



## Full wwPDB EM Validation Report ⓘ

Oct 22, 2025 – 10:58 PM JST

PDB ID : 9UWH / pdb\_00009uwh  
EMDB ID : EMD-64554  
Title : human mitoribosome trapped by retapamulin  
Authors : Ando, Y.; Nureki, O.; Itoh, Y.  
Deposited on : 2025-05-12  
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev129  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.46

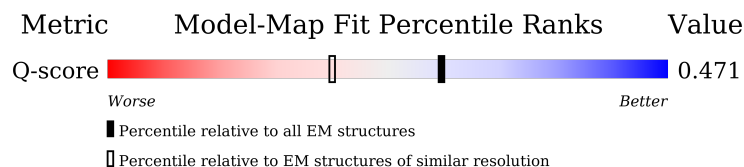
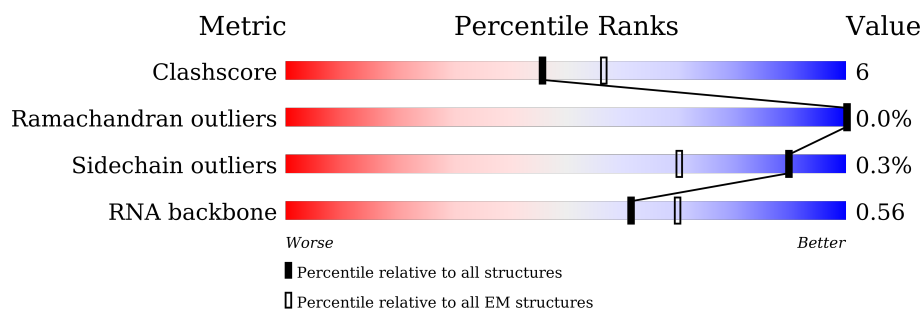
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.00 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
RNA backbone	6643	2191	-
Q-score	-	25397	14081 ( 2.50 - 3.50 )

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

Mol	Chain	Length	Quality of chain
1	A	1561	
2	B	72	
3	D	305	








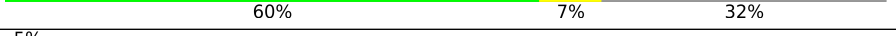
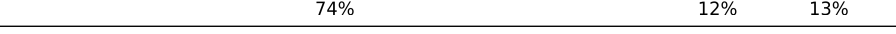








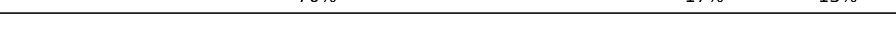


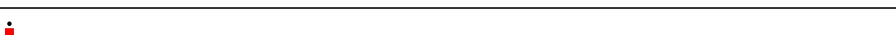




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Mol	Chain	Length	Quality of chain
4	E	348	
5	F	311	
6	H	267	
7	I	261	
8	J	192	
9	K	178	
10	L	145	
11	M	296	
12	N	251	
13	O	175	
14	P	180	
15	Q	292	
16	R	149	
17	S	205	
18	T	206	
19	U	153	
20	V	216	
21	W	148	
22	X	256	
23	Y	250	
24	Z	161	
25	AA	954	
26	AB	296	
27	AC	167	
28	AD	430	



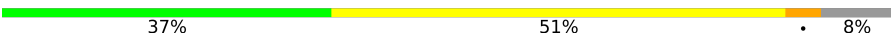






















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Mol	Chain	Length	Quality of chain
29	AE	125	
30	AF	242	
31	AG	396	
32	AH	201	
33	AI	194	
34	AJ	138	
35	AK	128	
36	AL	257	
37	AM	137	
38	AN	130	
39	AO	258	
40	AP	142	
41	AQ	87	
42	AR	360	
43	AS	190	
44	AT	173	
45	AU	205	
46	AV	414	
47	AW	187	
48	AX	398	
49	AY	395	
50	AZ	106	
51	A0	217	
52	A1	323	
53	A2	118	

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Mol	Chain	Length	Quality of chain
54	A3	199	
55	A4	689	
56	Ax	71	
57	Az	8	
58	0	188	
59	1	65	
60	2	92	
61	3	188	
62	4	103	
63	5	423	
64	6	380	
65	7	338	
66	8	206	
67	9	137	
68	a	142	
69	b	215	
70	c	332	
71	d	306	
72	e	279	
73	f	212	
74	g	166	
75	h	158	
76	i	128	
77	j	123	
78	k	112	

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Mol	Chain	Length	Quality of chain
79	l	138	
80	m	128	
81	o	102	
82	p	206	
83	q	222	
84	r	196	
85	s	439	
86	t	198	

## 2 Entry composition

There are 96 unique types of molecules in this entry. The entry contains 171472 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 16S mitochondrial rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1523	Total	C	N	O	P	0	0
			32331	14510	5827	10471	1523		

- Molecule 2 is a RNA chain called mitochondrial tRNAVal.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	72	Total	C	N	O	P	0	0
			1524	685	269	498	72		

- Molecule 3 is a protein called Large ribosomal subunit protein uL2m.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	238	Total	C	N	O	S	0	0
			1859	1157	376	317	9		

- Molecule 4 is a protein called Large ribosomal subunit protein uL3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	305	Total	C	N	O	S	0	0
			2406	1545	418	432	11		

- Molecule 5 is a protein called Large ribosomal subunit protein uL4m.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	252	Total	C	N	O	S	0	0
			2031	1305	370	350	6		

- Molecule 6 is a protein called Large ribosomal subunit protein bL9m.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	H	100	Total	C	N	O	0	0
			823	522	159	142		

- Molecule 7 is a protein called Large ribosomal subunit protein uL10m.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	169	Total	C	N	O	S	0	0
			1362	877	247	228	10		

- Molecule 8 is a protein called Large ribosomal subunit protein uL11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	175	Total	C	N	O	S	0	0
			1330	847	237	244	2		

- Molecule 9 is a protein called Large ribosomal subunit protein uL13m.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	178	Total	C	N	O	S	0	0
			1455	936	259	253	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	1	ACE	-	acetylation	UNP Q9BYD1

- Molecule 10 is a protein called Large ribosomal subunit protein uL14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	115	Total	C	N	O	S	0	0
			890	559	171	155	5		

- Molecule 11 is a protein called Large ribosomal subunit protein uL15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	289	Total	C	N	O	S	0	0
			2314	1476	427	405	6		

- Molecule 12 is a protein called Large ribosomal subunit protein uL16m.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	222	Total	C	N	O	S	0	0
			1786	1143	326	307	10		

- Molecule 13 is a protein called Large ribosomal subunit protein bL17m.



Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	154	Total	C	N	O	S	0	0
			1259	792	241	219	7		

- Molecule 14 is a protein called Large ribosomal subunit protein uL18m.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	144	Total	C	N	O	S	0	0
			1173	733	224	211	5		

- Molecule 15 is a protein called Large ribosomal subunit protein bL19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	239	Total	C	N	O	S	0	0
			1990	1277	353	351	9		

- Molecule 16 is a protein called Large ribosomal subunit protein bL20m.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	140	Total	C	N	O	S	0	0
			1154	732	231	187	4		

- Molecule 17 is a protein called Large ribosomal subunit protein bL21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	161	Total	C	N	O	S	0	0
			1293	835	227	227	4		

- Molecule 18 is a protein called Large ribosomal subunit protein uL22m.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	166	Total	C	N	O	S	0	0
			1369	875	254	233	7		

- Molecule 19 is a protein called Large ribosomal subunit protein uL23m.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	153	Total	C	N	O	S	0	0
			1251	788	234	226	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	1	ACE	-	acetylation	UNP Q16540

- Molecule 20 is a protein called Large ribosomal subunit protein uL24m.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	205	Total	C	N	O	S	0	0
			1676	1068	298	302	8		

- Molecule 21 is a protein called Large ribosomal subunit protein bL27m.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	116	Total	C	N	O	S	0	0
			904	577	171	153	3		

- Molecule 22 is a protein called Large ribosomal subunit protein bL28m.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	244	Total	C	N	O	S	0	0
			2044	1322	352	365	5		

- Molecule 23 is a protein called Large ribosomal subunit protein uL29m.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	181	Total	C	N	O	S	0	0
			1556	995	298	259	4		

- Molecule 24 is a protein called Large ribosomal subunit protein uL30m.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	122	Total	C	N	O	S	0	0
			996	636	186	171	3		

- Molecule 25 is a RNA chain called 12S mitochondrial rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AA	954	Total	C	N	O	P	0	0
			20260	9088	3647	6571	954		

- Molecule 26 is a protein called Small ribosomal subunit protein uS2m.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AB	225	Total	C	N	O	S	0	0
			1828	1164	331	323	10		

- Molecule 27 is a protein called Small ribosomal subunit protein uS3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	AC	132	Total	C	N	O	S	0	0
			1083	699	195	185	4		

- Molecule 28 is a protein called Small ribosomal subunit protein uS5m.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	AD	343	Total	C	N	O	S	0	0
			2731	1713	518	487	13		

- Molecule 29 is a protein called Small ribosomal subunit protein bS6m.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	AE	122	Total	C	N	O	S	0	0
			972	614	177	177	4		

- Molecule 30 is a protein called Small ribosomal subunit protein uS7m.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	AF	208	Total	C	N	O	S	0	0
			1725	1104	312	298	11		

- Molecule 31 is a protein called Small ribosomal subunit protein uS9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	AG	311	Total	C	N	O	S	0	0
			2561	1627	454	466	14		

- Molecule 32 is a protein called Small ribosomal subunit protein uS10m.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	AH	140	Total	C	N	O	S	0	0
			1152	745	194	210	3		

- Molecule 33 is a protein called Small ribosomal subunit protein uS11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	AI	137	Total	C	N	O	S	0	0
			1020	642	192	182	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	184	5F0	ASN	conflict	UNP P82912

- Molecule 34 is a protein called Small ribosomal subunit protein uS12m.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	AJ	108	Total	C	N	O	S	0	0
			839	521	169	143	6		

- Molecule 35 is a protein called Small ribosomal subunit protein uS14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	AK	101	Total	C	N	O	S	0	0
			862	537	179	141	5		

- Molecule 36 is a protein called Small ribosomal subunit protein uS15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	AL	174	Total	C	N	O	S	0	0
			1453	925	270	251	7		

- Molecule 37 is a protein called Small ribosomal subunit protein bS16m.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	AM	119	Total	C	N	O	S	0	0
			942	594	185	157	6		

- Molecule 38 is a protein called Small ribosomal subunit protein uS17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	AN	110	Total	C	N	O	S	0	0
			868	562	156	147	3		

- Molecule 39 is a protein called Small ribosomal subunit protein mS40.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	AO	193	Total	C	N	O	S	0	0
			1592	1014	294	277	7		

- Molecule 40 is a protein called Small ribosomal subunit protein bS18m.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	AP	97	Total	C	N	O	S	0	0
			781	501	134	138	8		

- Molecule 41 is a protein called MRPS21 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	AQ	87	Total	C	N	O	S	0	0
			744	460	150	126	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AQ	1	ACE	-	acetylation	UNP A0A2J8VEN6

- Molecule 42 is a protein called Small ribosomal subunit protein mS22.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	AR	295	Total	C	N	O	S	0	0
			2409	1533	413	455	8		

- Molecule 43 is a protein called Small ribosomal subunit protein mS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	AS	135	Total	C	N	O	S	0	0
			1111	716	198	196	1		

- Molecule 44 is a protein called Small ribosomal subunit protein mS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	AT	168	Total	C	N	O	S	0	0
			1371	877	239	244	11		

- Molecule 45 is a protein called Small ribosomal subunit protein mS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	AU	176	Total	C	N	O	S	0	0
			1488	916	301	267	4		

- Molecule 46 is a protein called Small ribosomal subunit protein mS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	AV	362	Total	C	N	O	S	0	0
			2969	1904	495	558	12		

- Molecule 47 is a protein called Small ribosomal subunit protein bS1m.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	AW	100	Total	C	N	O	S	0	0
			789	498	141	146	4		

- Molecule 48 is a protein called Small ribosomal subunit protein mS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	AX	352	Total	C	N	O	S	0	0
			2849	1822	499	517	11		

- Molecule 49 is a protein called Small ribosomal subunit protein mS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	AY	120	Total	C	N	O	S	0	0
			1016	657	167	190	2		

- Molecule 50 is a protein called Small ribosomal subunit protein mS33.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	AZ	100	Total	C	N	O	S	0	0
			839	534	153	148	4		

- Molecule 51 is a protein called Small ribosomal subunit protein mS34.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	A0	215	Total	C	N	O	S	0	0
			1787	1130	339	313	5		

- Molecule 52 is a protein called Small ribosomal subunit protein mS35.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	A1	277	Total	C	N	O	S	0	0
			2245	1424	382	428	11		

- Molecule 53 is a protein called Small ribosomal subunit protein mS37.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	A2	118	Total	C	N	O	S	0	0
			935	579	182	166	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A2	1	ACE	-	acetylation	UNP Q96BP2

- Molecule 54 is a protein called Small ribosomal subunit protein mS38.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	A3	70	Total	C	N	O	S	0	0
			625	401	134	89	1		

- Molecule 55 is a protein called Small ribosomal subunit protein mS39.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	A4	533	Total	C	N	O	S	0	0
			4329	2780	730	793	26		

- Molecule 56 is a RNA chain called P/P-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	Ax	65	Total	C	N	O	P	0	0
			1378	617	242	454	65		

- Molecule 57 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Az	8	Total	C	N	O	P	0	0
			167	75	25	59	8		

- Molecule 58 is a protein called Large ribosomal subunit protein bL32m.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	0	110	Total	C	N	O	S	0	0
			898	554	176	162	6		

- Molecule 59 is a protein called Large ribosomal subunit protein bL33m.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	1	53	Total	C	N	O	S	0	0
			440	281	84	73	2		

- Molecule 60 is a protein called Large ribosomal subunit protein bL34m.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	2	46	Total	C	N	O	S	0	0
			377	233	83	60	1		

- Molecule 61 is a protein called Large ribosomal subunit protein bL35m.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	3	95	Total	C	N	O	S	0	0
			832	539	162	128	3		

- Molecule 62 is a protein called Large ribosomal subunit protein bL36m.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	4	38	Total	C	N	O	S	0	0
			342	217	72	49	4		

- Molecule 63 is a protein called Large ribosomal subunit protein mL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	5	394	Total	C	N	O	S	0	0
			3210	2073	560	566	11		

- Molecule 64 is a protein called Large ribosomal subunit protein mL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	6	354	Total	C	N	O	S	0	0
			2948	1881	525	533	9		

- Molecule 65 is a protein called Large ribosomal subunit protein mL39.



Mol	Chain	Residues	Atoms					AltConf	Trace
65	7	294	Total	C	N	O	S	0	0
			2390	1529	405	438	18		

- Molecule 66 is a protein called Large ribosomal subunit protein mL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	8	140	Total	C	N	O	S	0	0
			1184	755	208	219	2		

- Molecule 67 is a protein called Large ribosomal subunit protein mL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	9	124	Total	C	N	O	S	0	0
			997	644	170	181	2		

- Molecule 68 is a protein called Large ribosomal subunit protein mL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	a	100	Total	C	N	O	S	0	0
			840	529	152	154	5		

- Molecule 69 is a protein called Large ribosomal subunit protein mL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	b	151	Total	C	N	O	S	0	0
			1196	744	231	218	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	1	ACE	-	acetylation	UNP Q8N983

- Molecule 70 is a protein called Large ribosomal subunit protein mL44.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	c	286	Total	C	N	O	S	0	0
			2299	1470	397	423	9		

- Molecule 71 is a protein called Large ribosomal subunit protein mL45.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	d	241	Total	C	N	O	S	0	0
			1985	1273	340	359	13		

- Molecule 72 is a protein called Large ribosomal subunit protein mL46.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	e	238	Total	C	N	O	S	0	0
			1931	1222	339	364	6		

- Molecule 73 is a protein called Large ribosomal subunit protein mL48.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	f	157	Total	C	N	O	S	0	0
			1252	799	207	242	4		

- Molecule 74 is a protein called Large ribosomal subunit protein mL49.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	g	134	Total	C	N	O	S	0	0
			1113	719	193	199	2		

- Molecule 75 is a protein called Large ribosomal subunit protein mL50.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	h	110	Total	C	N	O	S	0	0
			895	568	156	168	3		

- Molecule 76 is a protein called Large ribosomal subunit protein mL51.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	i	97	Total	C	N	O	S	0	0
			828	532	165	127	4		

- Molecule 77 is a protein called Large ribosomal subunit protein mL52.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	j	94	Total	C	N	O	S	0	0
			745	463	144	136	2		

- Molecule 78 is a protein called Large ribosomal subunit protein mL53.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	k	95	Total	C	N	O	S	0	0
			738	459	142	132	5		

- Molecule 79 is a protein called Large ribosomal subunit protein mL54.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	l	82	Total	C	N	O	S	0	0
			688	437	120	128	3		

- Molecule 80 is a protein called Large ribosomal subunit protein mL55.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	m	92	Total	C	N	O	S	0	0
			791	488	159	142	2		

- Molecule 81 is a protein called Large ribosomal subunit protein mL63.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	o	94	Total	C	N	O	S	0	0
			798	501	165	129	3		

- Molecule 82 is a protein called Large ribosomal subunit protein mL62.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	p	143	Total	C	N	O	S	0	0
			1179	735	222	218	4		

- Molecule 83 is a protein called Large ribosomal subunit protein mL64.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	q	133	Total	C	N	O	S	0	0
			1120	697	220	198	5		

- Molecule 84 is a protein called Large ribosomal subunit protein mL66.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	r	162	Total	C	N	O	S	0	0
			1322	839	252	223	8		

- Molecule 85 is a protein called Large ribosomal subunit protein mL65.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	s	383	Total	C	N	O	S	0	0
			3134	2010	556	554	14		

- Molecule 86 is a protein called Large ribosomal subunit protein bL12m.

Mol	Chain	Residues	Atoms				AltConf	Trace
86	t	11	Total	C	N	O	0	0
			72	44	12	16		

- Molecule 87 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
87	A	138	Total	Mg	0
			138	138	
87	D	2	Total	Mg	0
			2	2	
87	E	1	Total	Mg	0
			1	1	
87	AA	63	Total	Mg	0
			63	63	
87	AB	1	Total	Mg	0
			1	1	
87	AX	1	Total	Mg	0
			1	1	
87	A3	1	Total	Mg	0
			1	1	
87	g	1	Total	Mg	0
			1	1	

- Molecule 88 is POTASSIUM ION (CCD ID: K) (formula: K).

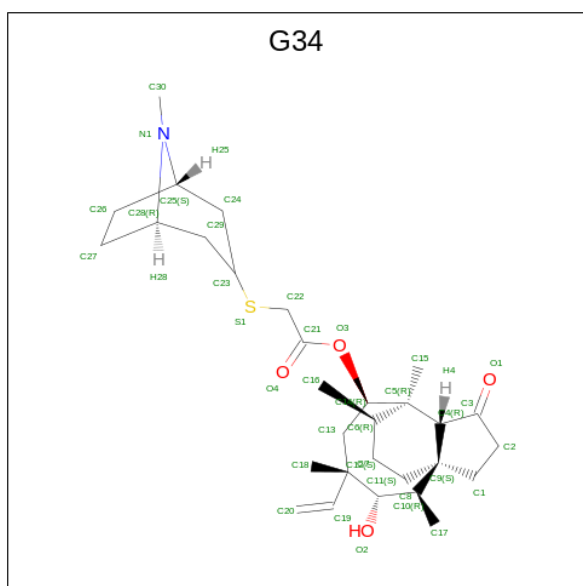
Mol	Chain	Residues	Atoms		AltConf
88	A	29	Total	K	0
			29	29	
88	D	1	Total	K	0
			1	1	
88	M	1	Total	K	0
			1	1	
88	W	1	Total	K	0
			1	1	
88	AA	18	Total	K	0
			18	18	

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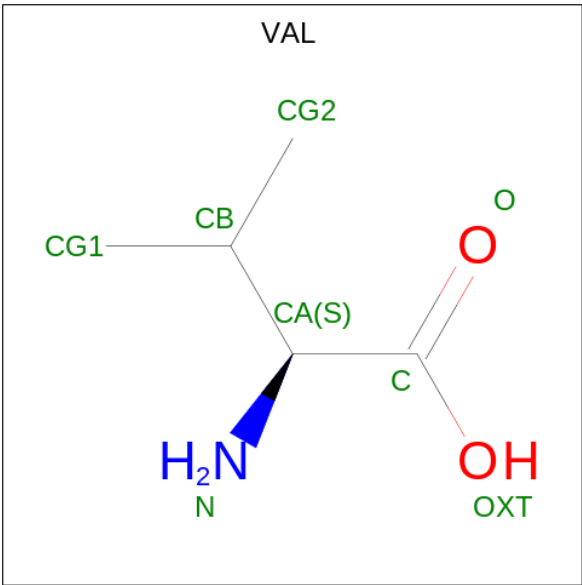
Mol	Chain	Residues	Atoms	AltConf
88	6	1	Total K 1 1	0
88	i	1	Total K 1 1	0
88	o	1	Total K 1 1	0

- Molecule 89 is Retapamulin (CCD ID: G34) (formula:  $C_{30}H_{47}NO_4S$ ) (labeled as "Ligand of Interest" by depositor).



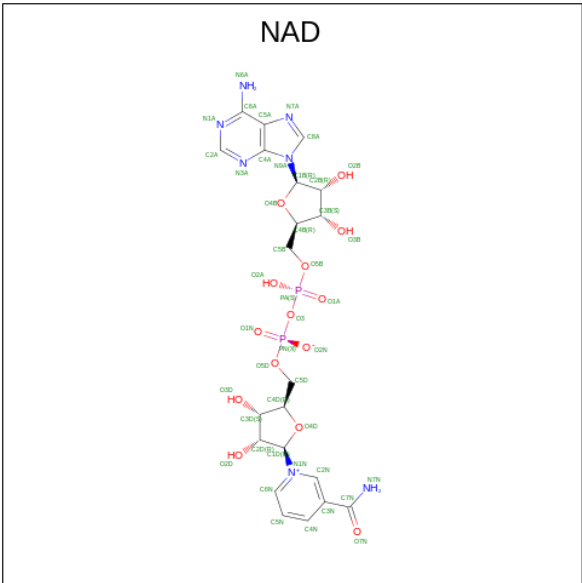
Mol	Chain	Residues	Atoms					AltConf
89	A	1	Total 36	C 30	N 1	O 4	S 1	0

- Molecule 90 is VALINE (CCD ID: VAL) (formula:  $\text{C}_5\text{H}_{11}\text{NO}_2$ ).



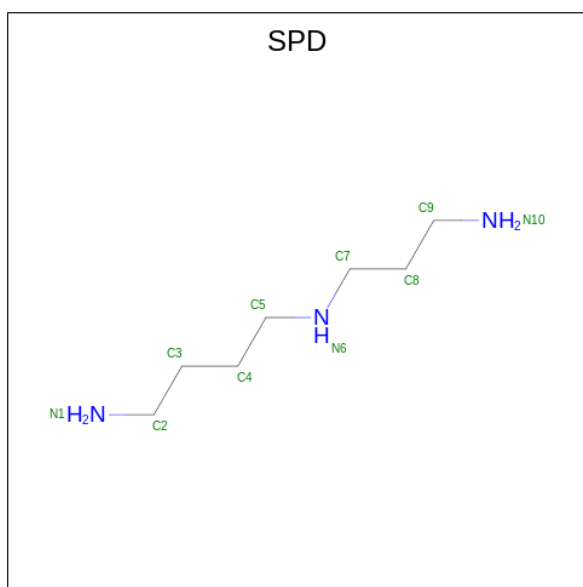
Mol	Chain	Residues	Atoms				AltConf
90	B	1	Total	C	N	O	0
			7	5	1	1	

- Molecule 91 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula:  $C_{21}H_{27}N_7O_{14}P_2$ ).



Mol	Chain	Residues	Atoms					AltConf
91	AA	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 92 is SPERMIDINE (CCD ID: SPD) (formula:  $C_7H_{19}N_3$ ).

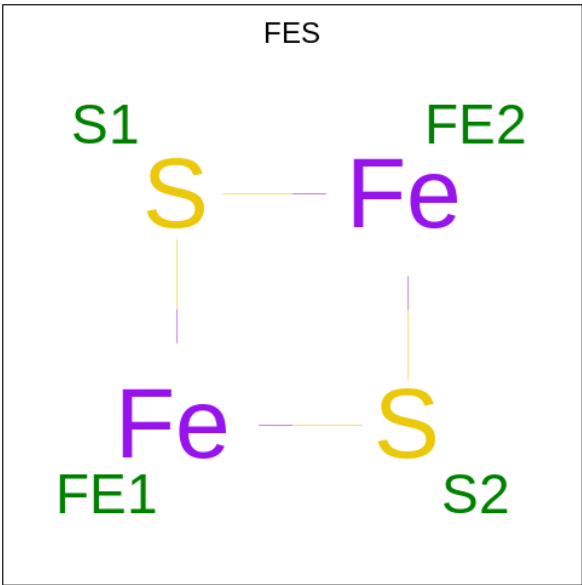


Mol	Chain	Residues	Atoms			AltConf
92	AA	1	Total	C	N	0
			10	7	3	

- Molecule 93 is ZINC ION (CCD ID: ZN) (formula: Zn).

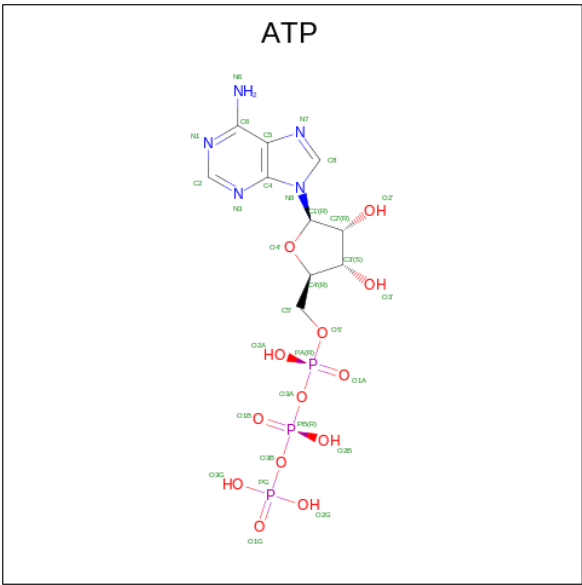
Mol	Chain	Residues	Atoms		AltConf
93	AO	1	Total	Zn	0
			1	1	
93	0	1	Total	Zn	0
			1	1	
93	4	1	Total	Zn	0
			1	1	

- Molecule 94 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



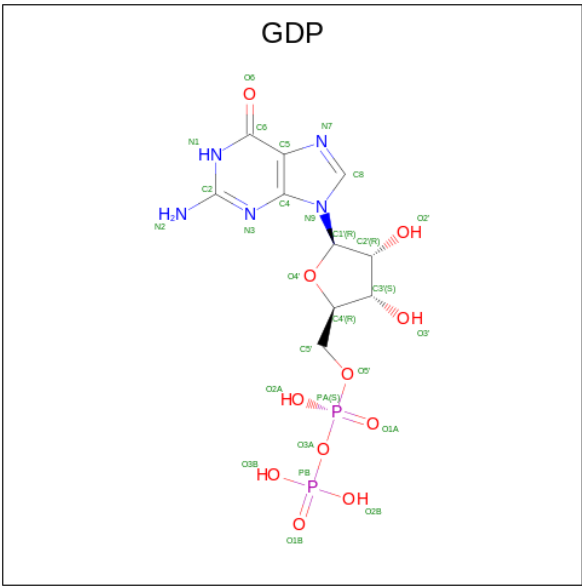
Mol	Chain	Residues	Atoms			AltConf
94	AP	1	Total	Fe	S	0
			4	2	2	
94	AT	1	Total	Fe	S	0
			4	2	2	
94	r	1	Total	Fe	S	0
			4	2	2	

- Molecule 95 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).





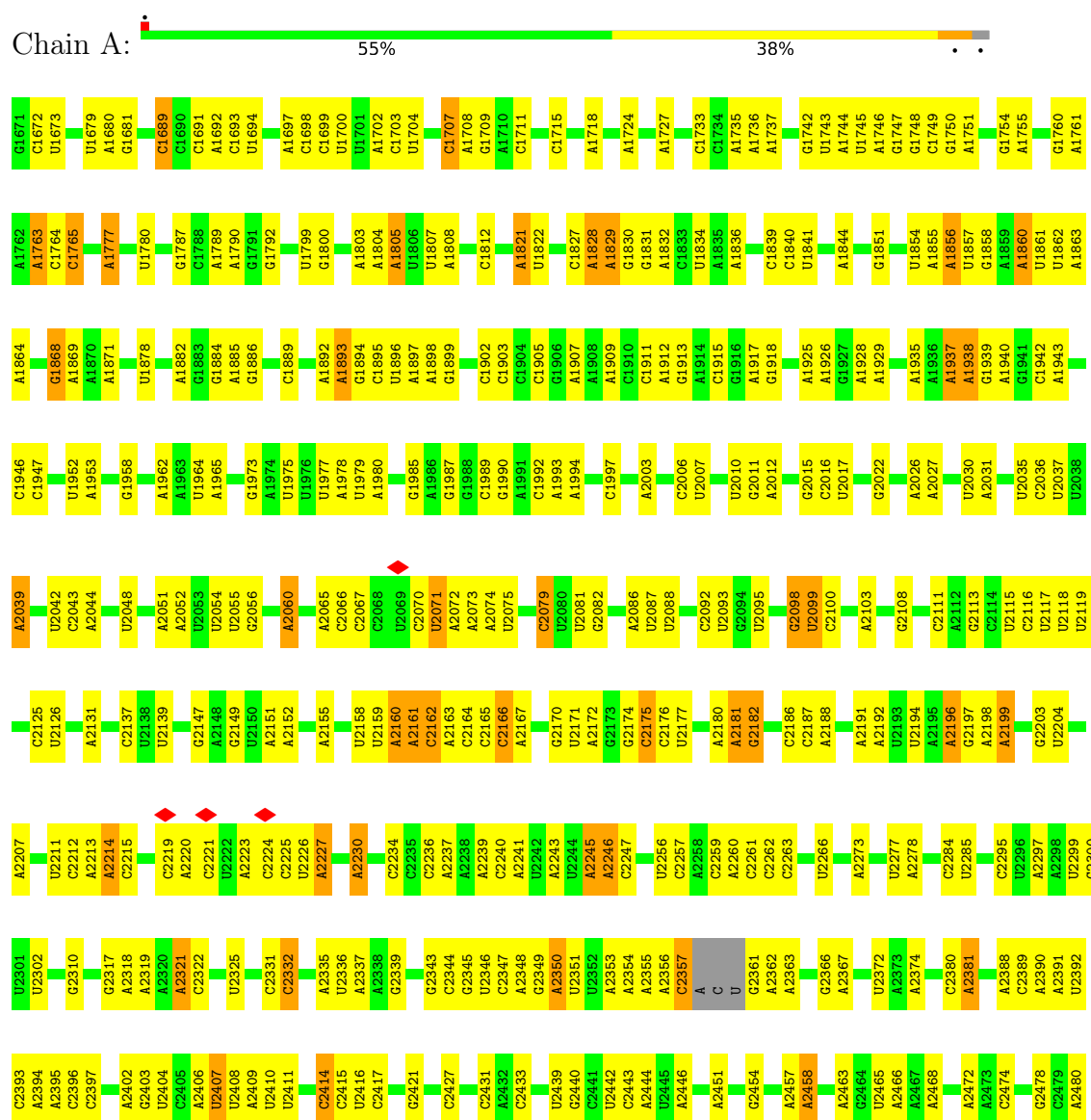
- Molecule 96 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).

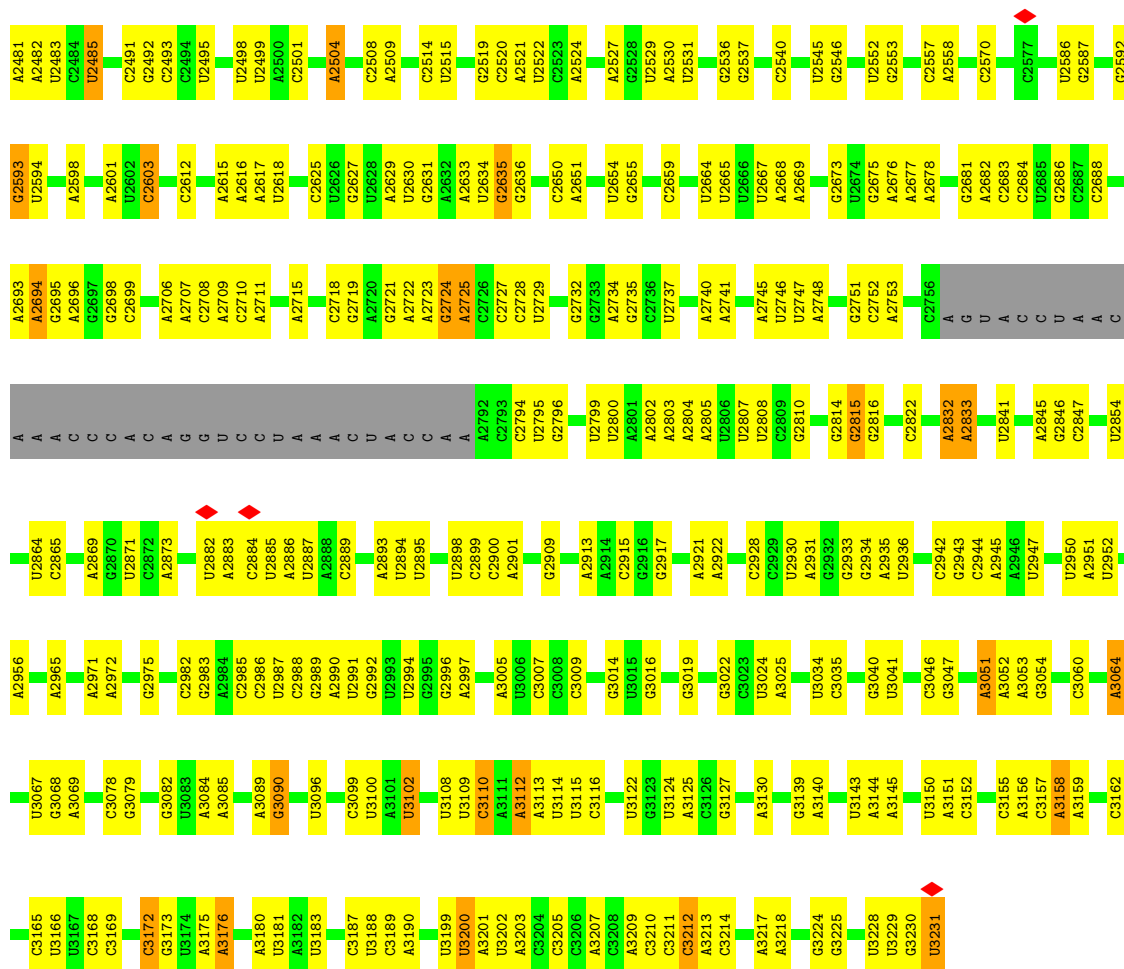


### 3 Residue-property plots

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: 16S mitochondrial rRNA

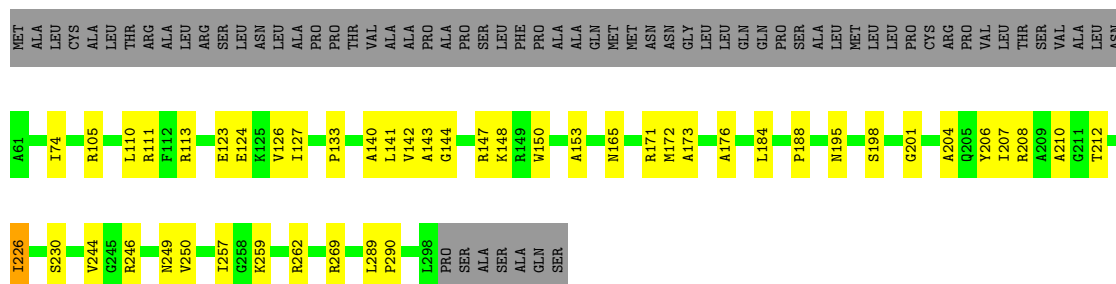





- Molecule 2: mitochondrial tRNA<sup>Val</sup>

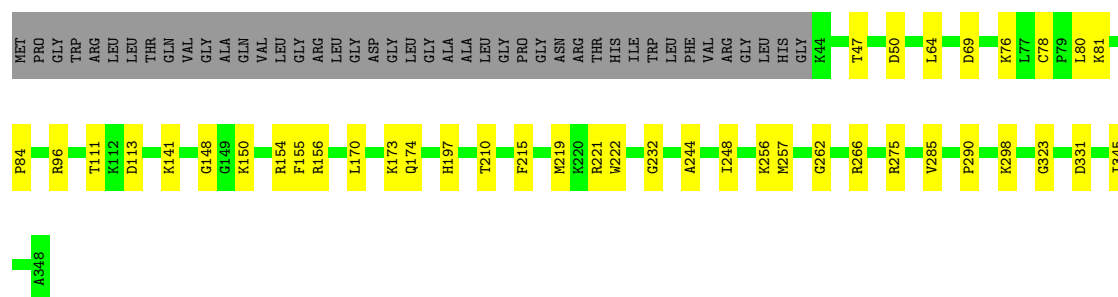


- Molecule 3: Large ribosomal subunit protein uL2m



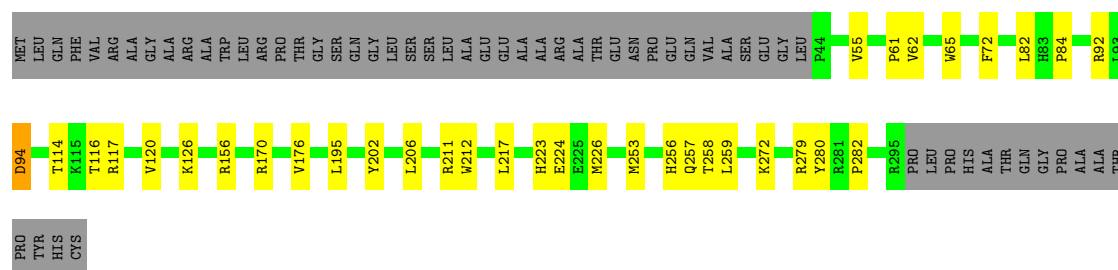
- Molecule 4: Large ribosomal subunit protein uL3m

Chain E:  76% 12% 12%



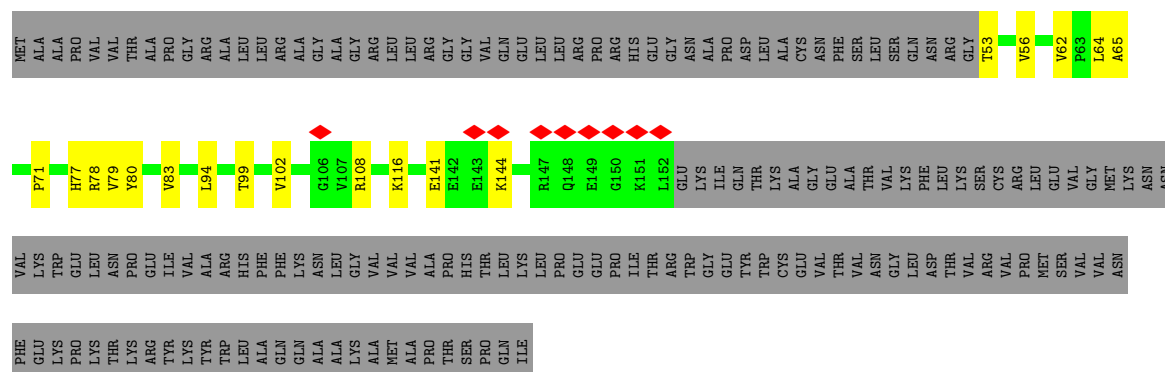
- Molecule 5: Large ribosomal subunit protein uL4m

Chain F:  70% 11% 19%



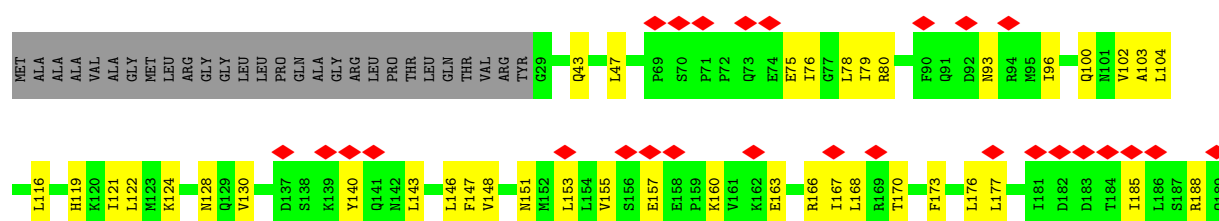
- Molecule 6: Large ribosomal subunit protein bL9m

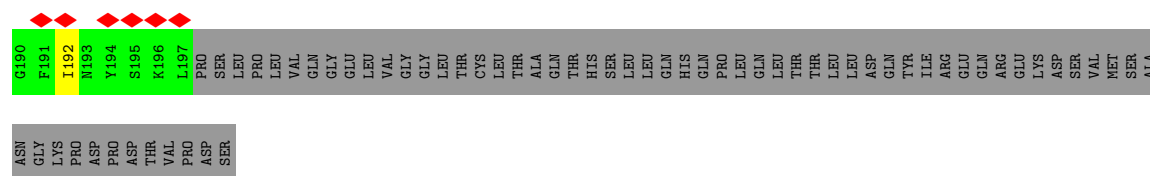
Chain H:  31% 7% 63%



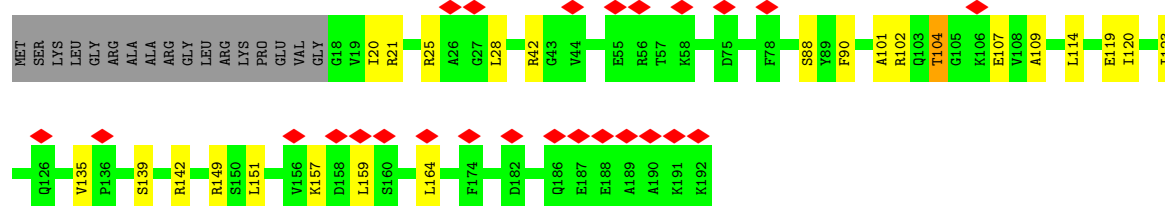
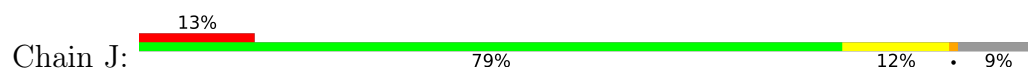
- Molecule 7: Large ribosomal subunit protein uL10m

Chain I:  13% 49% 16% 35%

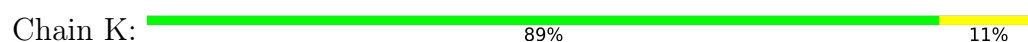




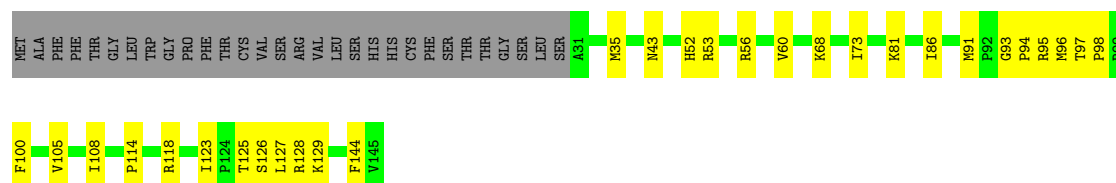
- Molecule 8: Large ribosomal subunit protein uL11m



