



Full wwPDB EM Validation Report ⓘ

Dec 1, 2025 – 03:18 PM EST

PDB ID : 9N7B / pdb_00009n7b
EMDB ID : EMD-49091
Title : SSU processome maturation and disassembly, State O
Authors : Buzovetsky, O.; Klinge, S.
Deposited on : 2025-02-05
Resolution : 3.25 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

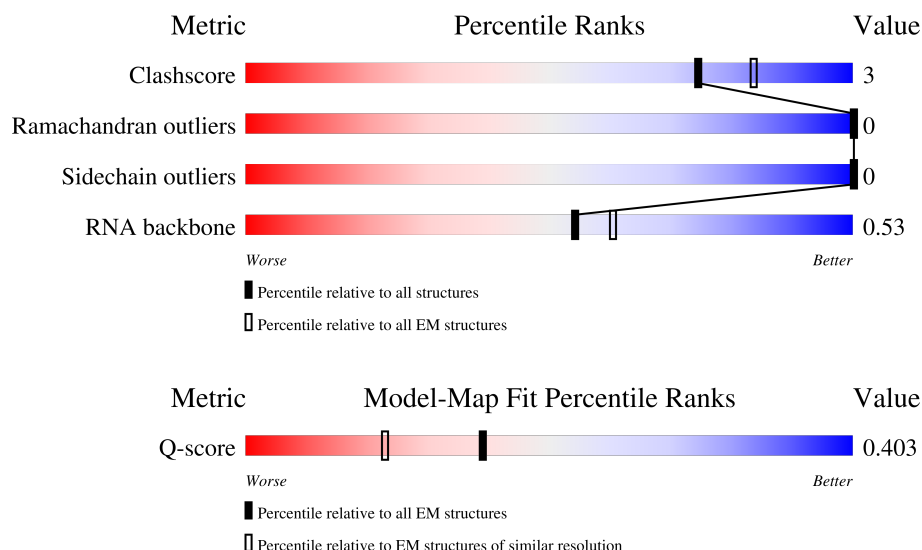
EMDB validation analysis : 0.0.1.dev129
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive 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 3.25 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.




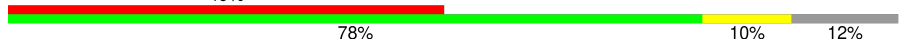




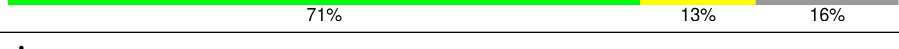
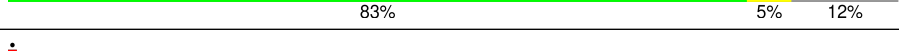
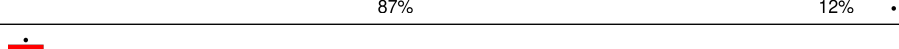

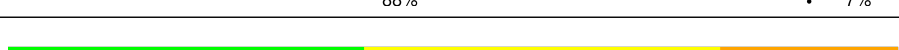


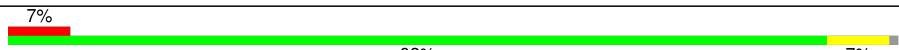
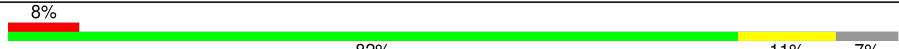






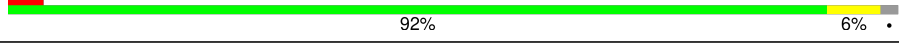



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
RNA backbone	6643	2191	-
Q-score	-	25397	14599 (2.75 - 3.75)

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

Mol	Chain	Length	Quality of chain
1	L1	1803	
2	L2	334	
3	L3	146	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	L4	261	
5	L5	225	
6	L6	236	
7	L7	190	
8	L8	200	
9	L9	197	
10	LC	143	
11	LD	156	
12	LE	130	
13	LF	135	
14	LG	67	
15	N2	5	
16	NA	593	
17	NB	610	
18	NF	151	
19	NG	137	
20	NL	318	
21	NM	255	
22	NP	144	
23	NQ	82	
24	NS	1267	
25	NW	108	
26	SH	367	
27	SI	1183	
28	SJ	252	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	SK	252	<p>91% 9% 6%</p>
29	SL	189	<p>68% 6% 26% 6%</p>
30	SM	290	<p>65% 10% 24% 33%</p>
31	SR	145	<p>91% 8% 7%</p>
32	SS	899	<p>15% 83%</p>
33	ST	810	<p>60% 39% 60%</p>
34	SU	552	<p>96% 96%</p>
35	SW	274	<p>59% 7% 35% 59%</p>
36	SZ	483	<p>54% 53% 46%</p>

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 85883 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L1	1401	Total	C	N	O	P	0	0
			29868	13354	5304	9809	1401		

- Molecule 2 is a RNA chain called U3 snoRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L2	23	Total	C	N	O	P	0	0
			496	220	87	165	24		

- Molecule 3 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L3	100	Total	C	N	O	S	0	0
			815	515	152	146	2		

- Molecule 4 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L4	258	Total	C	N	O	S	0	0
			2056	1308	387	358	3		

- Molecule 5 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L5	197	Total	C	N	O	S	0	0
			1558	975	291	289	3		

- Molecule 6 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L6	227	Total	C	N	O	S	0	0
			1831	1148	354	326	3		

- Molecule 7 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	L7	186	Total	C	N	O	0	0
			1492	957	267	268		

- Molecule 8 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L8	181	Total	C	N	O	S	0	0
			1437	892	287	256	2		

- Molecule 9 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L9	181	Total	C	N	O	S	0	0
			1470	930	285	254	1		

- Molecule 10 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	LC	120	Total	C	N	O	0	0
			930	598	165	167		

- Molecule 11 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LD	138	Total	C	N	O	S	0	0
			1119	718	213	185	3		

- Molecule 12 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LE	129	Total	C	N	O	S	0	0
			1022	650	188	181	3		

- Molecule 13 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	LF	130	Total	C	N	O	0	0
			1046	662	204	180		

- Molecule 14 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LG	62	Total	C	N	O	S	0	0
			490	302	98	89	1		

- Molecule 15 is a RNA chain called U3snoRNA segment.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N2	5	Total	C	N	O	P	0	0
			100	45	10	40	5		

- Molecule 16 is a protein called U3 small nucleolar RNA-associated protein MPP10.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	NA	103	Total	C	N	O	S	0	0
			843	522	147	173	1		

- Molecule 17 is a protein called Something about silencing protein 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	NB	54	Total	C	N	O	0	0
			460	289	95	76		

- Molecule 18 is a protein called 40S ribosomal protein S13.

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

- Molecule 19 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	NG	127	Total	C	N	O	S	0	0
			941	578	186	174	3		

- Molecule 20 is a protein called Dimethyladenosine transferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	NL	283	Total	C	N	O	S	0	0
			2262	1439	401	408	14		

- Molecule 21 is a protein called Small ribosomal subunit protein eS1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	NM	211	Total	C	N	O	S	0	0
			1688	1070	306	308	4		

- Molecule 22 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	NP	134	Total	C	N	O	S	0	0
			1040	653	193	192	2		

- Molecule 23 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	NQ	79	Total	C	N	O	S	0	0
			595	371	108	111	5		

- Molecule 24 is a protein called Probable ATP-dependent RNA helicase DHR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	NS	866	Total	C	N	O	S	0	0
			6446	4091	1147	1178	30		

- Molecule 25 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	NW	69	Total	C	N	O	0	0
			556	356	103	97		

- Molecule 26 is a protein called RNA 3'-terminal phosphate cyclase-like protein.

