594	G
1	D3	1620	C
1	D3	1632	C
2	D2	90	G
2	D2	370	U
2	D2	492	G
3	D4	312	U

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 1 is 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
62	GTP	CL	2001	-	26,34,34	1.17	2 (7%)	32,54,54	1.45	6 (18%)

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
62	GTP	CL	2001	-	-	5/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	CL	2001	GTP	C5-C6	-4.07	1.39	1.47
62	CL	2001	GTP	C2-N3	2.03	1.38	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	CL	2001	GTP	C5-C6-N1	3.23	119.66	113.95
62	CL	2001	GTP	C8-N7-C5	3.03	108.76	102.99
62	CL	2001	GTP	PA-O3A-PB	-3.01	122.51	132.83
62	CL	2001	GTP	C2-N1-C6	-2.87	119.81	125.10
62	CL	2001	GTP	C3'-C2'-C1'	2.80	105.19	100.98
62	CL	2001	GTP	PB-O3B-PG	-2.22	125.21	132.83

There are no chirality outliers.

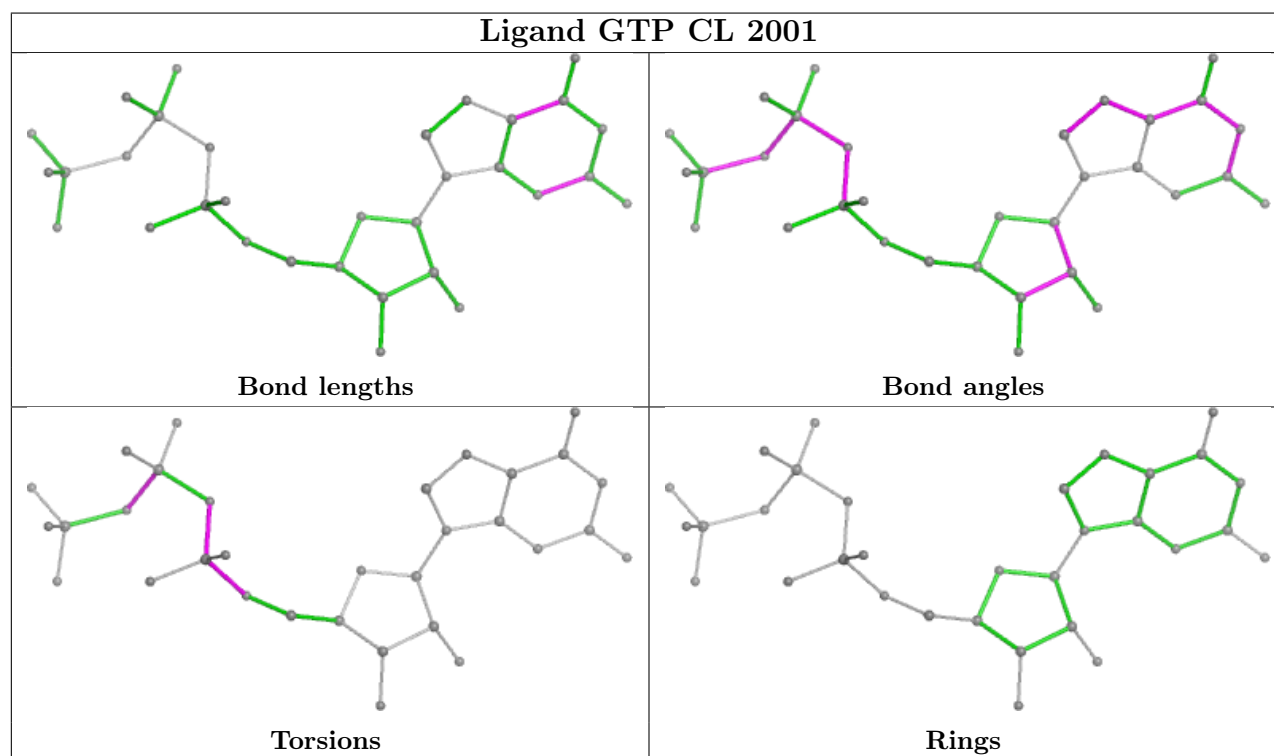
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
62	CL	2001	GTP	C5'-O5'-PA-O1A
62	CL	2001	GTP	C5'-O5'-PA-O2A
62	CL	2001	GTP	C5'-O5'-PA-O3A
62	CL	2001	GTP	PG-O3B-PB-O2B
62	CL	2001	GTP	PB-O3A-PA-O2A

There are no ring outliers.