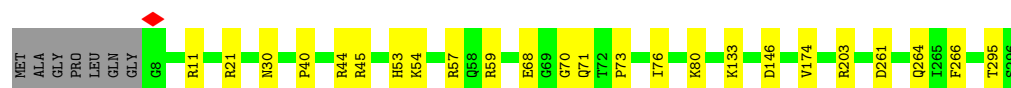
- Molecule 9: Large ribosomal subunit protein uL13m



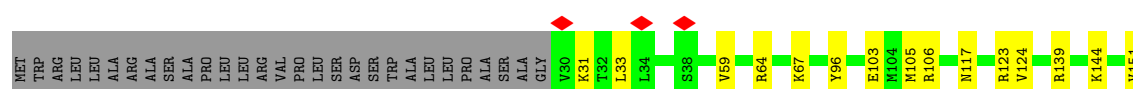
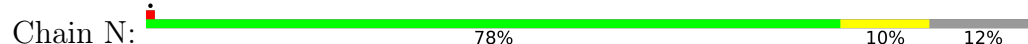
- Molecule 10: Large ribosomal subunit protein uL14m



- Molecule 11: Large ribosomal subunit protein uL15m

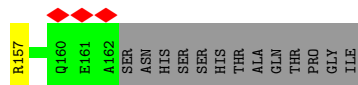


- Molecule 12: Large ribosomal subunit protein uL16m

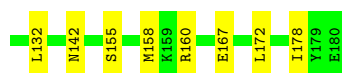
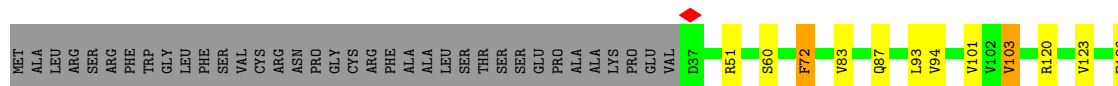




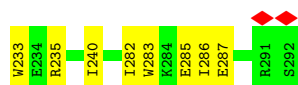
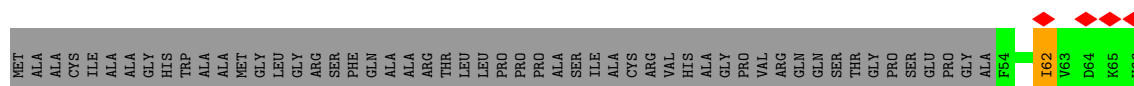
- Molecule 13: Large ribosomal subunit protein bL17m



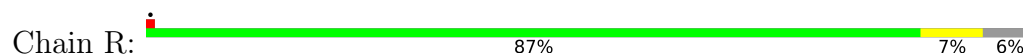
- Molecule 14: Large ribosomal subunit protein uL18m



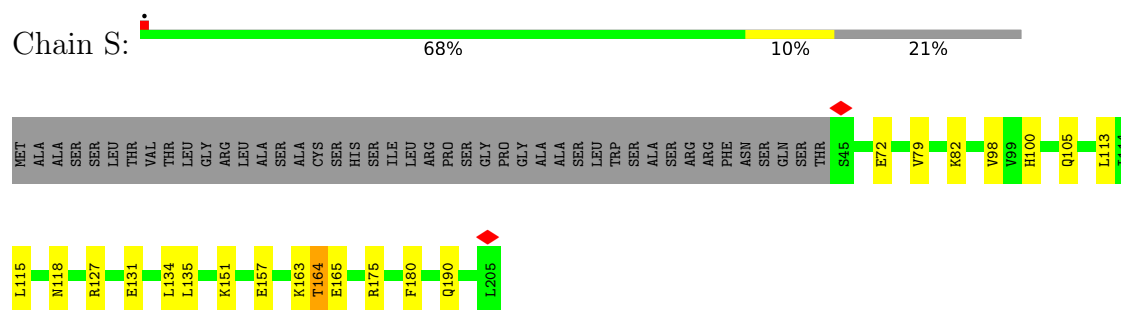
- Molecule 15: Large ribosomal subunit protein bL19m



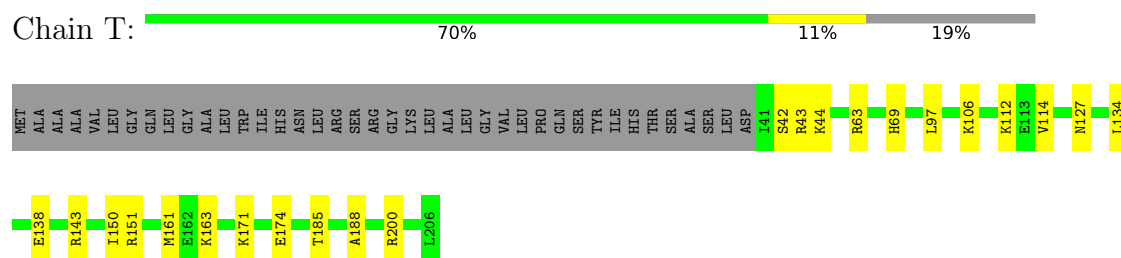
- Molecule 16: Large ribosomal subunit protein bL20m



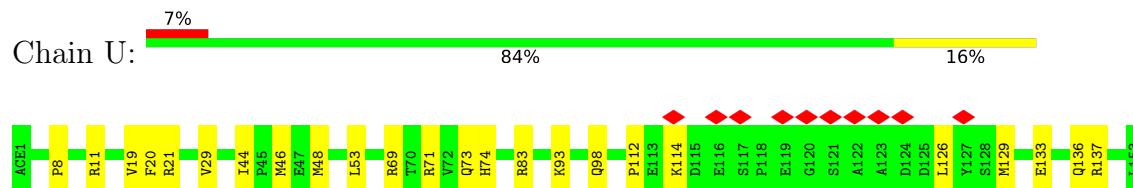
- Molecule 17: Large ribosomal subunit protein bL21m



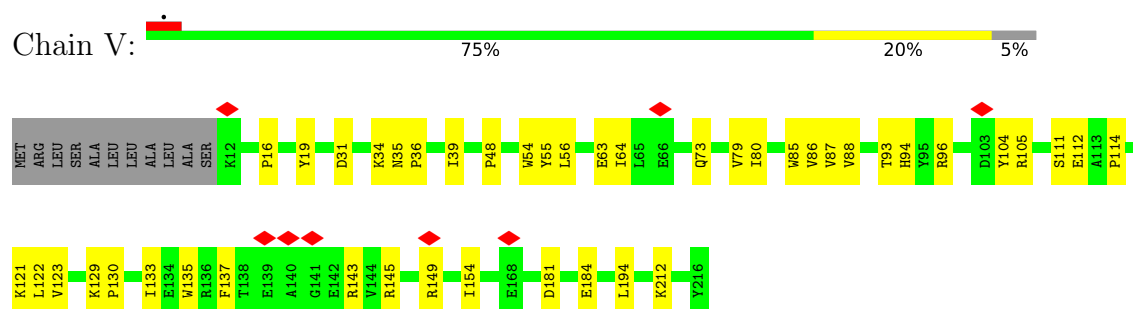
- Molecule 18: Large ribosomal subunit protein uL22m



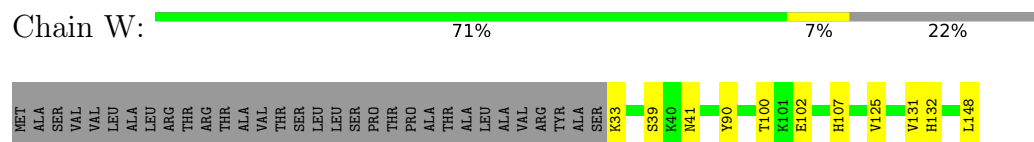
- Molecule 19: Large ribosomal subunit protein uL23m



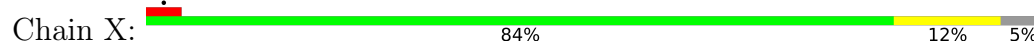
- Molecule 20: Large ribosomal subunit protein uL24m

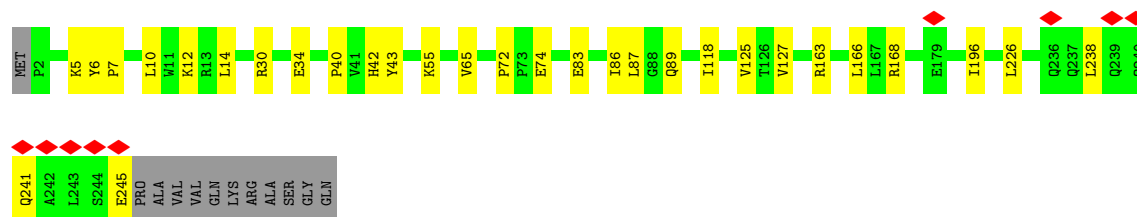


- Molecule 21: Large ribosomal subunit protein bL27m



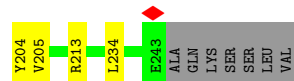
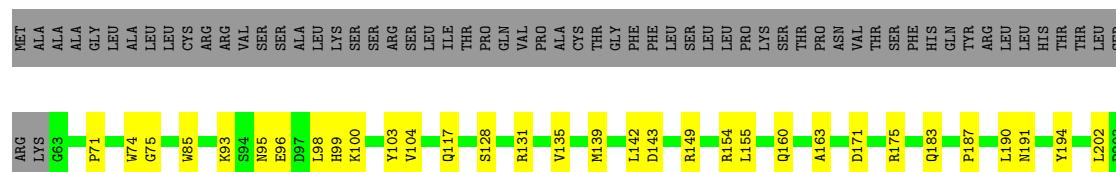
- Molecule 22: Large ribosomal subunit protein bL28m





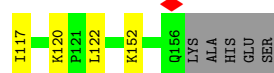
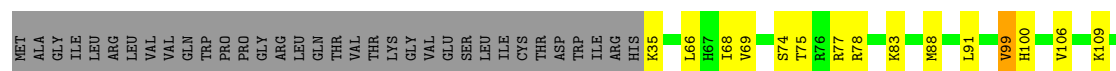
- Molecule 23: Large ribosomal subunit protein uL29m

Chain Y:



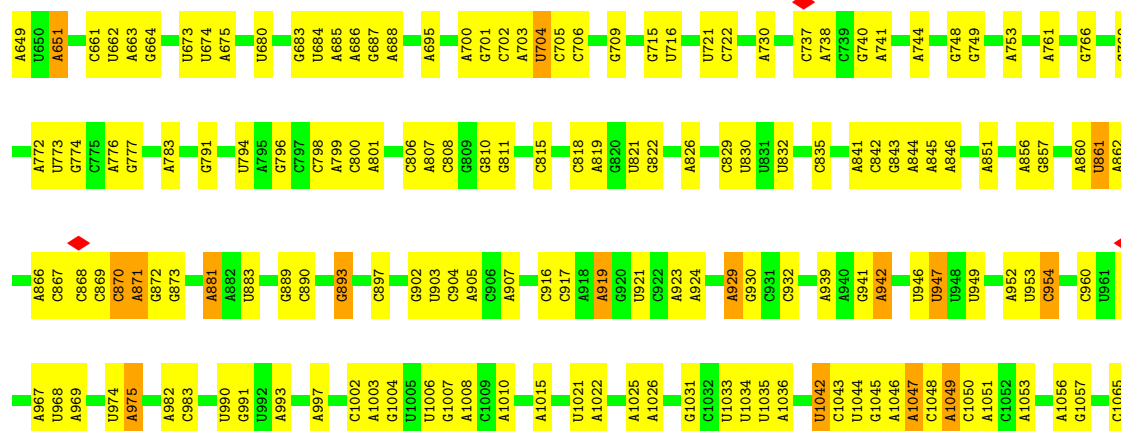
- Molecule 24: Large ribosomal subunit protein uL30m

Chain Z:

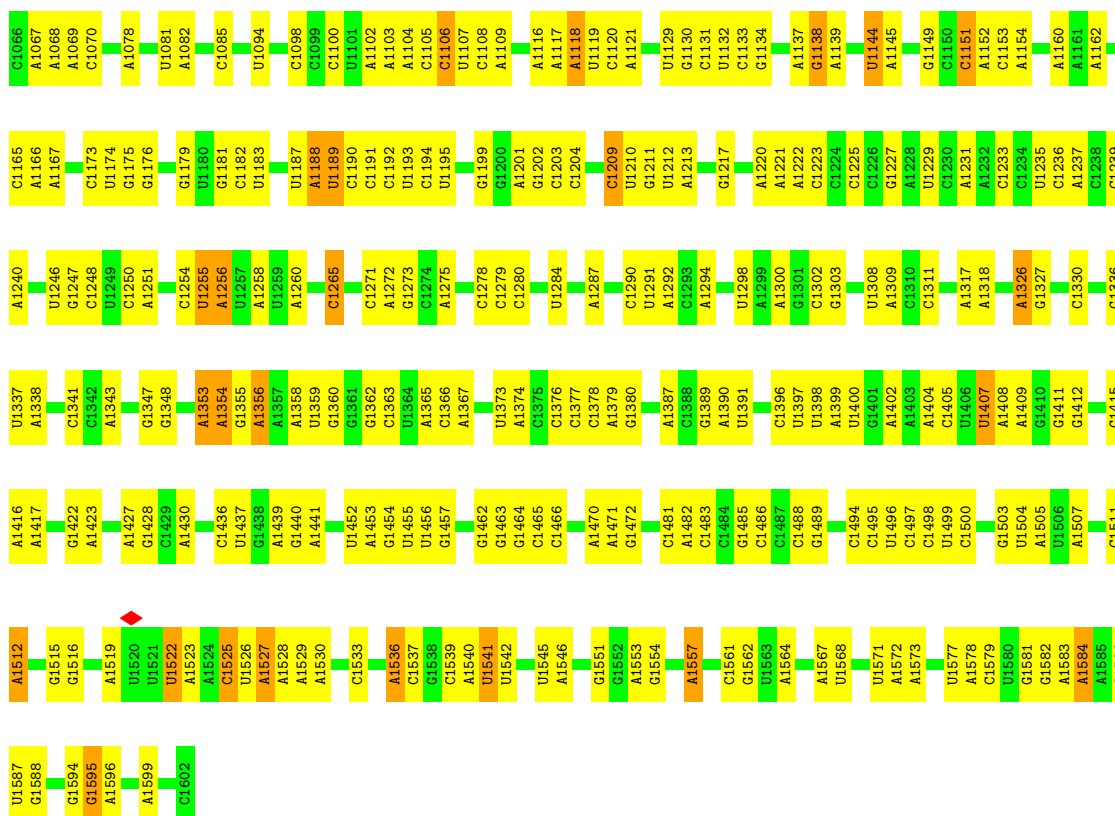


- Molecule 25: 12S mitochondrial rRNA

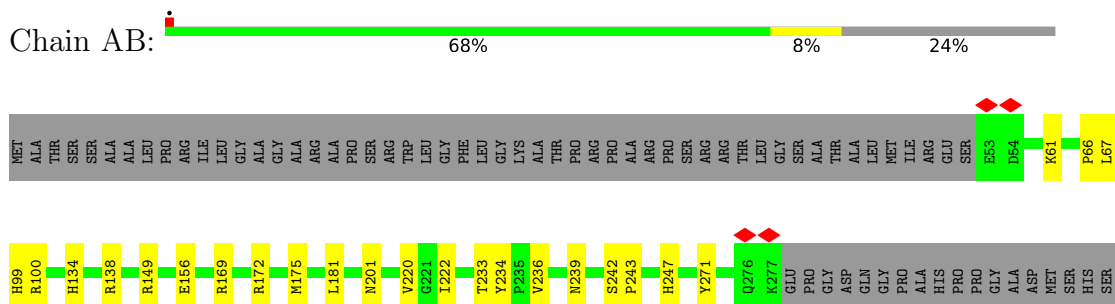
Chain AA:



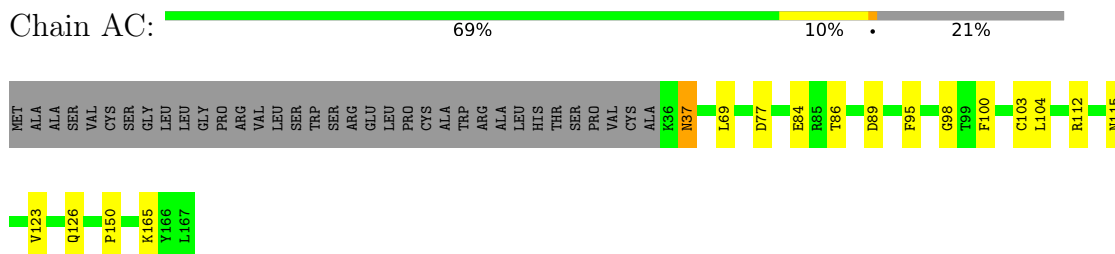




- Molecule 26: Small ribosomal subunit protein uS2m



- Molecule 27: Small ribosomal subunit protein uS3m



- Molecule 28: Small ribosomal subunit protein uS5m





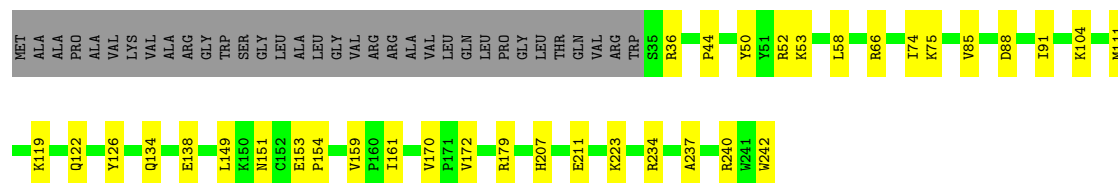
- Molecule 29: Small ribosomal subunit protein bS6m

Chain AE: 85% 13% .



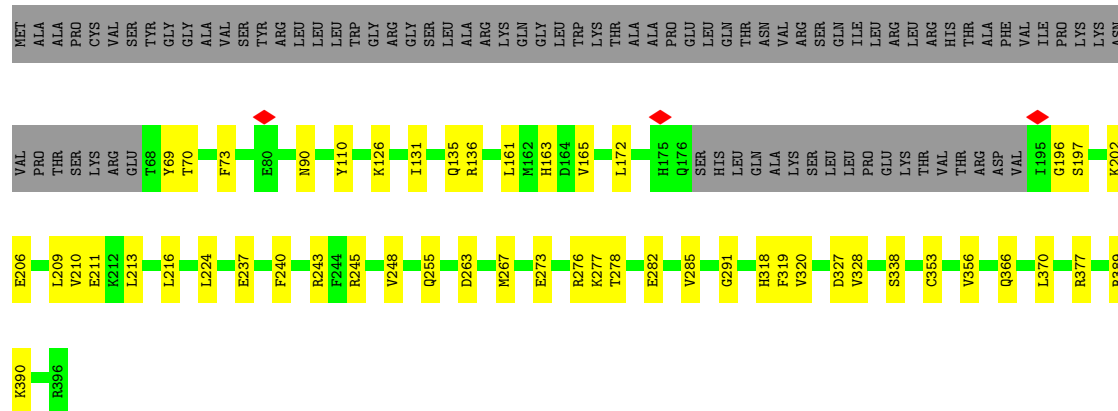
- Molecule 30: Small ribosomal subunit protein uS7m

Chain AF: 71% 14% 14%



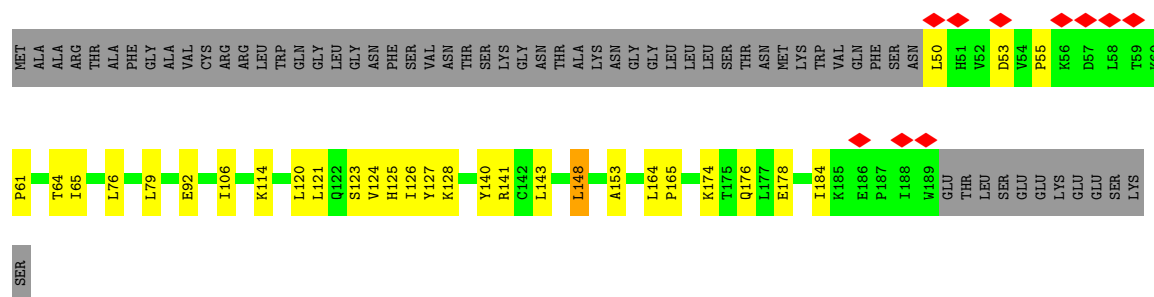
- Molecule 31: Small ribosomal subunit protein uS9m

Chain AG: 66% 13% 21%

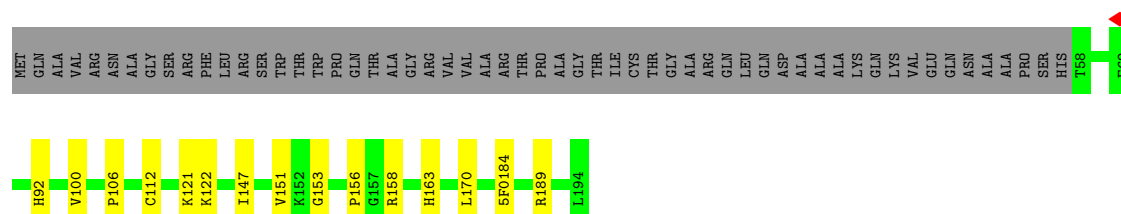


- Molecule 32: Small ribosomal subunit protein uS10m

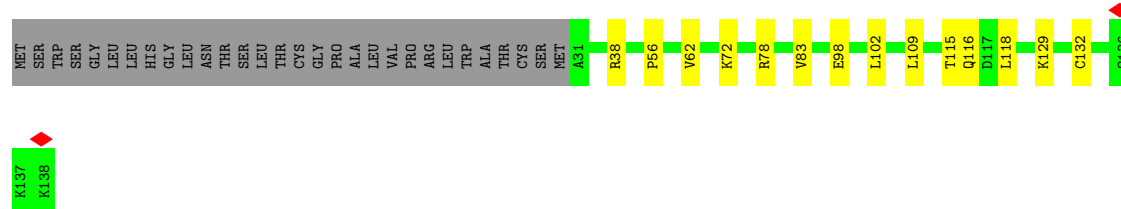
Chain AH: 5% 55% 14% 30%



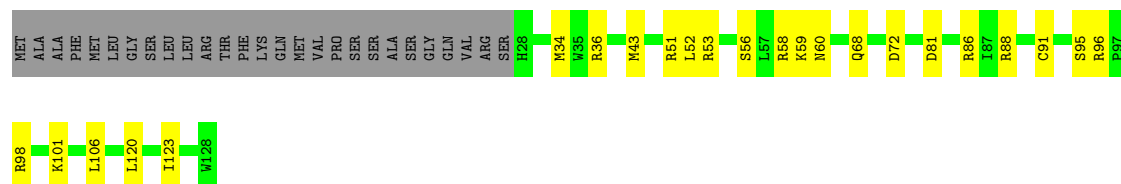
- Molecule 33: Small ribosomal subunit protein uS11m



- Molecule 34: Small ribosomal subunit protein uS12m

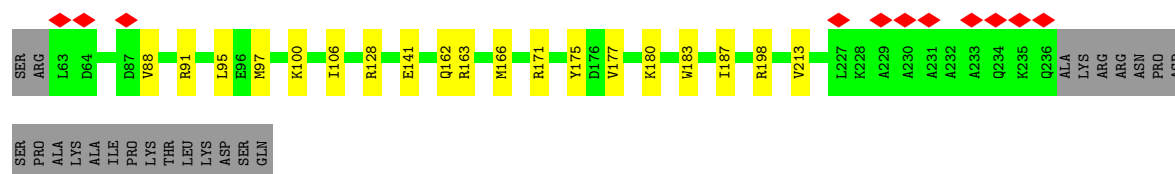


- Molecule 35: Small ribosomal subunit protein uS14m

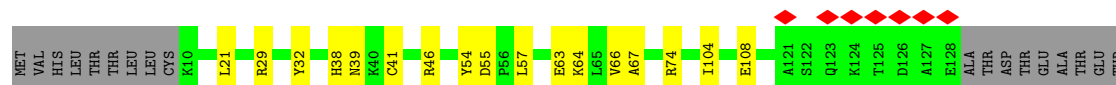
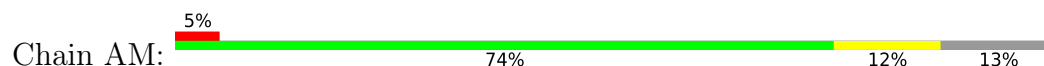


- Molecule 36: Small ribosomal subunit protein uS15m

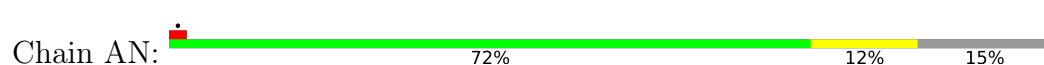




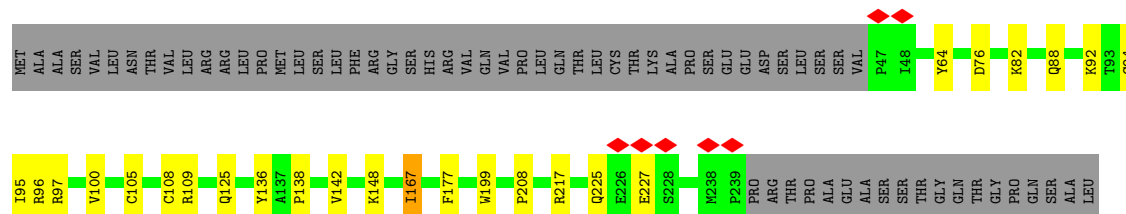
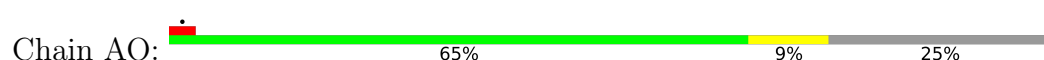
- Molecule 37: Small ribosomal subunit protein bS16m



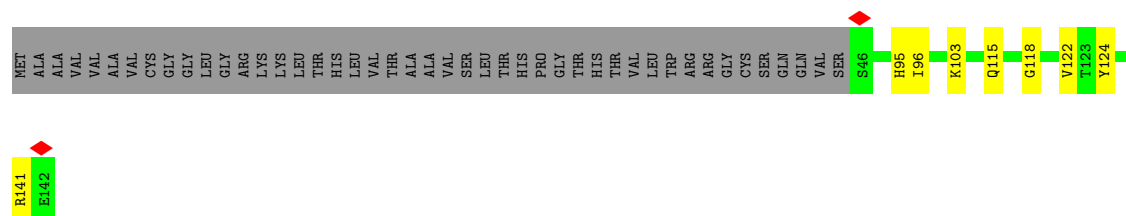
- Molecule 38: Small ribosomal subunit protein uS17m



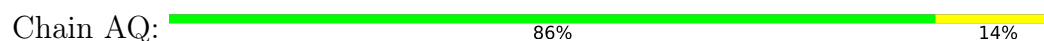
- Molecule 39: Small ribosomal subunit protein mS40



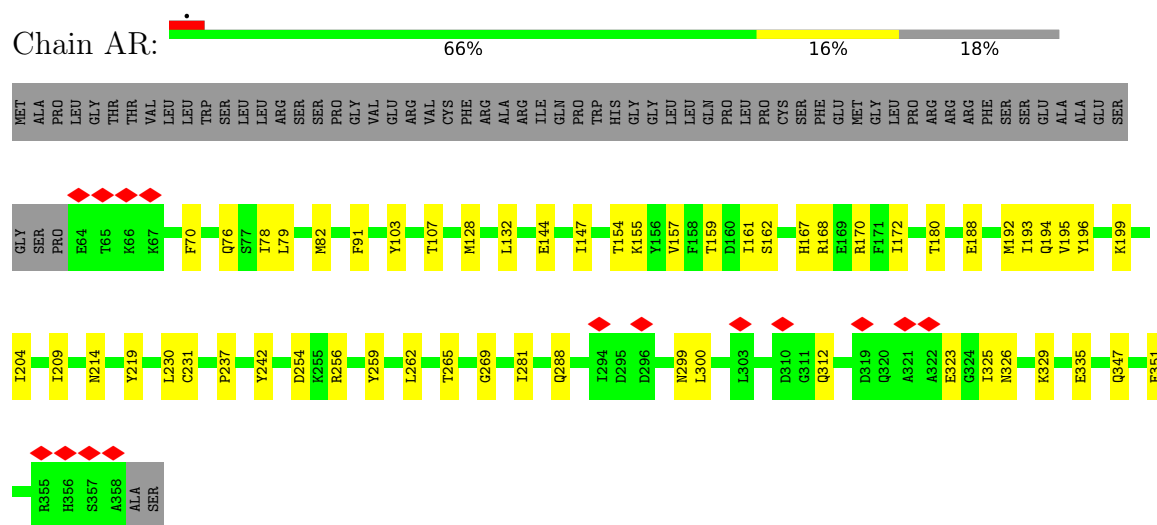
- Molecule 40: Small ribosomal subunit protein bS18m



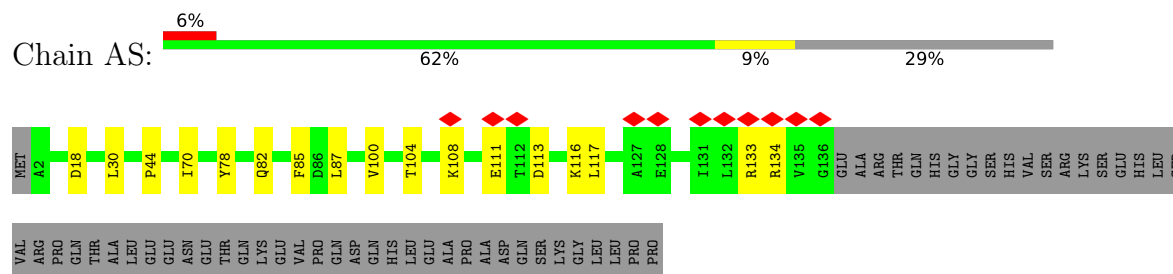
- Molecule 41: MRPS21 isoform 1



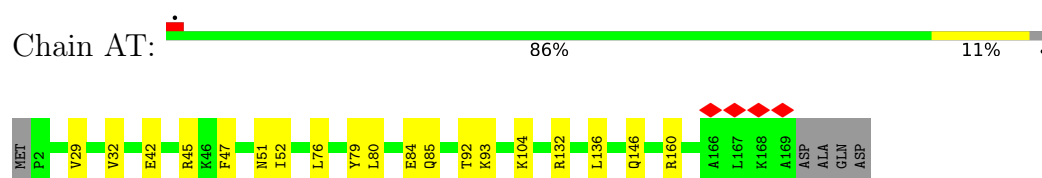
- Molecule 42: Small ribosomal subunit protein mS22



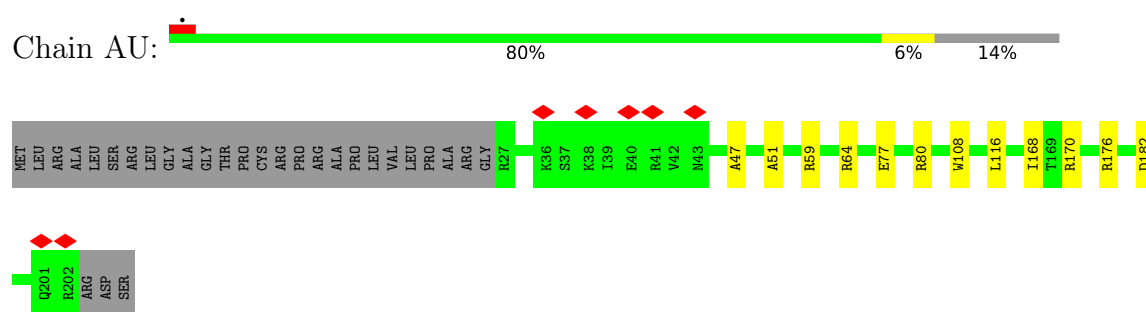
- Molecule 43: Small ribosomal subunit protein mS23



- Molecule 44: Small ribosomal subunit protein mS25

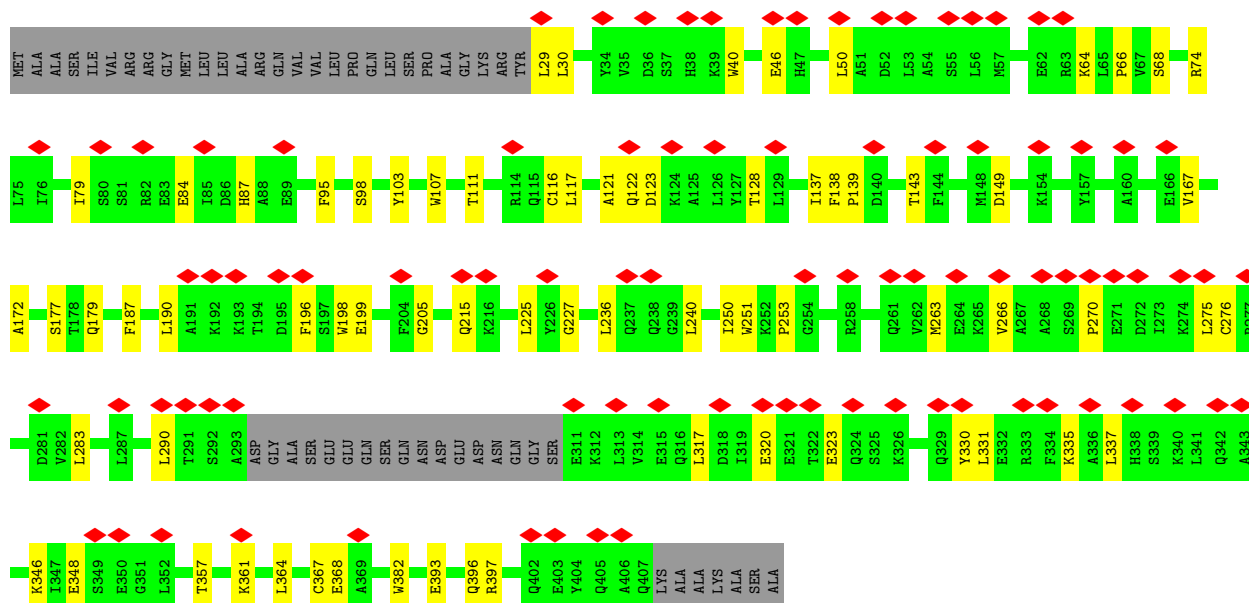


- Molecule 45: Small ribosomal subunit protein mS26



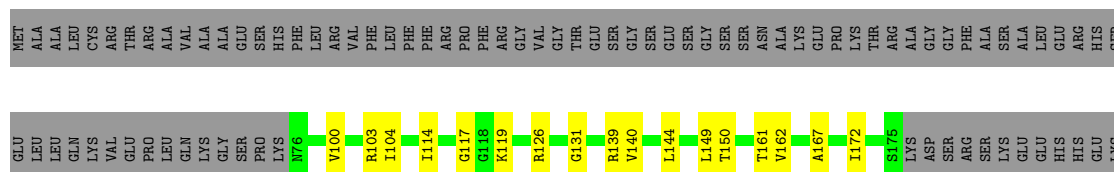
- Molecule 46: Small ribosomal subunit protein mS27





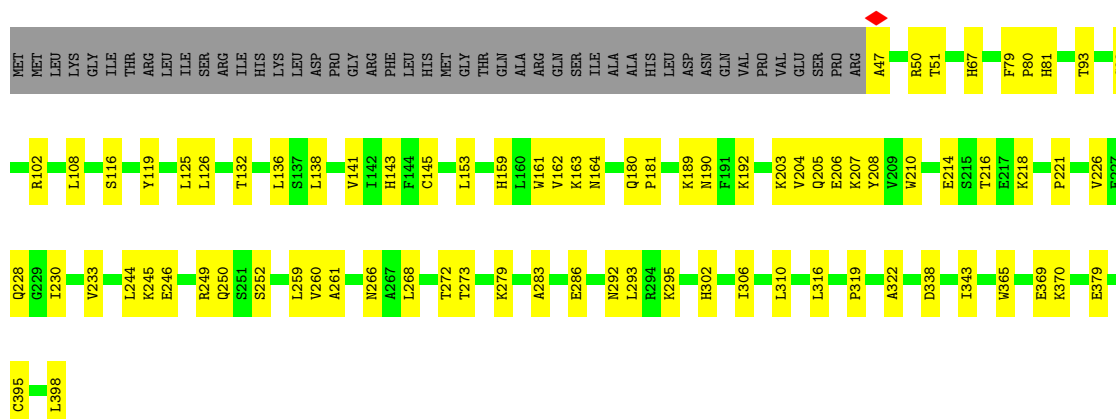
• Molecule 47: Small ribosomal subunit protein bS1m

Chain AW: 44% 9% 47%



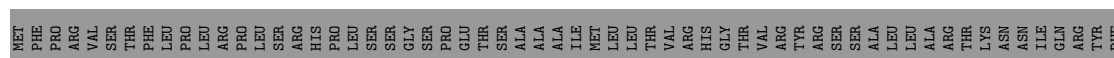
• Molecule 48: Small ribosomal subunit protein mS29

Chain AX: 68% 20% 12%

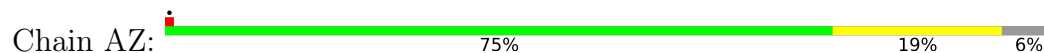


• Molecule 49: Small ribosomal subunit protein mS31

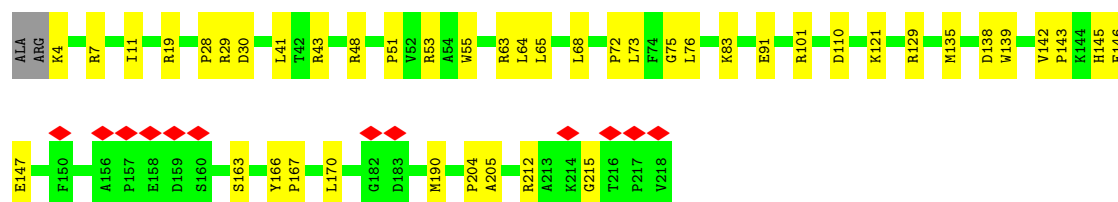
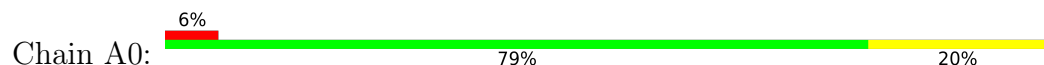
Chain AY: 29% 70%



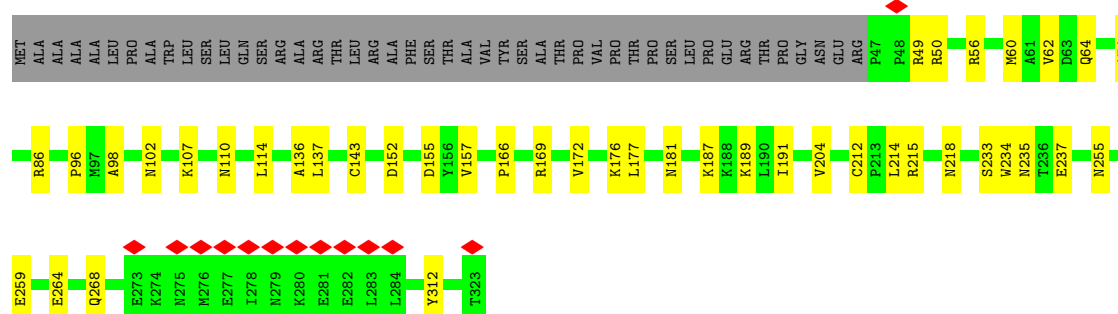
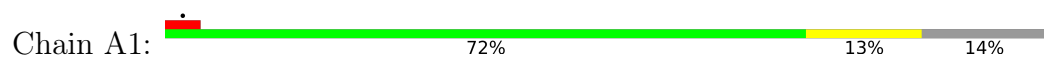
- Molecule 50: Small ribosomal subunit protein mS33



- Molecule 51: Small ribosomal subunit protein mS34



- Molecule 52: Small ribosomal subunit protein mS35



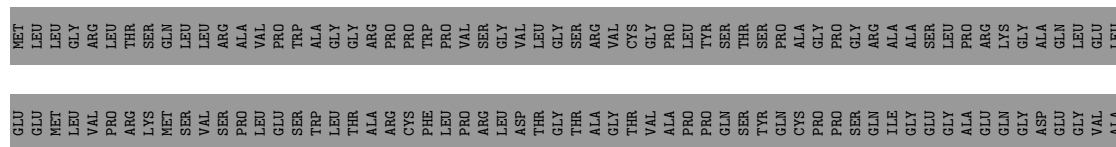
- Molecule 53: Small ribosomal subunit protein mS37





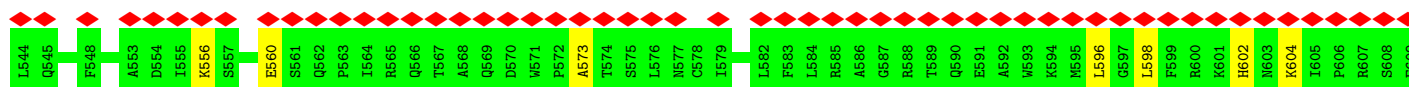
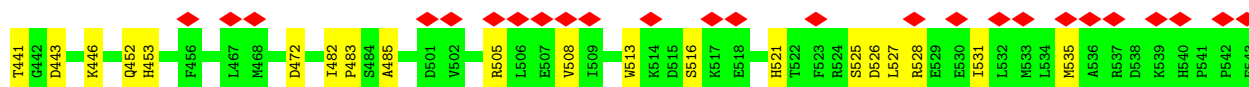
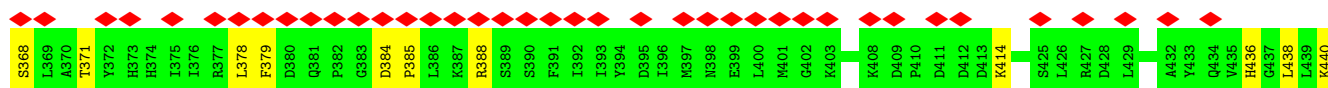
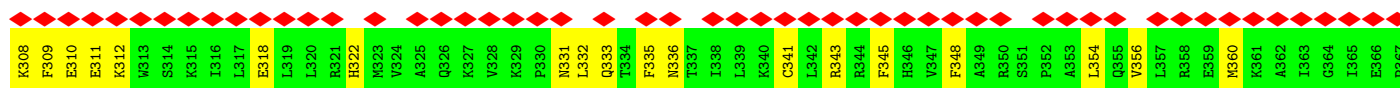
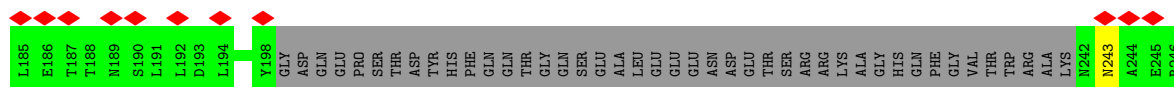
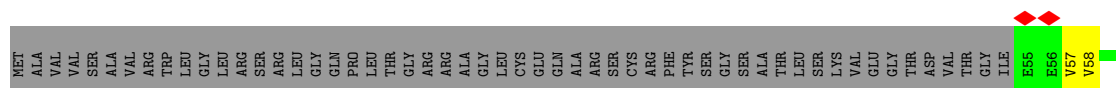
- Molecule 54: Small ribosomal subunit protein mS38