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

- Molecule 27 is a protein called Ribosome biogenesis protein BMS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	SI	707	Total	C	N	O	S	0	0
			5739	3687	1017	1008	27		

- Molecule 28 is a protein called Ribosomal RNA small subunit methyltransferase NEP1.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	SJ	213	Total	C	N	O	0	0
			1074	648	213	213		
28	SK	229	Total	C	N	O	0	0
			1160	702	229	229		

- Molecule 29 is a protein called rRNA-processing protein FCF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	SL	140	Total	C	N	O	S	0	0
			1108	712	196	190	10		

- Molecule 30 is a protein called U3 small nucleolar ribonucleoprotein protein IMP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	SM	219	Total	C	N	O	S	0	0
			1756	1107	325	318	6		

- Molecule 31 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	SR	134	Total	C	N	O	S	0	0
			1052	668	204	178	2		

- Molecule 32 is a protein called U3 small nucleolar RNA-associated protein 14.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	SS	153	Total	C	N	O	P	S	0	0
			1278	788	240	239	1	10		

- Molecule 33 is a protein called Nucleolar complex protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	ST	492	Total	C	N	O	S	0	0
			2669	1624	524	518	3		

- Molecule 34 is a protein called Nucleolar complex protein 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	SU	532	Total	C	N	O	0	0
			2703	1639	532	532		

- Molecule 35 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	SW	179	Total	C	N	O	S	0	0
			1415	906	255	250	4		

- Molecule 36 is a protein called Essential nuclear protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	SZ	259	Total	C	N	O		0	0
			1314	796	259	259			

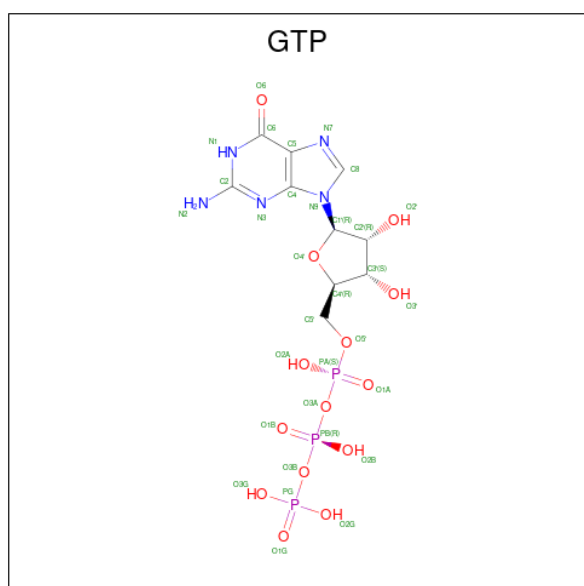
- Molecule 37 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
37	L1	46	Total	Mg	0
			46	46	
37	SI	1	Total	Mg	0
			1	1	

- Molecule 38 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
38	NQ	1	Total	Zn	0
			1	1	
38	SL	1	Total	Zn	0
			1	1	

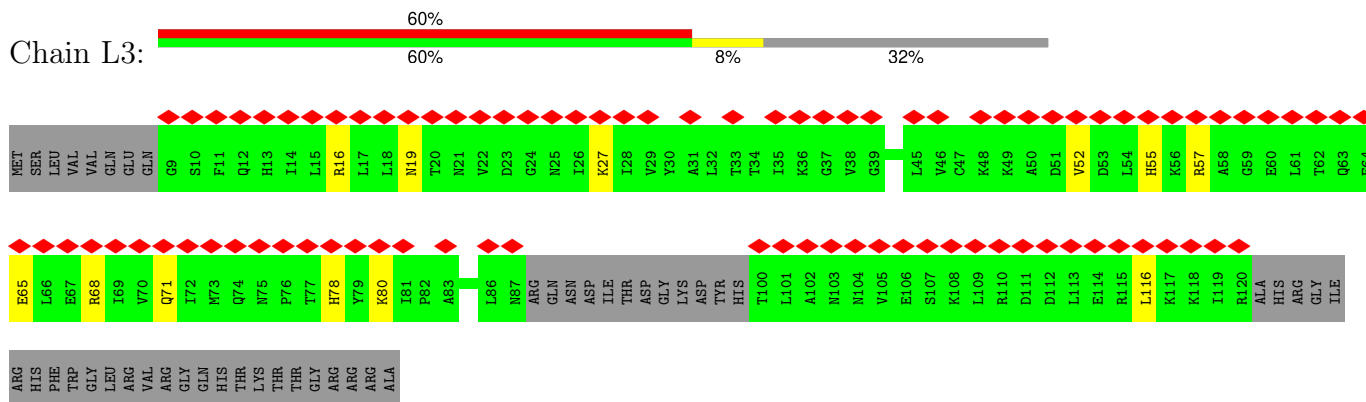
- Molecule 39 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



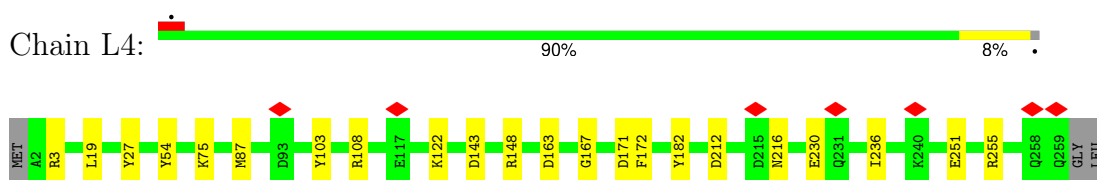
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
39	SI	1	32	10	5	14	3	0



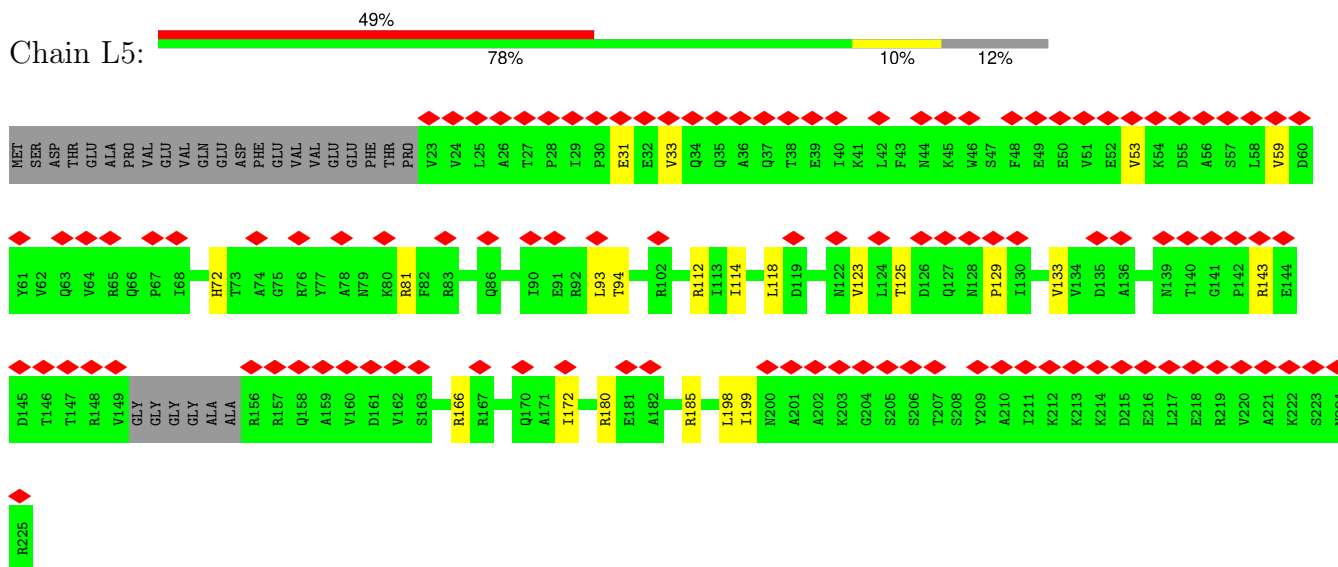
- Molecule 3: 40S ribosomal protein S18-A