No monomer is involved in short contacts.

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.

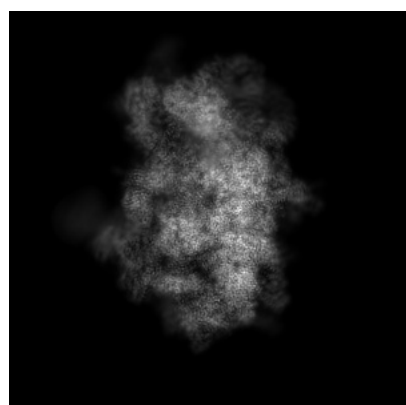
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50991. These allow visual inspection of the internal detail of the map and identification of artifacts.

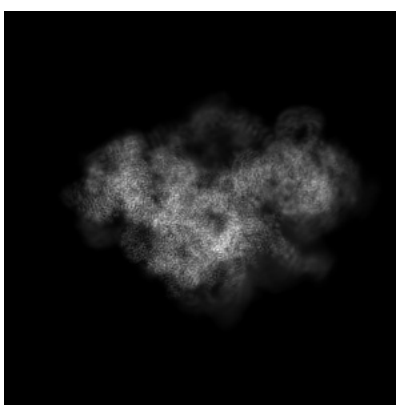
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

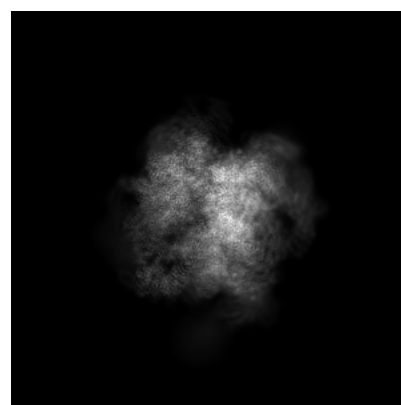
6.1.1 Primary map



X



Y

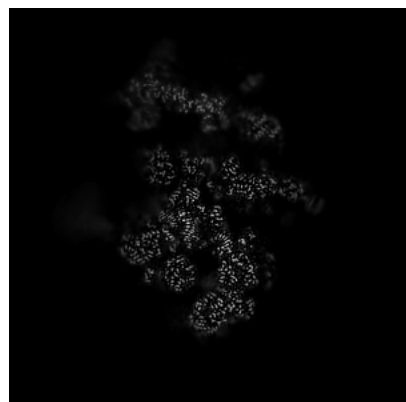


Z

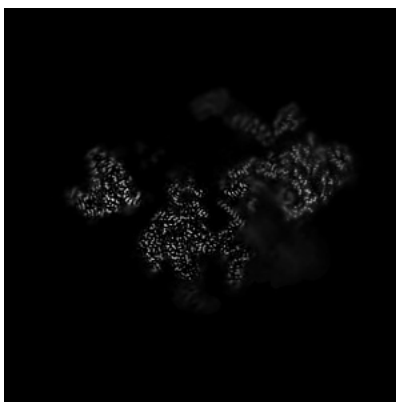
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

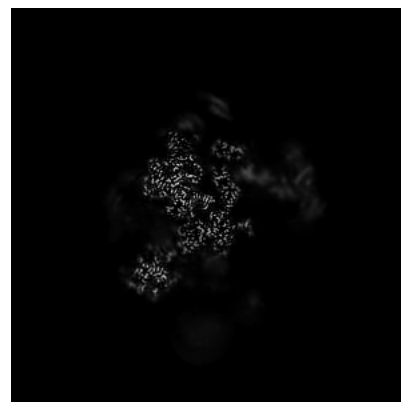
6.2.1 Primary map



X Index: 250



Y Index: 250

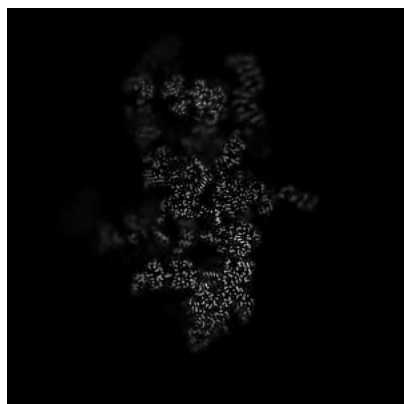


Z Index: 250

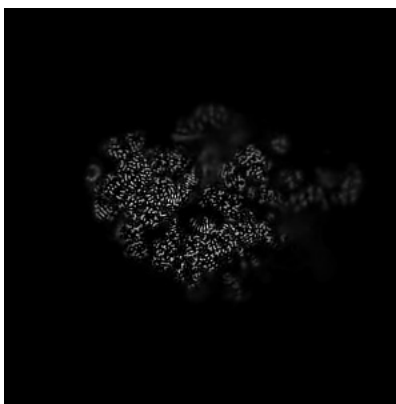
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