Chain A3: 31% 65%

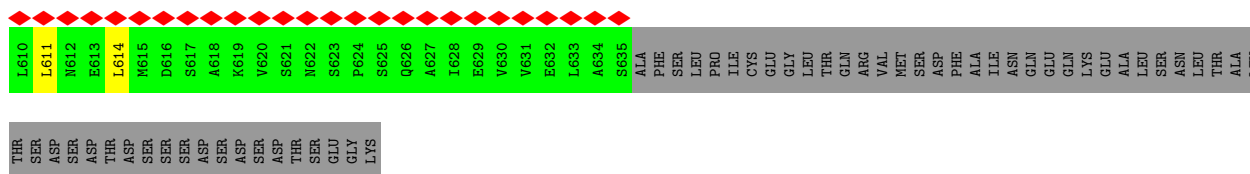


- Molecule 55: Small ribosomal subunit protein mS39

Chain A4: 43% 64% 13% 23%



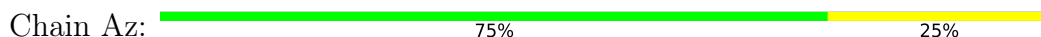




• Molecule 56: P/P-tRNA



• Molecule 57: mRNA



• Molecule 58: Large ribosomal subunit protein bL32m



• Molecule 59: Large ribosomal subunit protein bL33m

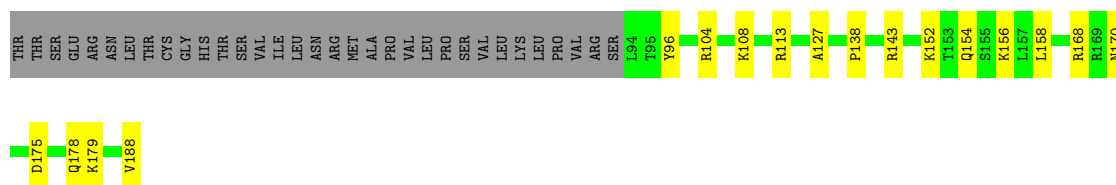


• Molecule 60: Large ribosomal subunit protein bL34m

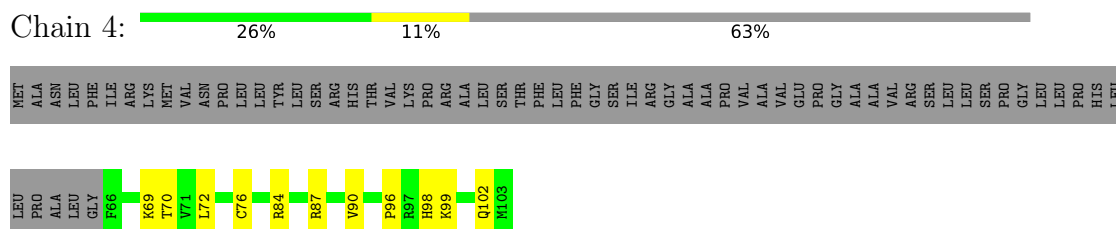


• Molecule 61: Large ribosomal subunit protein bL35m

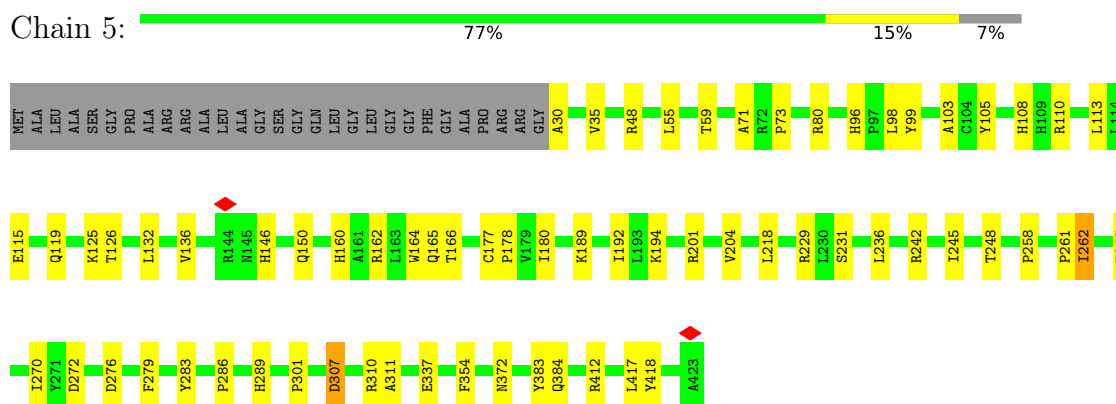




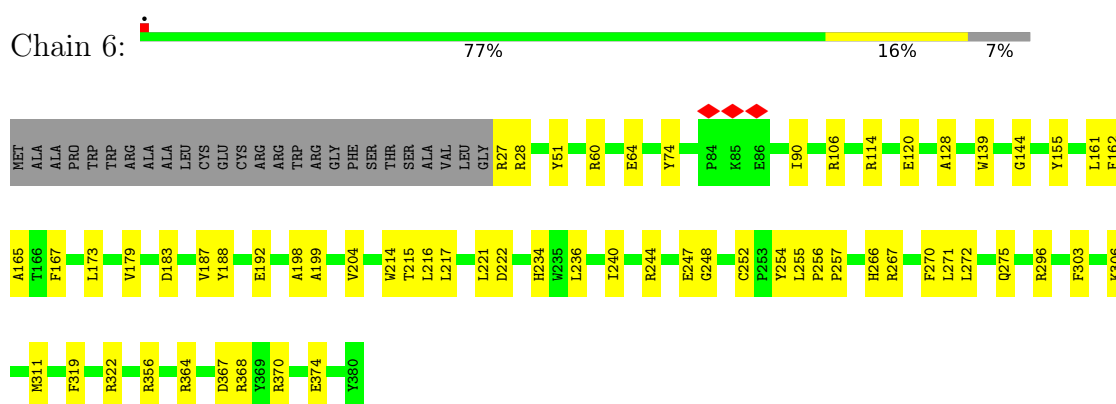
- Molecule 62: Large ribosomal subunit protein bL36m



- Molecule 63: Large ribosomal subunit protein mL37



- Molecule 64: Large ribosomal subunit protein mL38



- Molecule 65: Large ribosomal subunit protein mL39

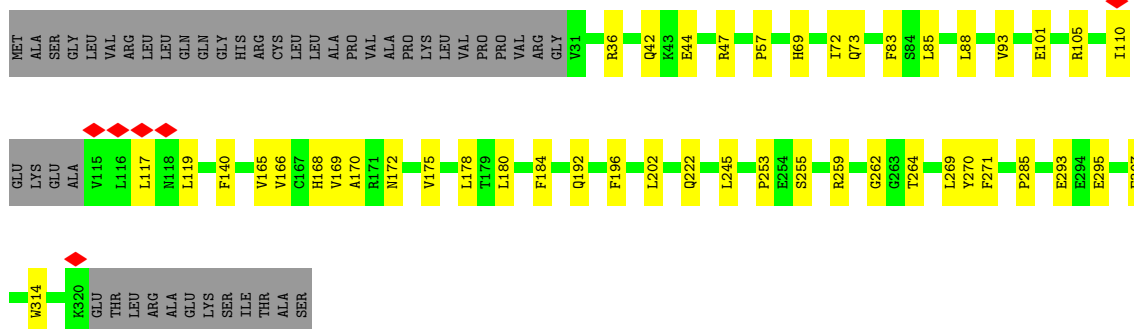




PRO ASP PRO PRO ASP PRO ASP PRO THR VAL ASP PRO PRO ILE SER SER SER THR THR ALA PRO ALA MET PRO MET LEU SER SER ALA VAL SER CYS LEU PRO PRO ILE VAL PRO PRO ALA ALA LEU THR THR VAL CYS SER ALA

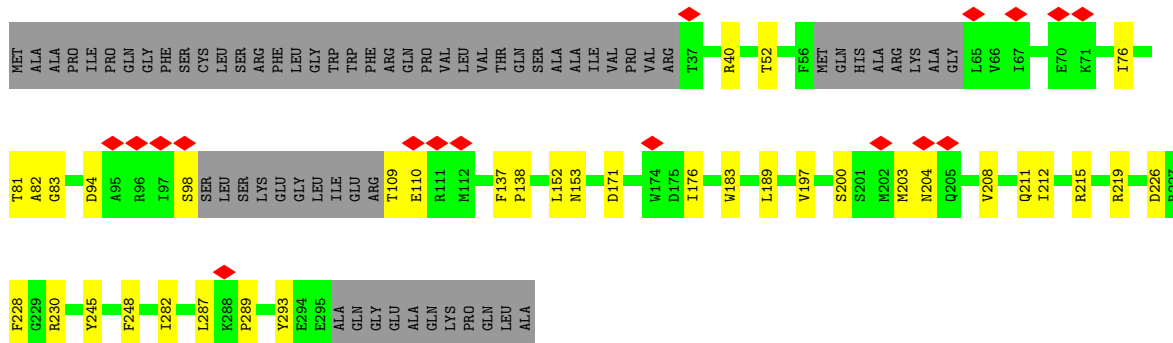
• Molecule 70: Large ribosomal subunit protein mL44

Chain c:



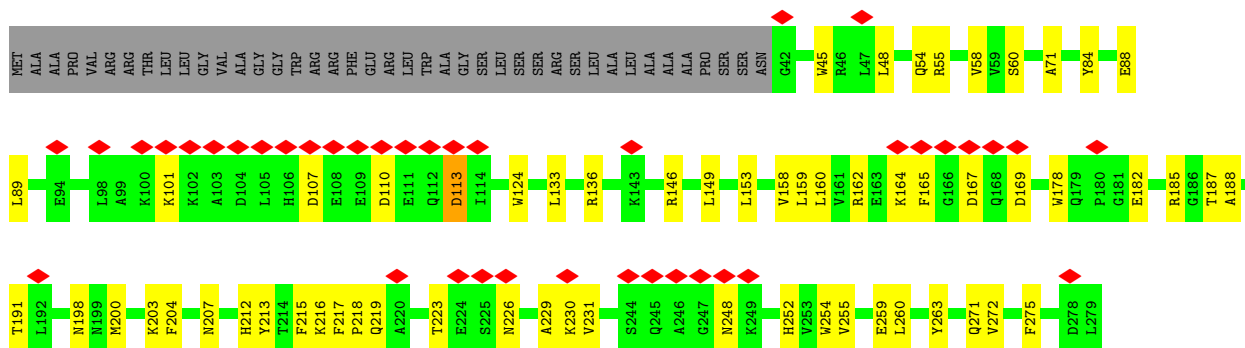
• Molecule 71: Large ribosomal subunit protein mL45

Chain d:



• Molecule 72: Large ribosomal subunit protein mL46

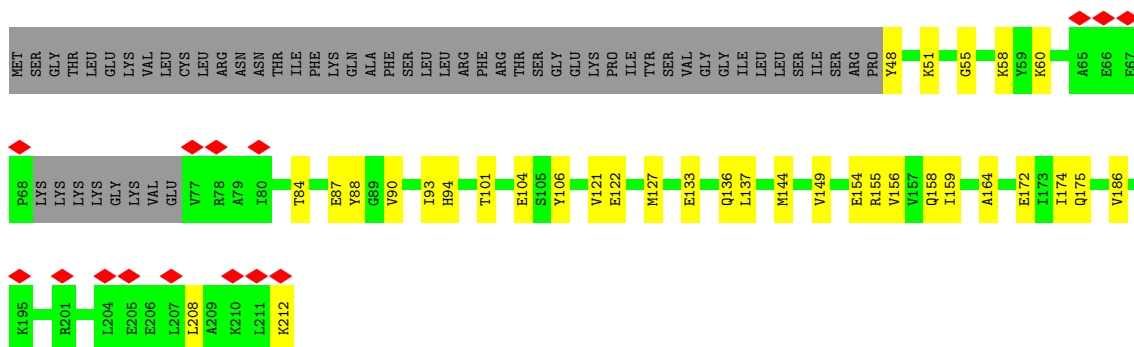
Chain e:



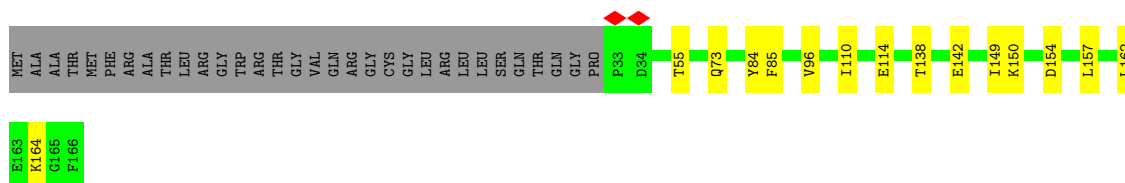
• Molecule 73: Large ribosomal subunit protein mL48

Chain f:

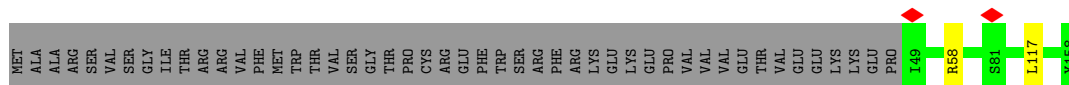




- Molecule 74: Large ribosomal subunit protein mL49



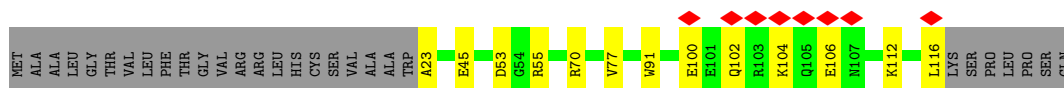
- Molecule 75: Large ribosomal subunit protein mL50



- Molecule 76: Large ribosomal subunit protein mL51

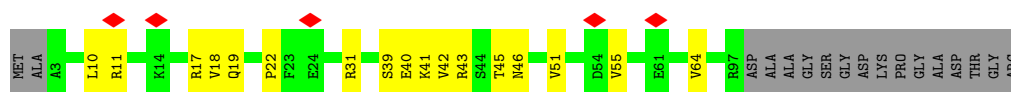


- Molecule 77: Large ribosomal subunit protein mL52



- Molecule 78: Large ribosomal subunit protein mL53

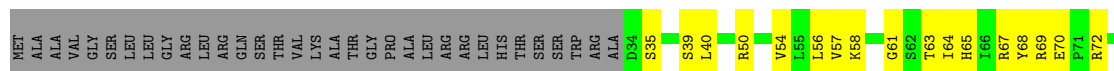




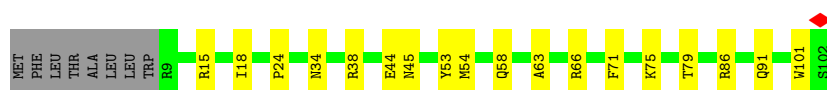
- Molecule 79: Large ribosomal subunit protein mL54



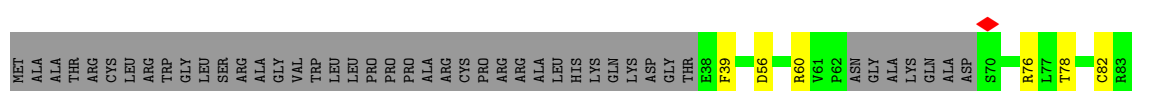
- Molecule 80: Large ribosomal subunit protein mL55



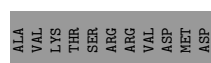
- Molecule 81: Large ribosomal subunit protein mL63

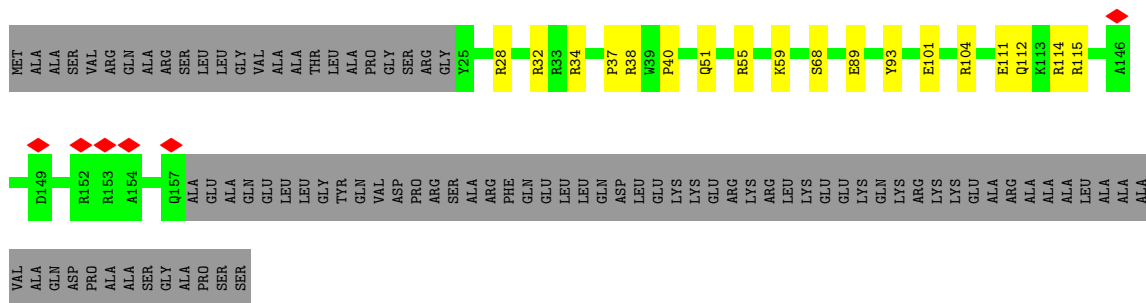


- Molecule 82: Large ribosomal subunit protein mL62

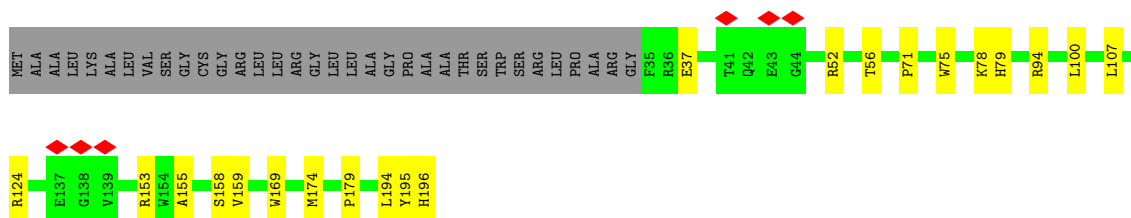


- Molecule 83: Large ribosomal subunit protein mL64

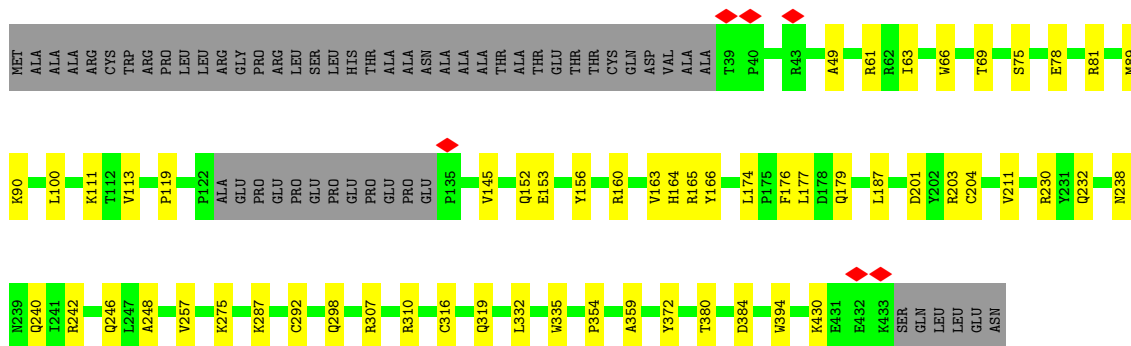




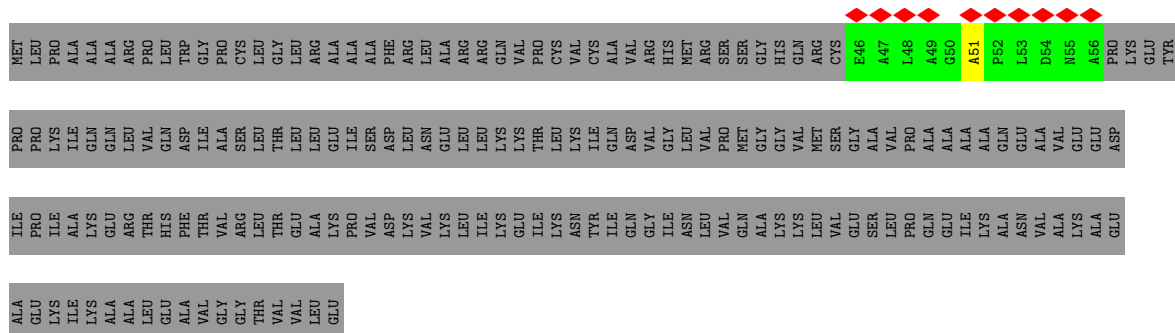
- Molecule 84: Large ribosomal subunit protein mL66



- Molecule 85: Large ribosomal subunit protein mL65



- Molecule 86: Large ribosomal subunit protein bL12m



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	114776	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 ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.321	Depositor
Minimum map value	-0.071	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	424.96, 424.96, 424.96	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PSU, NAD, ZN, ACE, SPD, 5MC, ATP, 1MA, MG, OMG, FES, GDP, 5F0, G34, B8T, K, 5MU, 2MG, RSQ, MA6, OMU

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	A	0.09	0/36048	0.21	0/56112
2	B	0.08	0/1627	0.20	0/2527
3	D	0.09	0/1896	0.24	0/2549
4	E	0.08	0/2475	0.22	0/3355
5	F	0.08	0/2090	0.23	0/2842
6	H	0.07	0/837	0.19	0/1124
7	I	0.08	0/1392	0.23	0/1880
8	J	0.08	0/1348	0.19	0/1813
9	K	0.09	0/1497	0.23	0/2031
10	L	0.08	0/905	0.23	0/1218
11	M	0.09	0/2368	0.24	0/3195
12	N	0.09	0/1833	0.24	0/2468
13	O	0.09	0/1283	0.22	0/1727
14	P	0.09	0/1199	0.24	0/1623
15	Q	0.09	0/2039	0.23	0/2750
16	R	0.09	0/1175	0.19	0/1572
17	S	0.09	0/1320	0.25	0/1789
18	T	0.09	0/1403	0.23	0/1886
19	U	0.11	0/1280	0.25	0/1732
20	V	0.07	0/1721	0.22	0/2333
21	W	0.08	0/926	0.21	0/1244
22	X	0.08	0/2099	0.19	0/2837
23	Y	0.08	0/1593	0.18	0/2136
24	Z	0.08	0/1021	0.25	0/1378
25	AA	0.08	0/22537	0.20	0/35085
26	AB	0.07	0/1871	0.22	0/2531
27	AC	0.07	0/1113	0.20	0/1505
28	AD	0.07	0/2783	0.19	0/3724
29	AE	0.07	0/989	0.19	0/1335
30	AF	0.07	0/1767	0.19	0/2373
31	AG	0.06	0/2616	0.18	0/3505

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	AH	0.08	0/1178	0.23	0/1598
33	AI	0.08	0/1030	0.23	0/1386
34	AJ	0.07	0/855	0.21	0/1148
35	AK	0.06	0/880	0.18	0/1182
36	AL	0.06	0/1477	0.17	0/1974
37	AM	0.06	0/963	0.19	0/1295
38	AN	0.07	0/886	0.20	0/1199
39	AO	0.06	0/1648	0.19	0/2243
40	AP	0.07	0/798	0.18	0/1070
41	AQ	0.12	0/754	0.20	0/1003
42	AR	0.06	0/2456	0.18	0/3317
43	AS	0.06	0/1138	0.18	0/1533
44	AT	0.07	0/1402	0.20	0/1883
45	AU	0.05	0/1510	0.16	0/2025
46	AV	0.06	0/3030	0.17	0/4093
47	AW	0.08	0/801	0.20	0/1079
48	AX	0.06	0/2921	0.19	0/3954
49	AY	0.07	0/1046	0.18	0/1410
50	AZ	0.05	0/857	0.16	0/1141
51	A0	0.07	0/1834	0.20	0/2484
52	A1	0.06	0/2293	0.19	0/3102
53	A2	0.12	0/947	0.22	0/1266
54	A3	0.07	0/636	0.19	0/839
55	A4	0.07	0/4427	0.19	0/5987
56	Ax	0.08	0/1511	0.21	0/2341
57	Az	0.06	0/185	0.16	0/285
58	0	0.08	0/913	0.18	0/1224
59	1	0.07	0/445	0.20	0/591
60	2	0.07	0/383	0.18	0/507
61	3	0.08	0/853	0.21	0/1136
62	4	0.07	0/350	0.18	0/461
63	5	0.09	0/3305	0.23	0/4502
64	6	0.07	0/3043	0.21	0/4140
65	7	0.08	0/2447	0.22	0/3310
66	8	0.08	0/1209	0.20	0/1628
67	9	0.07	0/1025	0.20	0/1379
68	a	0.08	0/866	0.22	0/1174
69	b	0.07	0/1219	0.23	0/1651
70	c	0.08	0/2347	0.20	0/3171
71	d	0.07	0/2039	0.21	0/2759
72	e	0.07	0/1970	0.22	0/2658
73	f	0.07	0/1273	0.21	0/1716
74	g	0.08	0/1151	0.21	0/1569

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
75	h	0.07	0/918	0.18	0/1249
76	i	0.08	0/850	0.20	0/1135
77	j	0.08	0/760	0.18	0/1023
78	k	0.07	0/749	0.18	0/1010
79	l	0.06	0/707	0.19	0/960
80	m	0.06	0/805	0.19	0/1081
81	o	0.08	0/819	0.22	0/1097
82	p	0.07	0/1197	0.18	0/1606
83	q	0.09	0/1151	0.19	0/1556
84	r	0.07	0/1362	0.20	0/1846
85	s	0.09	0/3217	0.22	0/4369
86	t	0.04	0/72	0.17	0/98
All	All	0.08	0/179959	0.21	0/255622

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
14	P	0	1
66	8	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
66	8	169	PHE	Peptide
14	P	72	PHE	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	A	32331	0	16416	412	0
2	B	1524	0	779	21	0
3	D	1859	0	1920	30	0
4	E	2406	0	2415	27	0
5	F	2031	0	2065	24	0
6	H	823	0	873	12	0
7	I	1362	0	1442	29	0
8	J	1330	0	1407	23	0
9	K	1455	0	1452	16	0
10	L	890	0	941	18	0
11	M	2314	0	2384	18	0
12	N	1786	0	1817	19	0
13	O	1259	0	1294	20	0
14	P	1173	0	1165	16	0
15	Q	1990	0	2031	28	0
16	R	1154	0	1214	11	0
17	S	1293	0	1365	16	0
18	T	1369	0	1410	17	0
19	U	1251	0	1232	20	0
20	V	1676	0	1687	35	0
21	W	904	0	935	9	0
22	X	2044	0	2060	21	0
23	Y	1556	0	1597	27	0
24	Z	996	0	1044	15	0
25	AA	20260	0	10285	269	0
26	AB	1828	0	1815	18	0
27	AC	1083	0	1088	14	0
28	AD	2731	0	2804	35	0
29	AE	972	0	1000	13	0
30	AF	1725	0	1769	24	0
31	AG	2561	0	2545	34	0
32	AH	1152	0	1183	24	0
33	AI	1020	0	1053	9	0
34	AJ	839	0	887	11	0
35	AK	862	0	885	18	0
36	AL	1453	0	1540	12	0
37	AM	942	0	965	14	0
38	AN	868	0	928	11	0
39	AO	1592	0	1557	19	0
40	AP	781	0	806	7	0
41	AQ	744	0	758	11	0
42	AR	2409	0	2428	36	0
43	AS	1111	0	1115	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	AT	1371	0	1393	12	0
45	AU	1488	0	1499	11	0
46	AV	2969	0	2961	45	0
47	AW	789	0	802	11	0
48	AX	2849	0	2844	54	0
49	AY	1016	0	962	6	0
50	AZ	839	0	858	16	0
51	A0	1787	0	1796	32	0
52	A1	2245	0	2276	27	0
53	A2	935	0	971	10	0
54	A3	625	0	699	5	0
55	A4	4329	0	4350	59	0
56	Ax	1378	0	703	26	0
57	Az	167	0	83	1	0
58	0	898	0	916	14	0
59	1	440	0	480	5	0
60	2	377	0	406	4	0
61	3	832	0	883	13	0
62	4	342	0	361	7	0
63	5	3210	0	3206	45	0
64	6	2948	0	2841	42	0
65	7	2390	0	2397	40	0
66	8	1184	0	1210	18	0
67	9	997	0	987	17	0
68	a	840	0	810	8	0
69	b	1196	0	1195	16	0
70	c	2299	0	2320	31	0
71	d	1985	0	1976	25	0
72	e	1931	0	1916	42	0
73	f	1252	0	1269	22	0
74	g	1113	0	1097	10	0
75	h	895	0	881	2	0
76	i	828	0	857	14	0
77	j	745	0	746	10	0
78	k	738	0	753	12	0
79	l	688	0	674	14	0
80	m	791	0	796	25	0
81	o	798	0	804	17	0
82	p	1179	0	1203	21	0
83	q	1120	0	1099	12	0
84	r	1322	0	1348	18	0
85	s	3134	0	3121	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	t	72	0	67	1	0
87	A	138	0	0	0	0
87	A3	1	0	0	0	0
87	AA	63	0	0	0	0
87	AB	1	0	0	0	0
87	AX	1	0	0	0	0
87	D	2	0	0	0	0
87	E	1	0	0	0	0
87	g	1	0	0	0	0
88	6	1	0	0	0	0
88	A	29	0	0	0	0
88	AA	18	0	0	0	0
88	D	1	0	0	0	0
88	M	1	0	0	0	0
88	W	1	0	0	0	0
88	i	1	0	0	0	0
88	o	1	0	0	0	0
89	A	36	0	47	3	0
90	B	7	0	8	2	0
91	AA	44	0	26	1	0
92	AA	10	0	19	0	0
93	0	1	0	0	0	0
93	4	1	0	0	0	0
93	AO	1	0	0	0	0
94	AP	4	0	0	0	0
94	AT	4	0	0	0	0
94	r	4	0	0	0	0
95	AX	31	0	12	1	0
96	AX	28	0	12	1	0
All	All	171472	0	145296	1877	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 6.