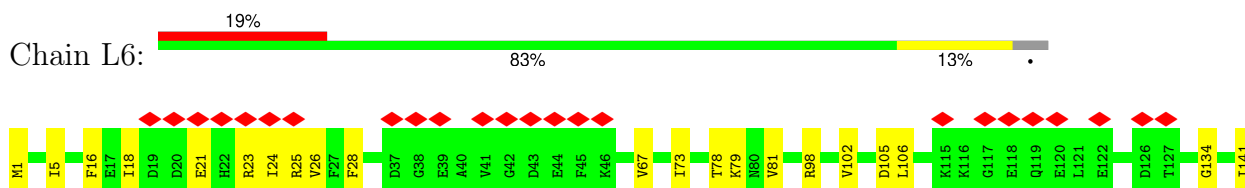
- Molecule 4: 40S ribosomal protein S4-A



- Molecule 5: 40S ribosomal protein S5

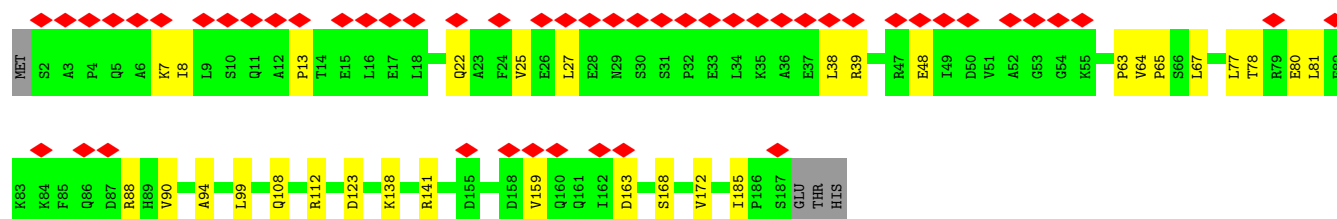
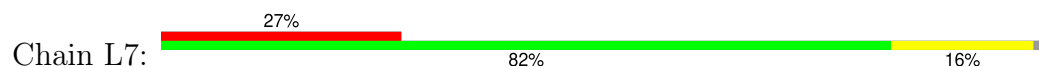


- Molecule 6: 40S ribosomal protein S6-A

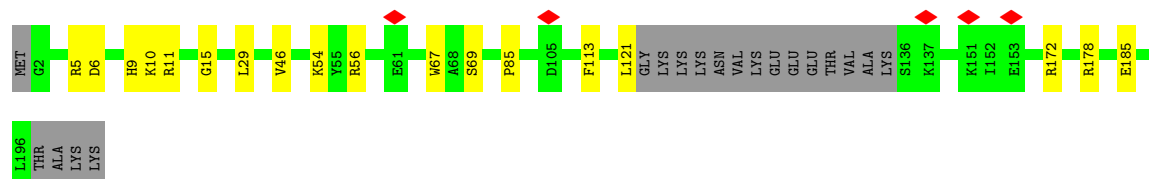
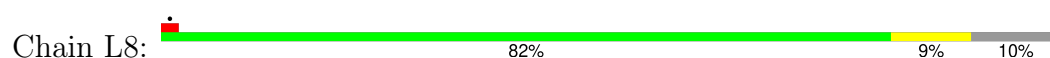




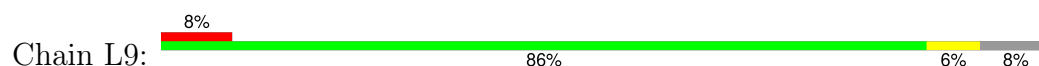
• Molecule 7: 40S ribosomal protein S7-A



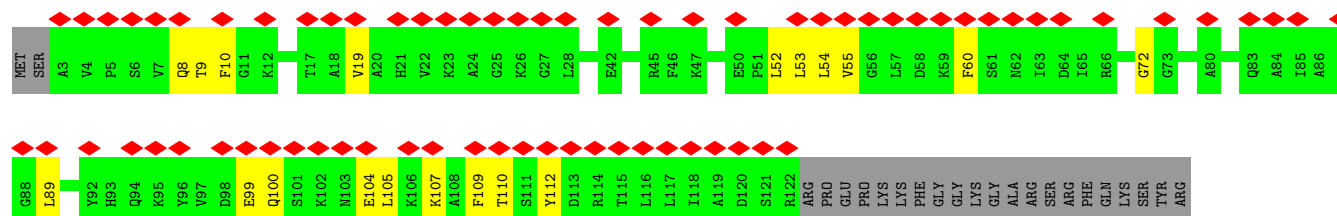
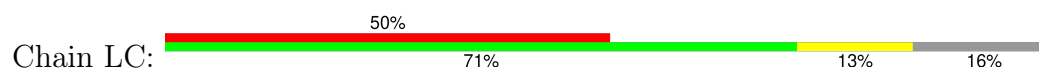
• Molecule 8: 40S ribosomal protein S8-A



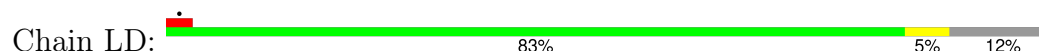
• Molecule 9: 40S ribosomal protein S9-A



• Molecule 10: 40S ribosomal protein S16-A



• Molecule 11: 40S ribosomal protein S11-A

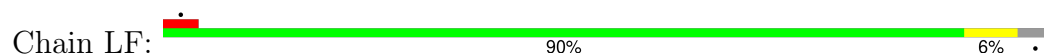




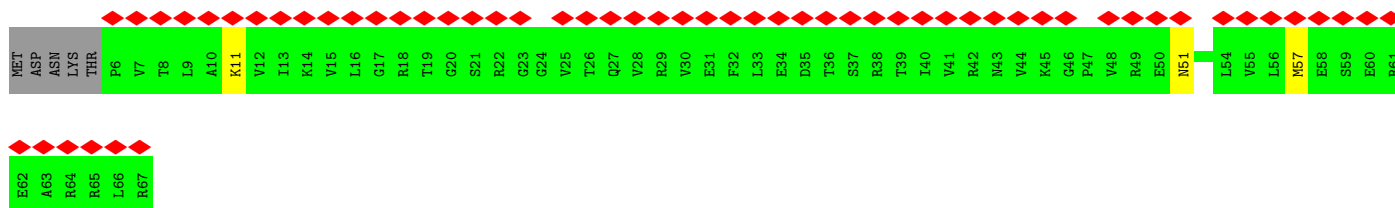
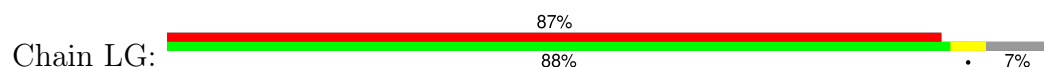
- Molecule 12: 40S ribosomal protein S22-A