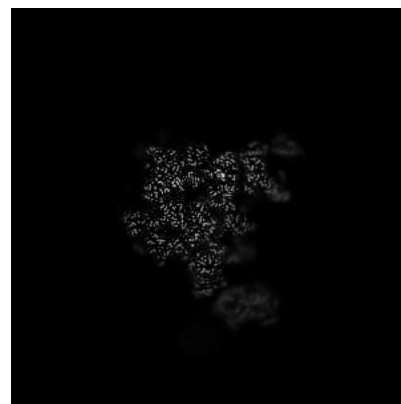
6.3.1 Primary map



X Index: 265



Y Index: 290

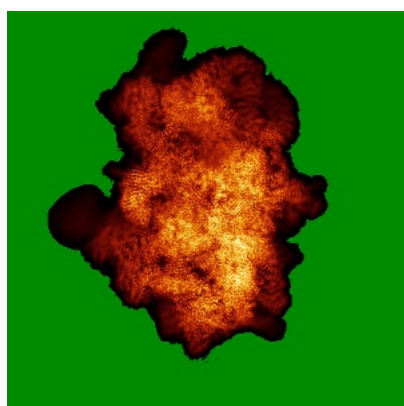


Z Index: 210

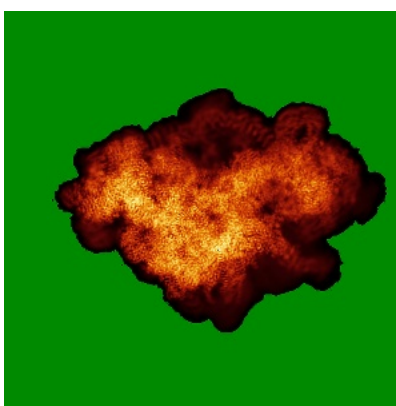
The images above show the largest variance slices of the map in three orthogonal directions.

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

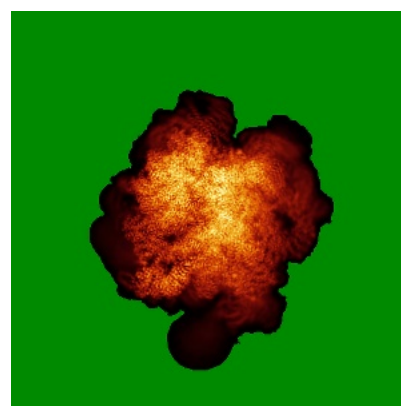
6.4.1 Primary map



X



Y

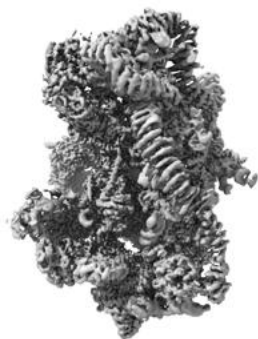


Z

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](#)

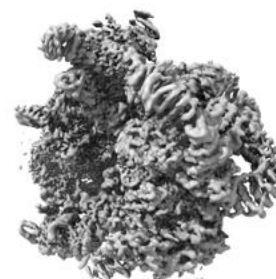
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.45. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