All (1877) 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)
1:A:2485:U:H3	1:A:2650:C:N4	1.52	1.06
1:A:2234:C:HO2'	1:A:2688:C:HO2'	1.30	0.80
64:6:179:VAL:O	64:6:183:ASP:HB2	1.82	0.78
9:K:74:GLN:HE21	84:r:159:VAL:HG21	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:p:84:SER:HB3	82:p:98:LYS:HB2	1.65	0.76
25:AA:1021:U:OP2	53:A2:9:ARG:NH2	2.19	0.74
25:AA:1053:A:N1	25:AA:1100:C:O2'	2.22	0.72
65:7:163:MET:H	65:7:186:ASP:HB2	1.54	0.72
2:B:44:A:H62	14:P:120:ARG:HH12	1.38	0.72
25:AA:1562:G:H1'	25:AA:1583:MA6:H2	1.70	0.72
8:J:20:ILE:HD11	8:J:42:ARG:HD3	1.72	0.72
1:A:1777:A:N6	1:A:1780:U:OP2	2.23	0.72
7:I:47:LEU:HD22	12:N:226:ILE:HG12	1.71	0.72
25:AA:1422:G:H21	56:Ax:41:C:H1'	1.54	0.71
1:A:1884:G:H1'	1:A:1895:C:H1'	1.70	0.71
1:A:2139:U:H5''	24:Z:74:SER:HB2	1.72	0.71
12:N:124:VAL:HG12	12:N:158:ARG:HE	1.53	0.71
30:AF:52:ARG:HH22	31:AG:320:VAL:HA	1.54	0.71
70:c:259:ARG:HB2	70:c:271:PHE:HB2	1.72	0.71
56:Ax:5:A:H2	56:Ax:68:G:H22	1.36	0.71
65:7:247:ASN:HD22	65:7:251:ILE:H	1.39	0.70
1:A:2499:U:OP2	1:A:2504:A:N6	2.21	0.70
1:A:2137:C:H5''	7:I:43:GLN:HE21	1.58	0.69
9:K:178:LEU:HD11	84:r:94:ARG:HA	1.75	0.69
22:X:7:PRO:HD2	22:X:10:LEU:HD12	1.73	0.69
1:A:2259:C:O2'	1:A:2261:C:OP2	2.09	0.69
48:AX:319:PRO:HG2	48:AX:322:ALA:HB2	1.75	0.68
11:M:44:ARG:HG3	11:M:45:ARG:HG3	1.73	0.68
25:AA:1557:A:H5''	34:AJ:72:LYS:HG3	1.75	0.68
1:A:1763:A:N7	83:q:38:ARG:NH1	2.42	0.68
65:7:112:PRO:HB2	65:7:267:PRO:HG2	1.74	0.68
10:L:68:LYS:NZ	10:L:91:MET:SD	2.67	0.68
63:5:204:VAL:HG11	63:5:279:PHE:HZ	1.58	0.68
1:A:1805:A:OP2	20:V:94:HIS:NE2	2.25	0.67
51:A0:28:PRO:HG3	51:A0:215:GLY:HA2	1.76	0.67
85:s:177:LEU:HD23	85:s:238:ASN:HD22	1.58	0.67
48:AX:80:PRO:HG2	48:AX:81:HIS:HD2	1.59	0.67
1:A:2603:C:H4'	1:A:3090:G:H1'	1.76	0.67
36:AL:180:LYS:HD2	36:AL:183:TRP:HE1	1.60	0.67
64:6:367:ASP:OD1	64:6:370:ARG:NH1	2.28	0.67
31:AG:90:ASN:HD21	52:A1:64:GLN:H	1.43	0.67
1:A:2545:U:H5''	1:A:2546:G:H5'	1.75	0.67
25:AA:773:U:H2'	25:AA:774:G:H8	1.60	0.67
25:AA:1355:G:N2	25:AA:1356:A:N7	2.41	0.67
2:B:26:A:N6	14:P:87:GLN:OE1	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:31:ASP:O	20:V:34:LYS:O	2.12	0.66
25:AA:929:A:H4'	28:AD:420:SER:HA	1.76	0.66
1:A:1763:A:H5''	83:q:34:ARG:HH21	1.59	0.66
25:AA:1294:A:OP1	26:AB:201:ASN:ND2	2.28	0.66
6:H:99:THR:O	6:H:108:ARG:NH1	2.29	0.66
1:A:2108:G:N7	12:N:67:LYS:NZ	2.43	0.66
17:S:175:ARG:HB2	17:S:180:PHE:HB3	1.78	0.66
68:a:41:ASP:HB3	68:a:46:ASN:HD22	1.59	0.66
24:Z:78:ARG:O	24:Z:83:LYS:NZ	2.29	0.66
72:e:110:ASP:HB3	72:e:113:ASP:HB2	1.78	0.66
82:p:111:ILE:O	82:p:116:ARG:NH1	2.28	0.66
1:A:2192:A:OP2	79:l:119:ARG:NH1	2.28	0.65
25:AA:821:U:H2'	25:AA:822:G:H8	1.61	0.65
20:V:31:ASP:OD1	20:V:35:ASN:ND2	2.29	0.65
1:A:1689:C:O2	23:Y:213:ARG:NH2	2.29	0.65
17:S:164:THR:HG23	69:b:107:GLN:HG2	1.79	0.65
9:K:178:LEU:HD13	84:r:100:LEU:HD21	1.78	0.65
22:X:163:ARG:HE	63:5:55:LEU:HD11	1.62	0.65
28:AD:103:LEU:HD11	28:AD:123:ARG:HB2	1.77	0.65
3:D:176:ALA:HB1	3:D:244:VAL:HG11	1.78	0.65
74:g:84:TYR:OH	74:g:164:LYS:NZ	2.30	0.65
1:A:2067:C:H4'	73:f:60:LYS:HD2	1.79	0.65
56:Ax:9:C:O2'	56:Ax:10:A:N7	2.27	0.65
1:A:2677:A:H2'	1:A:2678:A:C8	2.32	0.65
26:AB:239:ASN:OD1	47:AW:119:LYS:NZ	2.30	0.64
64:6:252:CYS:SG	64:6:296:ARG:NH1	2.70	0.64
72:e:101:LYS:HZ1	72:e:107:ASP:HB3	1.62	0.64
19:U:129:MET:HG3	71:d:82:ALA:HB2	1.79	0.64
50:AZ:66:ARG:NH2	50:AZ:77:ASP:OD1	2.29	0.64
1:A:2082:G:N2	24:Z:88:MET:SD	2.71	0.64
1:A:1800:G:N1	1:A:1803:A:OP2	2.30	0.64
4:E:69:ASP:OD1	4:E:154:ARG:NH1	2.31	0.64
46:AV:177:SER:HB2	46:AV:367:CYS:HB3	1.80	0.64
72:e:178:TRP:NE1	72:e:182:GLU:O	2.30	0.64
16:R:122:ARG:NH1	17:S:72:GLU:OE2	2.30	0.64
29:AE:26:ILE:HG23	29:AE:36:VAL:HG21	1.78	0.64
30:AF:44:PRO:HD3	30:AF:75:LYS:HB2	1.80	0.64
25:AA:942:A:N6	25:AA:1047:A:OP2	2.30	0.64
30:AF:172:VAL:HG12	30:AF:240:ARG:HD3	1.80	0.64
85:s:174:LEU:HD11	85:s:203:ARG:HD3	1.79	0.64
19:U:11:ARG:NH2	20:V:212:LYS:O	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:93:THR:HG22	20:V:112:GLU:HG3	1.79	0.63
20:V:133:ILE:HD13	20:V:145:ARG:HD2	1.81	0.63
71:d:98:SER:OG	71:d:215:ARG:NH2	2.32	0.63
1:A:2972:A:H5''	12:N:184:PRO:HA	1.80	0.63
65:7:159:LYS:NZ	68:a:92:LEU:O	2.31	0.63
1:A:2409:A:O2'	63:5:270:ILE:O	2.17	0.63
18:T:69:HIS:HD2	18:T:114:VAL:HG13	1.64	0.63
63:5:150:GLN:HE22	63:5:412:ARG:HG3	1.64	0.63
20:V:31:ASP:O	20:V:34:LYS:C	2.42	0.63
55:A4:263:ILE:HG23	55:A4:275:ALA:HB1	1.81	0.63
29:AE:35:ILE:HD13	36:AL:88:VAL:HG13	1.81	0.62
65:7:148:MET:HE2	65:7:257:ILE:HG12	1.79	0.62
15:Q:96:ARG:HH22	15:Q:285:GLU:HB3	1.64	0.62
25:AA:1046:A:O4'	91:AA:1701:NAD:N6A	2.32	0.62
31:AG:209:LEU:HD12	31:AG:213:LEU:HD11	1.82	0.62
7:I:167:ILE:O	7:I:170:THR:OG1	2.17	0.62
25:AA:1402:A:OP1	35:AK:51:ARG:NH2	2.30	0.62
55:A4:573:ALA:HB2	55:A4:604:LYS:HD2	1.82	0.62
85:s:63:ILE:HA	85:s:66:TRP:CD1	2.34	0.62
1:A:1886:G:H1	76:i:61:GLY:HA3	1.64	0.62
85:s:152:GLN:HA	85:s:156:TYR:HB2	1.81	0.62
1:A:3211:C:H4'	1:A:3212:C:H5	1.64	0.62
25:AA:1529:A:H1'	46:AV:66:PRO:HD3	1.80	0.62
1:A:1672:C:O2'	18:T:143:ARG:O	2.16	0.62
1:A:1745:U:O4	61:3:108:LYS:NZ	2.33	0.62
42:AR:162:SER:O	42:AR:170:ARG:NH1	2.31	0.62
48:AX:181:PRO:HB2	48:AX:233:VAL:HG12	1.81	0.62
5:F:55:VAL:HG21	5:F:61:PRO:HG3	1.82	0.62
25:AA:702:C:O2'	25:AA:842:C:O2	2.17	0.62
30:AF:50:TYR:O	30:AF:66:ARG:NH2	2.27	0.62
72:e:188:ALA:O	72:e:191:THR:OG1	2.15	0.62
25:AA:1199:G:N1	25:AA:1422:G:OP2	2.32	0.62
1:A:2103:A:HO2'	24:Z:35:LYS:N	1.98	0.62
7:I:128:ASN:ND2	7:I:147:PHE:O	2.33	0.62
30:AF:126:TYR:O	30:AF:134:GLN:NE2	2.33	0.62
84:r:71:PRO:HD2	84:r:107:LEU:HD23	1.81	0.62
1:A:1884:G:N3	1:A:1895:C:O2'	2.32	0.61
25:AA:704:U:H5''	51:A0:53:ARG:HB2	1.81	0.61
28:AD:307:LYS:NZ	42:AR:103:TYR:OH	2.32	0.61
1:A:2458:A:O2'	4:E:215:PHE:O	2.18	0.61
25:AA:949:U:O2'	38:AN:29:ARG:NH1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:124:VAL:HA	12:N:158:ARG:HH21	1.65	0.61
37:AM:64:LYS:HE3	42:AR:154:THR:HB	1.82	0.61
3:D:195:ASN:H	3:D:207:ILE:HB	1.66	0.61
33:AI:153:GLY:O	33:AI:158:ARG:NH1	2.33	0.61
4:E:78:CYS:HB3	4:E:81:LYS:HB2	1.83	0.61
41:AQ:49:CYS:SG	41:AQ:50:ARG:NH1	2.74	0.61
72:e:255:VAL:HB	72:e:259:GLU:HG3	1.83	0.61
17:S:127:ARG:NH2	17:S:157:GLU:OE1	2.34	0.61
1:A:2537:G:O2'	1:A:2634:U:OP2	2.18	0.61
25:AA:1470:A:H2'	25:AA:1471:A:H8	1.66	0.61
31:AG:389:ARG:NH1	31:AG:390:LYS:O	2.34	0.61
48:AX:125:LEU:HD11	48:AX:310:LEU:HG	1.82	0.61
52:A1:214:LEU:O	52:A1:218:ASN:ND2	2.34	0.61
1:A:3150:U:H2'	1:A:3151:A:H8	1.65	0.61
5:F:272:LYS:NZ	76:i:65:ASN:OD1	2.33	0.60
8:J:114:LEU:HD21	79:l:101:LEU:HD21	1.83	0.60
1:A:2055:U:H2'	1:A:2056:G:H8	1.65	0.60
48:AX:161:TRP:O	48:AX:180:GLN:NE2	2.34	0.60
48:AX:206:GLU:HG3	48:AX:249:ARG:HH12	1.66	0.60
78:k:10:LEU:O	78:k:46:ASN:ND2	2.34	0.60
25:AA:1239:C:H2'	25:AA:1240:A:H8	1.66	0.60
11:M:30:ASN:OD1	81:o:86:ARG:NH2	2.34	0.60
24:Z:99:VAL:HG11	77:j:77:VAL:HG22	1.82	0.60
25:AA:893:G:H4'	34:AJ:98:GLU:HG2	1.84	0.60
25:AA:952:A:N3	25:AA:954:C:N4	2.49	0.60
71:d:211:GLN:HA	71:d:248:PHE:O	2.01	0.60
1:A:3068:G:OP2	1:A:3068:G:N2	2.30	0.60
5:F:224:GLU:OE2	83:q:32:ARG:NH2	2.35	0.60
21:W:125:VAL:HG21	64:6:64:GLU:HG2	1.83	0.60
25:AA:1412:G:OP1	48:AX:279:LYS:NZ	2.34	0.60
9:K:143:GLU:OE1	69:b:136:LYS:NZ	2.34	0.60
20:V:79:VAL:HG12	20:V:86:VAL:HG12	1.82	0.60
1:A:1689:C:OP2	22:X:5:LYS:NZ	2.27	0.60
1:A:2909:G:OP1	59:1:63:ARG:NH1	2.34	0.60
46:AV:167:VAL:HG13	46:AV:172:ALA:HB3	1.83	0.60
1:A:1857:U:H2'	1:A:1858:G:C8	2.37	0.60
1:A:2197:G:H4'	79:l:127:TRP:HE1	1.67	0.60
25:AA:949:U:O2'	38:AN:46:ARG:NH1	2.35	0.60
82:p:94:LYS:HE2	82:p:96:ASN:HB2	1.83	0.60
1:A:2531:U:O4	3:D:246:ARG:NH2	2.35	0.59
25:AA:1530:A:OP1	51:A0:29:ARG:NH2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Q:183:LEU:HD21	15:Q:219:GLU:HG2	1.84	0.59
25:AA:1515:G:H2'	25:AA:1516:G:H8	1.68	0.59
32:AH:92:GLU:OE1	32:AH:141:ARG:NH1	2.35	0.59
55:A4:443:ASP:HB3	55:A4:446:LYS:HE2	1.84	0.59
85:s:111:LYS:NZ	85:s:384:ASP:OD1	2.36	0.59
20:V:129:LYS:HB2	20:V:149:ARG:HH12	1.68	0.59
25:AA:947:U:OP1	36:AL:162:GLN:NE2	2.34	0.59
1:A:2416:U:OP2	85:s:165:ARG:NH1	2.35	0.59
25:AA:744:A:OP1	37:AM:46:ARG:NH2	2.36	0.59
63:5:113:LEU:HD12	63:5:311:ALA:HB1	1.84	0.59
66:8:91:PRO:HB2	66:8:93:LYS:HG2	1.84	0.59
1:A:2182:G:N3	1:A:2199:A:O2'	2.33	0.59
1:A:2854:U:H4'	61:3:138:PRO:HG2	1.83	0.59
14:P:94:VAL:HB	14:P:103:VAL:HG23	1.84	0.59
65:7:83:LYS:NZ	65:7:120:THR:O	2.35	0.59
8:J:88:SER:HA	8:J:151:LEU:HD11	1.84	0.59
20:V:80:ILE:HB	20:V:85:TRP:HB2	1.84	0.59
55:A4:343:ARG:HA	55:A4:378:LEU:HD13	1.84	0.59
24:Z:117:ILE:O	81:o:45:ASN:ND2	2.35	0.59
34:AJ:62:VAL:HA	34:AJ:83:VAL:HG12	1.85	0.59
48:AX:268:LEU:HD21	48:AX:293:LEU:HD23	1.84	0.59
52:A1:187:LYS:HE3	52:A1:191:ILE:HD11	1.84	0.59
1:A:2277:U:H2'	1:A:2278:A:H8	1.67	0.59
55:A4:556:LYS:NZ	55:A4:560:GLU:OE2	2.36	0.59
50:AZ:54:ASN:ND2	50:AZ:57:THR:OG1	2.35	0.59
64:6:90:ILE:HA	77:j:112:LYS:HB2	1.82	0.59
66:8:99:ARG:HG2	72:e:89:LEU:HD11	1.84	0.59
55:A4:267:VAL:HG21	55:A4:296:ALA:HB1	1.85	0.59
68:a:75:ILE:HD13	70:c:255:SER:HB2	1.84	0.58
1:A:1871:A:N7	1:A:1902:C:N4	2.51	0.58
25:AA:1440:G:H2'	25:AA:1441:A:C8	2.38	0.58
26:AB:156:GLU:OE1	31:AG:163:HIS:ND1	2.35	0.58
63:5:307:ASP:OD1	63:5:310:ARG:NH2	2.35	0.58
70:c:42:GLN:NE2	76:i:36:LEU:O	2.35	0.58
79:l:76:ASN:ND2	79:l:83:ASP:OD1	2.37	0.58
8:J:28:LEU:HD13	79:l:56:LEU:HD22	1.84	0.58
15:Q:121:THR:HG22	15:Q:171:VAL:HA	1.85	0.58
25:AA:1132:U:H2'	25:AA:1133:C:H6	1.67	0.58
25:AA:1154:A:OP2	54:A3:155:ARG:NH2	2.37	0.58
28:AD:283:GLU:O	28:AD:356:GLN:NE2	2.37	0.58
39:AO:225:GLN:HE21	45:AU:47:ALA:HB3	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:a:77:ARG:NH2	70:c:293:GLU:OE1	2.33	0.58
1:A:1897:A:H2'	1:A:1898:A:H8	1.68	0.58
1:A:1905:C:OP1	5:F:117:ARG:NH1	2.35	0.58
1:A:2945:A:O2'	1:A:2947:U:O4	2.21	0.58
25:AA:1398:U:H2'	25:AA:1399:A:H8	1.69	0.58
30:AF:122:GLN:NE2	30:AF:138:GLU:O	2.35	0.58
45:AU:77:GLU:HG2	45:AU:80:ARG:HH22	1.68	0.58
69:b:15:LEU:HD22	70:c:222:GLN:HE22	1.68	0.58
46:AV:236:LEU:HD21	46:AV:323:GLU:HB2	1.85	0.58
1:A:2095:U:OP2	11:M:57:ARG:NH1	2.33	0.58
5:F:253:MET:HE3	5:F:259:LEU:HD22	1.85	0.58
25:AA:841:A:OP1	37:AM:39:ASN:ND2	2.35	0.58
38:AN:8:VAL:O	38:AN:11:ARG:NH1	2.37	0.58
43:AS:111:GLU:HB2	43:AS:117:LEU:HD13	1.85	0.58
48:AX:260:VAL:HB	48:AX:306:ILE:HG23	1.84	0.58
63:5:166:THR:O	85:s:287:LYS:NZ	2.33	0.58
65:7:220:GLU:HG2	65:7:253:LYS:HG2	1.85	0.58
85:s:242:ARG:NH1	85:s:292:CYS:O	2.36	0.58
25:AA:674:U:H2'	25:AA:675:A:H8	1.68	0.58
25:AA:1287:A:OP2	28:AD:260:LYS:NZ	2.33	0.58
42:AR:194:GLN:HE22	42:AR:199:LYS:H	1.51	0.58
63:5:115:GLU:HB2	63:5:119:GLN:HB2	1.86	0.58
77:j:100:GLU:HG2	77:j:104:LYS:HE3	1.85	0.58
64:6:255:LEU:HD12	64:6:256:PRO:HD2	1.85	0.58
72:e:164:LYS:HE2	72:e:167:ASP:HA	1.85	0.58
1:A:2737:U:O2'	1:A:3084:A:N3	2.37	0.58
1:A:2408:U:H2'	1:A:2409:A:H8	1.69	0.58
1:A:3188:U:OP2	62:4:84:ARG:NE	2.36	0.58
25:AA:1440:G:H2'	25:AA:1441:A:H8	1.69	0.58
30:AF:119:LYS:NZ	48:AX:398:LEU:O	2.36	0.58
64:6:214:TRP:HB3	64:6:272:LEU:HD11	1.86	0.58
65:7:51:GLU:OE2	65:7:54:ARG:NH1	2.37	0.58
78:k:42:VAL:O	78:k:45:THR:OG1	2.20	0.58
1:A:1697:A:N3	1:A:1703:C:O2'	2.37	0.57
7:I:122:LEU:HB3	7:I:124:LYS:HE2	1.86	0.57
26:AB:243:PRO:O	26:AB:247:HIS:ND1	2.31	0.57
61:3:179:LYS:O	64:6:370:ARG:NH2	2.37	0.57
25:AA:1132:U:H2'	25:AA:1133:C:C6	2.39	0.57
25:AA:1455:U:OP1	31:AG:278:THR:OG1	2.22	0.57
31:AG:126:LYS:H	31:AG:131:ILE:HD11	1.69	0.57
1:A:2519:G:N7	3:D:230:SER:OG	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:AA:897:C:OP2	34:AJ:116:GLN:NE2	2.36	0.57
25:AA:1587:U:H2'	25:AA:1588:G:H8	1.68	0.57
31:AG:273:GLU:HG2	31:AG:282:GLU:HG2	1.86	0.57
48:AX:108:LEU:HD23	48:AX:141:VAL:HG21	1.86	0.57
48:AX:214:GLU:OE1	48:AX:228:GLN:NE2	2.37	0.57
3:D:173:ALA:HB1	3:D:188:PRO:HG3	1.87	0.57
14:P:94:VAL:HG23	14:P:132:LEU:HD21	1.85	0.57
20:V:135:TRP:HB3	20:V:143:ARG:HD2	1.85	0.57
19:U:21:ARG:NH1	23:Y:143:ASP:OD1	2.34	0.57
20:V:123:VAL:HA	20:V:130:PRO:HA	1.85	0.57
25:AA:808:C:OP1	51:A0:19:ARG:NH1	2.37	0.57
65:7:284:HIS:HB3	65:7:323:MET:HE2	1.87	0.57
1:A:1871:A:N3	61:3:104:ARG:NH2	2.52	0.57
1:A:1990:G:OP1	3:D:269:ARG:NH2	2.37	0.57
1:A:2325:U:O2'	13:O:82:GLU:OE2	2.21	0.57
16:R:96:GLU:O	17:S:105:GLN:NE2	2.32	0.57
28:AD:244:LEU:HD22	28:AD:343:LEU:HD23	1.86	0.57
50:AZ:86:LYS:HG2	50:AZ:89:ARG:HH22	1.67	0.57
65:7:114:ASP:HB2	65:7:117:LYS:HB2	1.86	0.57
85:s:246:GLN:NE2	85:s:354:PRO:O	2.38	0.57
1:A:2395:A:O2'	63:5:384:GLN:NE2	2.38	0.57
2:B:43:G:H2'	2:B:44:A:C8	2.39	0.57
19:U:133:GLU:OE2	19:U:137:ARG:NH2	2.37	0.57
22:X:238:LEU:HD11	67:9:101:GLU:HG2	1.86	0.57
43:AS:78:TYR:HA	43:AS:134:ARG:HA	1.87	0.57
1:A:2191:A:H4'	8:J:142:ARG:HG2	1.87	0.57
56:Ax:69:U:H2'	56:Ax:70:A:H8	1.70	0.57
1:A:3127:G:N2	1:A:3130:A:OP2	2.38	0.57
15:Q:96:ARG:NH1	15:Q:285:GLU:OE1	2.38	0.57
56:Ax:67:C:H2'	56:Ax:68:G:C8	2.40	0.57
74:g:110:ILE:HD11	74:g:157:LEU:HD13	1.86	0.57
1:A:1672:C:OP1	18:T:44:LYS:N	2.36	0.56
1:A:1746:A:OP2	22:X:55:LYS:NZ	2.35	0.56
1:A:2410:U:HO2'	63:5:96:HIS:HD1	1.53	0.56
4:E:50:ASP:O	13:O:138:ARG:NH2	2.37	0.56
1:A:1799:U:O4	20:V:34:LYS:NZ	2.38	0.56
1:A:2822:C:O2'	1:A:2915:C:OP2	2.23	0.56
7:I:103:ALA:HB3	78:k:39:SER:HA	1.86	0.56
7:I:147:PHE:HE1	7:I:153:LEU:HD21	1.70	0.56
9:K:174:GLU:HG2	84:r:56:THR:HG21	1.87	0.56
42:AR:323:GLU:H	42:AR:326:ASN:HB2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:9:113:ASN:HB3	67:9:116:LYS:HB3	1.87	0.56
74:g:73:GLN:HB3	74:g:162:LEU:HD11	1.85	0.56
1:A:2421:G:H5''	67:9:24:LYS:HG2	1.88	0.56
18:T:127:ASN:O	71:d:230:ARG:NH2	2.38	0.56
33:AI:112:CYS:HB2	33:AI:122:LYS:HG3	1.86	0.56
34:AJ:109:LEU:HD22	34:AJ:129:LYS:HG2	1.86	0.56
35:AK:60:ASN:O	35:AK:68:GLN:NE2	2.38	0.56
38:AN:83:GLU:OE1	44:AT:85:GLN:NE2	2.38	0.56
44:AT:42:GLU:OE1	44:AT:45:ARG:NH2	2.36	0.56
46:AV:317:LEU:HB2	46:AV:320:GLU:HG3	1.88	0.56
48:AX:210:TRP:NE1	48:AX:216:THR:OG1	2.33	0.56
59:1:13:SER:HB3	59:1:36:ARG:HH21	1.69	0.56
62:4:87:ARG:NH2	62:4:102:GLN:O	2.35	0.56
72:e:213:TYR:HD1	72:e:271:GLN:HG3	1.71	0.56
85:s:145:VAL:HG21	85:s:187:LEU:HD11	1.88	0.56
1:A:2256:U:O2'	17:S:118:ASN:ND2	2.38	0.56
1:A:2273:A:O2'	16:R:16:ASP:OD2	2.22	0.56
3:D:257:ILE:HG23	3:D:262:ARG:HB3	1.87	0.56
36:AL:95:LEU:HD11	36:AL:106:ILE:HD12	1.87	0.56
44:AT:93:LYS:HE3	45:AU:116:LEU:HD11	1.87	0.56
1:A:2361:G:H3'	1:A:2362:A:H8	1.70	0.56
3:D:201:GLY:O	63:5:30:ALA:N	2.39	0.56
64:6:222:ASP:O	64:6:266:HIS:ND1	2.39	0.56
1:A:2871:U:OP2	61:3:143:ARG:NH2	2.38	0.56
4:E:275:ARG:NH2	4:E:331:ASP:OD2	2.39	0.56
25:AA:919:A:OP1	39:AO:92:LYS:NZ	2.31	0.56
25:AA:1398:U:OP1	50:AZ:29:LYS:NZ	2.29	0.56
55:A4:302:VAL:HA	55:A4:312:LYS:HD2	1.88	0.56
1:A:3175:A:OP2	1:A:3187:C:N4	2.37	0.56
48:AX:295:LYS:NZ	96:AX:503:GDP:O1A	2.38	0.56
1:A:2194:U:O2'	79:I:115:ARG:NH1	2.37	0.56
12:N:123:ARG:O	12:N:158:ARG:NH2	2.39	0.56
22:X:118:ILE:O	22:X:168:ARG:NH1	2.39	0.56
37:AM:104:ILE:HG23	42:AR:147:ILE:HG12	1.87	0.56
44:AT:29:VAL:HB	44:AT:79:TYR:HB2	1.88	0.56
73:f:208:LEU:HG	73:f:212:LYS:HE3	1.88	0.56
85:s:49:ALA:O	85:s:61:ARG:NH1	2.39	0.56
52:A1:235:ASN:ND2	52:A1:237:GLU:OE2	2.38	0.56
64:6:139:TRP:O	64:6:144:GLY:N	2.39	0.56
69:b:49:ARG:HG3	69:b:50:GLU:HG2	1.88	0.56
73:f:122:GLU:N	73:f:158:GLN:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2752:C:H2'	1:A:2753:A:H8	1.71	0.56
1:A:2804:A:H2'	1:A:2805:A:H8	1.70	0.56
14:P:93:LEU:HD21	14:P:101:VAL:HG22	1.88	0.56
21:W:148:LEU:HB3	82:p:128:ASN:HA	1.88	0.56
25:AA:1235:U:OP1	35:AK:36:ARG:NH2	2.36	0.56
26:AB:239:ASN:ND2	26:AB:242:SER:OG	2.39	0.56
52:A1:50:ARG:NH1	55:A4:94:TYR:O	2.39	0.56
63:5:160:HIS:HA	63:5:164:TRP:HB2	1.89	0.56
1:A:2137:C:OP2	24:Z:77:ARG:NH1	2.39	0.55
1:A:2175:C:H2'	1:A:2176:C:C6	2.41	0.55
17:S:115:LEU:HD11	17:S:190:GLN:HB3	1.87	0.55
48:AX:102:ARG:NH1	48:AX:132:THR:O	2.39	0.55
49:AY:353:LEU:HD21	50:AZ:26:THR:HG21	1.87	0.55
63:5:229:ARG:NH1	63:5:231:SER:OG	2.39	0.55
70:c:101:GLU:HG2	70:c:117:LEU:HD13	1.88	0.55
78:k:40:GLU:OE1	78:k:43:ARG:NH2	2.38	0.55
1:A:2740:A:N3	1:A:2921:A:O2'	2.34	0.55
19:U:126:LEU:HD22	71:d:76:ILE:HD12	1.88	0.55
25:AA:1003:A:H2'	25:AA:1004:G:H8	1.71	0.55
31:AG:70:THR:HG23	31:AG:73:PHE:H	1.71	0.55
48:AX:67:HIS:HB3	48:AX:98:CYS:HB3	1.88	0.55
1:A:1749:C:O2'	11:M:80:LYS:NZ	2.32	0.55
18:T:63:ARG:NH1	71:d:228:PHE:O	2.39	0.55
27:AC:84:GLU:OE1	27:AC:84:GLU:N	2.36	0.55
42:AR:347:GLN:NE2	42:AR:351:GLU:OE2	2.39	0.55
10:L:96:MET:HE1	15:Q:121:THR:HG21	1.87	0.55
15:Q:74:ARG:NH2	15:Q:287:GLU:OE2	2.35	0.55
25:AA:1528:A:OP1	51:A0:101:ARG:NH2	2.39	0.55
51:A0:65:LEU:HD23	51:A0:68:LEU:HD12	1.89	0.55
56:Ax:28:C:H42	56:Ax:42:G:H1	1.54	0.55
65:7:92:ALA:O	65:7:95:LEU:C	2.50	0.55
1:A:2027:A:O2'	1:A:2048:U:OP1	2.23	0.55
1:A:2043:C:C2	1:A:2044:A:C8	2.95	0.55
4:E:244:ALA:HB1	4:E:248:ILE:HD11	1.88	0.55
43:AS:85:PHE:HB2	47:AW:100:VAL:HG12	1.88	0.55
48:AX:283:ALA:HB3	48:AX:286:GLU:HG3	1.89	0.55
55:A4:611:LEU:HA	55:A4:614:LEU:HD12	1.89	0.55
1:A:2353:A:N6	1:A:2357:C:OP2	2.38	0.55
1:A:2655:G:N2	1:A:2659:C:O2'	2.40	0.55
7:I:188:ARG:HD2	78:k:55:VAL:HB	1.89	0.55
35:AK:58:ARG:NE	35:AK:72:ASP:OD1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:A0:68:LEU:HD22	51:A0:75:GLY:HA3	1.89	0.55
63:5:105:TYR:CZ	63:5:262:ILE:HD12	2.41	0.55
65:7:282:ALA:HB3	65:7:298:GLN:HB2	1.89	0.55
80:m:56:LEU:HD23	80:m:64:ILE:HD11	1.89	0.55
85:s:316:CYS:HB3	85:s:319:GLN:HB2	1.88	0.55
15:Q:233:TRP:HB3	15:Q:240:ILE:HD12	1.89	0.55
32:AH:120:LEU:HD21	35:AK:101:LYS:HD3	1.89	0.55
47:AW:150:THR:HG22	47:AW:161:THR:HB	1.89	0.55
1:A:2740:A:H2'	1:A:2741:A:H8	1.71	0.55
1:A:3189:C:O2'	84:r:155:ALA:N	2.39	0.55
6:H:94:LEU:HB2	6:H:116:LYS:HD3	1.89	0.55
13:O:154:GLN:HG2	13:O:157:ARG:HH21	1.72	0.55
63:5:126:THR:HB	63:5:372:ASN:HB2	1.89	0.55
64:6:90:ILE:HG13	64:6:167:PHE:HB3	1.88	0.55
66:8:99:ARG:HA	72:e:84:TYR:HB2	1.89	0.55
1:A:2246:A:H2'	1:A:2247:C:H6	1.72	0.55
7:I:75:GLU:O	7:I:80:ARG:NH1	2.39	0.55
55:A4:74:LEU:O	55:A4:77:THR:OG1	2.23	0.55
69:b:28:ARG:NH1	69:b:78:GLU:OE1	2.39	0.55
73:f:101:THR:OG1	80:m:67:ARG:NH1	2.39	0.55
4:E:47:THR:HG21	65:7:307:ARG:HD2	1.89	0.55
4:E:76:LYS:HG3	4:E:170:LEU:HD21	1.87	0.55
13:O:49:VAL:HG11	13:O:121:ALA:HB3	1.87	0.55
25:AA:1102:A:OP2	25:AA:1104:A:N6	2.38	0.55
32:AH:176:GLN:NE2	32:AH:178:GLU:OE2	2.38	0.55
11:M:11:ARG:NH2	74:g:142:GLU:OE2	2.40	0.54
17:S:100:HIS:HB2	17:S:134:LEU:HD11	1.89	0.54
25:AA:826:A:C6	34:AJ:56:PRO:HD2	2.41	0.54
42:AR:219:TYR:O	42:AR:256:ARG:NH2	2.38	0.54
55:A4:129:GLN:NE2	55:A4:144:TYR:OH	2.40	0.54
10:L:100:PHE:HB3	15:Q:158:GLN:HE21	1.73	0.54
25:AA:1162:A:N3	25:AA:1497:C:O2'	2.39	0.54
27:AC:86:THR:HG21	35:AK:106:LEU:HD11	1.88	0.54
55:A4:156:ALA:HB3	55:A4:172:MET:HE1	1.89	0.54
1:A:1749:C:OP2	1:A:2899:C:O2'	2.22	0.54
1:A:3046:C:H2'	1:A:3047:G:H8	1.71	0.54
28:AD:392:ARG:NH1	28:AD:396:GLU:OE2	2.40	0.54
30:AF:74:ILE:HG13	31:AG:366:GLN:HA	1.90	0.54
73:f:106:TYR:OH	73:f:174:ILE:O	2.24	0.54
1:A:2093:U:O2	1:A:2266:U:O2'	2.24	0.54
63:5:119:GLN:NE2	63:5:261:PRO:O	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1707:C:N3	63:5:80:ARG:NH1	2.51	0.54
1:A:1828:A:H4'	1:A:1829:A:C8	2.43	0.54
4:E:210:THR:OG1	4:E:262:GLY:O	2.22	0.54
7:I:148:VAL:O	78:k:31:ARG:NH2	2.40	0.54
25:AA:1464:G:H21	25:AA:1466:C:H41	1.55	0.54
29:AE:37:ARG:NH1	29:AE:69:TYR:OH	2.41	0.54
51:A0:163:SER:HB3	51:A0:190:MET:HB3	1.89	0.54
63:5:245:ILE:O	63:5:248:THR:OG1	2.25	0.54
25:AA:990:U:H3	25:AA:997:A:H61	1.56	0.54
46:AV:128:THR:HB	46:AV:137:ILE:HG13	1.89	0.54
1:A:1829:A:H2'	1:A:1830:G:H8	1.72	0.54
1:A:2795:U:H2'	1:A:2796:G:H8	1.72	0.54
25:AA:1239:C:H2'	25:AA:1240:A:C8	2.42	0.54
31:AG:196:GLY:O	31:AG:248:VAL:N	2.41	0.54
34:AJ:78:ARG:HG3	34:AJ:118:LEU:HD21	1.90	0.54
1:A:2694:A:N3	1:A:2942:C:O2'	2.36	0.54
14:P:126:GLU:OE1	14:P:160:ARG:NH2	2.37	0.54
25:AA:1085:C:OP1	33:AI:189:ARG:NH1	2.36	0.54
39:AO:217:ARG:NH1	39:AO:227:GLU:OE2	2.40	0.54
44:AT:32:VAL:HG22	44:AT:76:LEU:HD22	1.88	0.54
1:A:2454:G:OP1	13:O:48:ARG:NH2	2.39	0.54
2:B:74:C:OP1	72:e:219:GLN:NE2	2.41	0.54
10:L:93:GLY:O	10:L:95:ARG:NH2	2.41	0.54
28:AD:316:CYS:HB3	28:AD:334:ALA:HB3	1.89	0.54
48:AX:273:THR:HG23	48:AX:316:LEU:HD13	1.89	0.54
72:e:71:ALA:HB2	80:m:40:LEU:HD22	1.89	0.54
1:A:2950:U:H2'	1:A:2951:A:H8	1.73	0.53
1:A:3200:U:H2'	1:A:3201:A:C2	2.43	0.53
1:A:3205:C:OP2	4:E:298:LYS:NZ	2.35	0.53
2:B:23:A:H2'	2:B:24:G:C8	2.44	0.53
25:AA:701:G:O6	51:A0:48:ARG:NH1	2.41	0.53
25:AA:1454:G:OP2	31:AG:377:ARG:NH1	2.41	0.53
32:AH:50:LEU:HD22	55:A4:80:ARG:HB3	1.89	0.53
42:AR:78:ILE:HG23	42:AR:299:ASN:HB3	1.90	0.53
63:5:146:HIS:O	63:5:194:LYS:NZ	2.41	0.53
64:6:215:THR:OG1	64:6:275:GLN:OE1	2.26	0.53
1:A:2740:A:H2'	1:A:2741:A:C8	2.42	0.53
3:D:126:VAL:HA	3:D:142:VAL:HG12	1.90	0.53
5:F:94:ASP:OD1	81:o:91:GLN:NE2	2.42	0.53
42:AR:70:PHE:O	42:AR:76:GLN:NE2	2.41	0.53
55:A4:308:LYS:HE3	55:A4:310:GLU:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:s:89:MET:HE3	85:s:275:LYS:HB3	1.91	0.53
1:A:2747:U:H2'	1:A:2748:A:H8	1.73	0.53
1:A:3082:G:N2	1:A:3085:A:OP2	2.27	0.53
19:U:46:MET:HB3	67:9:36:ARG:HB3	1.89	0.53
54:A3:159:GLU:OE2	54:A3:163:ARG:NH1	2.41	0.53
10:L:60:VAL:HA	10:L:73:ILE:HG22	1.91	0.53
25:AA:1050:C:H2'	25:AA:1051:A:C8	2.44	0.53
28:AD:224:GLU:OE2	28:AD:226:ARG:NH2	2.41	0.53
29:AE:9:ILE:HD12	29:AE:90:ARG:HB2	1.89	0.53
61:3:175:ASP:HB3	61:3:178:GLN:HB2	1.90	0.53
73:f:55:GLY:HA3	73:f:58:LYS:HE3	1.91	0.53
1:A:2093:U:H4'	76:i:126:LYS:HE2	1.90	0.53
1:A:2175:C:H2'	1:A:2176:C:H6	1.74	0.53
19:U:74:HIS:HB2	67:9:24:LYS:HE3	1.91	0.53
25:AA:889:G:N2	25:AA:902:G:OP1	2.40	0.53
25:AA:917:C:O2'	25:AA:921:U:OP1	2.27	0.53
25:AA:1046:A:O2'	25:AA:1048:C:OP2	2.24	0.53
25:AA:1578:A:H2'	25:AA:1579:C:C6	2.42	0.53
32:AH:55:PRO:HA	55:A4:440:LYS:HB3	1.90	0.53
42:AR:82:MET:HE3	42:AR:288:GLN:HE22	1.73	0.53
1:A:2485:U:H3	1:A:2650:C:H42	0.72	0.53
1:A:2491:C:H2'	1:A:2492:G:C8	2.43	0.53
8:J:119:GLU:HB3	79:l:75:VAL:HG21	1.90	0.53
25:AA:1078:A:OP1	56:Ax:38:C:O2'	2.24	0.53
25:AA:1452:U:H2'	25:AA:1453:A:H8	1.73	0.53
25:AA:1470:A:H2'	25:AA:1471:A:C8	2.43	0.53
26:AB:99:HIS:ND1	26:AB:100:ARG:O	2.41	0.53
41:AQ:68:MET:HE2	53:A2:29:LEU:HD22	1.89	0.53
48:AX:81:HIS:CD2	48:AX:190:ASN:HB3	2.44	0.53
1:A:1780:U:H1'	19:U:83:ARG:HH22	1.72	0.53
1:A:1803:A:H4'	1:A:1804:A:H3'	1.90	0.53
1:A:2403:G:OP2	3:D:105:ARG:NH2	2.40	0.53
1:A:3201:A:H2'	1:A:3202:U:O4'	2.09	0.53
25:AA:843:G:N2	25:AA:846:A:OP2	2.26	0.53
51:A0:135:MET:N	51:A0:135:MET:SD	2.81	0.53
1:A:2586:U:H2'	1:A:2587:G:H8	1.73	0.53
6:H:79:VAL:HG22	22:X:89:GLN:HB2	1.90	0.53
7:I:119:HIS:CD2	7:I:163:GLU:HG2	2.44	0.53
14:P:123:VAL:HG11	64:6:128:ALA:HB3	1.89	0.53
25:AA:773:U:H2'	25:AA:774:G:C8	2.44	0.53
25:AA:1365:A:H4'	25:AA:1389:G:H4'	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:AX:47:ALA:HB1	48:AX:50:ARG:HB2	1.89	0.53
56:Ax:4:A:H2'	56:Ax:5:A:C8	2.43	0.53
64:6:240:ILE:HG12	64:6:248:GLY:HA3	1.90	0.53
1:A:1821:A:OP2	58:0:95:ARG:NH1	2.41	0.53
1:A:2086:A:H2'	1:A:2087:U:C6	2.43	0.53
1:A:2295:C:OP2	16:R:17:ARG:NH2	2.40	0.53
2:B:72:G:C2	2:B:73:A:C8	2.96	0.53
46:AV:46:GLU:OE2	46:AV:74:ARG:NE	2.42	0.53
51:A0:30:ASP:OD1	51:A0:212:ARG:NH2	2.35	0.53
63:5:98:LEU:HD13	63:5:272:ASP:HB2	1.90	0.53
1:A:2402:A:H2'	3:D:133:PRO:HG3	1.90	0.53
8:J:142:ARG:HH11	79:l:99:MET:HE1	1.74	0.53
10:L:94:PRO:O	10:L:97:THR:OG1	2.22	0.53
37:AM:21:LEU:HB3	37:AM:32:TYR:HB3	1.91	0.53
51:A0:63:ARG:NH2	51:A0:110:ASP:OD2	2.42	0.53
64:6:161:LEU:HD13	64:6:271:LEU:HD11	1.90	0.53
20:V:36:PRO:HG2	20:V:39:ILE:HB	1.90	0.52
25:AA:1347:G:OP1	35:AK:36:ARG:NH1	2.33	0.52
25:AA:1396:C:H5''	80:m:90:ARG:HE	1.73	0.52
55:A4:525:SER:HA	55:A4:528:ARG:HE	1.73	0.52
69:b:26:LEU:HD22	69:b:105:ALA:HA	1.91	0.52
1:A:2344:C:H1'	1:A:2362:A:H4'	1.91	0.52
7:l:173:PHE:HD1	78:k:51:VAL:HB	1.73	0.52
25:AA:663:A:H2'	25:AA:664:G:C8	2.45	0.52
25:AA:706:C:OP1	51:A0:43:ARG:NE	2.42	0.52
28:AD:294:ILE:HB	28:AD:305:MET:HE3	1.91	0.52
39:AO:199:TRP:NE1	51:A0:166:TYR:O	2.33	0.52
46:AV:179:GLN:OE1	46:AV:215:GLN:NE2	2.42	0.52
46:AV:266:VAL:HG11	46:AV:275:LEU:HG	1.91	0.52
65:7:194:PRO:HG3	65:7:283:VAL:HB	1.90	0.52
70:c:72:ILE:HD13	70:c:178:LEU:HD13	1.90	0.52
81:o:24:PRO:HG2	84:r:169:TRP:HB2	1.90	0.52
7:I:102:VAL:HG23	7:I:104:LEU:HG	1.91	0.52
13:O:87:PRO:O	13:O:91:GLN:HB2	2.10	0.52
26:AB:172:ARG:HB2	26:AB:175:MET:HE2	1.92	0.52
46:AV:357:THR:HG22	46:AV:361:LYS:HE3	1.91	0.52
1:A:1907:A:OP1	5:F:126:LYS:NZ	2.33	0.52
1:A:2347:C:H2'	1:A:2348:A:H8	1.73	0.52
11:M:264:GLN:NE2	11:M:266:PHE:O	2.41	0.52
25:AA:842:C:N4	25:AA:843:G:O6	2.42	0.52
1:A:2407:U:H2'	1:A:2408:U:H6	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3152:C:OP1	15:Q:141:SER:OG	2.24	0.52
2:B:40:U:H5''	14:P:155:SER:HB3	1.91	0.52
19:U:19:VAL:HB	67:9:136:LEU:HD23	1.90	0.52
25:AA:1025:A:H2'	25:AA:1026:A:C8	2.44	0.52
30:AF:240:ARG:NH1	30:AF:242:TRP:OXT	2.43	0.52
32:AH:64:THR:OG1	55:A4:64:THR:OG1	2.24	0.52
63:5:162:ARG:NH1	63:5:383:TYR:OH	2.39	0.52
72:e:48:LEU:HB2	72:e:231:VAL:HG12	1.92	0.52
1:A:2042:U:H2'	1:A:2043:C:H6	1.75	0.52
1:A:2192:A:O2'	8:J:135:VAL:HG11	2.10	0.52
25:AA:1515:G:H2'	25:AA:1516:G:C8	2.45	0.52
29:AE:96:HIS:HB3	29:AE:99:THR:HG23	1.91	0.52
59:1:24:ALA:HB2	59:1:54:VAL:HG11	1.92	0.52
70:c:245:LEU:HD12	70:c:253:PRO:HD3	1.92	0.52
80:m:103:ARG:HB3	80:m:108:GLN:HE21	1.74	0.52
1:A:3115:U:H2'	1:A:3116:C:H6	1.73	0.52
15:Q:80:PHE:O	15:Q:282:ILE:HD13	2.09	0.52
23:Y:171:ASP:OD1	23:Y:175:ARG:N	2.43	0.52
25:AA:1415:G:OP2	25:AA:1415:G:N2	2.20	0.52
32:AH:79:LEU:HD11	32:AH:140:TYR:HB3	1.91	0.52
48:AX:210:TRP:HB2	48:AX:214:GLU:HB2	1.90	0.52
72:e:58:VAL:N	72:e:153:LEU:O	2.41	0.52
83:q:112:GLN:OE1	83:q:115:ARG:NH2	2.41	0.52
1:A:2522:U:H1'	63:5:35:VAL:HG12	1.90	0.52
5:F:72:PHE:HA	5:F:206:LEU:HD13	1.92	0.52
5:F:211:ARG:HD3	75:h:58:ARG:HH21	1.75	0.52
25:AA:740:G:H2'	25:AA:741:A:H8	1.74	0.52
25:AA:872:G:H2'	25:AA:873:G:H8	1.75	0.52
25:AA:1278:C:H1'	26:AB:181:LEU:HD22	1.91	0.52
39:AO:167:ILE:HD12	42:AR:230:LEU:HG	1.91	0.52
50:AZ:13:ARG:NH1	80:m:109:GLU:O	2.43	0.52
51:A0:167:PRO:HG2	51:A0:170:LEU:HB2	1.90	0.52
55:A4:472:ASP:OD1	55:A4:505:ARG:NH1	2.43	0.52
1:A:3024:U:H2'	1:A:3025:A:H8	1.75	0.52
4:E:148:GLY:HA3	4:E:173:LYS:HG3	1.92	0.52
13:O:106:ARG:HE	13:O:126:LYS:HE2	1.75	0.52
24:Z:68:ILE:HD11	24:Z:122:LEU:HD13	1.91	0.52
25:AA:872:G:H2'	25:AA:873:G:C8	2.45	0.52
25:AA:1380:G:N3	48:AX:164:ASN:ND2	2.55	0.52
31:AG:263:ASP:OD1	31:AG:267:MET:N	2.42	0.52
32:AH:148:LEU:HD13	32:AH:153:ALA:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:AR:159:THR:HG23	42:AR:172:ILE:HG12	1.91	0.52
52:A1:155:ASP:OD1	52:A1:215:ARG:NH1	2.31	0.52
1:A:1750:G:H2'	1:A:1751:A:C8	2.45	0.52
1:A:1886:G:N7	5:F:170:ARG:NH2	2.58	0.52
1:A:1979:U:H2'	1:A:1980:A:C8	2.45	0.52
1:A:2082:G:OP1	81:o:66:ARG:NH2	2.42	0.52
1:A:2682:A:H5''	16:R:34:ARG:HH21	1.74	0.52
9:K:136:ASP:OD1	70:c:264:THR:OG1	2.24	0.52
31:AG:90:ASN:ND2	52:A1:62:VAL:O	2.43	0.52
42:AR:157:VAL:HG11	42:AR:192:MET:HE3	1.91	0.52
56:Ax:66:C:H2'	56:Ax:67:C:H6	1.74	0.52
1:A:3115:U:H2'	1:A:3116:C:C6	2.45	0.51
17:S:98:VAL:HB	17:S:135:LEU:HB3	1.91	0.51
31:AG:353:CYS:HA	31:AG:356:VAL:HG22	1.92	0.51
64:6:216:LEU:HD11	64:6:270:PHE:HB3	1.93	0.51
1:A:2160:A:N6	62:4:70:THR:O	2.40	0.51
5:F:279:ARG:HH12	5:F:282:PRO:HD3	1.74	0.51
33:AI:151:VAL:HG21	33:AI:158:ARG:HG3	1.93	0.51
42:AR:281:ILE:HB	42:AR:300:LEU:HD21	1.90	0.51
65:7:240:ILE:HG23	65:7:252:VAL:HG21	1.90	0.51
1:A:2175:C:H4'	8:J:102:ARG:HG2	1.90	0.51
1:A:2187:C:H2'	1:A:2188:A:C8	2.45	0.51
1:A:2332:C:H41	1:A:2442:U:H3	1.58	0.51
3:D:127:ILE:HD11	3:D:143:ALA:HB2	1.92	0.51
22:X:241:GLN:NE2	22:X:245:GLU:OE2	2.43	0.51
42:AR:312:GLN:HB2	42:AR:335:GLU:HG3	1.91	0.51
55:A4:332:LEU:HD21	55:A4:368:SER:HB3	1.92	0.51
72:e:58:VAL:HB	72:e:153:LEU:HB3	1.91	0.51
78:k:18:VAL:HG22	78:k:64:VAL:HG22	1.90	0.51
1:A:1895:C:H2'	1:A:1896:U:H6	1.76	0.51
20:V:54:TRP:NE1	20:V:56:LEU:O	2.43	0.51
25:AA:1022:A:OP2	53:A2:17:ARG:NE	2.42	0.51
1:A:1829:A:H2'	1:A:1830:G:C8	2.46	0.51
1:A:2196:A:O2'	1:A:2213:A:N1	2.42	0.51
1:A:2530:A:H5''	3:D:212:THR:HG21	1.92	0.51
5:F:195:LEU:HD22	5:F:202:TYR:HE2	1.75	0.51
47:AW:126:ARG:NH1	47:AW:131:GLY:O	2.34	0.51
48:AX:369:GLU:HG3	48:AX:370:LYS:HG2	1.93	0.51
73:f:48:TYR:HB3	73:f:51:LYS:HG2	1.93	0.51
25:AA:1211:G:H2'	25:AA:1212:U:C6	2.46	0.51
25:AA:1272:A:N1	25:AA:1303:G:O2'	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:AP:124:TYR:HE2	41:AQ:4:HIS:HB3	1.75	0.51
50:AZ:18:LEU:HD21	80:m:114:LEU:HD11	1.92	0.51
56:Ax:27:U:H2'	56:Ax:28:C:C6	2.45	0.51
1:A:1911:C:H2'	1:A:1912:A:H8	1.75	0.51
1:A:2017:U:OP2	11:M:59:ARG:NH2	2.41	0.51
46:AV:250:ILE:HB	51:A0:146:GLU:HG3	1.91	0.51
19:U:48:MET:HE2	19:U:53:LEU:HA	1.93	0.51
23:Y:187:PRO:HD2	23:Y:190:LEU:HD12	1.91	0.51
25:AA:1456:U:OP1	31:AG:338:SER:OG	2.25	0.51
31:AG:165:VAL:HG11	31:AG:224:LEU:HB3	1.93	0.51
46:AV:236:LEU:HD12	46:AV:290:LEU:HD13	1.92	0.51
55:A4:345:PHE:HB3	55:A4:348:PHE:HD2	1.76	0.51
65:7:247:ASN:ND2	65:7:251:ILE:HG12	2.26	0.51
67:9:16:ASP:N	67:9:16:ASP:OD1	2.44	0.51
1:A:1789:A:N3	1:A:1915:C:O2'	2.40	0.51
8:J:25:ARG:NH1	79:l:58:ASP:OD1	2.31	0.51
8:J:101:ALA:HB1	8:J:107:GLU:HG3	1.92	0.51
13:O:33:LEU:HD21	13:O:59:LEU:HD22	1.93	0.51
13:O:64:LYS:NZ	13:O:100:GLN:O	2.43	0.51
24:Z:120:LYS:NZ	81:o:44:GLU:OE2	2.38	0.51
35:AK:34:MET:HE3	35:AK:95:SER:HB2	1.92	0.51
45:AU:168:ILE:HG12	45:AU:176:ARG:HG3	1.93	0.51
52:A1:56:ARG:HG3	52:A1:60:MET:HE3	1.93	0.51
72:e:54:GLN:HG2	72:e:158:VAL:HG22	1.92	0.51
2:B:21:A:OP2	64:6:106:ARG:NH1	2.41	0.51
5:F:212:TRP:O	5:F:258:THR:OG1	2.25	0.51
27:AC:126:GLN:O	52:A1:49:ARG:NH2	2.44	0.51
48:AX:163:LYS:HB3	48:AX:316:LEU:HD11	1.92	0.51
63:5:354:PHE:HB3	63:5:417:LEU:HD11	1.93	0.51
73:f:127:MET:HB2	73:f:154:GLU:HB3	1.93	0.51
1:A:2310:G:N2	1:A:2676:A:OP2	2.35	0.50
1:A:2803:A:H2'	1:A:2804:A:O4'	2.11	0.50
5:F:94:ASP:OD1	5:F:94:ASP:N	2.34	0.50
7:I:76:ILE:HG22	7:I:78:LEU:H	1.76	0.50