- Molecule 13: 40S ribosomal protein S24-A



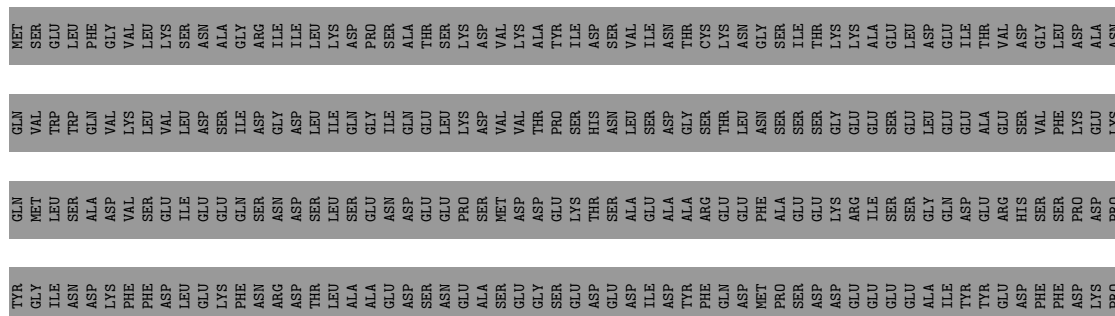
- Molecule 14: 40S ribosomal protein S28-A



- Molecule 15: U3snoRNA segment

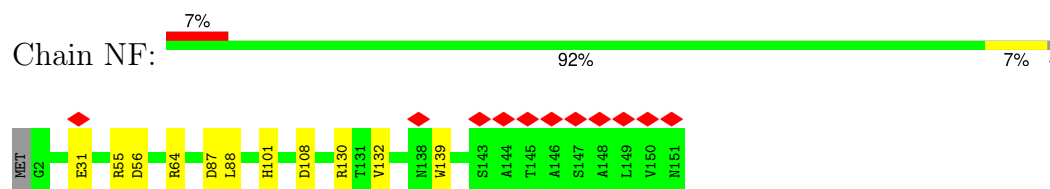


- Molecule 16: U3 small nucleolar RNA-associated protein MPP10

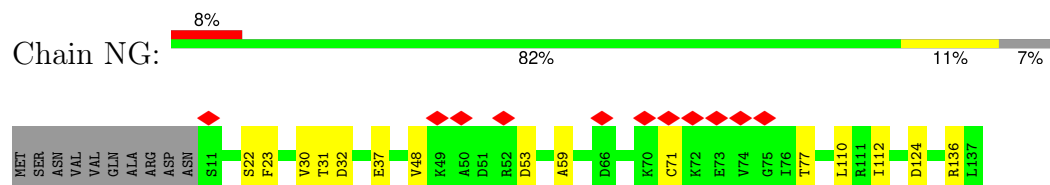




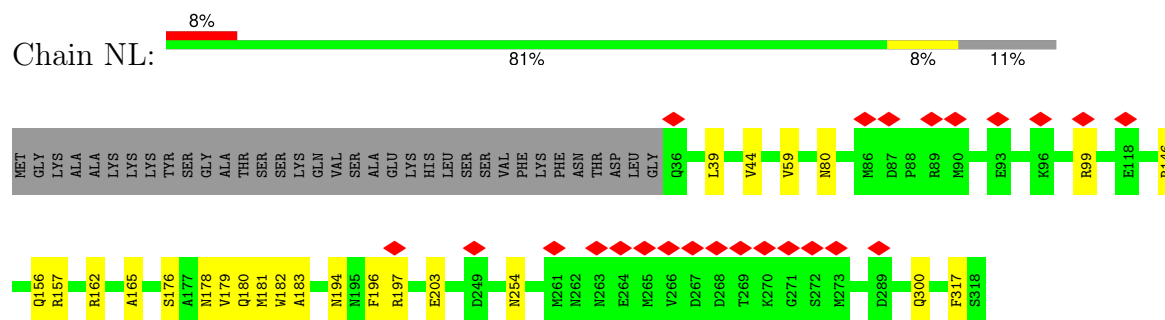
- Molecule 18: 40S ribosomal protein S13



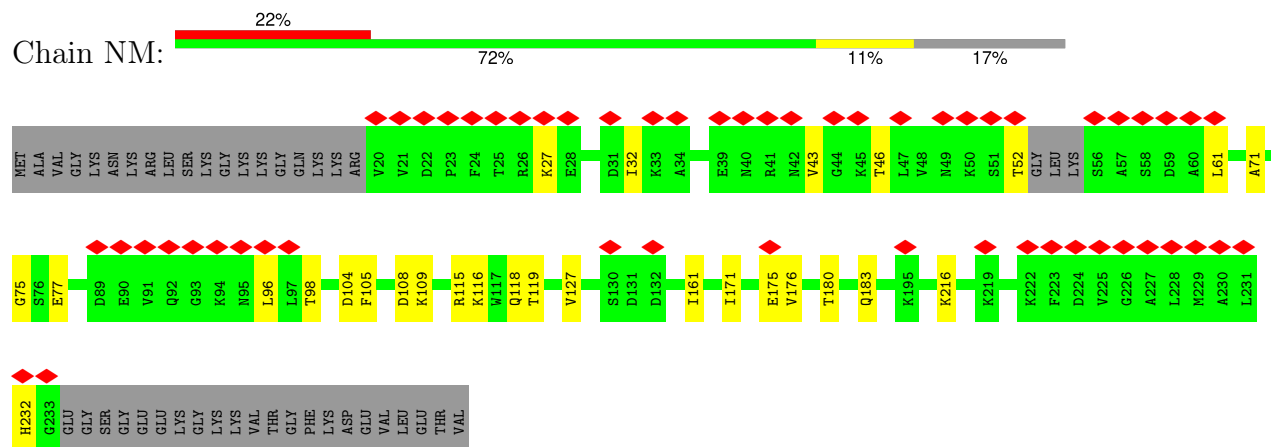
- Molecule 19: 40S ribosomal protein S14-A



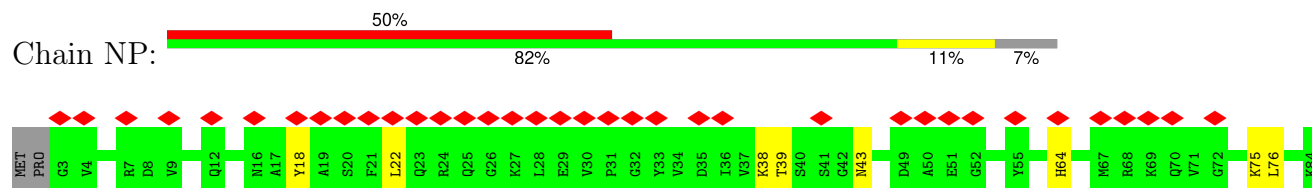
- Molecule 20: Dimethyladenosine transferase