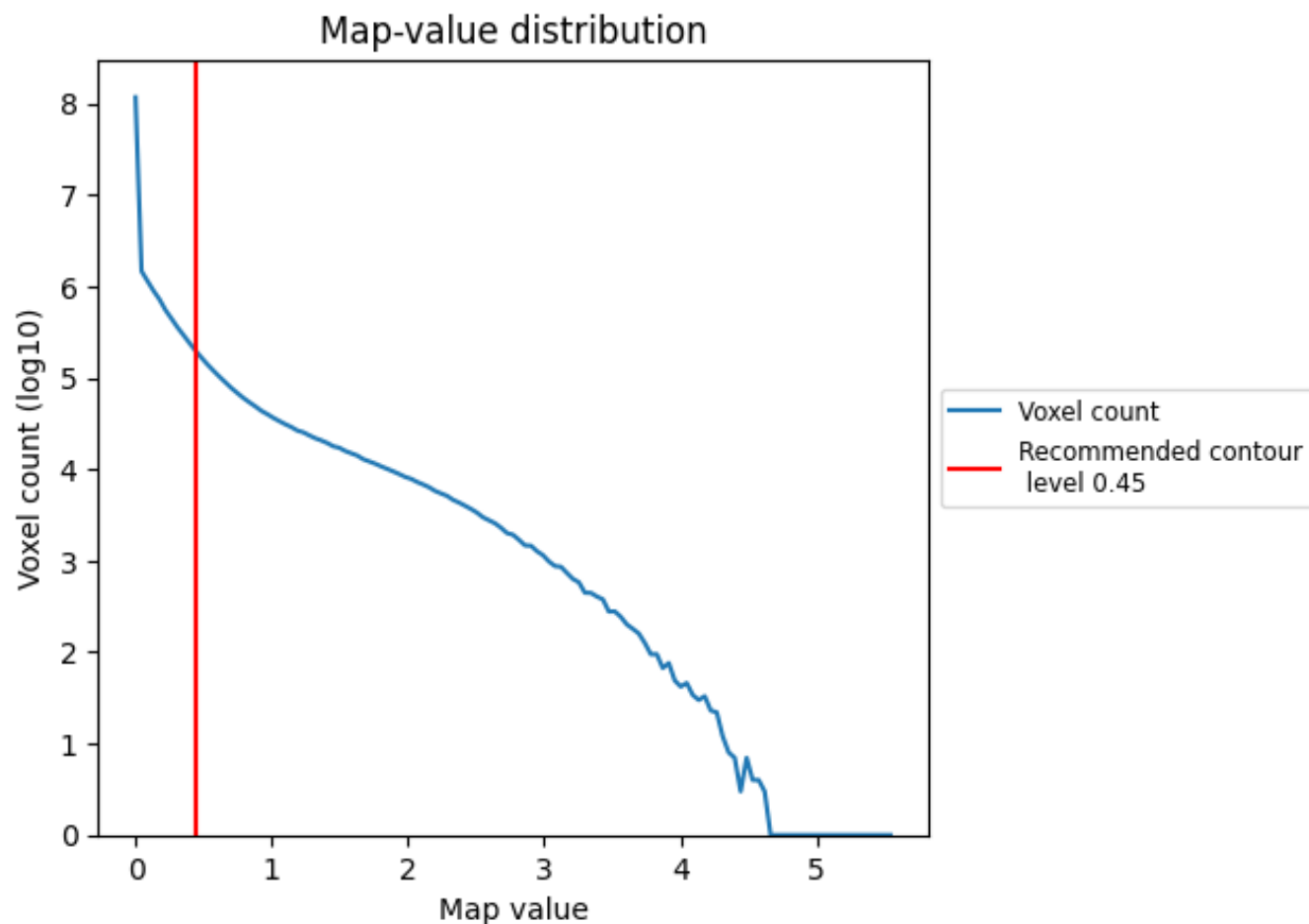
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