7:I:140:TYR:HB3	7:I:143:LEU:HD12	1.91	0.50
35:AK:52:LEU:HD11	50:AZ:36:LEU:HB3	1.92	0.50
77:j:53:ASP:OD2	77:j:55:ARG:NH2	2.43	0.50
1:A:2442:U:OP1	85:s:81:ARG:NH2	2.30	0.50
5:F:62:VAL:HG23	5:F:82:LEU:HB2	1.93	0.50
10:L:98:PRO:HA	15:Q:162:ILE:HG12	1.91	0.50
16:R:16:ASP:OD1	16:R:16:ASP:N	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:102:GLU:OE2	64:6:74:TYR:N	2.44	0.50
55:A4:516:SER:HB3	55:A4:521:HIS:HB2	1.92	0.50
74:g:150:LYS:NZ	81:o:79:THR:O	2.43	0.50
1:A:1897:A:H2'	1:A:1898:A:C8	2.46	0.50
25:AA:1042:U:H2'	25:AA:1043:C:H6	1.76	0.50
25:AA:1471:A:H2'	25:AA:1472:G:H8	1.75	0.50
32:AH:65:ILE:HG12	55:A4:63:LYS:HG2	1.93	0.50
38:AN:29:ARG:HD3	38:AN:46:ARG:HD2	1.94	0.50
55:A4:526:ASP:OD1	55:A4:527:LEU:N	2.44	0.50
64:6:236:LEU:HB3	64:6:252:CYS:HB3	1.94	0.50
69:b:48:GLU:OE2	81:o:101:TRP:NE1	2.39	0.50
1:A:1742:G:O2'	1:A:1754:G:O6	2.28	0.50
1:A:2457:A:O2'	13:O:17:ARG:NH1	2.43	0.50
1:A:2673:G:H5''	18:T:106:LYS:HB2	1.93	0.50
1:A:3019:G:O2'	1:A:3125:A:N1	2.43	0.50
63:5:177:CYS:HB3	63:5:178:PRO:HD3	1.92	0.50
64:6:311:MET:O	77:j:112:LYS:NZ	2.44	0.50
1:A:2051:A:H2'	1:A:2052:A:C8	2.47	0.50
2:B:29:C:H2'	2:B:30:A:H8	1.76	0.50
25:AA:889:G:N1	25:AA:905:A:OP2	2.35	0.50
32:AH:164:LEU:HD12	32:AH:165:PRO:HD2	1.92	0.50
54:A3:174:ARG:HA	54:A3:177:TRP:CE2	2.46	0.50
56:Ax:22:A:H2'	56:Ax:23:G:H8	1.76	0.50
73:f:172:GLU:OE1	73:f:175:GLN:NE2	2.44	0.50
1:A:2215:C:OP2	12:N:31:LYS:NZ	2.44	0.50
1:A:2335:A:H2'	1:A:2336:U:H6	1.76	0.50
1:A:2416:U:H3	85:s:166:TYR:HD1	1.59	0.50
18:T:150:ILE:HB	71:d:52:THR:HG21	1.92	0.50
32:AH:64:THR:HG1	55:A4:64:THR:HG1	1.50	0.50
54:A3:170:GLU:OE2	54:A3:193:LYS:NZ	2.45	0.50
64:6:198:ALA:O	64:6:254:TYR:OH	2.28	0.50
71:d:200:SER:HB2	71:d:204:ASN:HD21	1.77	0.50
76:i:57:TYR:OH	83:q:28:ARG:O	2.23	0.50
1:A:1787:G:N2	1:A:1790:A:OP2	2.28	0.50
1:A:3231:U:H3	13:O:106:ARG:HG2	1.76	0.50
18:T:185:THR:HG23	18:T:188:ALA:H	1.77	0.50
23:Y:85:TRP:HH2	67:9:70:LEU:HD22	1.76	0.50
25:AA:798:C:H2'	25:AA:799:A:C8	2.47	0.50
28:AD:380:LEU:HD12	28:AD:381:PRO:HD2	1.94	0.50
37:AM:67:ALA:HB1	42:AR:161:ILE:HD13	1.93	0.50
53:A2:49:MET:HG2	53:A2:53:MET:HE2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:f:90:VAL:HG11	73:f:158:GLN:HE21	1.77	0.50
1:A:2246:A:H2'	1:A:2247:C:C6	2.47	0.50
1:A:2727:C:H2'	1:A:2728:C:C6	2.47	0.50
25:AA:916:C:H2'	25:AA:917:C:C6	2.46	0.50
25:AA:1411:G:H2'	25:AA:1412:G:H8	1.77	0.50
55:A4:531:ILE:HG22	55:A4:535:MET:HE2	1.94	0.50
64:6:188:TYR:OH	82:p:190:GLN:NE2	2.45	0.50
6:H:62:VAL:HG22	6:H:77:HIS:HD2	1.77	0.50
17:S:131:GLU:HB3	17:S:151:LYS:HE2	1.93	0.50
21:W:100:THR:OG1	21:W:132:HIS:NE2	2.36	0.50
25:AA:1595:G:H2'	25:AA:1596:A:C8	2.47	0.50
29:AE:15:ARG:NH2	45:AU:182:ASP:OD1	2.45	0.50
46:AV:270:PRO:O	46:AV:346:LYS:NZ	2.45	0.50
1:A:2321:A:OP1	58:0:138:ARG:NH1	2.45	0.49
1:A:2321:A:N1	58:0:142:GLY:HA3	2.27	0.49
12:N:218:ILE:HG23	12:N:223:MET:HB2	1.93	0.49
25:AA:684:U:H2'	25:AA:685:A:H8	1.76	0.49
46:AV:139:PRO:HB2	46:AV:143:THR:HB	1.94	0.49
46:AV:240:LEU:HD22	46:AV:253:PRO:HB3	1.93	0.49
55:A4:596:LEU:HD11	55:A4:614:LEU:HD11	1.94	0.49
84:r:37:GLU:OE1	84:r:52:ARG:NH2	2.44	0.49
1:A:2816:G:O6	21:W:33:LYS:NZ	2.44	0.49
3:D:204:ALA:O	3:D:208:ARG:NH2	2.37	0.49
14:P:51:ARG:NH2	64:6:221:LEU:O	2.44	0.49
31:AG:209:LEU:O	31:AG:211:GLU:N	2.39	0.49
46:AV:331:LEU:HG	46:AV:335:LYS:HE3	1.94	0.49
80:m:79:ILE:HD11	80:m:84:LEU:HD21	1.94	0.49
1:A:1789:A:H2'	1:A:1790:A:C8	2.46	0.49
1:A:1792:G:OP2	60:2:85:LYS:NZ	2.45	0.49
1:A:1907:A:N3	1:A:2930:U:O2'	2.43	0.49
1:A:2236:C:N4	1:A:2688:C:O2	2.45	0.49
29:AE:40:GLU:HB2	29:AE:65:LEU:HB2	1.94	0.49
46:AV:29:LEU:N	46:AV:149:ASP:OD1	2.44	0.49
48:AX:79:PHE:HZ	48:AX:143:HIS:HB2	1.76	0.49
48:AX:126:LEU:HD23	48:AX:343:ILE:HB	1.93	0.49
72:e:45:TRP:CD2	72:e:230:LYS:HE3	2.47	0.49
1:A:1822:U:O2	1:A:2707:A:O2'	2.30	0.49
1:A:1939:G:O2'	1:A:1973:G:H4'	2.12	0.49
1:A:2380:C:H5''	1:A:2381:A:OP2	2.12	0.49
1:A:3051:A:H2'	1:A:3052:A:C8	2.47	0.49
2:B:44:A:OP1	64:6:114:ARG:NH2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:25:ARG:HD2	79:l:56:LEU:HB3	1.94	0.49
16:R:108:TYR:HD1	69:b:125:SER:HB2	1.77	0.49
25:AA:1056:A:H4'	25:AA:1588:G:N2	2.26	0.49
25:AA:1201:A:H2'	25:AA:1202:G:C8	2.47	0.49
28:AD:203:LEU:HD21	28:AD:222:ILE:HD11	1.94	0.49
37:AM:74:ARG:NH2	45:AU:77:GLU:OE1	2.45	0.49
48:AX:207:LYS:HB2	48:AX:218:LYS:HB2	1.93	0.49
73:f:137:LEU:HA	73:f:144:MET:HA	1.94	0.49
25:AA:769:G:OP2	38:AN:73:ARG:NH2	2.45	0.49
25:AA:1007:G:H2'	25:AA:1008:A:C8	2.48	0.49
25:AA:1527:A:H2'	25:AA:1528:A:O4'	2.13	0.49
55:A4:513:TRP:HB2	55:A4:531:ILE:HD13	1.94	0.49
61:3:168:ARG:NH1	61:3:170:ASN:OD1	2.45	0.49
64:6:155:TYR:O	64:6:267:ARG:NH1	2.45	0.49
1:A:1812:C:OP1	18:T:44:LYS:NZ	2.40	0.49
1:A:2734:A:H2'	1:A:2735:G:H8	1.77	0.49
10:L:35:MET:O	10:L:56:ARG:NH1	2.46	0.49
25:AA:1129:U:H2'	25:AA:1130:G:H8	1.76	0.49
1:A:2727:C:H2'	1:A:2728:C:H6	1.78	0.49
1:A:2751:G:H2'	1:A:2752:C:C6	2.48	0.49
4:E:221:ARG:NH1	4:E:257:MET:O	2.43	0.49
25:AA:1308:U:H2'	25:AA:1309:A:H8	1.78	0.49
25:AA:1462:G:H2'	25:AA:1463:G:H8	1.77	0.49
42:AR:209:ILE:HA	42:AR:214:ASN:HD22	1.77	0.49
47:AW:103:ARG:HG2	47:AW:139:ARG:HG2	1.94	0.49
63:5:165:GLN:HG2	63:5:166:THR:HG23	1.95	0.49
63:5:242:ARG:NH2	63:5:337:GLU:O	2.45	0.49
1:A:1980:A:OP1	60:2:56:SER:OG	2.31	0.49
1:A:2612:C:O2'	25:AA:1503:G:O2'	2.30	0.49
10:L:43:ASN:OD1	10:L:118:ARG:N	2.45	0.49
25:AA:1302:C:OP1	27:AC:165:LYS:NZ	2.39	0.49
36:AL:128:ARG:HH21	36:AL:166:MET:HE2	1.76	0.49
55:A4:598:LEU:O	55:A4:602:HIS:ND1	2.39	0.49
71:d:203:MET:H	71:d:208:VAL:HG22	1.78	0.49
1:A:2746:U:H2'	1:A:2747:U:C6	2.48	0.49
31:AG:202:LYS:O	31:AG:206:GLU:HG2	2.13	0.49
42:AR:262:LEU:O	42:AR:265:THR:OG1	2.25	0.49
43:AS:104:THR:HG22	43:AS:108:LYS:HE2	1.95	0.49
56:Ax:69:U:H2'	56:Ax:70:A:C8	2.48	0.49
85:s:152:GLN:NE2	85:s:179:GLN:OE1	2.46	0.49
1:A:1834:U:C4	18:T:200:ARG:HA	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Y:154:ARG:HA	67:9:130:LEU:HD13	1.95	0.49
25:AA:769:G:N2	25:AA:772:A:OP2	2.44	0.49
25:AA:1439:A:H2'	25:AA:1440:G:H8	1.78	0.49
25:AA:1471:A:H2'	25:AA:1472:G:C8	2.47	0.49
48:AX:365:TRP:NE1	48:AX:395:CYS:O	2.46	0.49
70:c:140:PHE:HB3	70:c:314:TRP:HH2	1.77	0.49
74:g:154:ASP:N	74:g:154:ASP:OD1	2.46	0.49
1:A:2443:C:O2	1:A:2444:A:N6	2.46	0.48
1:A:2616:A:O2'	1:A:3046:C:O2	2.30	0.48
1:A:3089:A:H5'	56:Ax:74:C:H5''	1.95	0.48
18:T:138:GLU:HB2	18:T:171:LYS:HB3	1.95	0.48
25:AA:1118:A:H4'	28:AD:355:ARG:HH12	1.76	0.48
26:AB:222:ILE:HD13	26:AB:236:VAL:HB	1.94	0.48
53:A2:100:LEU:HB3	53:A2:103:LYS:HG2	1.95	0.48
70:c:72:ILE:HG23	70:c:88:LEU:HD23	1.95	0.48
85:s:204:CYS:SG	85:s:240:GLN:NE2	2.86	0.48
1:A:2099:U:H2'	1:A:2100:C:C6	2.47	0.48
1:A:2392:U:H2'	1:A:2394:A:H62	1.78	0.48
1:A:3230:G:N7	4:E:156:ARG:NH2	2.60	0.48
6:H:141:GLU:HA	6:H:144:LYS:HE2	1.94	0.48
25:AA:798:C:H2'	25:AA:799:A:H8	1.79	0.48
32:AH:121:LEU:HD21	32:AH:128:LYS:HD2	1.95	0.48
55:A4:308:LYS:HG3	55:A4:311:GLU:H	1.78	0.48
56:Ax:66:C:H2'	56:Ax:67:C:C6	2.47	0.48
63:5:276:ASP:OD2	85:s:160:ARG:NH2	2.46	0.48
64:6:162:PHE:HB3	64:6:165:ALA:HB3	1.95	0.48
64:6:244:ARG:NH1	64:6:247:GLU:OE1	2.46	0.48
65:7:176:SER:O	65:7:319:ARG:NH2	2.46	0.48
81:o:71:PHE:CE2	81:o:75:LYS:HD2	2.47	0.48
1:A:1860:A:H5''	1:A:2681:G:H5''	1.94	0.48
15:Q:177:VAL:HG11	15:Q:204:MET:HG3	1.94	0.48
23:Y:202:LEU:HB2	23:Y:204:TYR:CE2	2.47	0.48
25:AA:1144:U:H2'	25:AA:1145:A:H8	1.78	0.48
33:AI:121:LYS:H	33:AI:121:LYS:HD2	1.78	0.48
67:9:68:PHE:CE2	67:9:70:LEU:HB2	2.48	0.48
85:s:248:ALA:HB2	85:s:430:LYS:HG3	1.96	0.48
1:A:1979:U:H2'	1:A:1980:A:H8	1.78	0.48
1:A:2468:A:H61	1:A:2659:C:H42	1.60	0.48
11:M:73:PRO:HG2	11:M:76:ILE:HB	1.96	0.48
13:O:29:LEU:HD22	13:O:52:MET:HB3	1.94	0.48
18:T:42:SER:O	18:T:43:ARG:NH1	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:AA:844:A:H4'	45:AU:64:ARG:HH12	1.79	0.48
25:AA:1003:A:H2'	25:AA:1004:G:C8	2.48	0.48
31:AG:255:GLN:HG2	31:AG:370:LEU:HD13	1.96	0.48
32:AH:53:ASP:OD2	55:A4:80:ARG:NH1	2.46	0.48
36:AL:175:TYR:HB2	38:AN:89:GLY:HA3	1.96	0.48
48:AX:162:VAL:HB	48:AX:272:THR:HB	1.96	0.48
49:AY:349:HIS:CD2	50:AZ:24:ARG:HD2	2.48	0.48
51:A0:41:LEU:HD13	51:A0:55:TRP:CG	2.49	0.48
63:5:229:ARG:NH2	63:5:286:PRO:O	2.45	0.48
73:f:136:GLN:HG2	80:m:78:PRO:HG3	1.94	0.48
1:A:2485:U:O2	1:A:2650:C:N3	2.46	0.48
1:A:3202:U:OP2	4:E:141:LYS:NZ	2.43	0.48
3:D:113:ARG:O	3:D:147:ARG:NH1	2.37	0.48
5:F:114:THR:O	5:F:156:ARG:NH1	2.46	0.48
12:N:33:LEU:HD22	79:l:125:ASN:HD22	1.78	0.48
19:U:44:ILE:HG13	19:U:93:LYS:HB3	1.95	0.48
25:AA:1050:C:H2'	25:AA:1051:A:H8	1.78	0.48
25:AA:1134:G:OP2	34:AJ:38:ARG:NH2	2.46	0.48
28:AD:296:LEU:HD11	28:AD:303:ILE:HD12	1.95	0.48
31:AG:197:SER:O	31:AG:245:ARG:NH2	2.45	0.48
42:AR:195:VAL:HG22	42:AR:204:ILE:HD13	1.96	0.48
83:q:40:PRO:HG2	83:q:51:GLN:HB3	1.95	0.48
1:A:2081:U:O2	24:Z:109:LYS:NZ	2.45	0.48
1:A:2431:C:OP2	1:A:2433:C:N4	2.38	0.48
1:A:2900:C:H2'	1:A:2901:A:H8	1.79	0.48
1:A:3110:C:O2'	4:E:266:ARG:NH1	2.46	0.48
1:A:3144:A:H2'	1:A:3145:A:H8	1.78	0.48
3:D:111:ARG:NH2	3:D:165:ASN:OD1	2.35	0.48
8:J:159:LEU:HD21	8:J:164:LEU:HD13	1.94	0.48
25:AA:1149:G:OP2	54:A3:165:LYS:NZ	2.39	0.48
25:AA:1408:A:H2'	25:AA:1409:A:H8	1.79	0.48
44:AT:132:ARG:NH1	44:AT:136:LEU:O	2.45	0.48
56:Ax:8:U:H5'	56:Ax:49:G:H5'	1.95	0.48
63:5:283:TYR:HE1	85:s:152:GLN:HB2	1.78	0.48
1:A:2668:A:H2'	1:A:2669:A:C8	2.48	0.48
2:B:55:U:C4	2:B:56:U:H1'	2.49	0.48
7:I:168:LEU:HD13	7:I:176:LEU:HB2	1.96	0.48
19:U:20:PHE:O	23:Y:99:HIS:NE2	2.34	0.48
20:V:63:GLU:HB2	20:V:73:GLN:HG2	1.96	0.48
20:V:122:LEU:HD21	20:V:154:ILE:HG21	1.95	0.48
25:AA:705:C:H5'	51:A0:51:PRO:HG3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:AG:276:ARG:HG3	31:AG:277:LYS:H	1.78	0.48
76:i:83:TRP:HZ3	76:i:90:ARG:HG2	1.79	0.48
1:A:2016:C:OP2	11:M:59:ARG:NH1	2.47	0.48
1:A:2039:A:N6	1:A:2729:U:O2	2.47	0.48
1:A:2795:U:H2'	1:A:2796:G:C8	2.48	0.48
3:D:289:LEU:HD12	3:D:290:PRO:HD2	1.95	0.48
25:AA:715:G:H2'	25:AA:716:U:C6	2.49	0.48
25:AA:799:A:H2'	25:AA:800:C:C6	2.48	0.48
25:AA:1174:U:H2'	25:AA:1175:G:H8	1.79	0.48
26:AB:138:ARG:HB3	43:AS:30:LEU:HD11	1.95	0.48
47:AW:114:ILE:HD13	47:AW:140:VAL:HG21	1.96	0.48
52:A1:86:ARG:HB3	52:A1:96:PRO:HB2	1.95	0.48
1:A:1673:U:O2'	18:T:143:ARG:NH1	2.46	0.48
1:A:2051:A:H2'	1:A:2052:A:H8	1.78	0.48
1:A:2176:C:H5'	8:J:102:ARG:HH22	1.77	0.48
1:A:3165:C:H2'	1:A:3166:U:C6	2.49	0.48
12:N:103:GLU:OE1	12:N:106:ARG:NH2	2.37	0.48
25:AA:1118:A:H4'	28:AD:351:ARG:HH21	1.77	0.48
37:AM:63:GLU:HG2	42:AR:155:LYS:HE2	1.96	0.48
39:AO:105:CYS:HB2	39:AO:142:VAL:HA	1.96	0.48
46:AV:116:CYS:HA	46:AV:121:ALA:HB3	1.95	0.48
49:AY:315:ILE:HD12	52:A1:157:VAL:HG13	1.96	0.48
1:A:2167:A:N6	1:A:2212:C:OP2	2.47	0.48
20:V:19:TYR:OH	20:V:31:ASP:OD2	2.29	0.48
25:AA:686:A:H2'	25:AA:687:G:H8	1.79	0.48
44:AT:47:PHE:HD1	44:AT:51:ASN:HD22	1.62	0.48
46:AV:187:PHE:HD1	46:AV:190:LEU:HD12	1.78	0.48
56:Ax:27:U:H2'	56:Ax:28:C:H6	1.79	0.48
65:7:155:GLU:HA	65:7:164:VAL:HG11	1.95	0.48
84:r:124:ARG:NH1	84:r:153:ARG:O	2.45	0.48
1:A:1760:G:OP2	83:q:55:ARG:NH2	2.47	0.47
4:E:345:ILE:O	15:Q:172:GLN:NE2	2.47	0.47
25:AA:1456:U:H2'	25:AA:1457:G:O4'	2.15	0.47
25:AA:1462:G:H2'	25:AA:1463:G:C8	2.48	0.47
37:AM:54:TYR:HD1	37:AM:66:VAL:HG22	1.77	0.47
1:A:2075:U:O2'	1:A:2833:A:N7	2.41	0.47
22:X:226:LEU:HD12	23:Y:155:LEU:HB3	1.94	0.47
25:AA:686:A:H2'	25:AA:687:G:C8	2.48	0.47
25:AA:1529:A:O2'	46:AV:64:LYS:O	2.30	0.47
28:AD:148:LEU:HD21	55:A4:108:LEU:HB2	1.96	0.47
65:7:247:ASN:HD21	65:7:249:GLU:HB2	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2318:A:H2'	1:A:2319:A:C8	2.50	0.47
1:A:2804:A:H2'	1:A:2805:A:C8	2.48	0.47
11:M:146:ASP:HA	82:p:144:PHE:HE1	1.78	0.47
25:AA:700:A:N1	25:AA:709:G:O2'	2.41	0.47
25:AA:1006:U:H2'	25:AA:1007:G:H8	1.78	0.47
25:AA:1298:U:H4'	26:AB:172:ARG:HH21	1.78	0.47
25:AA:1504:U:H2'	25:AA:1505:A:C8	2.50	0.47
35:AK:53:ARG:O	35:AK:56:SER:OG	2.29	0.47
46:AV:95:PHE:O	46:AV:98:SER:OG	2.26	0.47
48:AX:138:LEU:HD11	48:AX:261:ALA:HB1	1.96	0.47
48:AX:153:LEU:HD21	48:AX:244:LEU:HD22	1.96	0.47
55:A4:331:ASN:HD21	55:A4:333:GLN:HB2	1.79	0.47
1:A:2598:A:H3'	1:A:2625:C:H42	1.79	0.47
1:A:3144:A:H2'	1:A:3145:A:C8	2.49	0.47
4:E:210:THR:HG22	4:E:290:PRO:HB3	1.95	0.47
8:J:114:LEU:HD13	79:l:97:PHE:HA	1.97	0.47
9:K:22:ASP:HB3	9:K:147:GLN:HE21	1.78	0.47
19:U:29:VAL:HG12	23:Y:117:GLN:HG2	1.96	0.47
25:AA:806:C:OP2	25:AA:807:A:N6	2.30	0.47
30:AF:161:ILE:HD12	30:AF:170:VAL:HG21	1.96	0.47
33:AI:163:HIS:NE2	41:AQ:20:GLU:OE2	2.47	0.47
73:f:93:ILE:HG12	73:f:186:VAL:HG22	1.96	0.47
1:A:2481:A:H2'	1:A:2482:A:C8	2.50	0.47
2:B:74:C:H2'	2:B:75:C:O4'	2.14	0.47
10:L:52:HIS:HD2	10:L:53:ARG:HG3	1.80	0.47
13:O:133:LEU:HD23	58:0:130:VAL:HG11	1.95	0.47
20:V:34:LYS:HG2	20:V:35:ASN:H	1.79	0.47
22:X:6:TYR:CG	22:X:14:LEU:HD11	2.49	0.47
24:Z:75:THR:HB	24:Z:83:LYS:HG2	1.96	0.47
25:AA:1572:A:H2'	25:AA:1573:A:C8	2.49	0.47
28:AD:425:LEU:HB3	39:AO:88:GLN:HE22	1.79	0.47
42:AR:254:ASP:OD1	42:AR:259:TYR:OH	2.32	0.47
47:AW:104:ILE:HG12	47:AW:114:ILE:HG12	1.96	0.47
55:A4:152:ILE:HA	55:A4:172:MET:HE3	1.96	0.47
76:i:79:TRP:CD1	76:i:80:LEU:HG	2.50	0.47
85:s:211:VAL:HG22	85:s:230:ARG:HG2	1.96	0.47
1:A:2071:U:O2'	64:6:28:ARG:NH2	2.47	0.47
2:B:8:U:O2	2:B:15:A:N6	2.47	0.47
3:D:124:GLU:HG2	3:D:144:GLY:HA3	1.97	0.47
20:V:48:PRO:HG3	23:Y:234:LEU:HD21	1.97	0.47
25:AA:829:C:H1'	25:AA:857:G:H22	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:AA:1337:U:H2'	25:AA:1338:A:H8	1.79	0.47
42:AR:167:HIS:HB3	42:AR:193:ILE:HD13	1.96	0.47
46:AV:251:TRP:HH2	51:A0:142:VAL:HG22	1.80	0.47
52:A1:264:GLU:HG2	52:A1:268:GLN:HE21	1.80	0.47
64:6:173:LEU:HD13	64:6:272:LEU:HD22	1.96	0.47
85:s:332:LEU:HD13	85:s:372:TYR:HB2	1.96	0.47
1:A:1977:U:H2'	1:A:1978:A:H8	1.79	0.47
1:A:2151:A:O3'	81:o:38:ARG:NH2	2.47	0.47
1:A:2245:A:H4'	1:A:2246:A:OP1	2.13	0.47
1:A:2336:U:C2	1:A:2337:A:C8	3.03	0.47
2:B:12:U:O2'	2:B:14:A:OP1	2.31	0.47
18:T:134:LEU:HD23	18:T:174:GLU:HA	1.95	0.47
25:AA:661:C:H2'	25:AA:662:U:C6	2.50	0.47
25:AA:982:A:H2'	25:AA:983:C:H6	1.80	0.47
28:AD:147:PRO:O	28:AD:155:GLN:NE2	2.48	0.47
33:AI:100:VAL:HG12	33:AI:106:PRO:HA	1.95	0.47
39:AO:96:ARG:HG3	39:AO:97:ARG:HG3	1.97	0.47
41:AQ:72:ILE:HD13	53:A2:104:LEU:HD21	1.96	0.47
64:6:204:VAL:HG11	64:6:216:LEU:HD22	1.97	0.47
74:g:85:PHE:N	74:g:114:GLU:O	2.47	0.47
31:AG:161:LEU:HD22	31:AG:209:LEU:HD21	1.96	0.47
1:A:1755:A:O2'	6:H:64:LEU:O	2.29	0.47
1:A:2491:C:H2'	1:A:2492:G:H8	1.80	0.47
1:A:2933:G:N2	1:A:2936:U:O2	2.43	0.47
22:X:42:HIS:CG	22:X:86:ILE:HD11	2.50	0.47
25:AA:1049:A:H5''	36:AL:198:ARG:HB2	1.97	0.47
25:AA:1217:G:H21	32:AH:126:ILE:HG22	1.79	0.47
31:AG:285:VAL:HG22	31:AG:328:VAL:HG22	1.97	0.47
32:AH:106:ILE:HD11	32:AH:143:LEU:HD23	1.97	0.47
38:AN:57:GLN:O	38:AN:87:LYS:NZ	2.48	0.47
64:6:303:PHE:HA	64:6:306:LYS:HE2	1.97	0.47
82:p:110:TRP:H	82:p:110:TRP:CD1	2.33	0.47
1:A:1718:A:N3	1:A:1911:C:O2'	2.41	0.47
7:I:100:GLN:HB2	7:I:177:LEU:HD11	1.96	0.47
19:U:71:ARG:NH1	19:U:73:GLN:OE1	2.44	0.47
55:A4:318:GLU:OE2	55:A4:322:HIS:NE2	2.48	0.47
56:Ax:4:A:H2'	56:Ax:5:A:H8	1.80	0.47
70:c:93:VAL:HG11	70:c:119:LEU:HG	1.97	0.47
73:f:84:THR:H	73:f:87:GLU:HB2	1.80	0.47
1:A:1889:C:OP1	11:M:133:LYS:NZ	2.48	0.46
1:A:1911:C:H2'	1:A:1912:A:C8	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3078:C:N4	1:A:3079:G:O6	2.48	0.46
17:S:164:THR:HG22	17:S:165:GLU:H	1.80	0.46
19:U:69:ARG:HH22	19:U:98:GLN:HE21	1.63	0.46
23:Y:98:LEU:HB3	23:Y:142:LEU:HD21	1.97	0.46
25:AA:1106:C:O2'	25:AA:1108:C:OP2	2.23	0.46
25:AA:1523:A:H5''	46:AV:68:SER:N	2.30	0.46
32:AH:76:LEU:HD22	32:AH:174:LYS:HD3	1.95	0.46
52:A1:177:LEU:HB2	52:A1:187:LYS:HZ2	1.80	0.46
72:e:160:LEU:HD11	72:e:260:LEU:HD12	1.97	0.46
1:A:2115:U:H2'	1:A:2116:C:H6	1.80	0.46
1:A:2389:C:P	63:5:301:PRO:HB3	2.55	0.46
23:Y:191:ASN:HB3	23:Y:194:TYR:HB3	1.97	0.46
25:AA:1201:A:O2'	25:AA:1417:A:N3	2.38	0.46
25:AA:1237:A:O2'	25:AA:1254:C:O2'	2.23	0.46
25:AA:1578:A:H2'	25:AA:1579:C:H6	1.80	0.46
71:d:197:VAL:HG22	71:d:212:ILE:HG23	1.97	0.46
72:e:55:ARG:NH1	72:e:149:LEU:O	2.48	0.46
80:m:58:LYS:HA	80:m:77:MET:HE2	1.96	0.46
85:s:298:GLN:HG3	85:s:335:TRP:CZ3	2.51	0.46
1:A:2708:C:O2'	58:0:96:ASN:OD1	2.23	0.46
8:J:104:THR:OG1	8:J:149:ARG:O	2.33	0.46
13:O:131:PRO:HD3	58:0:137:ILE:HD12	1.98	0.46
25:AA:974:U:O2'	25:AA:975:A:N7	2.47	0.46
25:AA:1525:C:H5	46:AV:103:TYR:HA	1.79	0.46
52:A1:136:ALA:HB3	55:A4:57:VAL:HG12	1.97	0.46
55:A4:438:LEU:O	55:A4:441:THR:OG1	2.33	0.46
64:6:187:VAL:HG13	64:6:319:PHE:HB3	1.97	0.46
80:m:69:ARG:HG3	80:m:70:GLU:HG3	1.97	0.46
1:A:3213:A:H2'	1:A:3214:C:C6	2.49	0.46
25:AA:1422:G:H2'	25:AA:1423:A:C8	2.51	0.46
39:AO:105:CYS:SG	39:AO:108:CYS:CB	2.92	0.46
66:8:167:ASN:O	72:e:203:LYS:NZ	2.48	0.46
82:p:104:HIS:HA	82:p:132:GLU:HA	1.96	0.46
83:q:89:GLU:HA	83:q:93:TYR:HD2	1.80	0.46
7:I:146:LEU:HD22	78:k:22:PRO:HB2	1.97	0.46
13:O:52:MET:HA	13:O:55:TYR:HD2	1.79	0.46
15:Q:62:ILE:HD13	46:AV:87:HIS:CD2	2.50	0.46
20:V:122:LEU:HD22	20:V:133:ILE:HD11	1.98	0.46
25:AA:649:A:H3'	28:AD:335:LYS:HE2	1.97	0.46
30:AF:85:VAL:HB	48:AX:370:LYS:HG3	1.97	0.46
55:A4:170:VAL:HG23	55:A4:247:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:A4:452:GLN:HG2	55:A4:453:HIS:HD2	1.81	0.46
63:5:99:TYR:HD1	63:5:270:ILE:HG12	1.81	0.46
82:p:56:ASP:O	82:p:60:ARG:HG3	2.15	0.46
10:L:108:ILE:HA	10:L:114:PRO:HA	1.98	0.46
25:AA:1035:U:H2'	25:AA:1036:A:C8	2.50	0.46
25:AA:1341:C:OP1	50:AZ:100:LYS:N	2.49	0.46
55:A4:598:LEU:HD22	55:A4:602:HIS:HE1	1.80	0.46
70:c:42:GLN:HG3	76:i:38:LEU:HG	1.98	0.46
1:A:1747:G:OP2	1:A:1749:C:N4	2.47	0.46
1:A:1839:C:H2'	1:A:1840:C:C6	2.50	0.46
1:A:2065:A:C4	1:A:2066:C:C5	3.04	0.46
1:A:2170:G:H2'	1:A:2171:U:C5	2.51	0.46
1:A:2950:U:H2'	1:A:2951:A:C8	2.50	0.46
4:E:80:LEU:HD12	4:E:323:GLY:HA3	1.97	0.46
10:L:126:SER:O	10:L:129:LYS:HG2	2.16	0.46
25:AA:1488:5MC:O2	25:AA:1584:MA6:O2'	2.27	0.46
28:AD:317:HIS:HD2	28:AD:318:ARG:H	1.63	0.46
40:AP:115:GLN:HB3	40:AP:122:VAL:HG22	1.97	0.46
46:AV:40:TRP:HE1	46:AV:111:THR:HG23	1.81	0.46
46:AV:263:MET:HB2	46:AV:337:LEU:HD13	1.97	0.46
64:6:120:GLU:OE2	66:8:119:LYS:NZ	2.48	0.46
71:d:153:ASN:ND2	71:d:183:TRP:H	2.14	0.46
7:I:96:ILE:HA	7:I:155:VAL:HG12	1.96	0.46
13:O:130:LEU:HD22	58:O:134:THR:HG23	1.97	0.46
15:Q:152:ARG:NH1	15:Q:161:GLU:OE2	2.48	0.46
22:X:166:LEU:HD13	22:X:196:ILE:HD11	1.98	0.46
25:AA:867:C:H2'	25:AA:870:C:H42	1.80	0.46
25:AA:982:A:H2'	25:AA:983:C:C6	2.51	0.46
25:AA:1483:C:O2	25:AA:1567:A:N6	2.49	0.46
42:AR:281:ILE:HD12	42:AR:300:LEU:HG	1.98	0.46
46:AV:276:CYS:HA	46:AV:348:GLU:HB3	1.98	0.46
51:A0:129:ARG:NH1	51:A0:205:ALA:O	2.42	0.46
55:A4:336:ASN:OD1	55:A4:371:THR:OG1	2.32	0.46
62:4:90:VAL:O	62:4:99:LYS:HA	2.16	0.46
71:d:153:ASN:ND2	71:d:183:TRP:O	2.46	0.46
81:o:15:ARG:HB3	81:o:18:ILE:HG12	1.98	0.46
85:s:66:TRP:O	85:s:69:THR:OG1	2.27	0.46
16:R:85:ALA:O	16:R:89:ASN:ND2	2.31	0.46
19:U:136:GLN:HE22	71:d:83:GLY:HA3	1.80	0.46
25:AA:1407:U:H2'	25:AA:1408:A:H8	1.81	0.46
46:AV:364:LEU:HG	46:AV:368:GLU:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:A0:91:GLU:HB2	51:A0:121:LYS:HA	1.98	0.46
56:Ax:41:C:H2'	56:Ax:42:G:C8	2.51	0.46
63:5:108:HIS:CE1	63:5:110:ARG:HB3	2.51	0.46
65:7:298:GLN:HE22	65:7:323:MET:HA	1.80	0.46
66:8:67:ARG:HG2	66:8:71:LYS:HE3	1.98	0.46
73:f:104:GLU:HG2	73:f:155:ARG:HE	1.80	0.46
1:A:1917:A:N1	1:A:1997:C:H1'	2.30	0.46
1:A:2586:U:H2'	1:A:2587:G:C8	2.50	0.46
25:AA:1188:A:H4'	25:AA:1189:U:H5'	1.98	0.46
39:AO:95:ILE:HG12	39:AO:100:VAL:HG12	1.98	0.46
42:AR:231:CYS:SG	42:AR:242:TYR:HA	2.56	0.46
48:AX:266:ASN:HB3	48:AX:310:LEU:HD22	1.98	0.46
50:AZ:46:LYS:HA	50:AZ:49:TYR:CE2	2.51	0.46
65:7:262:ASP:OD1	65:7:263:VAL:N	2.49	0.46
85:s:307:ARG:HG3	85:s:310:ARG:H	1.81	0.46
1:A:1912:A:H2'	1:A:1913:G:C8	2.51	0.45
1:A:2845:A:H2'	1:A:2846:G:C8	2.52	0.45
7:I:93:ASN:HA	7:I:157:GLU:HA	1.97	0.45
25:AA:649:A:O2'	25:AA:651:A:OP2	2.32	0.45
25:AA:702:C:H2'	25:AA:703:A:O4'	2.16	0.45
25:AA:1353:A:H5'	25:AA:1354:A:C8	2.50	0.45
31:AG:172:LEU:HD11	31:AG:237:GLU:HG2	1.98	0.45
42:AR:144:GLU:HG2	42:AR:180:THR:HG23	1.98	0.45
48:AX:116:SER:HB3	48:AX:119:TYR:HD2	1.81	0.45
66:8:171:PHE:HB3	73:f:186:VAL:HB	1.98	0.45
72:e:248:ASN:HA	72:e:252:HIS:HE1	1.81	0.45
1:A:1953:A:O2'	1:A:2463:A:OP1	2.33	0.45
6:H:65:ALA:HB2	6:H:71:PRO:HA	1.98	0.45
9:K:140:ASN:HB2	70:c:262:GLY:HA2	1.97	0.45
9:K:169:LEU:HD22	84:r:75:TRP:CD1	2.51	0.45
17:S:79:VAL:HA	17:S:82:LYS:HE2	1.98	0.45
20:V:105:ARG:NH2	71:d:171:ASP:OD1	2.49	0.45
25:AA:818:C:C2	25:AA:819:A:C8	3.04	0.45
25:AA:1174:U:H2'	25:AA:1175:G:C8	2.50	0.45
25:AA:1561:C:H2'	25:AA:1562:G:C8	2.51	0.45
27:AC:104:LEU:HD23	27:AC:123:VAL:HG12	1.98	0.45
34:AJ:102:LEU:HD21	34:AJ:132:CYS:HA	1.98	0.45
46:AV:225:LEU:HD11	46:AV:283:LEU:HD22	1.98	0.45
67:9:115:GLU:HG2	67:9:121:PRO:HD3	1.98	0.45
83:q:37:PRO:HG2	83:q:68:SER:HA	1.96	0.45
1:A:2192:A:H4'	8:J:139:SER:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:P:142:ASN:OD1	82:p:184:ASN:ND2	2.42	0.45
25:AA:1512:A:N6	25:AA:1536:A:O4'	2.49	0.45
28:AD:282:ILE:HG13	28:AD:327:ILE:HD13	1.98	0.45
31:AG:240:PHE:HA	31:AG:243:ARG:HD3	1.98	0.45
53:A2:94:GLY:C	53:A2:95:GLU:HG3	2.41	0.45
65:7:193:MET:HE3	65:7:194:PRO:HD2	1.98	0.45
1:A:1928:A:H2'	1:A:1929:A:H8	1.80	0.45
1:A:2187:C:H2'	1:A:2188:A:H8	1.80	0.45
1:A:2869:A:OP1	61:3:127:ALA:N	2.43	0.45
7:I:100:GLN:HA	7:I:151:ASN:HD22	1.81	0.45
25:AA:1007:G:H2'	25:AA:1008:A:H8	1.81	0.45
25:AA:1047:A:H2'	25:AA:1047:A:N3	2.32	0.45
25:AA:1376:C:H4'	25:AA:1377:C:H5'	1.98	0.45
25:AA:1485:G:H2'	25:AA:1486:B8T:O4'	2.17	0.45
39:AO:94:CYS:HB2	39:AO:108:CYS:SG	2.56	0.45
64:6:199:ALA:HA	64:6:256:PRO:HB3	1.99	0.45
83:q:55:ARG:HE	83:q:59:LYS:HE3	1.81	0.45
85:s:90:LYS:HD2	85:s:232:GLN:HB2	1.98	0.45
1:A:1862:U:H2'	1:A:1863:A:H8	1.81	0.45
1:A:2016:C:H2'	1:A:2017:U:C6	2.51	0.45
1:A:2930:U:H2'	1:A:2931:A:H8	1.82	0.45
65:7:78:VAL:HB	71:d:282:ILE:HB	1.99	0.45
70:c:93:VAL:HG22	70:c:180:LEU:HD12	1.99	0.45
82:p:78:THR:HB	82:p:102:ARG:HG3	1.99	0.45
1:A:2081:U:H2'	1:A:2082:G:C8	2.52	0.45
7:I:185:ILE:HG22	86:t:51:ALA:HB2	1.98	0.45
10:L:86:ILE:HA	10:L:105:VAL:HG12	1.98	0.45
12:N:64:ARG:NH1	12:N:144:LYS:O	2.49	0.45
25:AA:1399:A:H2'	25:AA:1400:U:H6	1.81	0.45
25:AA:1457:G:H5''	30:AF:104:LYS:HD2	1.98	0.45
27:AC:100:PHE:HB3	27:AC:103:CYS:HB2	1.98	0.45
43:AS:113:ASP:HB2	43:AS:116:LYS:HB3	1.99	0.45
48:AX:203:LYS:HA	48:AX:221:PRO:HA	1.98	0.45
48:AX:245:LYS:HE2	48:AX:249:ARG:HH21	1.82	0.45
56:Ax:65:C:H2'	56:Ax:66:C:C6	2.51	0.45
80:m:82:ASP:O	80:m:89:ARG:NH2	2.49	0.45
1:A:1698:C:O2'	1:A:1702:A:N3	2.40	0.45
1:A:1790:A:OP1	60:2:82:ARG:NH1	2.49	0.45
1:A:1831:G:O6	69:b:4:ARG:NH2	2.48	0.45
1:A:2060:A:C8	1:A:2079:C:C4	3.05	0.45
1:A:2898:U:O2'	61:3:113:ARG:NH2	2.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3139:G:H2'	1:A:3140:A:C8	2.52	0.45
3:D:110:LEU:HD22	63:5:30:ALA:HB2	1.99	0.45
3:D:184:LEU:HD13	3:D:226:ILE:HD11	1.99	0.45
3:D:246:ARG:HH21	3:D:250:VAL:HG13	1.82	0.45
4:E:155:PHE:HA	65:7:309:HIS:CE1	2.52	0.45
7:I:176:LEU:HD23	7:I:188:ARG:HG3	1.98	0.45
23:Y:95:ASN:OD1	23:Y:149:ARG:NH1	2.50	0.45
25:AA:1317:A:H3'	25:AA:1318:A:H8	1.80	0.45
25:AA:1577:U:H2'	25:AA:1578:A:C8	2.52	0.45
30:AF:151:ASN:O	30:AF:223:LYS:NZ	2.40	0.45
32:AH:123:SER:OG	32:AH:124:VAL:N	2.49	0.45
39:AO:136:TYR:HD2	39:AO:138:PRO:HD2	1.82	0.45
66:8:145:GLU:HG2	72:e:212:HIS:HE1	1.81	0.45
77:j:91:TRP:CD2	81:o:58:GLN:HG2	2.51	0.45
1:A:2725:A:H5'	71:d:40:ARG:HH22	1.81	0.45
1:A:2794:C:H2'	1:A:2795:U:H6	1.81	0.45
1:A:3181:U:OP1	84:r:94:ARG:NH2	2.48	0.45
13:O:80:LEU:HD12	13:O:86:ILE:HG12	1.98	0.45
37:AM:55:ASP:OD2	44:AT:146:GLN:NE2	2.50	0.45
38:AN:67:ARG:NH1	38:AN:80:GLU:OE2	2.50	0.45
66:8:188:PRO:HG2	80:m:78:PRO:HB3	1.99	0.45
1:A:1856:A:OP2	1:A:2986:C:O2'	2.35	0.45
1:A:2118:U:C2	1:A:2119:U:C5	3.05	0.45
1:A:3155:C:H2'	1:A:3156:A:C8	2.52	0.45
1:A:3172:C:H1'	1:A:3173:G:N2	2.32	0.45
25:AA:748:G:H2'	25:AA:749:G:H8	1.82	0.45
25:AA:1399:A:H2'	25:AA:1400:U:C6	2.52	0.45
29:AE:31:ASP:OD1	45:AU:170:ARG:NH2	2.50	0.45
47:AW:140:VAL:HG12	47:AW:172:ILE:HG12	1.99	0.45
85:s:153:GLU:HG3	85:s:176:PHE:HB2	1.99	0.45
1:A:2380:C:O2'	67:9:46:SER:HB3	2.17	0.45
1:A:2894:U:H5''	1:A:2895:U:O4'	2.16	0.45
8:J:101:ALA:HB2	8:J:109:ALA:HB2	1.99	0.45
10:L:52:HIS:CD2	10:L:53:ARG:HG3	2.51	0.45
25:AA:1194:C:H2'	25:AA:1195:U:C6	2.51	0.45
25:AA:1265:C:O2'	32:AH:123:SER:HB2	2.17	0.45
28:AD:380:LEU:HB2	42:AR:91:PHE:CD2	2.52	0.45
35:AK:56:SER:O	35:AK:60:ASN:ND2	2.50	0.45
51:A0:73:LEU:O	51:A0:76:LEU:HG	2.17	0.45
64:6:234:HIS:CE1	64:6:257:PRO:HA	2.52	0.45
65:7:192:TRP:O	65:7:295:ARG:NH2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:8:147:LEU:HB3	66:8:158:HIS:HE1	1.82	0.45
66:8:182:ILE:H	80:m:61:GLY:HA3	1.81	0.45
1:A:1737:A:O2'	76:i:93:ARG:NH2	2.44	0.44
1:A:2230:A:H62	1:A:2975:G:H1'	1.81	0.44
1:A:2746:U:H2'	1:A:2747:U:H6	1.82	0.44
22:X:40:PRO:HB3	22:X:43:TYR:CZ	2.52	0.44
25:AA:1006:U:H2'	25:AA:1007:G:C8	2.52	0.44
25:AA:1541:U:H2'	25:AA:1542:U:C6	2.52	0.44
33:AI:147:ILE:HG21	33:AI:170:LEU:HD13	1.99	0.44
48:AX:189:LYS:HE2	48:AX:230:ILE:HG23	1.99	0.44
55:A4:414:LYS:HG2	55:A4:453:HIS:CE1	2.52	0.44
64:6:51:TYR:OH	64:6:60:ARG:HG2	2.17	0.44
70:c:57:PRO:HB2	70:c:184:PHE:HE2	1.82	0.44
72:e:146:ARG:HH11	72:e:263:TYR:HE2	1.64	0.44
72:e:159:LEU:HD11	72:e:252:HIS:HB2	1.99	0.44
1:A:3009:C:O2'	1:A:3115:U:OP1	2.31	0.44
6:H:78:ARG:NH1	22:X:87:LEU:O	2.50	0.44
25:AA:740:G:H2'	25:AA:741:A:C8	2.50	0.44
46:AV:50:LEU:HD13	46:AV:84:GLU:HB3	1.97	0.44
46:AV:117:LEU:HD23	46:AV:122:GLN:HG2	2.00	0.44
49:AY:329:HIS:CE1	49:AY:330:GLU:HG3	2.52	0.44
59:1:19:ARG:HB2	59:1:62:ILE:HD11	1.98	0.44
65:7:51:GLU:HG2	65:7:221:VAL:HG12	1.98	0.44
1:A:1863:A:H2'	1:A:1864:A:H8	1.83	0.44
2:B:75:C:C4	72:e:216:LYS:HB2	2.52	0.44
15:Q:96:ARG:NH2	15:Q:285:GLU:HB3	2.30	0.44
20:V:56:LEU:HD13	20:V:86:VAL:HG21	1.99	0.44
25:AA:1227:G:H1'	32:AH:125:HIS:CD2	2.53	0.44
25:AA:1416:A:H2'	25:AA:1417:A:C8	2.53	0.44
30:AF:170:VAL:HG13	30:AF:237:ALA:HA	1.99	0.44
32:AH:61:PRO:HG3	55:A4:73:ALA:HB2	1.98	0.44
39:AO:76:ASP:HB2	39:AO:109:ARG:HH22	1.82	0.44
69:b:85:ARG:NE	69:b:87:GLU:OE2	2.44	0.44
70:c:165:VAL:HG13	70:c:222:GLN:HG3	2.00	0.44
1:A:1896:U:C2	1:A:1897:A:C8	3.06	0.44
1:A:2072:A:H2'	1:A:2073:A:C8	2.53	0.44
1:A:2472:A:N3	1:A:2474:C:N4	2.66	0.44
1:A:2514:C:H2'	1:A:2515:U:H6	1.83	0.44
6:H:62:VAL:HG11	22:X:65:VAL:HG21	1.99	0.44
7:I:188:ARG:O	7:I:192:ILE:HG12	2.17	0.44
15:Q:182:ARG:HD2	15:Q:218:ASN:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:AA:1033:U:H4'	29:AE:94:VAL:HG12	1.99	0.44
25:AA:1213:A:H1'	25:AA:1239:C:O2'	2.17	0.44
26:AB:67:LEU:HD11	26:AB:138:ARG:HH21	1.82	0.44
32:AH:76:LEU:HG	32:AH:148:LEU:HD11	1.99	0.44
48:AX:93:THR:HG21	48:AX:365:TRP:HZ3	1.82	0.44
63:5:103:ALA:HB1	63:5:267:GLU:HG3	1.99	0.44
66:8:90:THR:HG23	66:8:94:PHE:HD2	1.83	0.44
72:e:187:THR:O	72:e:191:THR:HG23	2.17	0.44
80:m:54:VAL:HG11	80:m:75:LEU:HG	1.98	0.44
81:o:53:TYR:HD2	81:o:54:MET:HG3	1.82	0.44
1:A:1861:U:H2'	1:A:1862:U:C6	2.53	0.44
1:A:3158:A:H2'	1:A:3159:A:H8	1.82	0.44
4:E:111:THR:OG1	4:E:113:ASP:OD1	2.28	0.44
46:AV:138:PHE:CG	51:A0:72:PRO:HA	2.52	0.44
64:6:217:LEU:HB3	64:6:236:LEU:HD13	1.98	0.44
68:a:46:ASN:O	68:a:63:PRO:HD2	2.18	0.44
1:A:2117:U:C2	1:A:2118:U:C5	3.05	0.44
6:H:53:THR:OG1	22:X:83:GLU:OE2	2.29	0.44
7:I:116:LEU:HB3	7:I:121:ILE:HB	2.00	0.44
22:X:125:VAL:HG23	22:X:127:VAL:HG13	1.99	0.44
23:Y:104:VAL:HG12	67:9:72:PRO:HG3	1.98	0.44
25:AA:1042:U:H2'	25:AA:1043:C:C6	2.52	0.44
30:AF:234:ARG:HB2	53:A2:53:MET:HE1	2.00	0.44
32:AH:123:SER:HB3	32:AH:127:TYR:HB2	1.99	0.44
40:AP:124:TYR:HB3	41:AQ:9:ALA:HB2	2.00	0.44
52:A1:137:LEU:HD22	52:A1:143:CYS:HA	2.00	0.44
55:A4:308:LYS:HE2	55:A4:311:GLU:HG2	2.00	0.44
55:A4:354:LEU:HD11	55:A4:388:ARG:HH22	1.83	0.44
56:Ax:8:U:H3	56:Ax:14:A:H62	1.64	0.44
59:1:34:ARG:HD3	59:1:41:LEU:HG	1.99	0.44
64:6:192:GLU:OE2	64:6:322:ARG:NH1	2.49	0.44
66:8:110:GLU:OE2	66:8:113:ARG:NH2	2.46	0.44
1:A:1902:C:H1'	76:i:126:LYS:HB3	1.99	0.44
1:A:2099:U:H2'	1:A:2100:C:H6	1.83	0.44
1:A:2466:A:OP1	15:Q:235:ARG:NH1	2.49	0.44
1:A:2495:U:O4	1:A:2509:A:H2	2.00	0.44
1:A:2668:A:H2'	1:A:2669:A:H8	1.82	0.44
1:A:2693:A:OP1	81:o:15:ARG:NH1	2.51	0.44
6:H:62:VAL:HG22	6:H:77:HIS:CD2	2.51	0.44
25:AA:942:A:N6	25:AA:1047:A:H5'	2.32	0.44
25:AA:1044:U:H2'	25:AA:1045:G:O4'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:AD:364:ASP:OD2	28:AD:388:ARG:NH1	2.50	0.44
1:A:2166:C:H2'	1:A:2167:A:C8	2.53	0.44
5:F:116:THR:O	5:F:120:VAL:HG23	2.18	0.44
15:Q:96:ARG:HH21	15:Q:286:ILE:HG13	1.82	0.44
25:AA:800:C:H2'	25:AA:801:A:C8	2.52	0.44
25:AA:867:C:H2'	25:AA:870:C:N4	2.33	0.44
25:AA:1175:G:H2'	25:AA:1176:G:H8	1.83	0.44
25:AA:1373:U:H2'	25:AA:1374:A:H8	1.82	0.44
48:AX:132:THR:N	95:AX:501:ATP:O2B	2.48	0.44
64:6:374:GLU:OE2	82:p:140:SER:OG	2.28	0.44
72:e:162:ARG:HD2	72:e:169:ASP:HB3	1.99	0.44
74:g:96:VAL:HG22	74:g:110:ILE:HG12	2.00	0.44
1:A:1894:G:H2'	1:A:1895:C:H6	1.83	0.44
1:A:2016:C:H2'	1:A:2017:U:H6	1.82	0.44
1:A:2414:C:N4	85:s:163:VAL:O	2.38	0.44
1:A:2883:A:H61	14:P:172:LEU:HB3	1.82	0.44
8:J:114:LEU:HD12	8:J:157:LYS:HG3	1.99	0.44
12:N:105:MET:HG2	12:N:179:VAL:HG13	2.00	0.44
16:R:141:ILE:HG22	68:a:51:LEU:HD12	2.00	0.44
19:U:8:PRO:HA	23:Y:183:GLN:HE22	1.83	0.44
25:AA:881:A:N6	39:AO:82:LYS:HB3	2.33	0.44
25:AA:1034:U:H2'	25:AA:1035:U:H6	1.83	0.44
25:AA:1035:U:H2'	25:AA:1036:A:H8	1.82	0.44
55:A4:80:ARG:HH22	55:A4:485:ALA:HB2	1.81	0.44
55:A4:100:SER:OG	55:A4:104:ARG:NH1	2.51	0.44
63:5:59:THR:HG22	63:5:71:ALA:HB3	1.99	0.44
78:k:11:ARG:HH11	78:k:46:ASN:HA	1.83	0.44
80:m:54:VAL:HG21	80:m:68:TYR:HB3	1.99	0.44
82:p:82:CYS:O	82:p:97:SER:OG	2.34	0.44
83:q:111:GLU:HG3	83:q:114:ARG:HH21	1.83	0.44
85:s:119:PRO:HG3	85:s:394:TRP:CD2	2.53	0.44
1:A:2728:C:H2'	1:A:2729:U:H6	1.82	0.43
1:A:2942:C:H2'	1:A:2943:G:H8	1.83	0.43