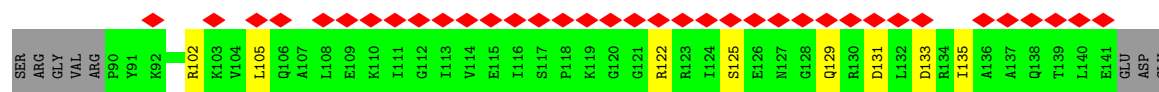


- Molecule 21: Small ribosomal subunit protein eS1A

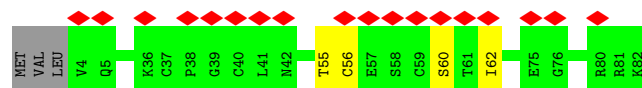


- Molecule 22: 40S ribosomal protein S19-A

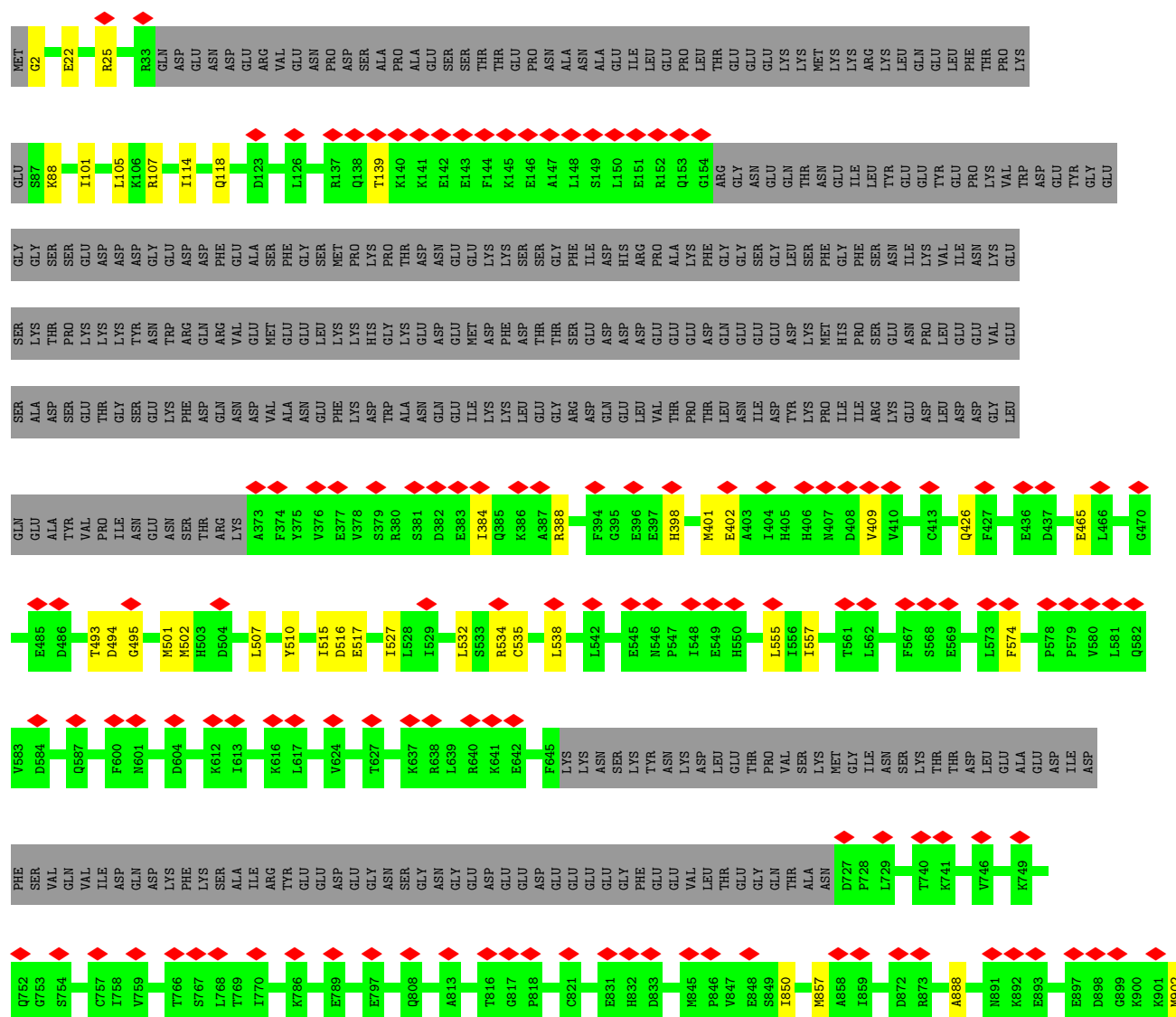


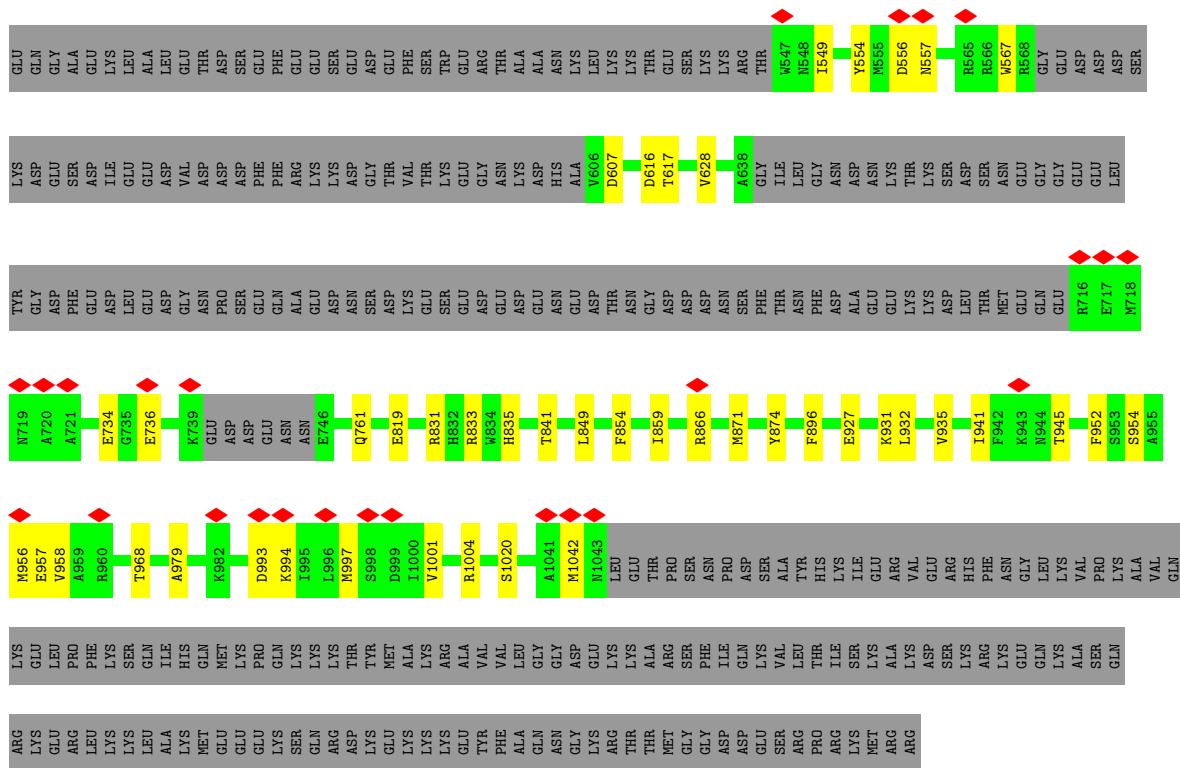


- Molecule 23: 40S ribosomal protein S27-A

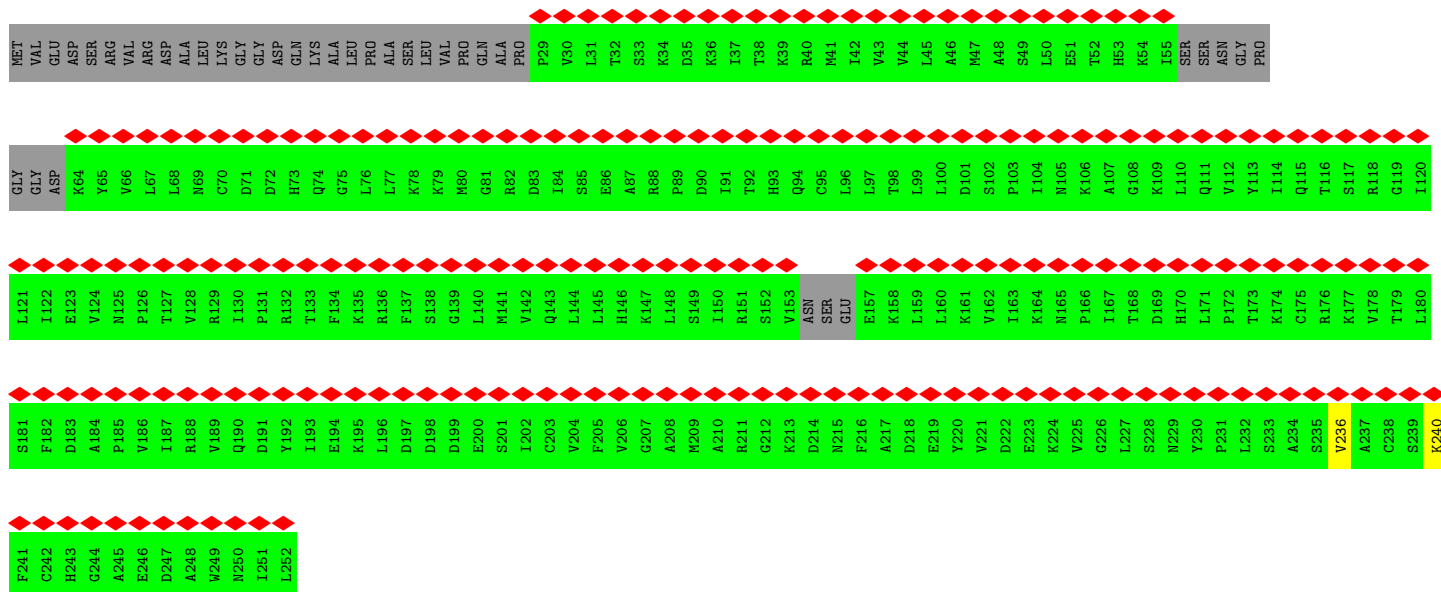
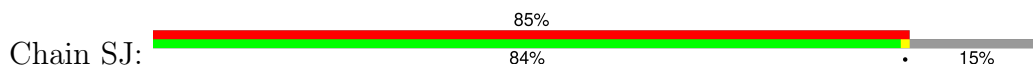