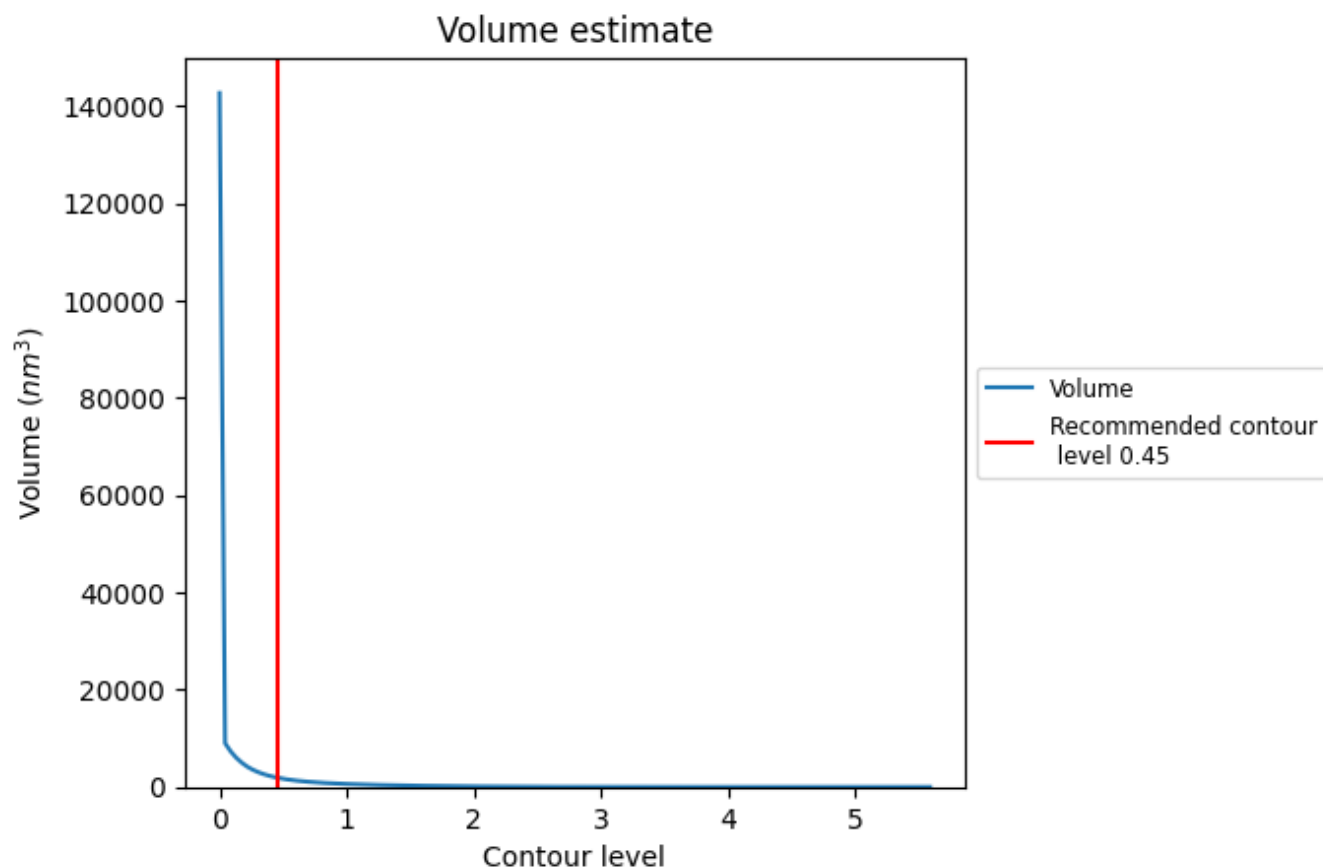
This section contains the results of statistical analysis of the map.

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.

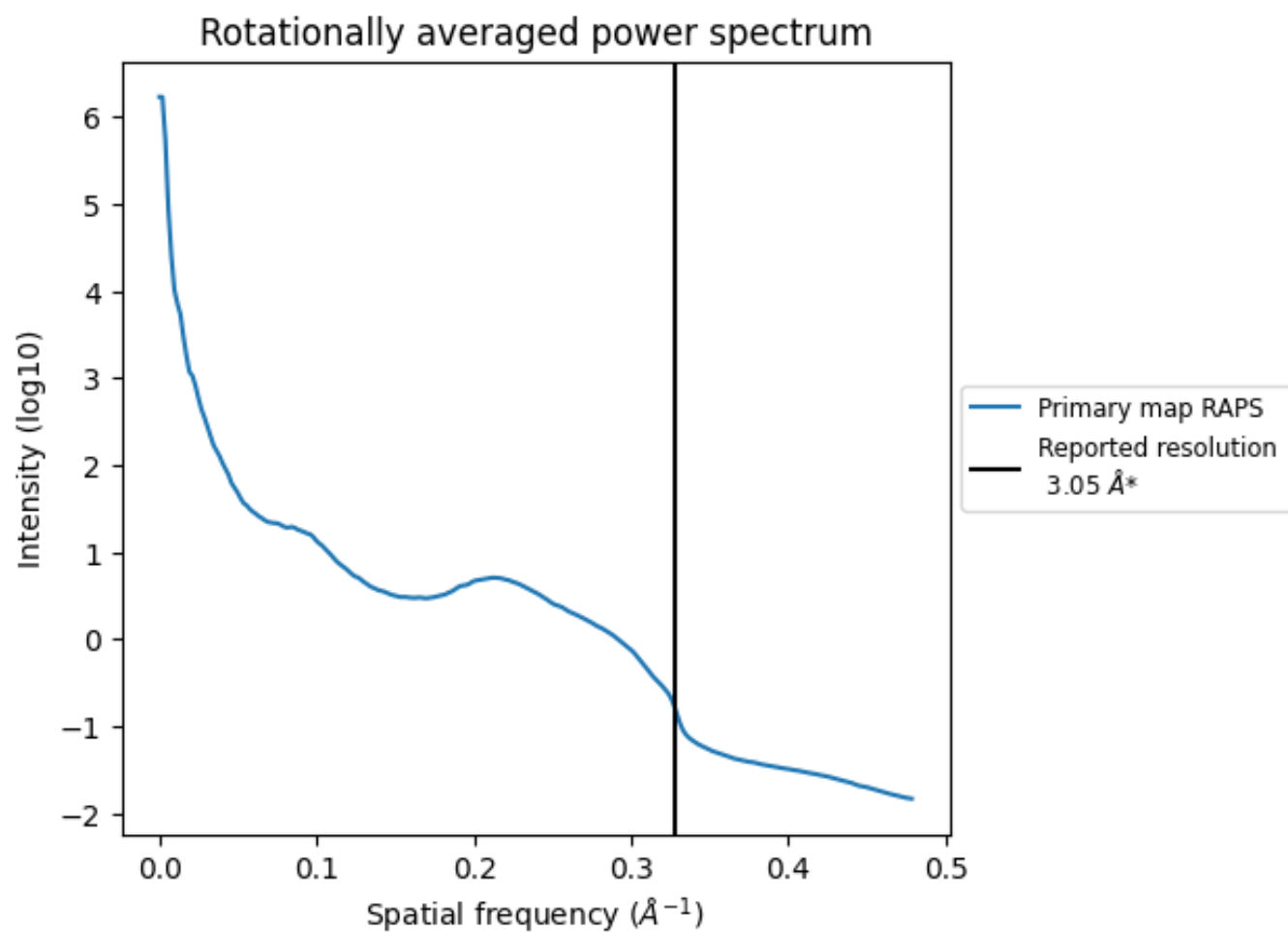
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1930 nm^3 ; this corresponds to an approximate mass of 1743 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 0.328 Å⁻¹