1:A:3112:A:N7	1:A:3200:U:O2	2.51	0.43
3:D:140:ALA:HB2	3:D:153:ALA:HB2	1.99	0.43
25:AA:1326:A:O4'	28:AD:114:ARG:NH1	2.51	0.43
25:AA:1366:C:H3'	25:AA:1367:A:H5'	1.99	0.43
25:AA:1464:G:H2'	25:AA:1465:C:C6	2.53	0.43
29:AE:37:ARG:N	29:AE:67:ASP:O	2.50	0.43
39:AO:64:TYR:OH	39:AO:125:GLN:NE2	2.44	0.43
72:e:159:LEU:HD13	72:e:254:TRP:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:m:57:VAL:HG22	80:m:63:THR:HG22	1.99	0.43
85:s:113:VAL:HG11	85:s:257:VAL:HG21	2.00	0.43
1:A:1993:A:H8	1:A:2498:U:HO2'	1.66	0.43
1:A:2011:G:O6	76:i:113:ARG:NH1	2.40	0.43
1:A:2346:U:H2'	1:A:2347:C:C6	2.52	0.43
1:A:2593:G:O2'	1:A:2631:G:O6	2.35	0.43
1:A:2710:C:H2'	1:A:2711:A:H8	1.83	0.43
4:E:150:LYS:O	4:E:174:GLN:N	2.44	0.43
24:Z:100:HIS:HB3	24:Z:106:VAL:HG11	2.00	0.43
26:AB:149:ARG:NH2	41:AQ:84:TRP:O	2.52	0.43
31:AG:291:GLY:N	31:AG:327:ASP:OD1	2.51	0.43
48:AX:145:CYS:SG	48:AX:259:LEU:HD22	2.58	0.43
61:3:154:GLN:O	61:3:158:LEU:HG	2.19	0.43
71:d:109:THR:OG1	71:d:110:GLU:N	2.49	0.43
83:q:101:GLU:HG3	83:q:104:ARG:HH21	1.83	0.43
1:A:1765:C:O3'	76:i:75:ARG:NH2	2.50	0.43
1:A:1863:A:H2'	1:A:1864:A:C8	2.53	0.43
1:A:2152:A:OP1	81:o:34:ASN:HB3	2.18	0.43
18:T:97:LEU:HD22	18:T:112:LYS:HG3	1.99	0.43
20:V:137:PHE:HA	20:V:143:ARG:HA	2.01	0.43
25:AA:1553:A:H2'	25:AA:1554:G:C8	2.53	0.43
27:AC:37:ASN:N	27:AC:37:ASN:OD1	2.52	0.43
48:AX:338:ASP:OD1	52:A1:312:TYR:OH	2.27	0.43
50:AZ:81:GLU:OE2	50:AZ:84:ARG:NH2	2.34	0.43
63:5:218:LEU:HD13	63:5:262:ILE:HD13	2.00	0.43
65:7:184:VAL:HG22	65:7:294:ILE:HG12	1.99	0.43
70:c:105:ARG:HG3	70:c:110:ILE:HB	2.00	0.43
72:e:124:TRP:CE2	80:m:72:ARG:HG2	2.53	0.43
72:e:198:ASN:HB2	72:e:200:MET:HE2	1.99	0.43
73:f:94:HIS:HB3	73:f:156:VAL:HG22	2.00	0.43
1:A:1953:A:OP1	4:E:232:GLY:HA2	2.19	0.43
1:A:2164:C:H2'	1:A:2165:C:C6	2.53	0.43
1:A:2350:A:H1'	1:A:2351:U:H5	1.83	0.43
1:A:2408:U:C2	1:A:2409:A:N7	2.87	0.43
2:B:23:A:H2'	2:B:24:G:H8	1.81	0.43
12:N:96:TYR:HB3	12:N:151:VAL:HB	2.00	0.43
25:AA:856:A:C2	25:AA:857:G:C8	3.06	0.43
25:AA:924:A:N3	34:AJ:56:PRO:HB3	2.34	0.43
25:AA:1488:5MC:H2'	25:AA:1489:G:C8	2.54	0.43
27:AC:115:ASN:ND2	49:AY:309:LYS:O	2.51	0.43
30:AF:53:LYS:HD2	30:AF:58:LEU:HD23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:7:106:ALA:O	65:7:113:TRP:N	2.52	0.43
72:e:124:TRP:CD2	80:m:72:ARG:HG2	2.53	0.43
78:k:17:ARG:HH12	78:k:19:GLN:HB2	1.83	0.43
1:A:2409:A:H2'	1:A:2410:U:C6	2.54	0.43
1:A:2465:U:H2'	1:A:2466:A:C8	2.53	0.43
1:A:2841:U:OP2	21:W:39:SER:OG	2.35	0.43
5:F:92:ARG:HB2	5:F:176:VAL:HG21	2.00	0.43
7:I:119:HIS:O	7:I:160:LYS:HD2	2.19	0.43
13:O:82:GLU:OE1	13:O:82:GLU:N	2.52	0.43
24:Z:69:VAL:HG23	24:Z:91:LEU:HD21	2.01	0.43
29:AE:35:ILE:HG13	36:AL:97:MET:HE1	2.00	0.43
1:A:2256:U:H2'	1:A:2257:C:C6	2.54	0.43
1:A:2508:C:H2'	1:A:2509:A:C8	2.53	0.43
19:U:112:PRO:HD2	23:Y:75:GLY:HA3	1.99	0.43
25:AA:806:C:C2	51:A0:11:ILE:HB	2.54	0.43
25:AA:1173:C:H2'	25:AA:1174:U:C6	2.54	0.43
25:AA:1311:C:O2	30:AF:36:ARG:NH2	2.52	0.43
26:AB:233:THR:HA	43:AS:44:PRO:HG3	2.00	0.43
46:AV:107:TRP:HB3	46:AV:382:TRP:CG	2.54	0.43
47:AW:144:LEU:HD23	47:AW:167:ALA:HB2	2.00	0.43
48:AX:204:VAL:HG12	48:AX:246:GLU:HG3	2.00	0.43
72:e:113:ASP:N	72:e:113:ASP:OD1	2.50	0.43
72:e:217:PHE:HE2	72:e:226:ASN:HB3	1.83	0.43
1:A:2987:U:O2'	1:A:2991:U:OP1	2.33	0.43
6:H:56:VAL:HB	6:H:80:TYR:HB3	2.00	0.43
9:K:5:SER:HB2	9:K:8:PRO:HD2	2.00	0.43
14:P:178:ILE:HD13	82:p:174:LYS:HE2	2.00	0.43
25:AA:1175:G:H2'	25:AA:1176:G:C8	2.54	0.43
25:AA:1545:U:H2'	25:AA:1546:A:C8	2.54	0.43
28:AD:325:ARG:NH2	28:AD:430:THR:OXT	2.43	0.43
36:AL:163:ARG:HD2	36:AL:187:ILE:HD13	2.00	0.43
42:AR:194:GLN:NE2	42:AR:199:LYS:H	2.14	0.43
46:AV:30:LEU:HD23	46:AV:364:LEU:HD21	2.00	0.43
48:AX:205:GLN:HB2	48:AX:249:ARG:HH11	1.83	0.43
51:A0:145:HIS:ND1	51:A0:146:GLU:HG2	2.34	0.43
66:8:178:TYR:CG	80:m:65:HIS:HE1	2.37	0.43
71:d:287:LEU:HD11	71:d:293:TYR:HB2	2.00	0.43
73:f:133:GLU:HG2	73:f:149:VAL:HG22	2.01	0.43
1:A:1946:C:H2'	1:A:1947:C:H6	1.83	0.43
1:A:2186:C:H2'	1:A:2187:C:H6	1.83	0.43
1:A:2191:A:N6	1:A:2197:G:OP2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:AA:1292:A:C5	31:AG:216:LEU:HD12	2.54	0.43
25:AA:1522:U:O2'	46:AV:66:PRO:O	2.31	0.43
27:AC:77:ASP:OD1	32:AH:114:LYS:NZ	2.36	0.43
47:AW:149:LEU:HB2	47:AW:162:VAL:HG22	2.01	0.43
52:A1:74:ALA:O	52:A1:110:ASN:ND2	2.42	0.43
65:7:276:PHE:CD2	65:7:277:GLN:HG3	2.54	0.43
72:e:185:ARG:HH21	72:e:204:PHE:HB2	1.83	0.43
1:A:2529:U:OP2	3:D:208:ARG:HD3	2.18	0.43
5:F:223:HIS:HA	5:F:226:MET:HE3	2.00	0.43
19:U:137:ARG:HD2	20:V:104:TYR:HE1	1.83	0.43
25:AA:1233:C:O2	35:AK:86:ARG:HG2	2.18	0.43
28:AD:317:HIS:CD2	28:AD:318:ARG:H	2.37	0.43
43:AS:82:GLN:HE21	43:AS:133:ARG:HD3	1.82	0.43
66:8:182:ILE:HB	66:8:185:TYR:HB2	1.99	0.43
85:s:332:LEU:HD21	85:s:359:ALA:HB2	2.00	0.43
1:A:2841:U:H3'	21:W:41:ASN:HD21	1.84	0.43
1:A:3158:A:H2'	1:A:3159:A:C8	2.54	0.43
3:D:123:GLU:HG3	63:5:258:PRO:HG3	2.01	0.43
3:D:171:ARG:HD3	3:D:172:MET:HE2	2.01	0.43
25:AA:1116:A:H2'	25:AA:1117:A:C8	2.54	0.43
25:AA:1165:C:H2'	25:AA:1166:A:C8	2.54	0.43
25:AA:1452:U:H2'	25:AA:1453:A:C8	2.53	0.43
25:AA:1499:U:H2'	25:AA:1500:C:H6	1.84	0.43
52:A1:189:LYS:HD3	52:A1:233:SER:HA	2.01	0.43
69:b:76:VAL:HG22	69:b:86:GLU:HG3	2.01	0.43
84:r:179:PRO:HA	84:r:194:LEU:HD13	2.01	0.43
1:A:2081:U:H5''	81:o:63:ALA:HB3	2.01	0.42
1:A:2203:G:H2'	1:A:2204:U:C6	2.54	0.42
1:A:2747:U:H2'	1:A:2748:A:C8	2.51	0.42
20:V:16:PRO:HD2	20:V:19:TYR:HB2	2.01	0.42
23:Y:99:HIS:NE2	23:Y:103:TYR:HE2	2.17	0.42
24:Z:66:LEU:HD12	24:Z:122:LEU:HD23	1.99	0.42
25:AA:845:A:H2'	25:AA:846:A:C8	2.54	0.42
25:AA:1033:U:H2'	25:AA:1034:U:H6	1.84	0.42
25:AA:1255:U:H2'	25:AA:1256:A:C8	2.53	0.42
25:AA:1553:A:H2'	25:AA:1554:G:H8	1.84	0.42
35:AK:59:LYS:HB3	50:AZ:32:LYS:HD3	2.01	0.42
39:AO:177:PHE:HA	42:AR:168:ARG:NE	2.34	0.42
46:AV:275:LEU:O	46:AV:348:GLU:N	2.40	0.42
80:m:35:SER:O	80:m:39:SER:HB3	2.18	0.42
1:A:2799:U:H2'	1:A:2800:U:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2943:G:H2'	1:A:2944:C:C6	2.54	0.42
8:J:123:ILE:HG13	79:I:75:VAL:HG13	2.00	0.42
12:N:31:LYS:HE3	12:N:31:LYS:HB2	1.82	0.42
23:Y:96:GLU:HG2	23:Y:100:LYS:HE3	2.02	0.42
25:AA:1067:A:H2'	25:AA:1068:A:O4'	2.18	0.42
25:AA:1260:A:C6	25:AA:1336:G:C5	3.08	0.42
27:AC:150:PRO:HG3	49:AY:309:LYS:HB3	2.00	0.42
43:AS:70:ILE:HB	43:AS:100:VAL:HG22	2.01	0.42
53:A2:56:TRP:HE1	53:A2:70:ILE:HD11	1.84	0.42
58:0:125:TYR:CZ	71:d:289:PRO:HA	2.53	0.42
70:c:192:GLN:HE21	70:c:196:PHE:HE2	1.68	0.42
72:e:60:SER:O	72:e:136:ARG:NH2	2.42	0.42
72:e:215:PHE:CZ	72:e:229:ALA:HB3	2.54	0.42
79:I:107:LEU:HG	79:I:117:TYR:CE2	2.54	0.42
81:o:53:TYR:CD2	81:o:54:MET:HG3	2.55	0.42
85:s:380:THR:O	85:s:384:ASP:HB2	2.20	0.42
1:A:1868:G:H2'	11:M:40:PRO:HG3	2.00	0.42
1:A:1989:C:H2'	1:A:1990:G:C8	2.54	0.42
1:A:2343:G:N3	1:A:2343:G:H3'	2.33	0.42
1:A:2615:A:H1'	10:L:81:LYS:HD3	2.01	0.42
1:A:2807:U:H2'	1:A:2808:U:C6	2.54	0.42
2:B:68:C:H2'	2:B:69:U:C6	2.54	0.42
17:S:163:LYS:HZ2	17:S:163:LYS:HB3	1.84	0.42
20:V:64:ILE:HD11	20:V:88:VAL:HG21	2.00	0.42
25:AA:1373:U:H2'	25:AA:1374:A:C8	2.53	0.42
25:AA:1404:A:C8	25:AA:1407:U:C4	3.07	0.42
25:AA:1511:C:OP1	51:A0:7:ARG:NH2	2.52	0.42
30:AF:91:ILE:HG23	30:AF:111:MET:HE2	2.00	0.42
35:AK:91:CYS:HB3	35:AK:96:ARG:H	1.84	0.42
40:AP:95:HIS:CD2	40:AP:96:ILE:HG13	2.54	0.42
42:AR:128:MET:SD	42:AR:269:GLY:HA3	2.59	0.42
46:AV:79:ILE:HG23	46:AV:84:GLU:HB2	2.01	0.42
50:AZ:24:ARG:HG2	80:m:110:LEU:HD22	2.00	0.42
55:A4:262:MET:HG3	55:A4:266:MET:HE3	2.00	0.42
56:Ax:45:A:H5'	56:Ax:46:A:OP2	2.19	0.42
63:5:136:VAL:HG11	63:5:417:LEU:HD23	2.02	0.42
80:m:98:ALA:HB1	80:m:101:GLN:HE21	1.84	0.42
1:A:2213:A:H3'	1:A:2214:A:H5''	2.01	0.42
1:A:3151:A:H4'	15:Q:146:GLY:O	2.19	0.42
89:A:6456:G34:H222	89:A:6456:G34:H241	1.59	0.42
11:M:68:GLU:OE1	11:M:71:GLN:NE2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:R:101:VAL:HG11	17:S:98:VAL:HG11	2.02	0.42
20:V:184:GLU:O	23:Y:93:LYS:NZ	2.48	0.42
25:AA:810:G:C2	25:AA:811:G:C5	3.08	0.42
25:AA:1057:G:H4'	25:AA:1578:A:H4'	2.01	0.42
63:5:125:LYS:HE3	63:5:125:LYS:HB3	1.88	0.42
76:i:98:VAL:O	76:i:102:MET:HG3	2.18	0.42
1:A:1937:A:H2	1:A:1938:A:C5	2.38	0.42
1:A:1939:G:C8	3:D:259:LYS:HE3	2.55	0.42
1:A:2482:A:H2'	1:A:2483:U:C6	2.54	0.42
1:A:2951:A:H2'	1:A:2952:U:C6	2.53	0.42
8:J:90:PHE:HB3	8:J:120:ILE:HD13	2.01	0.42
13:O:46:TRP:HD1	13:O:121:ALA:HB2	1.83	0.42
25:AA:1359:U:H2'	25:AA:1360:G:H8	1.84	0.42
28:AD:317:HIS:HD2	28:AD:318:ARG:N	2.17	0.42
42:AR:188:GLU:O	42:AR:192:MET:HG2	2.20	0.42
55:A4:356:VAL:O	55:A4:360:MET:HG3	2.19	0.42
61:3:152:LYS:HE2	61:3:156:LYS:HE3	2.01	0.42
61:3:188:VAL:O	64:6:356:ARG:NH2	2.41	0.42
63:5:59:THR:HB	63:5:73:PRO:HG3	2.01	0.42
67:9:126:LYS:HB3	67:9:126:LYS:HE2	1.78	0.42
72:e:101:LYS:NZ	72:e:107:ASP:O	2.52	0.42
77:j:45:GLU:OE2	77:j:70:ARG:NH2	2.33	0.42
85:s:100:LEU:HD22	85:s:319:GLN:HG3	2.00	0.42
1:A:1898:A:H2'	1:A:1899:G:H8	1.85	0.42
1:A:1962:A:OP2	1:A:2501:C:N4	2.53	0.42
1:A:2227:A:H2'	1:A:2227:A:N3	2.35	0.42
1:A:2698:G:H5''	1:A:2699:C:H5	1.84	0.42
1:A:3046:C:H2'	1:A:3047:G:C8	2.54	0.42
89:A:6456:G34:H4	89:A:6456:G34:H11	1.86	0.42
9:K:36:SER:OG	9:K:40:GLN:NE2	2.51	0.42
23:Y:128:SER:HB3	23:Y:131:ARG:NE	2.35	0.42
25:AA:1347:G:H2'	25:AA:1348:G:H8	1.85	0.42
32:AH:53:ASP:OD1	55:A4:436:HIS:NE2	2.46	0.42
34:AJ:72:LYS:HD2	57:Az:9:U:H5'	2.02	0.42
46:AV:123:ASP:OD1	46:AV:123:ASP:N	2.52	0.42
48:AX:252:SER:O	48:AX:302:HIS:NE2	2.52	0.42
55:A4:255:ASN:O	55:A4:258:SER:OG	2.35	0.42
72:e:133:LEU:HD22	80:m:63:THR:HG21	2.01	0.42
1:A:1840:C:H2'	1:A:1841:U:C6	2.55	0.42
1:A:2067:C:H5''	73:f:60:LYS:HB2	2.01	0.42
1:A:2982:C:H5''	12:N:139:ARG:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3034:U:H2'	1:A:3035:C:C6	2.54	0.42
1:A:3064:A:O4'	1:A:3099:C:N4	2.52	0.42
1:A:3143:U:H2'	1:A:3144:A:H8	1.84	0.42
25:AA:1354:A:H2'	25:AA:1355:G:C8	2.54	0.42
28:AD:160:ARG:NH2	28:AD:165:GLN:OE1	2.44	0.42
30:AF:207:HIS:NE2	30:AF:211:GLU:OE2	2.52	0.42
36:AL:100:LYS:NZ	36:AL:141:GLU:OE1	2.47	0.42
39:AO:208:PRO:HG3	45:AU:51:ALA:HA	2.01	0.42
42:AR:209:ILE:HD12	42:AR:214:ASN:HB3	2.01	0.42
51:A0:110:ASP:OD1	51:A0:110:ASP:N	2.47	0.42
65:7:88:PRO:HB3	65:7:125:ILE:HD11	2.02	0.42
72:e:185:ARG:NH1	72:e:207:ASN:OD1	2.52	0.42
72:e:272:VAL:HA	72:e:275:PHE:CE2	2.55	0.42
84:r:174:MET:N	84:r:196:HIS:OXT	2.47	0.42
1:A:2667:U:C2	1:A:2668:A:C8	3.08	0.42
4:E:80:LEU:HA	4:E:84:PRO:HB3	2.00	0.42
15:Q:74:ARG:HG2	15:Q:283:TRP:CZ2	2.55	0.42
20:V:55:TYR:CD1	20:V:133:ILE:HD12	2.55	0.42
25:AA:1209:C:H2'	25:AA:1210:U:C6	2.54	0.42
25:AA:1427:A:H2'	25:AA:1428:G:C8	2.55	0.42
25:AA:1497:C:H2'	25:AA:1498:C:C6	2.55	0.42
25:AA:1497:C:H2'	25:AA:1498:C:H6	1.85	0.42
26:AB:66:PRO:HB2	26:AB:134:HIS:HE1	1.85	0.42
48:AX:203:LYS:O	48:AX:250:GLN:NE2	2.53	0.42
51:A0:129:ARG:HH22	51:A0:204:PRO:HB2	1.84	0.42
55:A4:302:VAL:HG21	55:A4:341:CYS:HB3	2.01	0.42
55:A4:452:GLN:HG2	55:A4:453:HIS:CD2	2.55	0.42
65:7:139:ASN:HB3	65:7:174:VAL:HG21	2.01	0.42
71:d:94:ASP:OD2	71:d:245:TYR:OH	2.27	0.42
71:d:152:LEU:HD22	71:d:176:ILE:HD11	2.02	0.42
71:d:226:ASP:OD1	71:d:230:ARG:N	2.51	0.42
82:p:84:SER:OG	82:p:96:ASN:O	2.37	0.42
1:A:1743:U:H2'	1:A:1744:A:H8	1.85	0.42
1:A:1925:A:H2'	1:A:1926:A:C8	2.54	0.42
1:A:2006:C:H2'	1:A:2007:U:C6	2.55	0.42
1:A:2026:A:H2'	1:A:2027:A:C8	2.55	0.42
1:A:2339:G:H21	1:A:2427:C:H5'	1.85	0.42
89:A:6456:G34:H4	89:A:6456:G34:H131	1.83	0.42
14:P:83:VAL:HG11	14:P:158:MET:HE1	2.02	0.42
25:AA:1069:A:H5''	25:AA:1070:C:H5	1.85	0.42
30:AF:154:PRO:O	30:AF:179:ARG:HD2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:AV:323:GLU:OE1	46:AV:330:TYR:OH	2.30	0.42
51:A0:143:PRO:O	51:A0:147:GLU:HG3	2.20	0.42
65:7:192:TRP:CD1	68:a:91:VAL:HG21	2.54	0.42
1:A:2408:U:H2'	1:A:2409:A:C8	2.51	0.42
1:A:2635:G:H2'	1:A:2636:G:H8	1.85	0.42
1:A:2724:G:H2'	1:A:2988:C:O2'	2.20	0.42
1:A:3024:U:H2'	1:A:3025:A:C8	2.54	0.42
25:AA:871:A:O4'	25:AA:919:A:N6	2.53	0.42
25:AA:990:U:H2'	25:AA:991:G:O4'	2.20	0.42
25:AA:1203:C:H2'	25:AA:1204:C:H6	1.84	0.42
25:AA:1255:U:O2'	25:AA:1256:A:OP1	2.34	0.42
33:AI:92:HIS:HA	33:AI:156:PRO:HD2	2.02	0.42
37:AM:38:HIS:HB2	37:AM:41:CYS:SG	2.60	0.42
46:AV:205:GLY:HA2	46:AV:227:GLY:HA2	2.01	0.42
55:A4:170:VAL:HG21	55:A4:243:ASN:HB3	2.02	0.42
85:s:152:GLN:OE1	85:s:179:GLN:NE2	2.43	0.42
1:A:1799:U:H2'	1:A:1800:G:O4'	2.20	0.41
1:A:2366:G:H2'	1:A:2367:A:C8	2.55	0.41
1:A:2407:U:H2'	1:A:2408:U:C6	2.53	0.41
9:K:27:PRO:HG2	9:K:30:LYS:HD2	2.02	0.41
9:K:34:MET:O	9:K:38:ARG:HG2	2.20	0.41
14:P:167:GLU:O	82:p:187:ARG:NH1	2.35	0.41
17:S:163:LYS:HB2	69:b:106:ASP:HB3	2.02	0.41
22:X:72:PRO:HB2	22:X:74:GLU:HG2	2.02	0.41
25:AA:1495:C:H2'	25:AA:1496:U:C6	2.55	0.41
30:AF:149:LEU:O	30:AF:153:GLU:HG3	2.19	0.41
38:AN:6:SER:OG	38:AN:69:LEU:O	2.35	0.41
55:A4:160:ARG:NH1	55:A4:172:MET:SD	2.93	0.41
55:A4:335:PHE:CD2	55:A4:360:MET:HG2	2.54	0.41
63:5:132:LEU:HD21	63:5:354:PHE:HB2	2.01	0.41
73:f:88:TYR:HE2	73:f:164:ALA:HA	1.84	0.41
82:p:113:GLU:OE1	82:p:116:ARG:NH2	2.33	0.41
1:A:2035:U:O2'	11:M:70:GLY:HA3	2.20	0.41
1:A:2355:A:H2'	1:A:2356:A:O4'	2.19	0.41
1:A:2675:G:OP1	18:T:163:LYS:HA	2.20	0.41
1:A:2677:A:H2'	1:A:2678:A:H8	1.82	0.41
1:A:2795:U:C2	1:A:2796:G:C8	3.08	0.41
2:B:63:G:H2'	2:B:64:A:H8	1.85	0.41
3:D:141:LEU:HD11	3:D:148:LYS:HG2	2.02	0.41
5:F:280:TYR:N	74:g:55:THR:O	2.45	0.41
7:I:79:ILE:HG23	7:I:130:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:123:ILE:HD12	10:L:127:LEU:HD12	2.02	0.41
10:L:128:ARG:HB2	15:Q:125:TYR:HB3	2.01	0.41
16:R:149:HIS:ND1	24:Z:152:LYS:O	2.53	0.41
25:AA:683:G:H5''	44:AT:160:ARG:NH2	2.35	0.41
25:AA:861:U:H2'	25:AA:862:A:H8	1.85	0.41
28:AD:281:TYR:CG	43:AS:18:ASP:HB3	2.55	0.41
44:AT:80:LEU:HD12	44:AT:84:GLU:HB3	2.01	0.41
48:AX:206:GLU:HA	48:AX:218:LYS:HE2	2.03	0.41
58:0:166:SER:O	58:0:170:GLN:HG3	2.20	0.41
64:6:364:ARG:O	64:6:368:ARG:HG3	2.20	0.41
66:8:165:ASP:HB3	66:8:168:LEU:HB2	2.02	0.41
71:d:137:PHE:N	71:d:138:PRO:HD2	2.36	0.41
1:A:1893:A:H1'	1:A:1894:G:C8	2.55	0.41
2:B:4:A:H2'	2:B:5:G:C8	2.55	0.41
90:B:101:VAL:HB	72:e:165:PHE:HB3	2.01	0.41
11:M:53:HIS:CG	11:M:54:LYS:H	2.37	0.41
12:N:191:SER:H	12:N:194:THR:HG1	1.63	0.41
22:X:125:VAL:HG12	63:5:48:ARG:NH1	2.34	0.41
42:AR:325:ILE:HG22	42:AR:329:LYS:HE2	2.02	0.41
44:AT:104:LYS:HD3	45:AU:108:TRP:CH2	2.55	0.41
46:AV:190:LEU:HD23	46:AV:196:PHE:CZ	2.55	0.41
48:AX:205:GLN:HB2	48:AX:249:ARG:NH1	2.35	0.41
63:5:236:LEU:HD21	63:5:289:HIS:CD2	2.56	0.41
65:7:97:GLU:O	65:7:101:ARG:HG2	2.21	0.41
70:c:170:ALA:HB1	70:c:175:VAL:HB	2.02	0.41
85:s:75:SER:HB2	85:s:78:GLU:HG3	2.01	0.41
1:A:1860:A:H2'	1:A:1861:U:C6	2.55	0.41
1:A:2087:U:H2'	1:A:2088:U:C6	2.55	0.41
3:D:74:ILE:HB	3:D:150:TRP:HE1	1.86	0.41
25:AA:1034:U:H2'	25:AA:1035:U:C6	2.56	0.41
25:AA:1118:A:N1	28:AD:297:ARG:NH1	2.69	0.41
27:AC:89:ASP:OD1	27:AC:112:ARG:NH2	2.45	0.41
28:AD:289:THR:HG21	28:AD:308:GLN:O	2.20	0.41
30:AF:52:ARG:NH2	31:AG:319:PHE:O	2.53	0.41
30:AF:88:ASP:HB3	30:AF:91:ILE:HB	2.02	0.41
48:AX:159:HIS:O	48:AX:163:LYS:HG2	2.20	0.41
52:A1:176:LYS:HG2	52:A1:204:VAL:HG22	2.03	0.41
52:A1:181:ASN:O	52:A1:234:TRP:NE1	2.46	0.41
65:7:204:LYS:HD3	68:a:99:LYS:HZ3	1.85	0.41
69:b:103:LYS:O	69:b:107:GLN:HG3	2.20	0.41
70:c:69:HIS:HE1	70:c:85:LEU:HD13	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:e:88:GLU:OE2	80:m:50:ARG:NH1	2.42	0.41
78:k:41:LYS:O	78:k:45:THR:HG23	2.20	0.41
1:A:1993:A:H8	1:A:2498:U:O2'	2.04	0.41
1:A:2650:C:H2'	1:A:2651:A:C8	2.55	0.41
1:A:2815:OMG:OP1	12:N:139:ARG:NH1	2.54	0.41
1:A:2832:A:N1	64:6:27:ARG:N	2.69	0.41
1:A:2930:U:H2'	1:A:2931:A:C8	2.55	0.41
3:D:210:ALA:HB1	3:D:249:ASN:HB2	2.03	0.41
7:I:76:ILE:HG22	7:I:78:LEU:N	2.35	0.41
15:Q:165:GLU:HB2	15:Q:168:ASN:HB2	2.03	0.41
23:Y:163:ALA:HB1	67:9:133:ARG:HB2	2.03	0.41
25:AA:776:A:O3'	25:AA:777:G:H8	2.03	0.41
25:AA:1133:C:H2'	25:AA:1134:G:H8	1.85	0.41
25:AA:1203:C:H2'	25:AA:1204:C:C6	2.54	0.41
25:AA:1439:A:H2'	25:AA:1440:G:C8	2.55	0.41
31:AG:69:TYR:H	31:AG:135:GLN:HE22	1.68	0.41
51:A0:64:LEU:HB2	51:A0:139:TRP:CD2	2.56	0.41
55:A4:482:ILE:HA	55:A4:483:PRO:HA	1.95	0.41
65:7:103:SER:HA	65:7:129:THR:HG22	2.01	0.41
1:A:2010:U:O4'	1:A:2012:A:H5'	2.21	0.41
1:A:2175:C:O2'	8:J:102:ARG:NH2	2.53	0.41
1:A:2212:C:H2'	1:A:2213:A:H8	1.85	0.41
1:A:2734:A:H2'	1:A:2735:G:C8	2.55	0.41
1:A:2951:A:H2'	1:A:2952:U:H6	1.86	0.41
12:N:117:ASN:OD1	12:N:166:ARG:NH2	2.54	0.41
20:V:105:ARG:H	20:V:105:ARG:HG2	1.69	0.41
25:AA:1138:G:H2'	25:AA:1139:A:H8	1.84	0.41
25:AA:1191:C:H2'	25:AA:1192:C:C6	2.56	0.41
26:AB:169:ARG:NH1	41:AQ:87:CYS:HA	2.36	0.41
28:AD:294:ILE:HD11	28:AD:356:GLN:HB3	2.02	0.41
35:AK:120:LEU:HB3	35:AK:123:ILE:HD12	2.02	0.41
40:AP:103:LYS:HD3	40:AP:103:LYS:HA	1.86	0.41
42:AR:132:LEU:HD12	42:AR:237:PRO:HB2	2.02	0.41
55:A4:384:ASP:HB2	55:A4:385:PRO:HD3	2.02	0.41
62:4:69:LYS:HB2	62:4:72:LEU:HD23	2.02	0.41
67:9:43:PHE:HE1	67:9:53:ILE:HD11	1.86	0.41
82:p:76:ARG:NH1	82:p:109:GLU:OE1	2.50	0.41
82:p:115:VAL:HG13	82:p:161:ALA:HB3	2.02	0.41
84:r:78:LYS:HG2	84:r:79:HIS:CD2	2.55	0.41
1:A:2098:G:HO2'	1:A:2099:U:H6	1.66	0.41
1:A:2347:C:H2'	1:A:2348:A:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2552:U:H2'	1:A:2553:G:H8	1.86	0.41
1:A:2943:G:H2'	1:A:2944:C:H6	1.86	0.41
1:A:3224:G:H2'	1:A:3225:G:H8	1.86	0.41
15:Q:77:SER:HB3	15:Q:80:PHE:HD2	1.85	0.41
19:U:114:LYS:H	19:U:114:LYS:HG3	1.69	0.41
20:V:121:LYS:HD3	20:V:130:PRO:HB2	2.03	0.41
20:V:194:LEU:HA	23:Y:95:ASN:HD22	1.86	0.41
25:AA:663:A:H2'	25:AA:664:G:H8	1.86	0.41
25:AA:821:U:H2'	25:AA:822:G:C8	2.48	0.41
25:AA:1504:U:H2'	25:AA:1505:A:H8	1.85	0.41
29:AE:35:ILE:HD11	36:AL:91:ARG:HD3	2.02	0.41
30:AF:159:VAL:HG23	30:AF:172:VAL:HG21	2.02	0.41
48:AX:192:LYS:HB2	48:AX:226:VAL:HG11	2.02	0.41
61:3:96:TYR:OH	76:i:128:ARG:O	2.31	0.41
1:A:1851:G:H2'	1:A:2693:A:N7	2.36	0.41
1:A:1894:G:H2'	1:A:1895:C:C6	2.55	0.41
1:A:1942:C:H2'	1:A:1943:A:O4'	2.20	0.41
1:A:2172:A:OP2	8:J:21:ARG:NH2	2.54	0.41
1:A:2181:A:C4	1:A:2207:A:H4'	2.56	0.41
1:A:2814:G:O2'	1:A:2983:G:OP1	2.34	0.41
1:A:2971:A:O2'	12:N:182:LYS:O	2.37	0.41
2:B:27:C:H4'	66:8:133:ARG:HH22	1.86	0.41
5:F:65:TRP:CD1	75:h:117:LEU:HD11	2.56	0.41
7:I:166:ARG:O	7:I:170:THR:HG23	2.20	0.41
9:K:138:LEU:HD11	69:b:146:ARG:HB2	2.02	0.41
11:M:203:ARG:NH2	11:M:261:ASP:O	2.53	0.41
20:V:87:VAL:HG22	20:V:114:PRO:HA	2.01	0.41
23:Y:160:GLN:HG3	67:9:131:TYR:CD2	2.56	0.41
25:AA:1255:U:H2'	25:AA:1256:A:H8	1.85	0.41
25:AA:1408:A:H2'	25:AA:1409:A:C8	2.55	0.41
27:AC:98:GLY:HA3	50:AZ:71:TYR:CE1	2.56	0.41
28:AD:289:THR:HG22	28:AD:331:ASP:O	2.21	0.41
39:AO:148:LYS:HE3	39:AO:148:LYS:HB2	1.85	0.41
41:AQ:72:ILE:HG23	53:A2:104:LEU:HD11	2.02	0.41
56:Ax:54:U:H2'	56:Ax:55:U:O4'	2.21	0.41
66:8:193:ASN:O	73:f:133:GLU:N	2.44	0.41
70:c:269:LEU:HD21	70:c:271:PHE:HE1	1.86	0.41
71:d:153:ASN:HD21	71:d:183:TRP:H	1.69	0.41
77:j:112:LYS:HA	77:j:116:LEU:HA	2.02	0.41
85:s:201:ASP:HB2	85:s:240:GLN:HG2	2.03	0.41
1:A:1928:A:H2'	1:A:1929:A:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2155:A:N6	84:r:169:TRP:O	2.54	0.41
1:A:2158:U:OP2	84:r:195:TYR:OH	2.27	0.41
1:A:2177:U:N3	1:A:2180:A:OP2	2.32	0.41
1:A:2321:A:C2	58:0:142:GLY:HA3	2.55	0.41
1:A:2410:U:H2'	1:A:2411:U:H6	1.86	0.41
1:A:2414:C:N3	85:s:164:HIS:HA	2.35	0.41
1:A:2417:C:H2'	85:s:310:ARG:HH21	1.86	0.41
1:A:2481:A:H2'	1:A:2482:A:H8	1.85	0.41
1:A:2552:U:C2	1:A:2553:G:C8	3.09	0.41
1:A:2664:U:H2'	1:A:2665:U:H6	1.86	0.41
1:A:3014:G:H5''	62:4:96:PRO:HB2	2.03	0.41
1:A:3102:U:C2	58:0:81:PRO:HA	2.56	0.41
1:A:3202:U:H2'	1:A:3203:A:H8	1.86	0.41
4:E:64:LEU:HD23	4:E:64:LEU:HA	1.90	0.41
15:Q:89:PRO:HA	15:Q:92:PHE:HD2	1.86	0.41
15:Q:95:GLU:OE2	15:Q:145:LEU:N	2.53	0.41
15:Q:148:THR:HG22	15:Q:165:GLU:HG2	2.03	0.41
23:Y:71:PRO:HA	23:Y:74:TRP:CD2	2.56	0.41
25:AA:1181:G:H2'	25:AA:1182:C:C6	2.56	0.41
25:AA:1358:A:O2'	56:Ax:30:G:OP1	2.39	0.41
25:AA:1407:U:H2'	25:AA:1408:A:C8	2.55	0.41
25:AA:1586:G:H2'	25:AA:1587:U:C6	2.56	0.41
27:AC:95:PHE:HD1	50:AZ:62:MET:HE1	1.86	0.41
29:AE:63:TYR:OH	40:AP:118:GLY:O	2.27	0.41
40:AP:141:ARG:HA	41:AQ:28:ARG:HH21	1.86	0.41
42:AR:79:LEU:HD22	42:AR:269:GLY:HA2	2.02	0.41
46:AV:198:TRP:NE1	46:AV:199:GLU:OE2	2.53	0.41
46:AV:393:GLU:OE2	46:AV:397:ARG:NE	2.46	0.41
48:AX:162:VAL:O	48:AX:272:THR:OG1	2.28	0.41
48:AX:208:TYR:O	48:AX:216:THR:N	2.54	0.41
56:Ax:39:C:C2	56:Ax:40:C:C5	3.09	0.41
56:Ax:70:A:H2'	56:Ax:71:C:C6	2.56	0.41
58:0:152:PRO:HG3	58:0:173:ARG:CZ	2.51	0.41
1:A:1679:U:H2'	1:A:1680:A:C8	2.56	0.41
1:A:1952:U:H2'	1:A:1953:A:C8	2.56	0.41
1:A:2026:A:H2'	1:A:2027:A:H8	1.86	0.41
1:A:2161:A:O2'	1:A:2162:C:O5'	2.33	0.41
1:A:2186:C:H2'	1:A:2187:C:C6	2.56	0.41
1:A:2285:U:H5''	70:c:36:ARG:HH12	1.86	0.41
1:A:2802:A:H2'	1:A:2803:A:O4'	2.20	0.41
1:A:2996:G:C2	1:A:2997:A:C8	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:217:LEU:HB2	5:F:256:HIS:CG	2.56	0.41
5:F:257:GLN:HG2	11:M:21:ARG:CZ	2.50	0.41
11:M:295:THR:HG22	82:p:39:PHE:HE1	1.85	0.41
25:AA:1130:G:H2'	25:AA:1131:C:C6	2.55	0.41
25:AA:1182:C:H2'	25:AA:1183:U:C6	2.55	0.41
25:AA:1396:C:H2'	25:AA:1397:U:H6	1.86	0.41
27:AC:69:LEU:HD23	52:A1:107:LYS:HD3	2.01	0.41
31:AG:318:HIS:NE2	48:AX:379:GLU:OE2	2.54	0.41
37:AM:67:ALA:HB2	42:AR:196:TYR:CZ	2.56	0.41
41:AQ:77:ARG:HG2	41:AQ:80:ARG:HH12	1.86	0.41
56:Ax:51:U:H2'	56:Ax:52:G:C8	2.55	0.41
69:b:15:LEU:HD11	70:c:169:VAL:HA	2.02	0.41
70:c:83:PHE:CE2	70:c:202:LEU:HB2	2.55	0.41
70:c:168:HIS:CE1	70:c:172:ASN:HD21	2.39	0.41
70:c:285:PRO:HD2	70:c:295:GLU:HG2	2.03	0.41
74:g:138:THR:HG22	74:g:149:ILE:HG12	2.01	0.41
77:j:102:GLN:O	77:j:106:GLU:HG3	2.21	0.41
1:A:3176:A:H62	1:A:3187:C:H1'	1.85	0.40
5:F:61:PRO:HA	5:F:84:PRO:HD3	2.03	0.40
13:O:148:LEU:HD22	65:7:177:GLY:HA2	2.02	0.40
18:T:151:ARG:HB2	18:T:161:MET:HE3	2.03	0.40
25:AA:722:C:H5'	51:A0:4:LYS:NZ	2.36	0.40
25:AA:871:A:H1'	25:AA:872:G:C8	2.56	0.40
25:AA:952:A:H2'	25:AA:953:U:C6	2.56	0.40
25:AA:1033:U:H2'	25:AA:1034:U:C6	2.56	0.40
25:AA:1151:C:H5'	25:AA:1152:A:N7	2.36	0.40
25:AA:1221:A:OP2	25:AA:1222:A:O2'	2.27	0.40
25:AA:1231:A:OP1	35:AK:88:ARG:NH2	2.52	0.40
25:AA:1436:C:H2'	25:AA:1437:U:C6	2.57	0.40
25:AA:1581:G:H2'	25:AA:1583:MA6:OP2	2.21	0.40
26:AB:61:LYS:HD2	26:AB:271:TYR:HE1	1.85	0.40
31:AG:110:TYR:OH	52:A1:114:LEU:O	2.27	0.40
35:AK:88:ARG:HH21	35:AK:98:ARG:HG3	1.86	0.40
38:AN:17:VAL:HG22	38:AN:28:VAL:HG22	2.03	0.40
51:A0:83:LYS:N	51:A0:138:ASP:OD1	2.50	0.40
65:7:276:PHE:HB2	65:7:304:VAL:HG22	2.03	0.40
85:s:63:ILE:HA	85:s:66:TRP:HD1	1.81	0.40
1:A:2873:A:H4'	21:W:90:TYR:CZ	2.56	0.40
1:A:3114:U:H2'	1:A:3115:U:C6	2.56	0.40
1:A:3124:U:H2'	1:A:3125:A:H8	1.85	0.40
1:A:3189:C:OP2	84:r:158:SER:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:198:SER:HB2	3:D:206:TYR:CE2	2.56	0.40
4:E:96:ARG:HD2	4:E:197:HIS:CE1	2.56	0.40
4:E:222:TRP:CD1	4:E:256:LYS:HB3	2.57	0.40
14:P:60:SER:HB3	82:p:177:ARG:HH11	1.86	0.40
22:X:30:ARG:O	22:X:34:GLU:HG3	2.21	0.40
25:AA:1470:A:C2	25:AA:1471:A:C5	3.09	0.40
28:AD:305:MET:HG2	28:AD:334:ALA:HB2	2.04	0.40
31:AG:136:ARG:HB3	31:AG:210:VAL:HG11	2.03	0.40
31:AG:206:GLU:OE1	31:AG:213:LEU:N	2.54	0.40
35:AK:43:MET:SD	35:AK:81:ASP:HB2	2.61	0.40
52:A1:166:PRO:O	52:A1:169:ARG:NH1	2.53	0.40
55:A4:414:LYS:HG2	55:A4:453:HIS:HE1	1.85	0.40
58:0:137:ILE:HD13	58:0:158:VAL:HG21	2.04	0.40
70:c:270:TYR:O	70:c:285:PRO:HA	2.21	0.40
1:A:1861:U:H2'	1:A:1862:U:H6	1.87	0.40
1:A:2149:G:OP1	77:j:23:ALA:N	2.54	0.40
1:A:2815:OMG:HM23	1:A:2815:OMG:H1'	1.86	0.40
9:K:118:ARG:O	9:K:122:MET:HG2	2.21	0.40
9:K:169:LEU:HD22	84:r:75:TRP:CG	2.56	0.40
15:Q:210:GLU:HB2	15:Q:213:GLN:HG3	2.02	0.40
17:S:113:LEU:HB2	69:b:120:HIS:HB3	2.04	0.40
20:V:96:ARG:HE	20:V:111:SER:HB2	1.86	0.40
25:AA:870:C:H5''	39:AO:97:ARG:NH1	2.36	0.40
44:AT:52:ILE:HD13	44:AT:52:ILE:HA	1.97	0.40
63:5:189:LYS:O	63:5:192:ILE:HG13	2.22	0.40
65:7:234:LYS:HA	65:7:237:VAL:HG22	2.03	0.40
70:c:44:GLU:HA	70:c:47:ARG:HD3	2.03	0.40
1:A:1964:U:H2'	1:A:1965:A:C8	2.57	0.40
1:A:2239:A:H2'	1:A:2240:C:C6	2.57	0.40
1:A:2439:U:H2'	1:A:2440:G:H8	1.86	0.40
1:A:2678:A:H2	58:0:80:ALA:HA	1.86	0.40
2:B:27:C:H2'	2:B:28:C:H6	1.86	0.40
4:E:219:MET:HE2	4:E:219:MET:HB3	1.99	0.40
20:V:181:ASP:O	23:Y:93:LYS:NZ	2.49	0.40
22:X:12:LYS:HA	22:X:12:LYS:HD3	1.89	0.40
25:AA:968:U:H2'	25:AA:969:A:H8	1.87	0.40
25:AA:1279:C:H2'	25:AA:1280:C:H6	1.85	0.40
25:AA:1523:A:N7	46:AV:396:GLN:NE2	2.55	0.40
26:AB:220:VAL:HG22	26:AB:234:TYR:HB2	2.04	0.40
28:AD:282:ILE:HG23	28:AD:353:LEU:HB3	2.03	0.40
36:AL:171:ARG:HG3	36:AL:175:TYR:HD1	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:AM:108:GLU:OE2	45:AU:59:ARG:NH2	2.33	0.40
48:AX:136:LEU:HD23	48:AX:136:LEU:HA	1.92	0.40
48:AX:244:LEU:HD12	48:AX:292:ASN:HB3	2.02	0.40
52:A1:152:ASP:HB2	52:A1:172:VAL:HB	2.04	0.40
55:A4:596:LEU:HD21	55:A4:614:LEU:HD13	2.03	0.40
63:5:201:ARG:NH1	63:5:418:TYR:O	2.39	0.40
65:7:180:CYS:HB2	65:7:296:ARG:HG3	2.04	0.40
1:A:1946:C:H2'	1:A:1947:C:C6	2.55	0.40
1:A:2339:G:H4'	60:2:55:PRO:HB2	2.02	0.40
1:A:2408:U:O2	1:A:2409:A:C8	2.74	0.40
1:A:2664:U:H2'	1:A:2665:U:C6	2.57	0.40
90:B:101:VAL:O	72:e:218:PRO:HD3	2.21	0.40
10:L:125:THR:HG22	10:L:144:PHE:HB3	2.03	0.40
14:P:72:PHE:HB2	21:W:107:HIS:HA	2.03	0.40
23:Y:135:VAL:O	23:Y:139:MET:HG3	2.21	0.40
25:AA:1362:G:H2'	25:AA:1363:C:C6	2.57	0.40
25:AA:1562:G:H1'	25:AA:1583:MA6:C2	2.46	0.40
37:AM:29:ARG:HD2	37:AM:57:LEU:HD12	2.03	0.40
43:AS:87:LEU:HB2	47:AW:117:GLY:HA3	2.03	0.40
52:A1:98:ALA:O	52:A1:102:ASN:HB2	2.21	0.40
52:A1:212:CYS:HB2	52:A1:218:ASN:CG	2.46	0.40
52:A1:255:ASN:N	52:A1:259:GLU:OE1	2.54	0.40
62:4:76:CYS:SG	62:4:98:HIS:CE1	3.14	0.40
65:7:152:CYS:HB2	65:7:260:PHE:CD2	2.57	0.40
70:c:69:HIS:NE2	70:c:73:GLN:OE1	2.54	0.40
70:c:166:VAL:HG11	70:c:192:GLN:HG3	2.03	0.40
71:d:189:LEU:HD21	71:d:219:ARG:NE	2.37	0.40
73:f:121:VAL:HG22	73:f:159:ILE:HG22	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	236/305 (77%)	227 (96%)	9 (4%)	0	100	100
4	E	303/348 (87%)	299 (99%)	4 (1%)	0	100	100
5	F	250/311 (80%)	247 (99%)	3 (1%)	0	100	100
6	H	98/267 (37%)	97 (99%)	1 (1%)	0	100	100
7	I	167/261 (64%)	162 (97%)	5 (3%)	0	100	100
8	J	173/192 (90%)	172 (99%)	1 (1%)	0	100	100
9	K	176/178 (99%)	173 (98%)	3 (2%)	0	100	100
10	L	113/145 (78%)	111 (98%)	2 (2%)	0	100	100
11	M	287/296 (97%)	280 (98%)	7 (2%)	0	100	100
12	N	220/251 (88%)	218 (99%)	2 (1%)	0	100	100
13	O	152/175 (87%)	149 (98%)	3 (2%)	0	100	100
14	P	142/180 (79%)	136 (96%)	6 (4%)	0	100	100
15	Q	237/292 (81%)	232 (98%)	4 (2%)	1 (0%)	30	66
16	R	138/149 (93%)	136 (99%)	2 (1%)	0	100	100
17	S	159/205 (78%)	156 (98%)	3 (2%)	0	100	100
18	T	164/206 (80%)	160 (98%)	4 (2%)	0	100	100
19	U	151/153 (99%)	150 (99%)	1 (1%)	0	100	100
20	V	203/216 (94%)	196 (97%)	7 (3%)	0	100	100
21	W	114/148 (77%)	113 (99%)	1 (1%)	0	100	100
22	X	242/256 (94%)	236 (98%)	6 (2%)	0	100	100
23	Y	179/250 (72%)	179 (100%)	0	0	100	100
24	Z	120/161 (74%)	119 (99%)	1 (1%)	0	100	100
26	AB	223/296 (75%)	217 (97%)	6 (3%)	0	100	100
27	AC	130/167 (78%)	129 (99%)	1 (1%)	0	100	100
28	AD	341/430 (79%)	335 (98%)	6 (2%)	0	100	100
29	AE	120/125 (96%)	119 (99%)	1 (1%)	0	100	100
30	AF	206/242 (85%)	204 (99%)	2 (1%)	0	100	100
31	AG	307/396 (78%)	300 (98%)	7 (2%)	0	100	100
32	AH	138/201 (69%)	135 (98%)	3 (2%)	0	100	100
33	AI	134/194 (69%)	130 (97%)	4 (3%)	0	100	100
34	AJ	106/138 (77%)	102 (96%)	4 (4%)	0	100	100
35	AK	99/128 (77%)	97 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	AL	172/257 (67%)	169 (98%)	3 (2%)	0	100	100
37	AM	117/137 (85%)	116 (99%)	1 (1%)	0	100	100
38	AN	108/130 (83%)	107 (99%)	1 (1%)	0	100	100
39	AO	191/258 (74%)	189 (99%)	2 (1%)	0	100	100
40	AP	95/142 (67%)	95 (100%)	0	0	100	100
41	AQ	85/87 (98%)	82 (96%)	3 (4%)	0	100	100
42	AR	293/360 (81%)	288 (98%)	5 (2%)	0	100	100
43	AS	133/190 (70%)	131 (98%)	2 (2%)	0	100	100
44	AT	166/173 (96%)	163 (98%)	3 (2%)	0	100	100
45	AU	174/205 (85%)	174 (100%)	0	0	100	100
46	AV	358/414 (86%)	355 (99%)	3 (1%)	0	100	100
47	AW	98/187 (52%)	98 (100%)	0	0	100	100
48	AX	350/398 (88%)	348 (99%)	2 (1%)	0	100	100
49	AY	118/395 (30%)	116 (98%)	2 (2%)	0	100	100
50	AZ	98/106 (92%)	96 (98%)	2 (2%)	0	100	100
51	A0	213/217 (98%)	207 (97%)	6 (3%)	0	100	100
52	A1	275/323 (85%)	272 (99%)	3 (1%)	0	100	100
53	A2	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
54	A3	68/199 (34%)	67 (98%)	1 (2%)	0	100	100
55	A4	527/689 (76%)	520 (99%)	7 (1%)	0	100	100
58	0	108/188 (57%)	107 (99%)	1 (1%)	0	100	100
59	1	51/65 (78%)	50 (98%)	1 (2%)	0	100	100
60	2	44/92 (48%)	44 (100%)	0	0	100	100
61	3	93/188 (50%)	93 (100%)	0	0	100	100
62	4	36/103 (35%)	36 (100%)	0	0	100	100
63	5	392/423 (93%)	386 (98%)	6 (2%)	0	100	100
64	6	352/380 (93%)	347 (99%)	5 (1%)	0	100	100
65	7	292/338 (86%)	282 (97%)	10 (3%)	0	100	100
66	8	138/206 (67%)	136 (99%)	2 (1%)	0	100	100
67	9	122/137 (89%)	121 (99%)	1 (1%)	0	100	100
68	a	96/142 (68%)	94 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
69	b	149/215 (69%)	145 (97%)	4 (3%)	0	100	100
70	c	282/332 (85%)	279 (99%)	3 (1%)	0	100	100
71	d	235/306 (77%)	232 (99%)	3 (1%)	0	100	100
72	e	236/279 (85%)	229 (97%)	7 (3%)	0	100	100
73	f	153/212 (72%)	151 (99%)	2 (1%)	0	100	100
74	g	132/166 (80%)	132 (100%)	0	0	100	100
75	h	108/158 (68%)	105 (97%)	3 (3%)	0	100	100
76	i	95/128 (74%)	94 (99%)	1 (1%)	0	100	100
77	j	92/123 (75%)	90 (98%)	2 (2%)	0	100	100
78	k	93/112 (83%)	93 (100%)	0	0	100	100
79	l	80/138 (58%)	79 (99%)	1 (1%)	0	100	100
80	m	90/128 (70%)	89 (99%)	1 (1%)	0	100	100
81	o	92/102 (90%)	91 (99%)	1 (1%)	0	100	100
82	p	137/206 (66%)	137 (100%)	0	0	100	100
83	q	131/222 (59%)	131 (100%)	0	0	100	100
84	r	160/196 (82%)	159 (99%)	1 (1%)	0	100	100
85	s	379/439 (86%)	372 (98%)	7 (2%)	0	100	100
86	t	9/198 (4%)	9 (100%)	0	0	100	100
All	All	13960/18169 (77%)	13735 (98%)	224 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	Q	62	ILE