- Molecule 24: Probable ATP-dependent RNA helicase DHR1

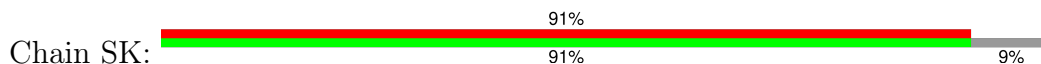


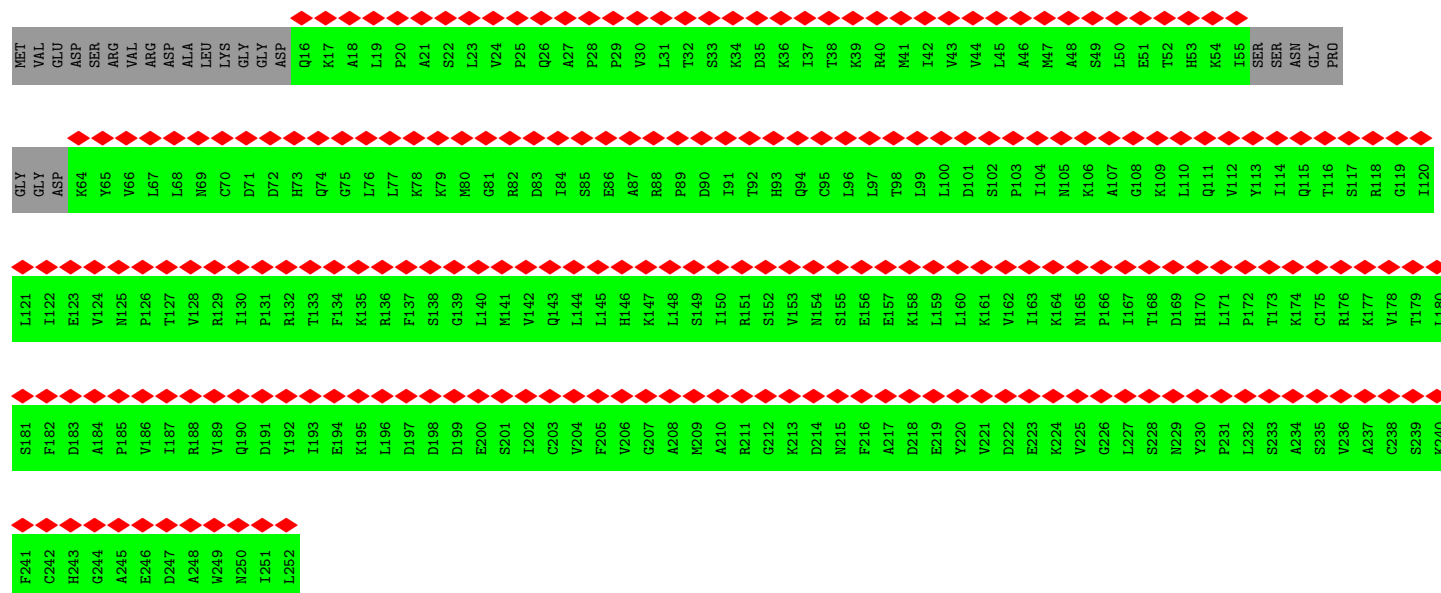


- Molecule 28: Ribosomal RNA small subunit methyltransferase NEP1

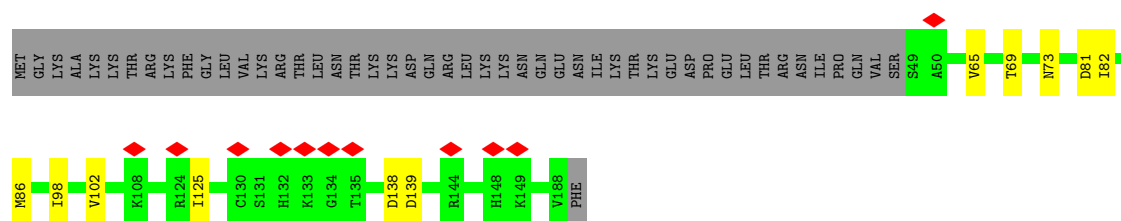


- Molecule 28: Ribosomal RNA small subunit methyltransferase NEP1

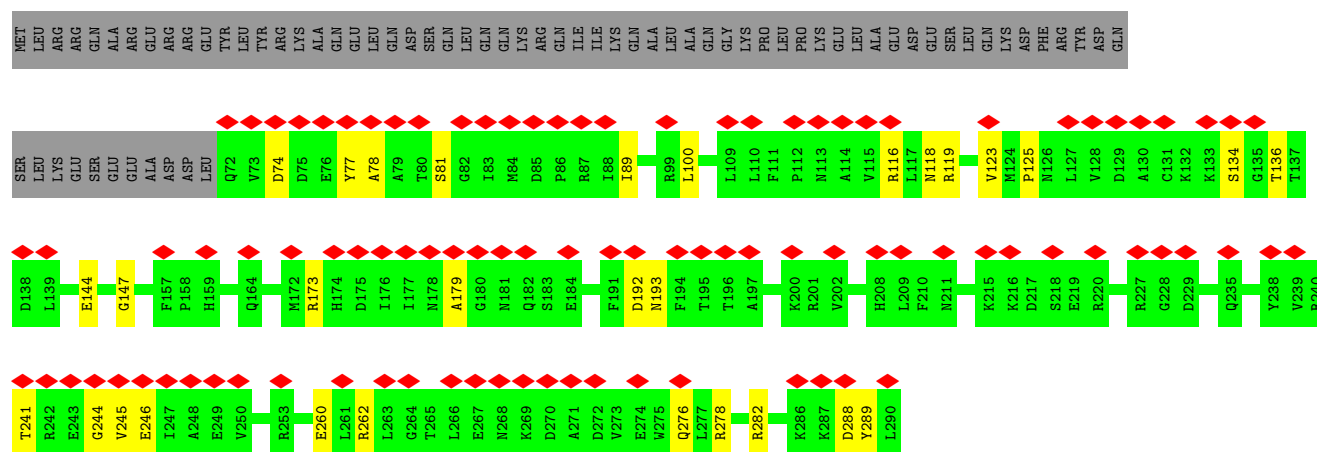




• Molecule 29: rRNA-processing protein FCF1

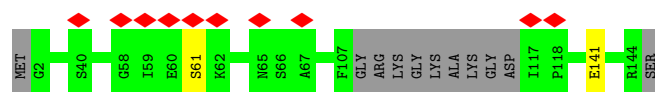


• Molecule 30: U3 small nucleolar ribonucleoprotein protein IMP4



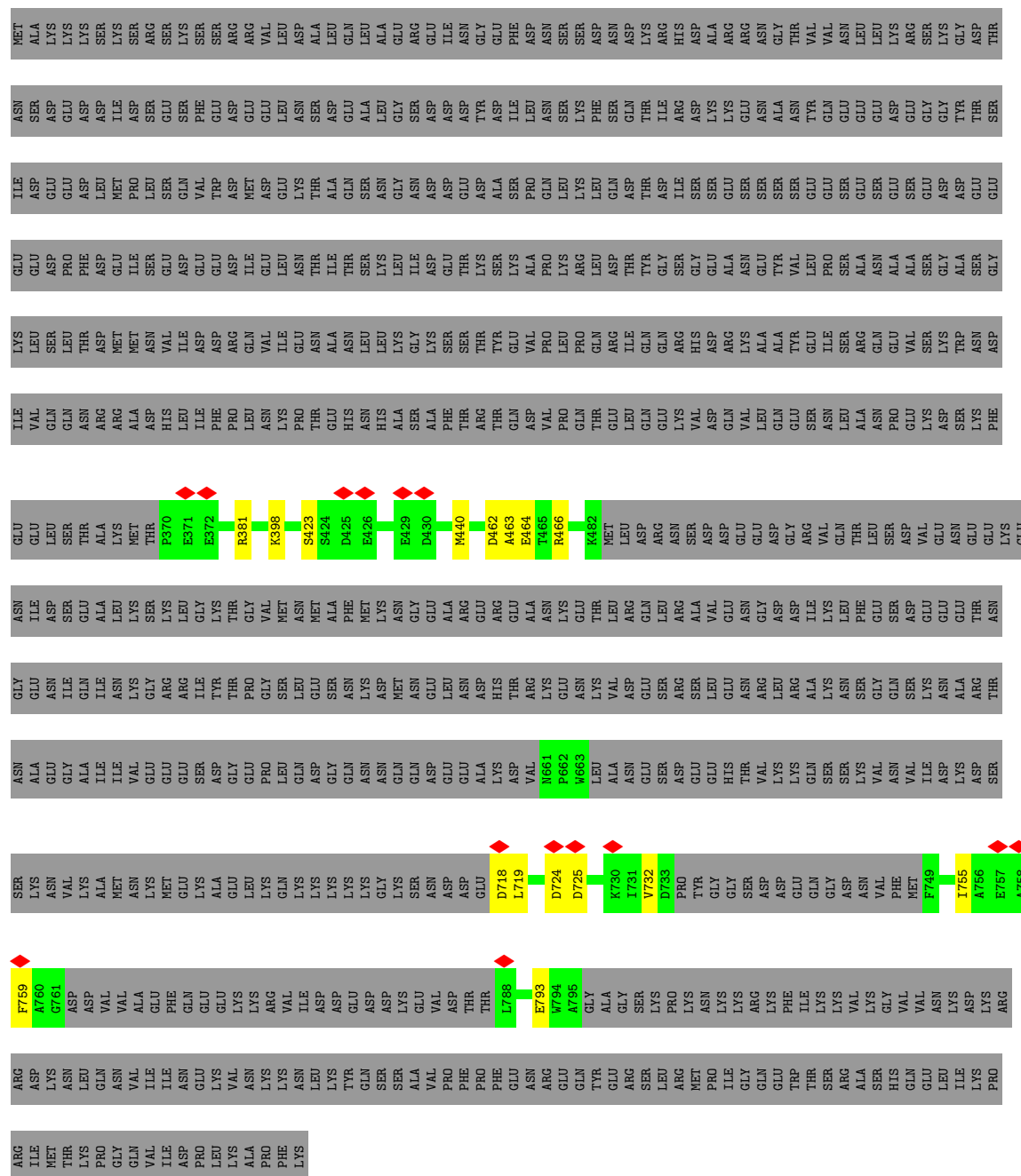
• Molecule 31: 40S ribosomal protein S23-A





- Molecule 32: U3 small nucleolar RNA-associated protein 14

Chain SS: 15% 83%



- Molecule 33: Nucleolar complex protein 14

Chain ST: 60% 39%

- Molecule 34: Nucleolar complex protein 4



Chain SZ:

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	131106	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 ($e^-/\text{\AA}^2$)	61.6	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	25000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.679	Depositor
Minimum map value	-0.292	Depositor
Average map value	0.044	Depositor
Map value standard deviation	0.108	Depositor
Recommended contour level	0.85	Depositor
Map size (\AA)	535.75195, 535.75195, 535.75195	wwPDB
Map dimensions	504, 504, 504	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.063, 1.063, 1.063	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: M7G, ZN, GTP, SEP, MG