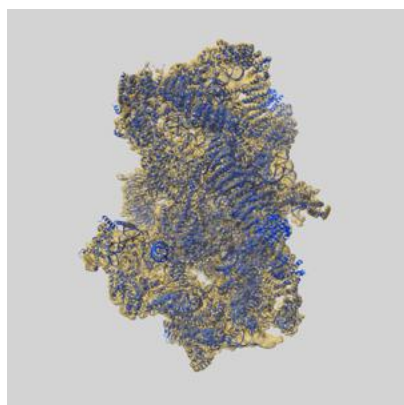
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

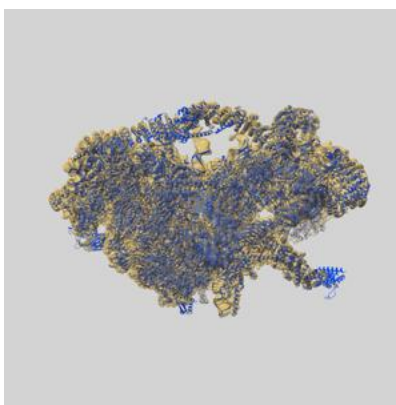
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-50991 and PDB model 9G33. Per-residue inclusion information can be found in section [3](#) on page [16](#).

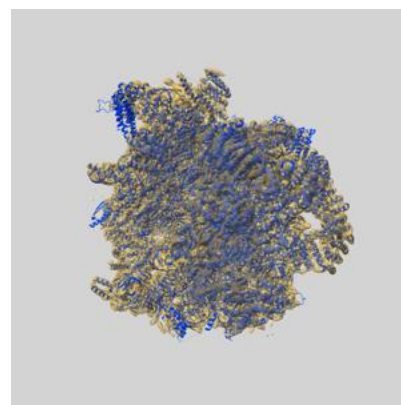
9.1 Map-model overlay [i](#)