### 5.3.2 Protein sidechains ⓘ

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

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



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	192/245 (78%)	191 (100%)	1 (0%)	86	94
4	E	260/290 (90%)	259 (100%)	1 (0%)	89	95
5	F	219/262 (84%)	218 (100%)	1 (0%)	86	94
6	H	90/228 (40%)	88 (98%)	2 (2%)	47	76
7	I	155/232 (67%)	155 (100%)	0	100	100
8	J	138/150 (92%)	137 (99%)	1 (1%)	81	91
9	K	155/155 (100%)	155 (100%)	0	100	100
10	L	98/124 (79%)	98 (100%)	0	100	100
11	M	245/249 (98%)	244 (100%)	1 (0%)	89	95
12	N	189/211 (90%)	188 (100%)	1 (0%)	86	94
13	O	134/150 (89%)	132 (98%)	2 (2%)	60	83
14	P	126/155 (81%)	125 (99%)	1 (1%)	79	90
15	Q	221/256 (86%)	220 (100%)	1 (0%)	86	94
16	R	118/126 (94%)	118 (100%)	0	100	100
17	S	146/180 (81%)	145 (99%)	1 (1%)	81	91
18	T	146/176 (83%)	146 (100%)	0	100	100
19	U	134/134 (100%)	134 (100%)	0	100	100
20	V	183/191 (96%)	183 (100%)	0	100	100
21	W	94/119 (79%)	93 (99%)	1 (1%)	70	87
22	X	220/229 (96%)	220 (100%)	0	100	100
23	Y	163/223 (73%)	162 (99%)	1 (1%)	84	93
24	Z	113/147 (77%)	112 (99%)	1 (1%)	75	89
26	AB	198/249 (80%)	198 (100%)	0	100	100
27	AC	115/143 (80%)	114 (99%)	1 (1%)	75	89
28	AD	286/357 (80%)	286 (100%)	0	100	100
29	AE	104/107 (97%)	104 (100%)	0	100	100
30	AF	185/209 (88%)	185 (100%)	0	100	100
31	AG	270/342 (79%)	270 (100%)	0	100	100
32	AH	130/180 (72%)	128 (98%)	2 (2%)	60	83
33	AI	104/146 (71%)	104 (100%)	0	100	100
34	AJ	93/118 (79%)	92 (99%)	1 (1%)	70	87
35	AK	91/113 (80%)	91 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	AL	158/226 (70%)	156 (99%)	2 (1%)	65	85
37	AM	97/113 (86%)	97 (100%)	0	100	100
38	AN	96/115 (84%)	95 (99%)	1 (1%)	73	88
39	AO	174/230 (76%)	173 (99%)	1 (1%)	84	93
40	AP	88/123 (72%)	88 (100%)	0	100	100
41	AQ	78/78 (100%)	78 (100%)	0	100	100
42	AR	264/318 (83%)	263 (100%)	1 (0%)	89	95
43	AS	116/164 (71%)	116 (100%)	0	100	100
44	AT	153/157 (98%)	152 (99%)	1 (1%)	81	91
45	AU	152/174 (87%)	152 (100%)	0	100	100
46	AV	325/364 (89%)	325 (100%)	0	100	100
47	AW	87/158 (55%)	87 (100%)	0	100	100
48	AX	311/351 (89%)	310 (100%)	1 (0%)	91	96
49	AY	111/357 (31%)	111 (100%)	0	100	100
50	AZ	90/95 (95%)	90 (100%)	0	100	100
51	A0	188/189 (100%)	188 (100%)	0	100	100
52	A1	255/291 (88%)	255 (100%)	0	100	100
53	A2	100/100 (100%)	100 (100%)	0	100	100
54	A3	65/166 (39%)	65 (100%)	0	100	100
55	A4	479/609 (79%)	475 (99%)	4 (1%)	79	90
58	0	99/164 (60%)	98 (99%)	1 (1%)	73	88
59	1	50/60 (83%)	50 (100%)	0	100	100
60	2	40/72 (56%)	39 (98%)	1 (2%)	42	73
61	3	88/166 (53%)	88 (100%)	0	100	100
62	4	37/89 (42%)	37 (100%)	0	100	100
63	5	353/368 (96%)	350 (99%)	3 (1%)	79	90
64	6	313/332 (94%)	313 (100%)	0	100	100
65	7	270/303 (89%)	269 (100%)	1 (0%)	89	95
66	8	129/190 (68%)	129 (100%)	0	100	100
67	9	104/112 (93%)	104 (100%)	0	100	100
68	a	96/133 (72%)	96 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
69	b	132/185 (71%)	132 (100%)	0	100	100
70	c	251/288 (87%)	250 (100%)	1 (0%)	89	95
71	d	223/274 (81%)	222 (100%)	1 (0%)	89	95
72	e	207/236 (88%)	205 (99%)	2 (1%)	73	88
73	f	139/188 (74%)	139 (100%)	0	100	100
74	g	124/148 (84%)	124 (100%)	0	100	100
75	h	104/148 (70%)	104 (100%)	0	100	100
76	i	86/110 (78%)	86 (100%)	0	100	100
77	j	74/97 (76%)	74 (100%)	0	100	100
78	k	81/90 (90%)	81 (100%)	0	100	100
79	l	76/116 (66%)	76 (100%)	0	100	100
80	m	85/113 (75%)	85 (100%)	0	100	100
81	o	80/87 (92%)	80 (100%)	0	100	100
82	p	132/181 (73%)	132 (100%)	0	100	100
83	q	114/178 (64%)	114 (100%)	0	100	100
84	r	147/169 (87%)	147 (100%)	0	100	100
85	s	338/381 (89%)	338 (100%)	0	100	100
86	t	6/158 (4%)	6 (100%)	0	100	100
All	All	12480/15710 (79%)	12439 (100%)	41 (0%)	90	96

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	226	ILE
4	E	285	VAL
5	F	94	ASP
6	H	83	VAL
6	H	102	VAL
8	J	104	THR
11	M	174	VAL
12	N	59	VAL
13	O	52	MET
13	O	93	LEU
14	P	103	VAL
15	Q	69	VAL
17	S	164	THR

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Mol	Chain	Res	Type
21	W	131	VAL
23	Y	205	VAL
24	Z	99	VAL
27	AC	37	ASN
32	AH	148	LEU
32	AH	184	ILE
34	AJ	115	THR
36	AL	177	VAL
36	AL	213	VAL
38	AN	88	VAL
39	AO	167	ILE
42	AR	107	THR
44	AT	92	THR
48	AX	51	THR
55	A4	58	VAL
55	A4	309	PHE
55	A4	379	PHE
55	A4	508	VAL
58	0	153	THR
60	2	92	HIS
63	5	180	ILE
63	5	262	ILE
63	5	307	ASP
65	7	62	THR
70	c	307	PHE
71	d	81	THR
72	e	113	ASP
72	e	223	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (151) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	168	HIS
3	D	276	HIS
4	E	52	HIS
4	E	63	GLN
4	E	174	GLN
4	E	280	HIS
5	F	223	HIS
6	H	121	ASN
7	I	36	HIS
7	I	43	GLN

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Mol	Chain	Res	Type
7	I	100	GLN
7	I	119	HIS
7	I	151	ASN
8	J	54	ASN
9	K	40	GLN
9	K	74	GLN
10	L	52	HIS
10	L	59	HIS
11	M	71	GLN
11	M	84	ASN
12	N	237	HIS
13	O	100	GLN
15	Q	139	GLN
15	Q	158	GLN
15	Q	172	GLN
18	T	73	GLN
18	T	204	HIS
19	U	74	HIS
19	U	98	GLN
19	U	136	GLN
20	V	18	HIS
22	X	240	GLN
23	Y	225	ASN
24	Z	100	HIS
26	AB	64	ASN
26	AB	134	HIS
26	AB	201	ASN
26	AB	228	ASN
27	AC	64	HIS
27	AC	130	HIS
27	AC	156	GLN
28	AD	155	GLN
28	AD	317	HIS
28	AD	415	GLN
30	AF	147	GLN
31	AG	77	GLN
31	AG	90	ASN
31	AG	135	GLN
31	AG	176	GLN
31	AG	261	GLN
31	AG	384	GLN
32	AH	125	HIS

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Mol	Chain	Res	Type
33	AI	98	GLN
34	AJ	100	HIS
34	AJ	105	HIS
34	AJ	116	GLN
34	AJ	134	HIS
35	AK	117	HIS
39	AO	111	HIS
39	AO	125	GLN
39	AO	130	HIS
39	AO	147	HIS
39	AO	169	GLN
39	AO	225	GLN
41	AQ	15	GLN
42	AR	110	GLN
42	AR	194	GLN
42	AR	214	ASN
42	AR	288	GLN
43	AS	66	HIS
43	AS	82	GLN
44	AT	14	GLN
44	AT	63	GLN
46	AV	78	ASN
46	AV	237	GLN
46	AV	238	GLN
46	AV	380	GLN
48	AX	81	HIS
48	AX	110	HIS
48	AX	235	ASN
48	AX	312	GLN
50	AZ	54	ASN
50	AZ	76	GLN
51	A0	133	HIS
53	A2	71	GLN
55	A4	90	GLN
55	A4	129	GLN
55	A4	136	HIS
55	A4	189	ASN
55	A4	257	HIS
55	A4	453	HIS
55	A4	545	GLN
58	0	115	HIS
58	0	120	HIS

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Mol	Chain	Res	Type
58	0	188	ASN
59	1	52	GLN
63	5	150	GLN
63	5	160	HIS
63	5	275	ASN
63	5	302	HIS
63	5	384	GLN
64	6	320	GLN
65	7	247	ASN
65	7	298	GLN
66	8	158	HIS
67	9	52	GLN
68	a	46	ASN
68	a	71	HIS
68	a	126	HIS
70	c	80	GLN
70	c	118	ASN
70	c	128	GLN
70	c	168	HIS
70	c	192	GLN
70	c	204	GLN
70	c	222	GLN
71	d	149	HIS
71	d	204	ASN
72	e	67	GLN
72	e	75	GLN
72	e	106	HIS
72	e	175	GLN
72	e	212	HIS
72	e	219	GLN
72	e	252	HIS
72	e	271	GLN
73	f	158	GLN
74	g	141	ASN
76	i	120	HIS
78	k	80	HIS
79	l	82	GLN
79	l	124	GLN
79	l	125	ASN
79	l	135	ASN
80	m	65	HIS
80	m	101	GLN

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Mol	Chain	Res	Type
80	m	108	GLN
81	o	21	HIS
81	o	58	GLN
81	o	85	HIS
81	o	94	HIS
82	p	123	HIS
82	p	190	GLN
83	q	81	GLN
84	r	79	HIS
84	r	96	HIS
85	s	152	GLN
85	s	179	GLN
85	s	240	GLN
85	s	358	GLN
85	s	397	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1520/1561 (97%)	258 (16%)	3 (0%)
2	B	71/72 (98%)	16 (22%)	0
25	AA	953/954 (99%)	148 (15%)	2 (0%)
56	Ax	62/71 (87%)	11 (17%)	0
57	Az	7/8 (87%)	1 (14%)	0
All	All	2613/2666 (98%)	434 (16%)	5 (0%)

All (434) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	1681	G
1	A	1689	C
1	A	1691	C
1	A	1693	C
1	A	1694	U
1	A	1699	C
1	A	1700	U
1	A	1704	U
1	A	1707	C
1	A	1708	A
1	A	1709	G
1	A	1711	C

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Mol	Chain	Res	Type
1	A	1715	C
1	A	1724	A
1	A	1727	A
1	A	1733	C
1	A	1735	A
1	A	1736	A
1	A	1748	G
1	A	1761	A
1	A	1763	A
1	A	1764	C
1	A	1765	C
1	A	1777	A
1	A	1805	A
1	A	1807	U
1	A	1808	A
1	A	1821	A
1	A	1827	C
1	A	1828	A
1	A	1829	A
1	A	1832	A
1	A	1836	A
1	A	1844	A
1	A	1854	U
1	A	1855	A
1	A	1856	A
1	A	1860	A
1	A	1868	G
1	A	1869	A
1	A	1878	U
1	A	1882	A
1	A	1885	A
1	A	1892	A
1	A	1893	A
1	A	1903	C
1	A	1909	A
1	A	1918	G
1	A	1935	A
1	A	1937	A
1	A	1938	A
1	A	1940	A
1	A	1958	G
1	A	1975	U

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Mol	Chain	Res	Type
1	A	1985	G
1	A	1987	G
1	A	1992	C
1	A	1994	A
1	A	2003	A
1	A	2015	G
1	A	2022	G
1	A	2030	U
1	A	2031	A
1	A	2036	C
1	A	2037	U
1	A	2039	A
1	A	2054	U
1	A	2060	A
1	A	2070	C
1	A	2071	U
1	A	2074	A
1	A	2079	C
1	A	2092	C
1	A	2098	G
1	A	2099	U
1	A	2111	C
1	A	2113	G
1	A	2125	C
1	A	2126	U
1	A	2131	A
1	A	2147	G
1	A	2159	U
1	A	2160	A
1	A	2161	A
1	A	2162	C
1	A	2163	A
1	A	2166	C
1	A	2174	G
1	A	2175	C
1	A	2181	A
1	A	2182	G
1	A	2196	A
1	A	2198	A
1	A	2199	A
1	A	2211	U
1	A	2214	A

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Mol	Chain	Res	Type
1	A	2219	C
1	A	2220	A
1	A	2221	C
1	A	2223	A
1	A	2224	C
1	A	2225	C
1	A	2226	U
1	A	2227	A
1	A	2230	A
1	A	2237	A
1	A	2241	A
1	A	2243	A
1	A	2245	A
1	A	2246	A
1	A	2260	A
1	A	2262	C
1	A	2263	C
1	A	2284	C
1	A	2297	A
1	A	2299	U
1	A	2300	G
1	A	2302	U
1	A	2317	G
1	A	2321	A
1	A	2322	C
1	A	2331	C
1	A	2332	C
1	A	2345	G
1	A	2349	G
1	A	2350	A
1	A	2354	A
1	A	2357	C
1	A	2363	A
1	A	2372	U
1	A	2374	A
1	A	2381	A
1	A	2388	A
1	A	2390	A
1	A	2391	A
1	A	2393	C
1	A	2396	C
1	A	2397	C

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Mol	Chain	Res	Type
1	A	2404	U
1	A	2406	A
1	A	2407	U
1	A	2414	C
1	A	2415	C
1	A	2446	A
1	A	2451	A
1	A	2458	A
1	A	2478	G
1	A	2480	A
1	A	2485	U
1	A	2493	C
1	A	2504	A
1	A	2520	C
1	A	2521	A
1	A	2524	A
1	A	2527	A
1	A	2536	G
1	A	2540	C
1	A	2557	C
1	A	2558	A
1	A	2570	C
1	A	2592	G
1	A	2593	G
1	A	2594	U
1	A	2601	A
1	A	2603	C
1	A	2618	U
1	A	2627	G
1	A	2629	A
1	A	2630	U
1	A	2633	A
1	A	2635	G
1	A	2654	U
1	A	2683	C
1	A	2684	C
1	A	2686	G
1	A	2694	A
1	A	2695	G
1	A	2696	A
1	A	2706	A
1	A	2709	A

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Mol	Chain	Res	Type
1	A	2715	A
1	A	2718	C
1	A	2719	G
1	A	2721	G
1	A	2722	A
1	A	2723	A
1	A	2724	G
1	A	2725	A
1	A	2732	G
1	A	2745	A
1	A	2810	G
1	A	2832	A
1	A	2833	A
1	A	2847	C
1	A	2864	U
1	A	2865	C
1	A	2882	U
1	A	2884	C
1	A	2885	U
1	A	2886	A
1	A	2887	U
1	A	2889	C
1	A	2893	A
1	A	2913	A
1	A	2917	G
1	A	2922	A
1	A	2928	C
1	A	2934	G
1	A	2935	A
1	A	2956	A
1	A	2965	A
1	A	2985	C
1	A	2989	G
1	A	2990	A
1	A	2992	G
1	A	2994	U
1	A	3005	A
1	A	3007	C
1	A	3016	G
1	A	3022	G
1	A	3041	U
1	A	3051	A

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Mol	Chain	Res	Type
1	A	3053	A
1	A	3054	G
1	A	3060	C
1	A	3064	A
1	A	3069	A
1	A	3090	G
1	A	3096	U
1	A	3100	U
1	A	3102	U
1	A	3108	U
1	A	3109	U
1	A	3110	C
1	A	3112	A
1	A	3113	A
1	A	3122	U
1	A	3157	C
1	A	3158	A
1	A	3162	C
1	A	3168	C
1	A	3169	C
1	A	3172	C
1	A	3176	A
1	A	3180	A
1	A	3183	U
1	A	3190	A
1	A	3199	U
1	A	3200	U
1	A	3207	A
1	A	3209	A
1	A	3210	C
1	A	3212	C
1	A	3217	A
1	A	3218	A
1	A	3228	U
1	A	3229	U
1	A	3231	U
2	B	7	G
2	B	8	U
2	B	10	2MG
2	B	16	C
2	B	21	A
2	B	45	G

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Mol	Chain	Res	Type
2	B	46	A
2	B	48	U
2	B	49	U
2	B	54	C
2	B	55	U
2	B	56	U
2	B	58	A
2	B	59	A
2	B	72	G
2	B	76	A
25	AA	651	A
25	AA	673	U
25	AA	680	U
25	AA	688	A
25	AA	695	A
25	AA	704	U
25	AA	721	U
25	AA	730	A
25	AA	737	C
25	AA	738	A
25	AA	753	A
25	AA	761	A
25	AA	766	G
25	AA	783	A
25	AA	791	G
25	AA	794	U
25	AA	796	G
25	AA	815	C
25	AA	830	U
25	AA	832	U
25	AA	835	C
25	AA	851	A
25	AA	860	A
25	AA	861	U
25	AA	866	A
25	AA	868	C
25	AA	869	C
25	AA	870	C
25	AA	871	A
25	AA	881	A
25	AA	883	U
25	AA	890	C

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Mol	Chain	Res	Type
25	AA	893	G
25	AA	903	U
25	AA	904	C
25	AA	907	A
25	AA	919	A
25	AA	923	A
25	AA	929	A
25	AA	930	G
25	AA	932	C
25	AA	939	A
25	AA	941	G
25	AA	942	A
25	AA	946	U
25	AA	947	U
25	AA	954	C
25	AA	960	C
25	AA	962	C
25	AA	967	A
25	AA	975	A
25	AA	993	A
25	AA	1002	C
25	AA	1010	A
25	AA	1015	A
25	AA	1031	G
25	AA	1042	U
25	AA	1047	A
25	AA	1049	A
25	AA	1065	C
25	AA	1081	U
25	AA	1082	A
25	AA	1094	U
25	AA	1098	C
25	AA	1103	A
25	AA	1105	C
25	AA	1106	C
25	AA	1107	U
25	AA	1109	A
25	AA	1118	A
25	AA	1119	U
25	AA	1120	C
25	AA	1121	A
25	AA	1137	A

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Mol	Chain	Res	Type
25	AA	1138	G
25	AA	1144	U
25	AA	1151	C
25	AA	1153	C
25	AA	1160	A
25	AA	1167	A
25	AA	1179	G
25	AA	1187	U
25	AA	1188	A
25	AA	1189	U
25	AA	1190	C
25	AA	1193	U
25	AA	1209	C
25	AA	1220	A
25	AA	1223	C
25	AA	1225	C
25	AA	1229	U
25	AA	1236	C
25	AA	1246	U
25	AA	1247	G
25	AA	1248	C
25	AA	1250	C
25	AA	1251	A
25	AA	1256	A
25	AA	1258	A
25	AA	1265	C
25	AA	1271	C
25	AA	1273	G
25	AA	1275	A
25	AA	1284	U
25	AA	1290	C
25	AA	1291	U
25	AA	1300	A
25	AA	1326	A
25	AA	1327	G
25	AA	1330	C
25	AA	1343	A
25	AA	1353	A
25	AA	1354	A
25	AA	1356	A
25	AA	1378	C
25	AA	1379	A

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Mol	Chain	Res	Type
25	AA	1387	A
25	AA	1390	A
25	AA	1391	U
25	AA	1405	C
25	AA	1407	U
25	AA	1430	A
25	AA	1481	C
25	AA	1482	A
25	AA	1494	C
25	AA	1507	A
25	AA	1512	A
25	AA	1519	A
25	AA	1522	U
25	AA	1525	C
25	AA	1526	U
25	AA	1527	A
25	AA	1533	C
25	AA	1536	A
25	AA	1537	C
25	AA	1539	C
25	AA	1540	A
25	AA	1541	U
25	AA	1551	G
25	AA	1557	A
25	AA	1564	A
25	AA	1568	U
25	AA	1571	U
25	AA	1582	G
25	AA	1584	MA6
25	AA	1594	G
25	AA	1595	G
25	AA	1599	A
56	Ax	2	G
56	Ax	3	U
56	Ax	34	RSQ
56	Ax	42	G
56	Ax	43	A
56	Ax	44	A
56	Ax	45	A
56	Ax	46	A
56	Ax	48	U
56	Ax	53	G

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Mol	Chain	Res	Type
56	Ax	76	A
57	Az	11	U

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1692	A
1	A	2245	A
1	A	2349	G
25	AA	1255	U
25	AA	1539	C

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

15 non-standard protein/DNA/RNA residues are modelled in this entry.

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
2	2MG	B	10	2	18,26,27	0.91	1 (5%)	16,38,41	0.70	0
33	5F0	AI	184	33	8,8,9	0.54	0	7,9,11	1.02	1 (14%)
1	OMG	A	3040	1	18,26,27	0.91	1 (5%)	19,38,41	0.61	0
1	PSU	A	3067	1	18,21,22	0.51	0	22,30,33	0.62	1 (4%)
2	PSU	B	39	2	18,21,22	0.49	0	22,30,33	0.57	0
25	B8T	AA	1486	25,87	19,22,23	0.30	0	26,31,34	0.32	0
56	RSQ	Ax	34	57,56	20,23,24	0.31	0	26,33,36	0.34	0
25	5MC	AA	1488	25	18,22,23	0.32	0	26,32,35	0.46	0
1	1MA	A	2617	1	16,25,26	1.17	2 (12%)	18,37,40	0.87	1 (5%)
1	OMU	A	3039	88,1	19,22,23	0.28	0	26,31,34	0.42	0
25	5MU	AA	1076	25	19,22,23	0.29	0	28,32,35	0.31	0
2	1MA	B	9	2	16,25,26	1.16	2 (12%)	18,37,40	0.85	1 (5%)
25	MA6	AA	1583	25	18,26,27	0.74	0	19,38,41	0.62	0
25	MA6	AA	1584	25	18,26,27	0.76	0	19,38,41	0.63	0
1	OMG	A	2815	88,56,1	18,26,27	0.92	1 (5%)	19,38,41	0.61	0

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
2	2MG	B	10	2	-	0/5/27/28	0/3/3/3
33	5F0	AI	184	33	-	7/9/9/10	-
1	OMG	A	3040	1	-	0/5/27/28	0/3/3/3
1	PSU	A	3067	1	-	0/7/25/26	0/2/2/2
2	PSU	B	39	2	-	0/7/25/26	0/2/2/2
25	B8T	AA	1486	25,87	-	0/7/27/28	0/2/2/2
56	RSQ	Ax	34	57,56	-	1/9/27/28	0/2/2/2
25	5MC	AA	1488	25	-	0/7/25/26	0/2/2/2
1	1MA	A	2617	1	-	0/3/25/26	0/3/3/3
1	OMU	A	3039	88,1	-	0/9/27/28	0/2/2/2
25	5MU	AA	1076	25	-	0/7/25/26	0/2/2/2
2	1MA	B	9	2	-	0/3/25/26	0/3/3/3
25	MA6	AA	1583	25	-	3/7/29/30	0/3/3/3
25	MA6	AA	1584	25	-	4/7/29/30	0/3/3/3
1	OMG	A	2815	88,56,1	-	0/5/27/28	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	9	1MA	C6-N6	3.20	1.35	1.27
1	A	2617	1MA	C6-N6	3.16	1.35	1.27
2	B	10	2MG	C5-C6	-2.30	1.42	1.47
1	A	2815	OMG	C5-C6	-2.27	1.42	1.47
1	A	3040	OMG	C5-C6	-2.19	1.43	1.47
1	A	2617	1MA	C5-C4	-2.12	1.37	1.43
2	B	9	1MA	C5-C4	-2.10	1.37	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	AI	184	5F0	O-C-CB	-2.29	118.75	125.43
1	A	3067	PSU	O4'-C1'-C2'	2.13	108.14	105.14
2	B	9	1MA	N1-C6-N6	2.08	125.07	119.77
1	A	2617	1MA	N1-C6-N6	2.07	125.04	119.77

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	AA	1583	MA6	C5-C6-N6-C9
25	AA	1584	MA6	C5-C6-N6-C9
25	AA	1584	MA6	C5-C6-N6-C10
33	AI	184	5F0	O1-C1-CA-CB
33	AI	184	5F0	OD1-C1-CA-CB
33	AI	184	5F0	N-CA-CB-C
33	AI	184	5F0	C1-CA-CB-C
33	AI	184	5F0	O-C-CB-CA
25	AA	1584	MA6	N1-C6-N6-C9
25	AA	1583	MA6	C5-C6-N6-C10
25	AA	1583	MA6	N1-C6-N6-C9
33	AI	184	5F0	O1-C1-CA-N
33	AI	184	5F0	OD1-C1-CA-N
25	AA	1584	MA6	C4'-C5'-O5'-P
56	Ax	34	RSQ	O4'-C4'-C5'-O5'

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	AA	1486	B8T	1	0
25	AA	1488	5MC	2	0
25	AA	1583	MA6	3	0
25	AA	1584	MA6	1	0
1	A	2815	OMG	2	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 273 ligands modelled in this entry, 264 are monoatomic - leaving 9 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
90	VAL	B	101	2	4,6,7	0.51	0	6,7,9	0.95	0
94	FES	AP	201	40,29	0,4,4	-	-	-		
92	SPD	AA	1703	-	9,9,9	0.29	0	8,8,8	0.85	0
96	GDP	AX	503	-	24,30,30	0.88	1 (4%)	30,47,47	0.62	0
91	NAD	AA	1701	87	42,48,48	0.57	0	50,73,73	0.57	1 (2%)
89	G34	A	6456	-	40,40,40	0.50	0	58,64,64	1.11	3 (5%)
94	FES	AT	201	44,37	0,4,4	-	-	-		
94	FES	r	201	7,84	0,4,4	-	-	-		
95	ATP	AX	501	87	26,33,33	0.75	0	31,52,52	0.66	0

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
90	VAL	B	101	2	-	1/5/6/8	-
94	FES	AP	201	40,29	-	-	0/1/1/1
92	SPD	AA	1703	-	-	0/7/7/7	-
96	GDP	AX	503	-	-	0/12/32/32	0/3/3/3
91	NAD	AA	1701	87	-	2/26/62/62	0/5/5/5
89	G34	A	6456	-	-	3/12/94/94	0/6/5/5
94	FES	AT	201	44,37	-	-	0/1/1/1
94	FES	r	201	7,84	-	-	0/1/1/1
95	ATP	AX	501	87	-	0/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
96	AX	503	GDP	C5-C6	-2.15	1.43	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
89	A	6456	G34	O1-C3-C2	-3.28	120.80	125.56
89	A	6456	G34	C15-C5-C14	-3.22	105.77	108.95
89	A	6456	G34	C1-C9-C10	-2.64	107.44	110.58
91	AA	1701	NAD	C5A-C6A-N6A	2.32	123.88	120.35

There are no chirality outliers.