X



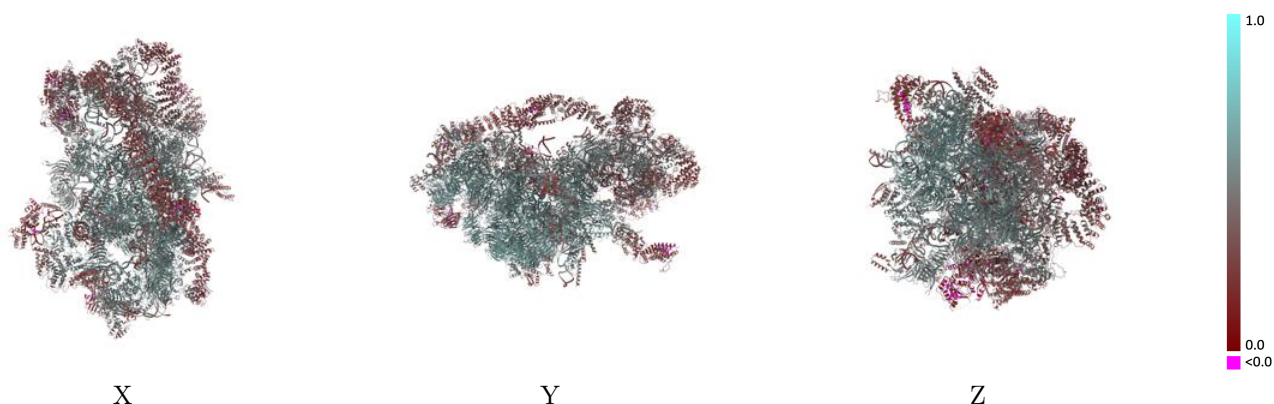
Y



Z

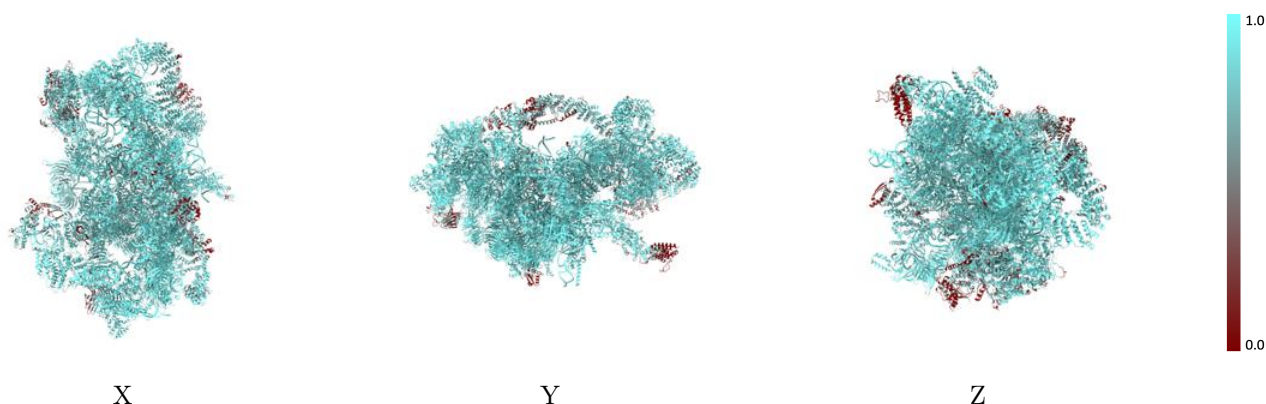
The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



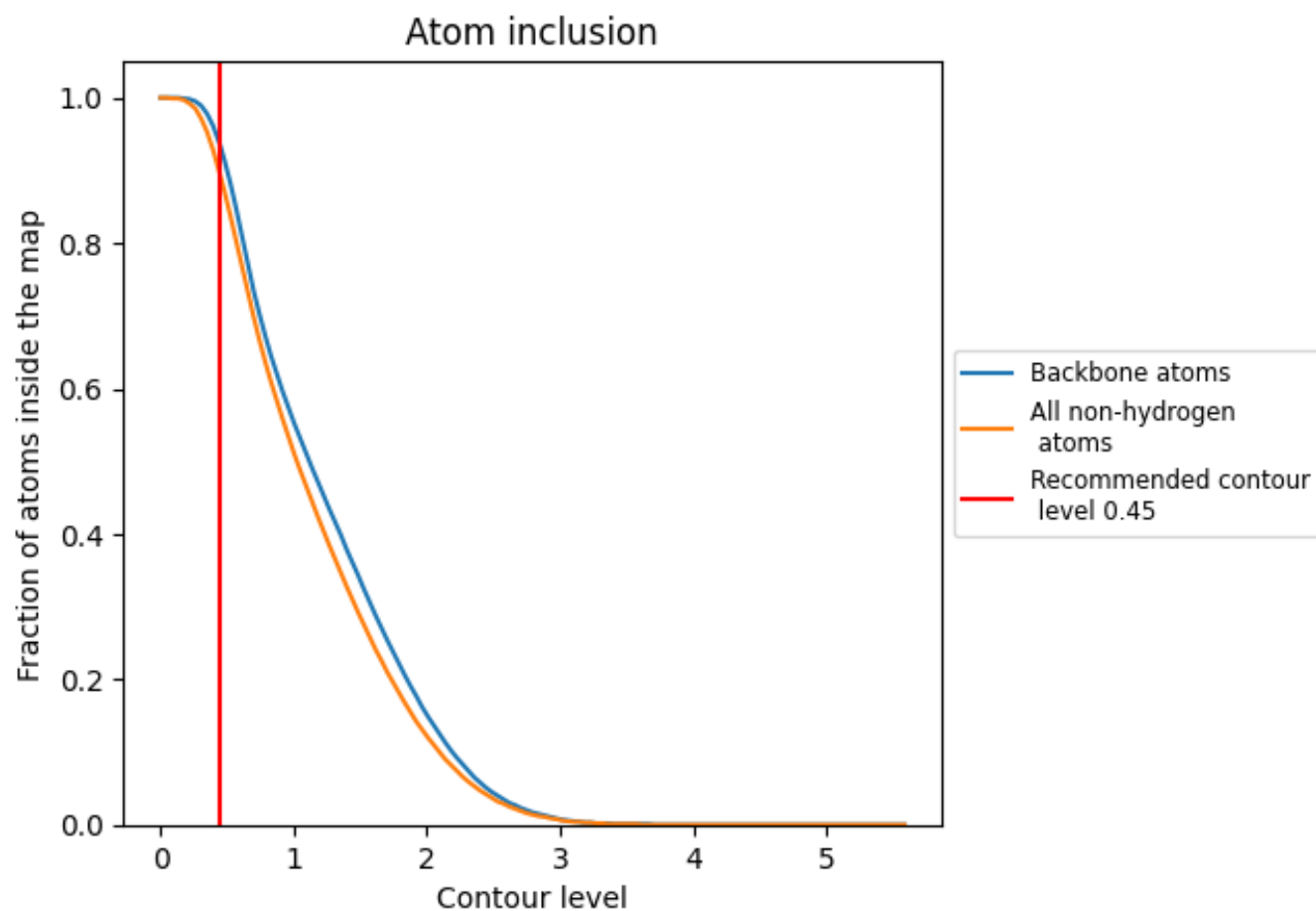
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.45).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 89% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8920	 0.4850
CA	 0.9520	 0.5910
CB	 0.9510	 0.5240
CD	 0.9090	 0.4920
CE	 0.9180	 0.4950
CF	 0.9700	 0.5890
CG	 0.9390	 0.5250
CH	 0.9230	 0.4930
CI	 0.9830	 0.6240
CJ	 0.9410	 0.5720
CK	 0.8680	 0.5210
CL	 0.9210	 0.5440
CM	 0.8940	 0.5180
D2	 0.9710	 0.5120
D3	 0.9220	 0.4450
D4	 0.9640	 0.5140
DE	 0.9170	 0.4680
DF	 0.9570	 0.5760
DG	 0.9020	 0.4660
DH	 0.8480	 0.4440
DI	 0.9380	 0.5130
DJ	 0.9430	 0.5450
DL	 0.9390	 0.4770
DQ	 0.9730	 0.6050
DS	 0.7850	 0.3810
DW	 0.9400	 0.5320
DX	 0.9480	 0.5790
DY	 0.8960	 0.4890
Dc	 0.9370	 0.5700
JA	 0.7910	 0.3960
JB	 0.5550	 0.2550
JC	 0.9300	 0.5020
JE	 0.8740	 0.4510
JF	 0.8840	 0.4790
JG	 0.9330	 0.5450



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Chain	Atom inclusion	Q-score
JH	 0.6530	 0.2360
JJ	 0.2860	 0.3190
JK	 0.8980	 0.4690
JM	 0.8630	 0.5240
JN	 0.9110	 0.5230
JO	 0.8650	 0.5030
JP	 0.9780	 0.5930
JQ	 0.7020	 0.3690
UA	 0.9640	 0.6110
UB	 0.8670	 0.4510
UC	 0.8610	 0.5040
UD	 0.9660	 0.5590
UE	 0.9460	 0.5630
UF	 0.9000	 0.4730
UG	 0.9630	 0.5980
UH	 0.6730	 0.3420
UI	 0.9090	 0.4200
UJ	 0.7650	 0.3700
UK	 0.9460	 0.5690
UL	 0.9390	 0.5010
UM	 0.9440	 0.5090
UN	 0.8980	 0.5270
UO	 0.9740	 0.5740
UP	 0.9440	 0.4920
UQ	 0.9560	 0.5620
UR	 0.9710	 0.5980
US	 0.9240	 0.4750
UT	 0.8020	 0.3350
UU	 0.9440	 0.6000
UX	 0.9690	 0.5900
UZ	 0.9030	 0.4890