All (6) torsion outliers are listed below:

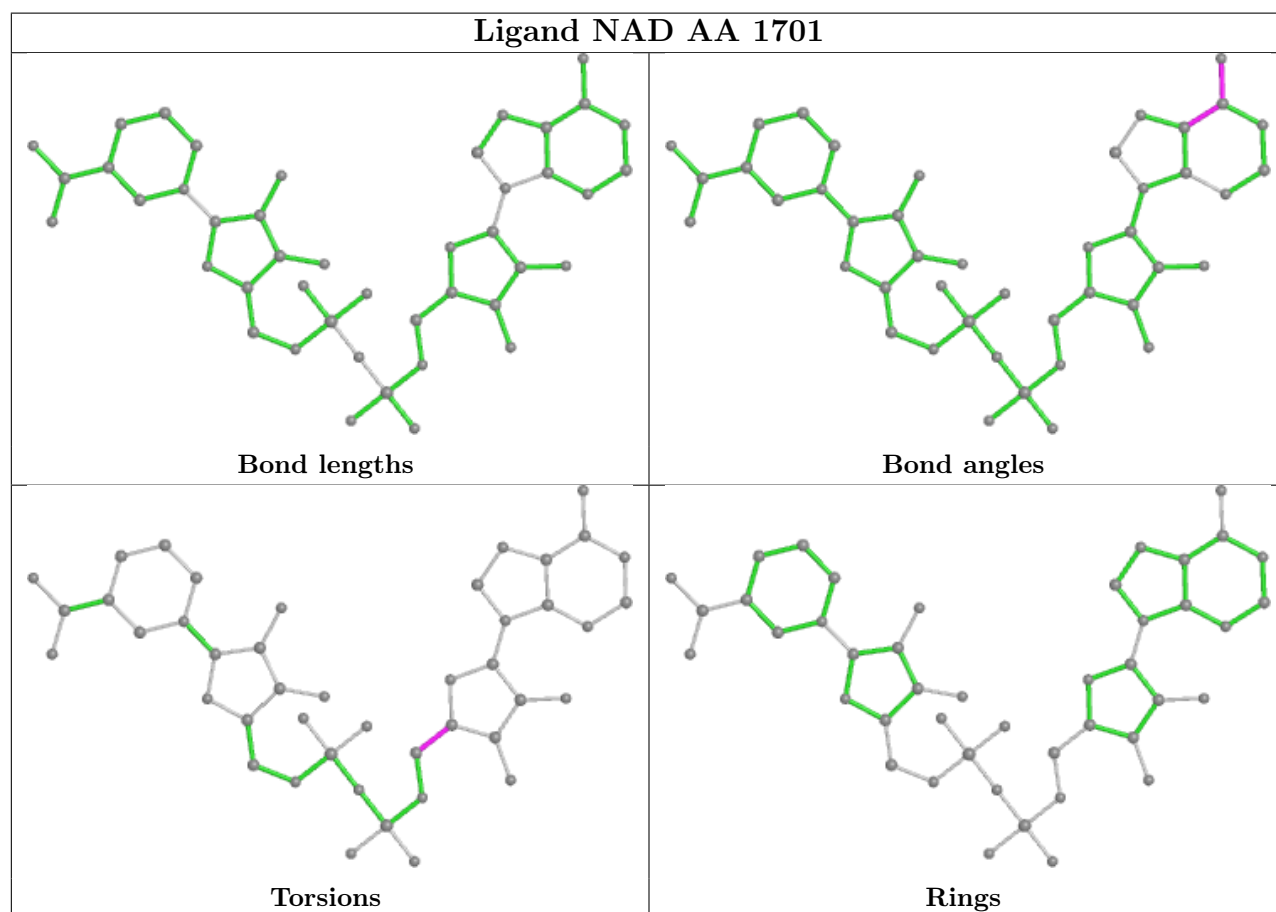
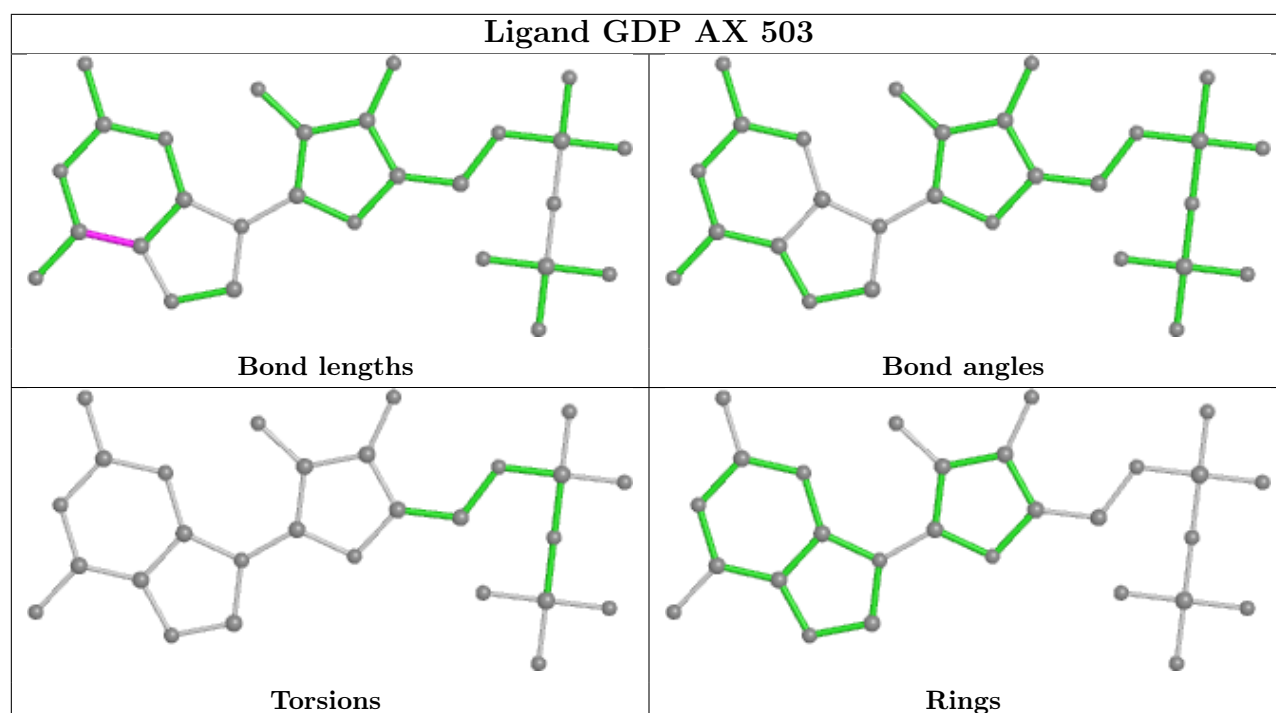
Mol	Chain	Res	Type	Atoms
89	A	6456	G34	C24-C23-S1-C22
91	AA	1701	NAD	O4B-C4B-C5B-O5B
91	AA	1701	NAD	C3B-C4B-C5B-O5B
89	A	6456	G34	C21-C22-S1-C23
89	A	6456	G34	C22-C21-O3-C14
90	B	101	VAL	O-C-CA-CB

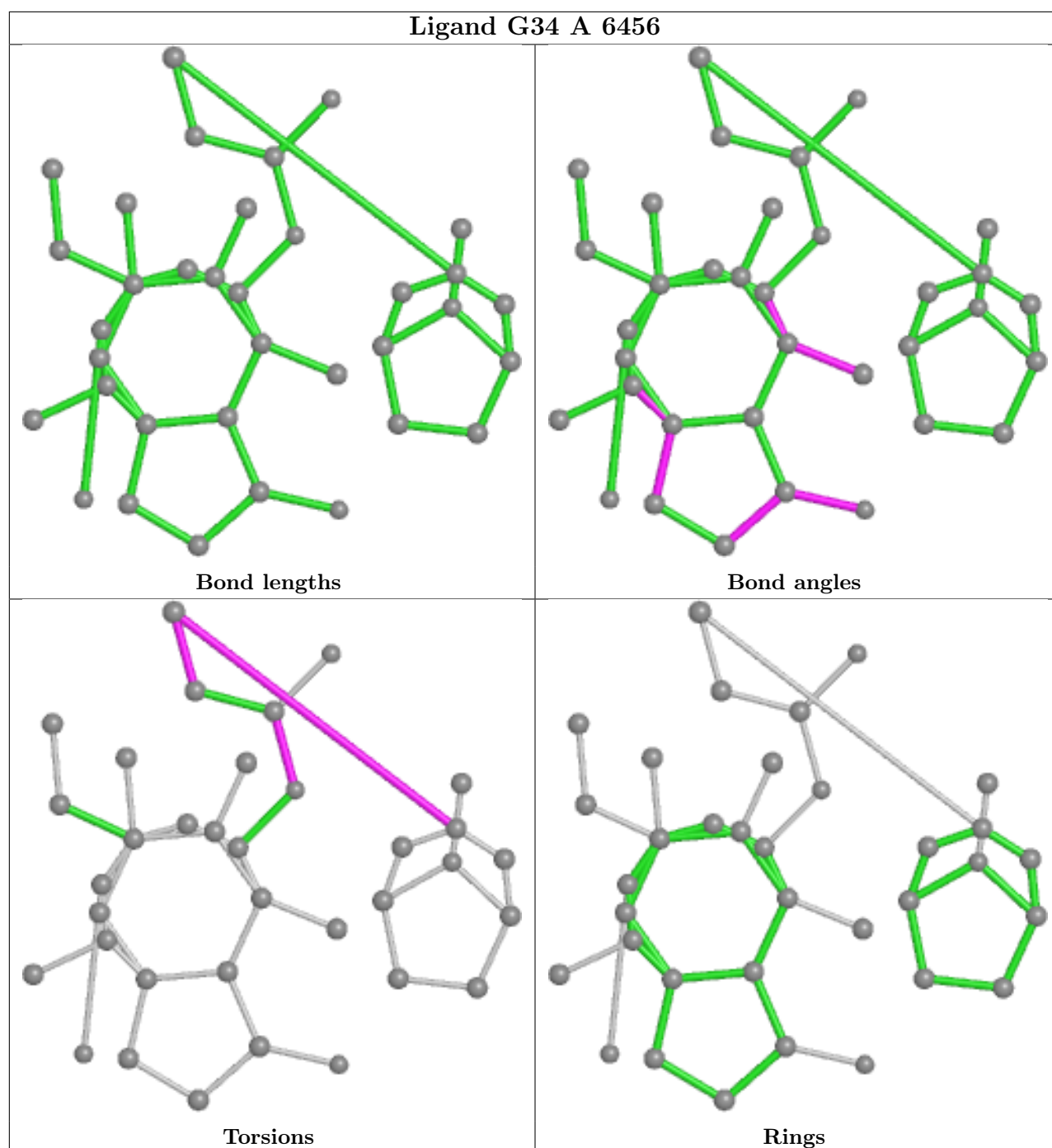
There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
90	B	101	VAL	2	0
96	AX	503	GDP	1	0
91	AA	1701	NAD	1	0
89	A	6456	G34	3	0
95	AX	501	ATP	1	0

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



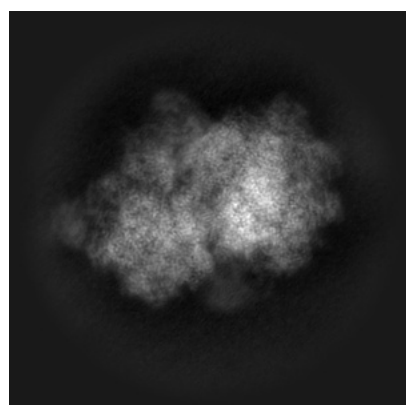
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64554. These allow visual inspection of the internal detail of the map and identification of artifacts.

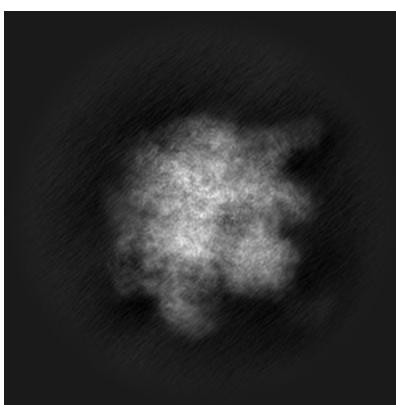
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

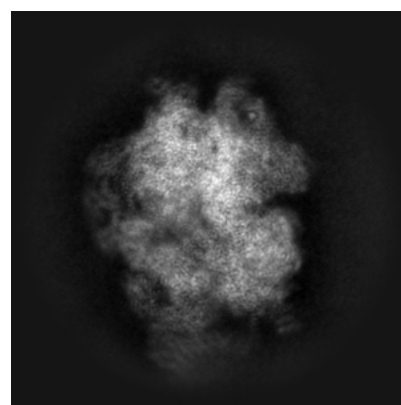
#### 6.1.1 Primary map



X



Y

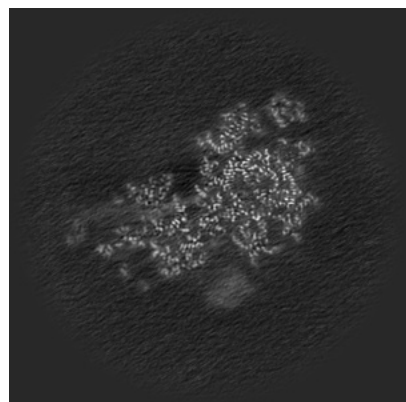


Z

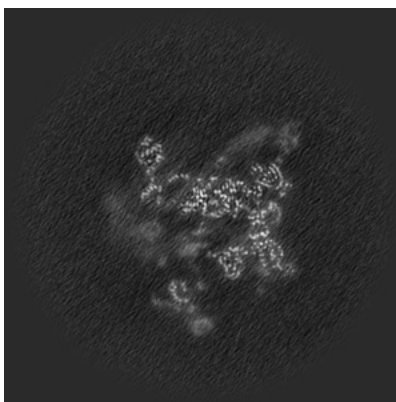
The images above show the map projected in three orthogonal directions.

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

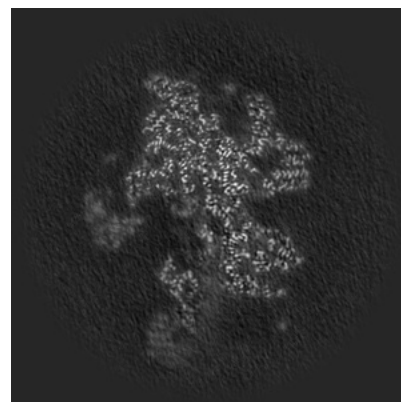
#### 6.2.1 Primary map



X Index: 256



Y Index: 256

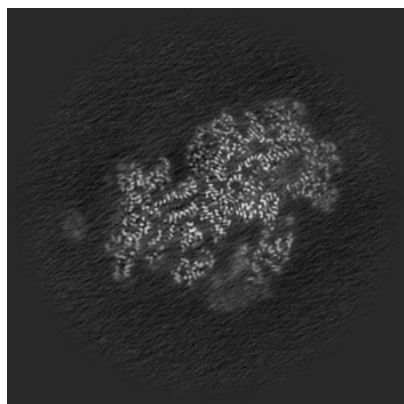


Z Index: 256

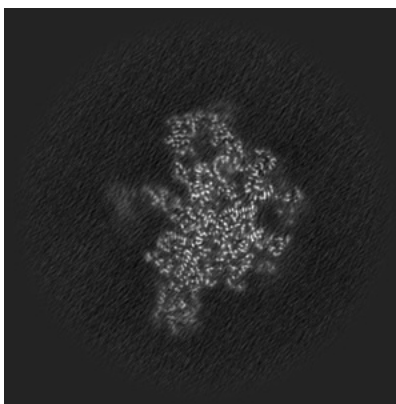
The images above show central slices of the map in three orthogonal directions.

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

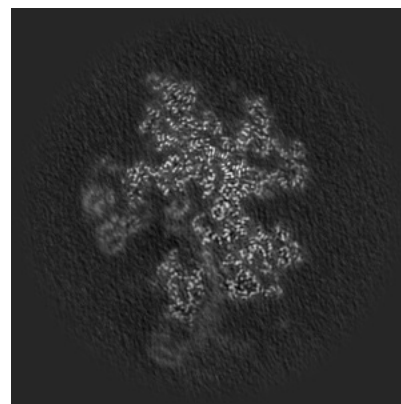
### 6.3.1 Primary map



X Index: 277



Y Index: 306

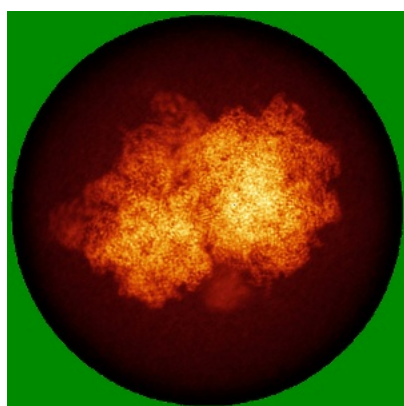


Z Index: 248

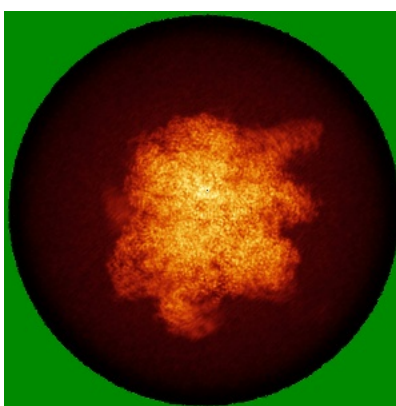
The images above show the largest variance slices of the map in three orthogonal directions.

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

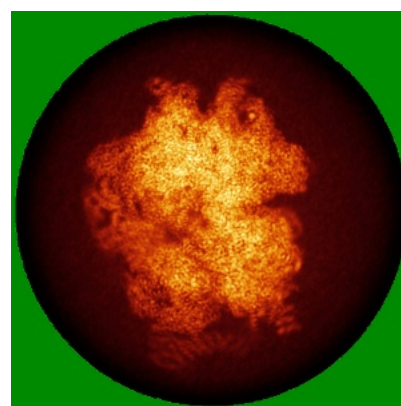
### 6.4.1 Primary map



X



Y

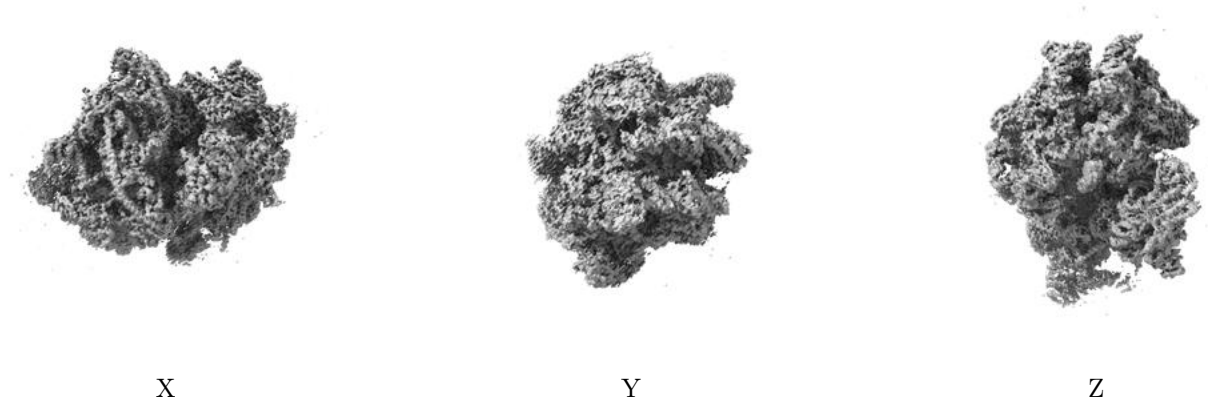


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

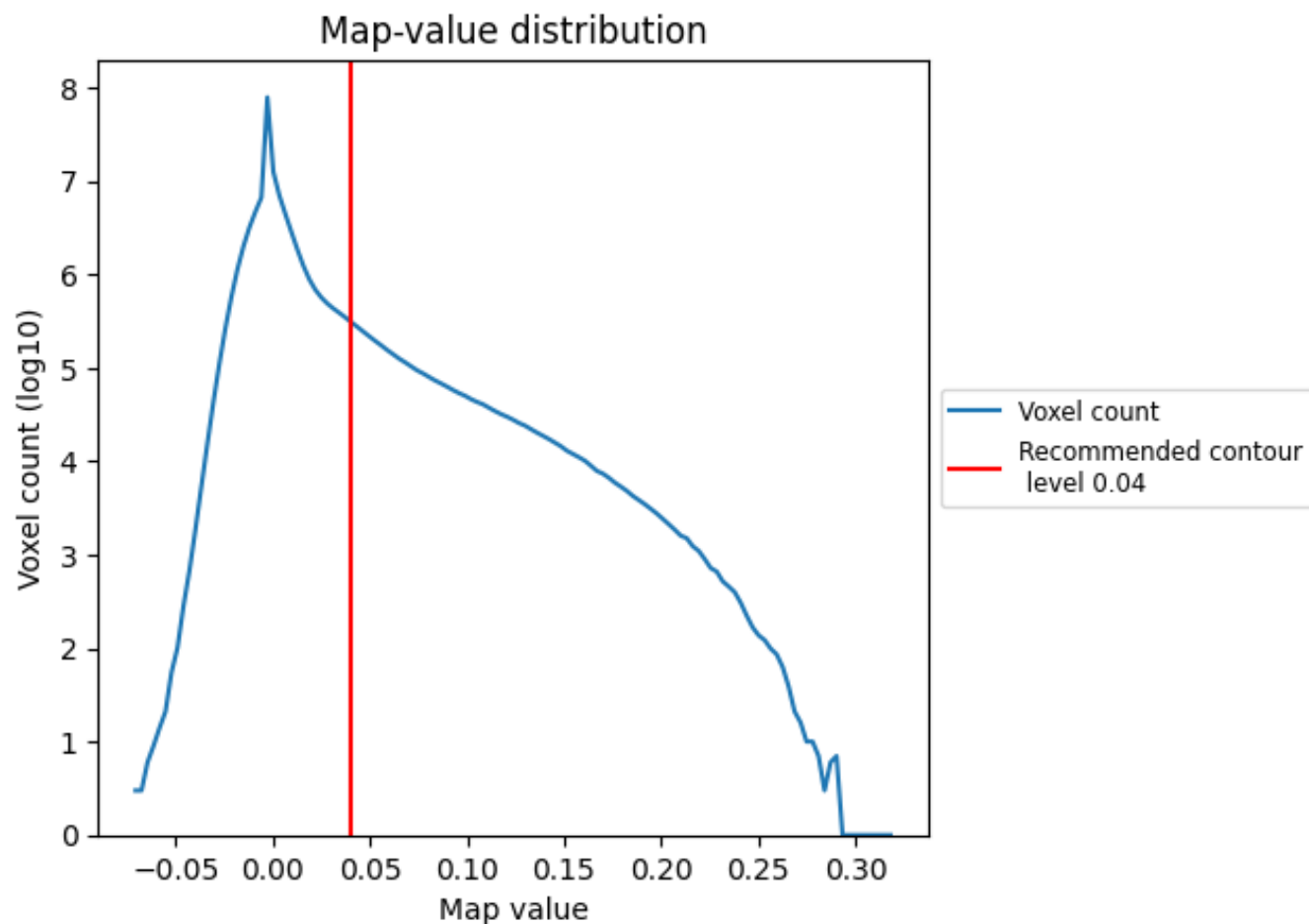
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

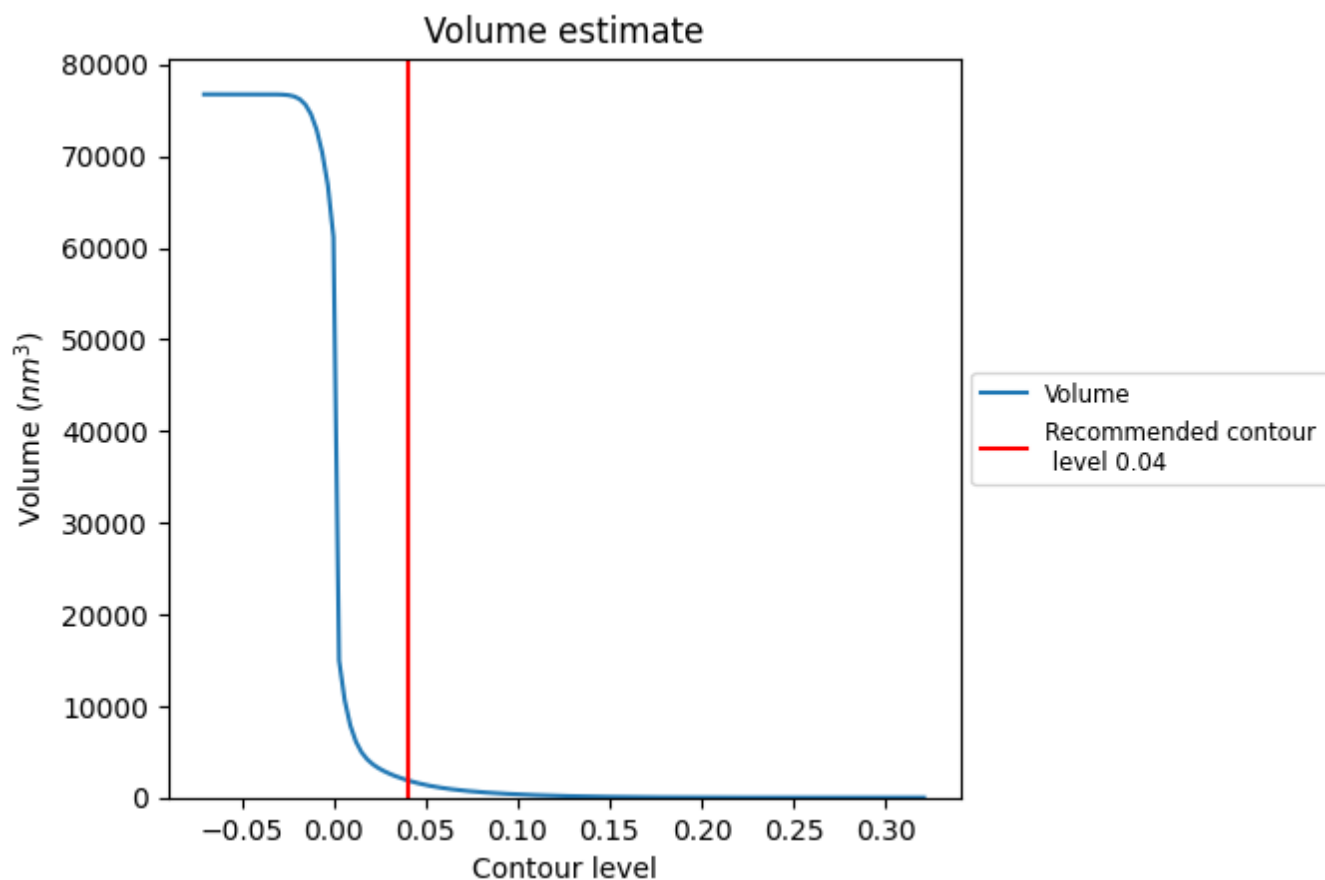
This section contains the results of statistical analysis of the map.

### 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.

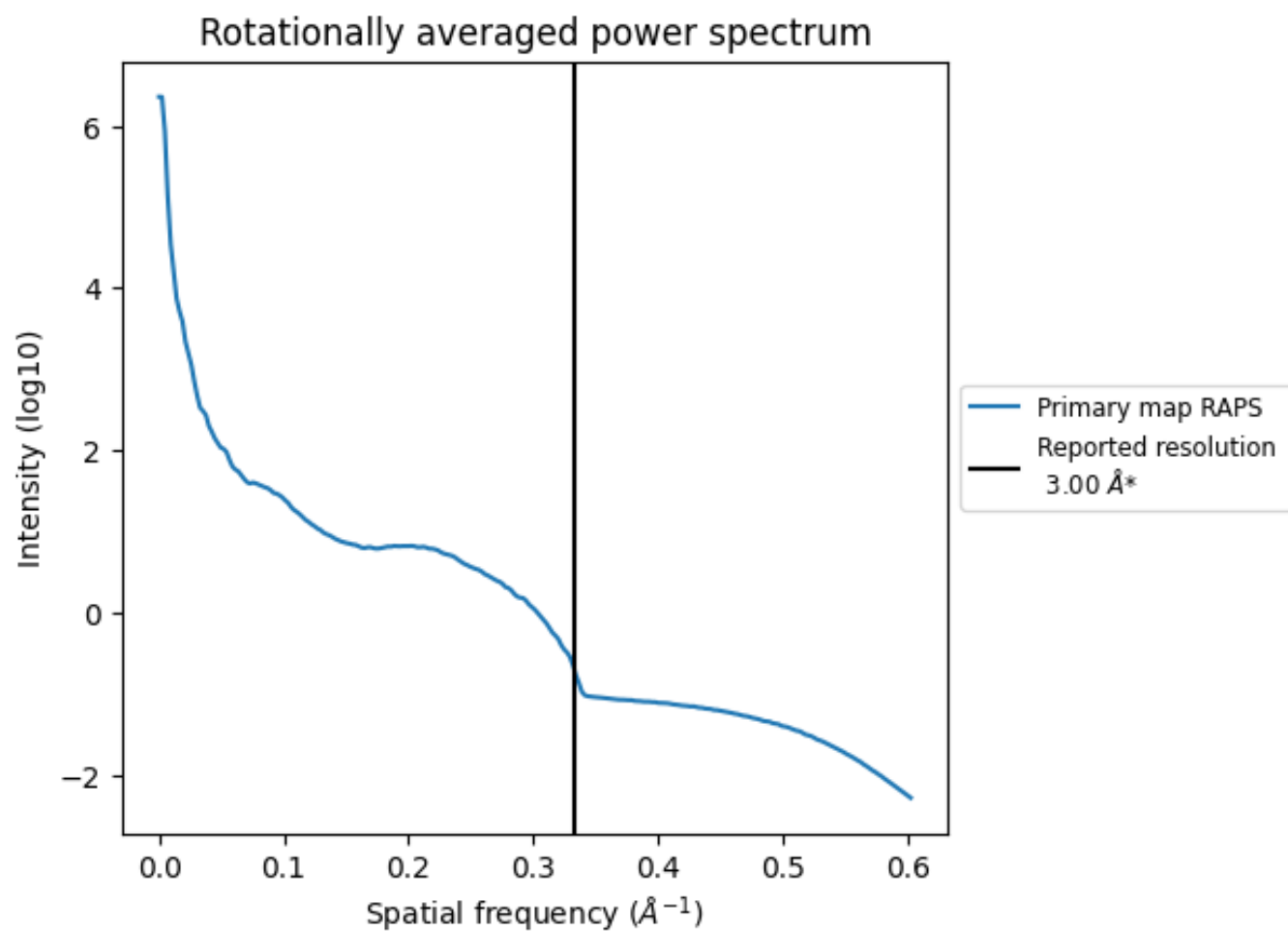
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1886 nm<sup>3</sup>; this corresponds to an approximate mass of 1704 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 0.333 Å<sup>-1</sup>

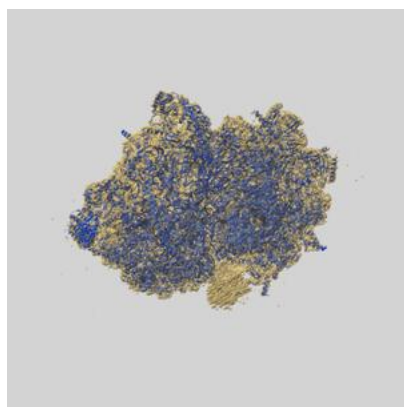
## 8 Fourier-Shell correlation

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

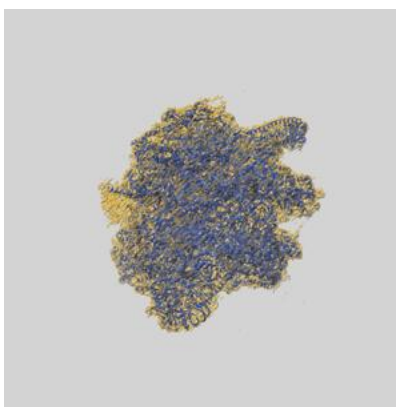
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-64554 and PDB model 9UWH. Per-residue inclusion information can be found in section [3](#) on page [26](#).

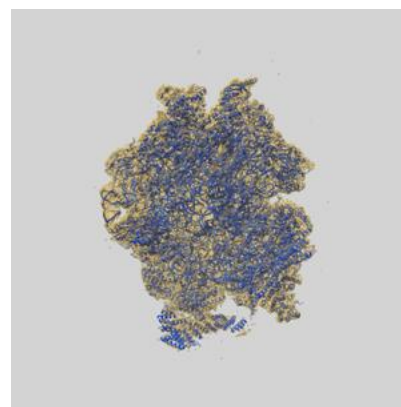
### 9.1 Map-model overlay [i](#)



X



Y

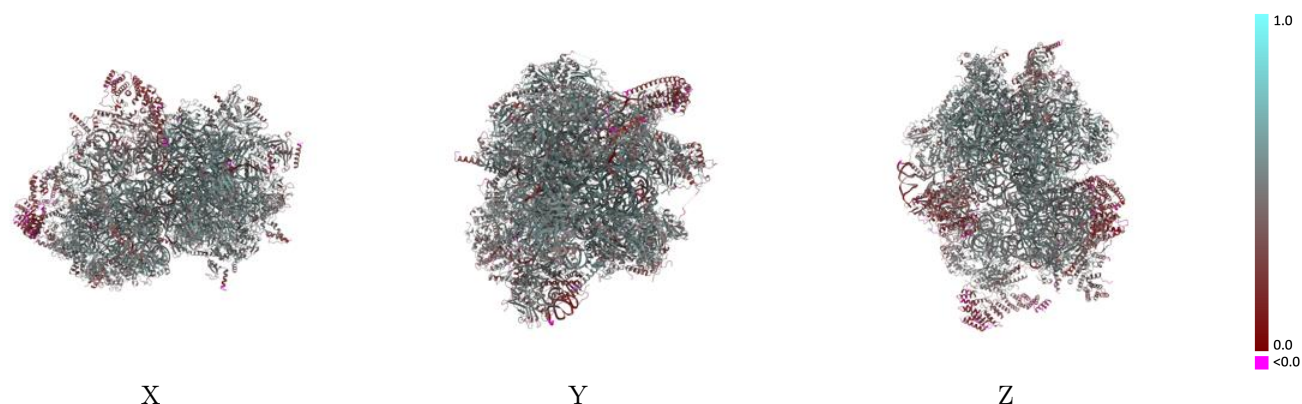


Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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.

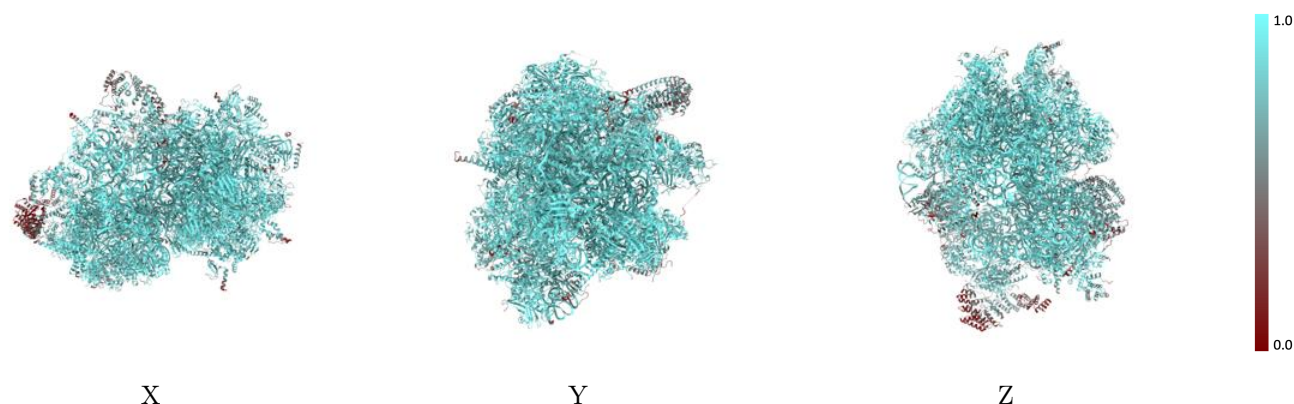


## 9.2 Q-score mapped to coordinate model [i](#)



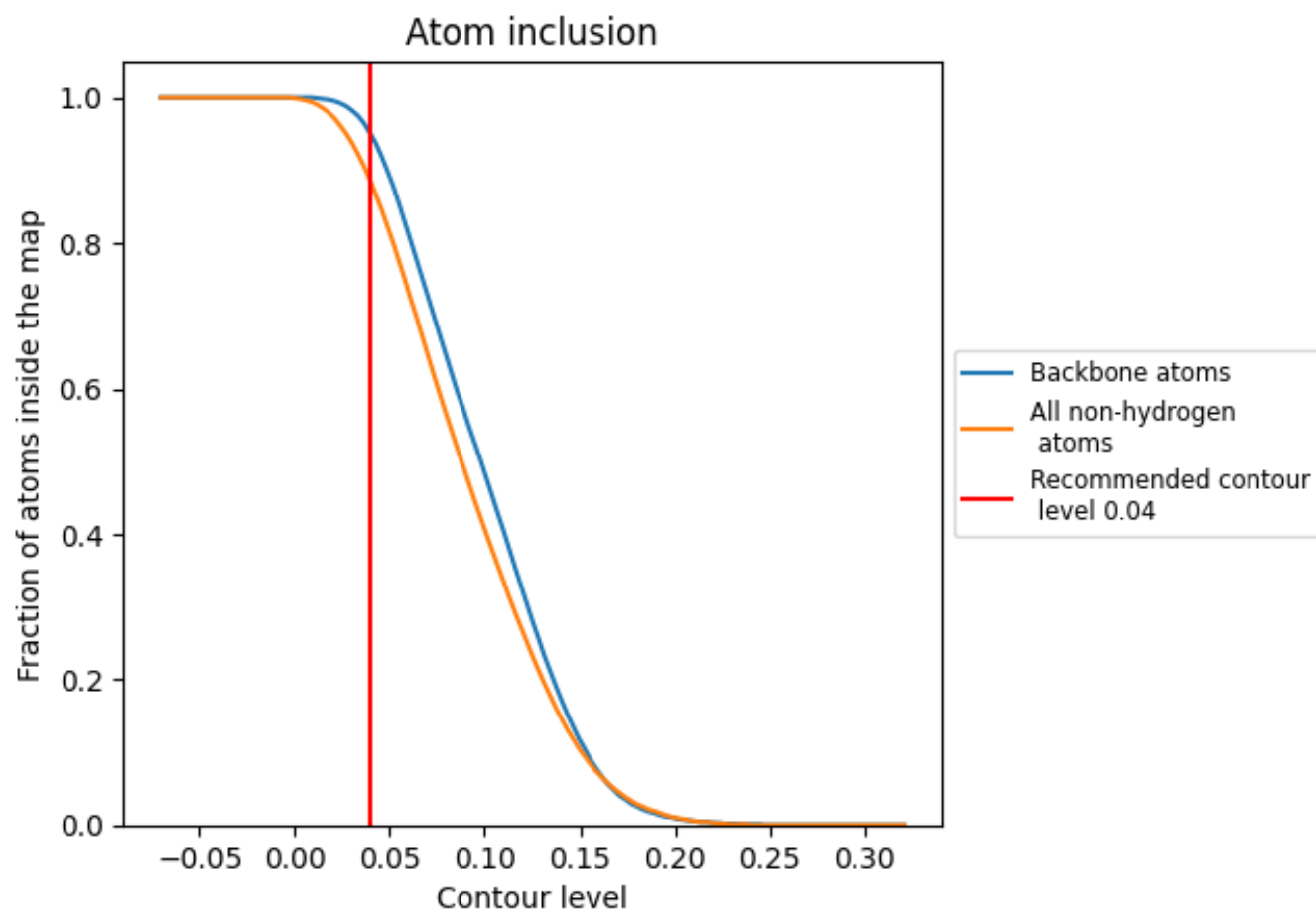
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 88% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8850	 0.4710
0	 0.9130	 0.5220
1	 0.9390	 0.5290
2	 0.9950	 0.5750
3	 0.9830	 0.5750
4	 0.9630	 0.5360
5	 0.9120	 0.5090
6	 0.8890	 0.4600
7	 0.8380	 0.4390
8	 0.6930	 0.3330
9	 0.8590	 0.4890
A	 0.9840	 0.5220
A0	 0.7440	 0.3630
A1	 0.7760	 0.4220
A2	 0.8930	 0.4710
A3	 0.9510	 0.5140
A4	 0.3840	 0.2300
AA	 0.9750	 0.5010
AB	 0.9250	 0.5080
AC	 0.8980	 0.5060
AD	 0.8690	 0.4840
AE	 0.9110	 0.5110
AF	 0.8960	 0.4600
AG	 0.8890	 0.4680
AH	 0.8020	 0.4500
AI	 0.9280	 0.5200
AJ	 0.8580	 0.4970
AK	 0.9180	 0.5110
AL	 0.8720	 0.4610
AM	 0.8330	 0.4450
AN	 0.9380	 0.5270
AO	 0.8300	 0.4260
AP	 0.9300	 0.5160
AQ	 0.9600	 0.5350
AR	 0.8000	 0.4000























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Chain	Atom inclusion	Q-score
AS	 0.8130	 0.4450
AT	 0.8970	 0.4800
AU	 0.7840	 0.4010
AV	 0.5680	 0.2350
AW	 0.9090	 0.4910
AX	 0.8420	 0.4410
AY	 0.7300	 0.3870
AZ	 0.8270	 0.4580
Ax	 0.9190	 0.3980
Az	 0.9640	 0.4310
B	 0.8860	 0.3270
D	 0.9630	 0.5520
E	 0.9410	 0.5260
F	 0.9600	 0.5390
H	 0.7680	 0.4240
I	 0.6510	 0.3370
J	 0.6600	 0.2330
K	 0.9560	 0.5300
L	 0.9070	 0.5240
M	 0.9400	 0.5310
N	 0.9200	 0.5100
O	 0.9100	 0.5130
P	 0.9190	 0.4990
Q	 0.8410	 0.4960
R	 0.9580	 0.5450
S	 0.9290	 0.5290
T	 0.9510	 0.5470
U	 0.8750	 0.4760
V	 0.8330	 0.4480
W	 0.9340	 0.5430
X	 0.8840	 0.4920
Y	 0.9280	 0.5120
Z	 0.9280	 0.5360
a	 0.8240	 0.4500
b	 0.9390	 0.5380
c	 0.8880	 0.4800
d	 0.7980	 0.4060
e	 0.6400	 0.2670
f	 0.7210	 0.3980
g	 0.9180	 0.5160
h	 0.8560	 0.4380
i	 0.9710	 0.5660

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Chain	Atom inclusion	Q-score
j	 0.8410	 0.4670
k	 0.7410	 0.3440
l	 0.6820	 0.2940
m	 0.6660	 0.3170
o	 0.9630	 0.5300
p	 0.7720	 0.4120
q	 0.8010	 0.4080
r	 0.9000	 0.4930
s	 0.9340	 0.5140
t	 0.2360	 0.2580