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	L1	0.18	0/33399	0.28	0/52011
2	L2	0.14	0/521	0.20	0/809
3	L3	0.13	0/825	0.32	0/1109
4	L4	0.18	0/2097	0.32	0/2823
5	L5	0.13	0/1575	0.31	0/2127
6	L6	0.16	0/1855	0.33	0/2478
7	L7	0.18	0/1517	0.39	0/2044
8	L8	0.18	0/1462	0.30	0/1955
9	L9	0.15	0/1495	0.28	0/2003
10	LC	0.24	0/945	0.53	0/1274
11	LD	0.19	0/1145	0.32	0/1543
12	LE	0.20	0/1039	0.35	0/1395
13	LF	0.16	0/1060	0.29	0/1412
14	LG	0.10	0/492	0.28	0/659
15	N2	0.14	0/109	0.31	0/166
16	NA	0.15	0/850	0.33	0/1138
17	NB	0.14	0/464	0.31	0/608
18	NF	0.16	0/1215	0.31	0/1638
19	NG	0.16	0/952	0.32	0/1279
20	NL	0.17	0/2305	0.35	0/3116
21	NM	0.17	0/1713	0.32	0/2305
22	NP	0.16	0/1056	0.33	0/1416
23	NQ	0.15	0/605	0.31	0/817
24	NS	0.17	0/6556	0.35	0/8856
25	NW	0.13	0/564	0.33	0/758
26	SH	0.15	0/2832	0.29	0/3825
27	SI	0.16	0/5870	0.31	0/7908
28	SJ	0.11	0/1080	0.30	0/1508
28	SK	0.12	0/1170	0.32	0/1639
29	SL	0.15	0/1129	0.32	0/1523
30	SM	0.13	0/1792	0.32	0/2425
31	SR	0.16	0/1069	0.29	0/1427

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	SS	0.18	0/1280	0.34	0/1692
33	ST	0.16	1/2688 (0.0%)	0.35	2/3727 (0.1%)
34	SU	0.16	0/2726	0.35	2/3825 (0.1%)
35	SW	0.16	0/1441	0.29	0/1943
36	SZ	0.13	0/1326	0.32	0/1859
All	All	0.17	1/90219 (0.0%)	0.31	4/129040 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	ST	681	PRO	CG-CD	-5.29	1.32	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	ST	681	PRO	N-CD-CG	-9.37	89.15	103.20
34	SU	335	PRO	CA-N-CD	-7.46	101.56	112.00
34	SU	335	PRO	N-CD-CG	-6.82	92.97	103.20
33	ST	681	PRO	CA-CB-CG	-6.38	92.38	104.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	L1	29868	0	15038	125	0
2	L2	496	0	253	5	0
3	L3	815	0	850	8	0
4	L4	2056	0	2140	16	0
5	L5	1558	0	1629	16	0
6	L6	1831	0	1931	22	0
7	L7	1492	0	1581	20	0
8	L8	1437	0	1458	14	0
9	L9	1470	0	1554	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	LC	930	0	983	21	0
11	LD	1119	0	1186	6	0
12	LE	1022	0	1060	11	0
13	LF	1046	0	1114	6	0
14	LG	490	0	529	2	0
15	N2	100	0	51	2	0
16	NA	843	0	848	19	0
17	NB	460	0	508	1	0
18	NF	1192	0	1255	7	0
19	NG	941	0	979	11	0
20	NL	2262	0	2330	15	0
21	NM	1688	0	1756	20	0
22	NP	1040	0	1057	12	0
23	NQ	595	0	613	2	0
24	NS	6446	0	6221	51	0
25	NW	556	0	596	8	0
26	SH	2781	0	2878	14	0
27	SI	5739	0	5867	49	0
28	SJ	1074	0	514	1	0
28	SK	1160	0	570	0	0
29	SL	1108	0	1163	8	0
30	SM	1756	0	1765	20	0
31	SR	1052	0	1120	2	0
32	SS	1278	0	1300	15	0
33	ST	2669	0	1505	4	0
34	SU	2703	0	1302	2	0
35	SW	1415	0	1494	13	0
36	SZ	1314	0	649	2	0
37	L1	46	0	0	0	0
37	SI	1	0	0	0	0
38	NQ	1	0	0	0	0
38	SL	1	0	0	0	0
39	SI	32	0	12	0	0
All	All	85883	0	67659	445	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 3.

All (445) 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)
10:LC:100:GLN:NE2	10:LC:104:GLU:OE2	2.00	0.95
1:L1:904:G:N2	1:L1:1000:C:O2	2.07	0.87
1:L1:622:A:O2'	1:L1:1032:G:OP2	1.95	0.83
1:L1:110:U:OP1	1:L1:753:A:O2'	1.98	0.81
1:L1:1034:C:HO2'	12:LE:2:THR:N	1.79	0.81
3:L3:16:ARG:NH2	3:L3:19:ASN:OD1	2.14	0.81
19:NG:31:THR:OG1	19:NG:37:GLU:O	1.97	0.80
1:L1:1483:A:N3	1:L1:1607:G:O2'	2.14	0.79
9:L9:112:GLN:NE2	9:L9:153:GLU:OE2	2.15	0.79
1:L1:1781:A:N3	20:NL:156:GLN:NE2	2.30	0.79
1:L1:221:A:OP2	1:L1:832:U:O2'	2.00	0.79
1:L1:1533:C:OP2	25:NW:77:ARG:NH2	2.15	0.79
10:LC:52:LEU:HD23	10:LC:60:PHE:CE2	2.19	0.78
20:NL:162:ARG:O	20:NL:176:SER:OG	2.00	0.78
16:NA:371:ARG:O	20:NL:99:ARG:NH2	2.17	0.78
1:L1:1471:A:OP1	5:L5:185:ARG:NH1	2.16	0.77
10:LC:55:VAL:HG11	10:LC:105:LEU:HD23	1.67	0.77
1:L1:1478:G:OP1	22:NP:39:THR:OG1	2.03	0.76
19:NG:32:ASP:OD1	21:NM:46:THR:OG1	2.03	0.76
1:L1:904:G:N1	1:L1:1000:C:N3	2.33	0.76
22:NP:129:GLN:NE2	22:NP:133:ASP:OD2	2.18	0.76
1:L1:330:G:OP2	8:L8:172:ARG:NH1	2.19	0.75
1:L1:72:A:N7	6:L6:167:LYS:NZ	2.35	0.75
1:L1:1003:A:OP1	35:SW:269:ARG:NH2	2.19	0.75
1:L1:935:U:OP2	1:L1:1075:C:O2'	2.05	0.74
35:SW:204:ARG:NH1	35:SW:250:LEU:O	2.20	0.74
20:NL:254:ASN:ND2	20:NL:317:PHE:O	2.21	0.74
1:L1:127:G:O6	6:L6:202:ARG:NH2	2.22	0.73
10:LC:52:LEU:HD23	10:LC:60:PHE:HE2	1.53	0.72
1:L1:1080:U:O2'	1:L1:1082:C:OP1	2.04	0.72
1:L1:927:C:O2'	19:NG:124:ASP:OD2	2.08	0.72
8:L8:6:ASP:OD1	8:L8:9:HIS:ND1	2.21	0.71
16:NA:367:ASP:OD1	16:NA:370:ARG:NH2	2.23	0.71
16:NA:301:GLU:O	16:NA:305:ILE:HD12	1.89	0.71
24:NS:888:ALA:HB2	24:NS:902:MET:HE1	1.72	0.71
1:L1:810:G:N2	7:L7:108:GLN:OE1	2.23	0.71
1:L1:539:G:OP2	1:L1:539:G:N2	2.17	0.70
13:LF:86:GLU:OE2	13:LF:90:ARG:NE	2.23	0.70
32:SS:724:ASP:OD1	32:SS:725:ASP:N	2.24	0.70
9:L9:106:GLU:OE1	9:L9:115:LYS:NZ	2.21	0.70
5:L5:93:LEU:HA	5:L5:172:ILE:HD11	1.74	0.69
6:L6:98:ARG:NH1	6:L6:105:ASP:OD1	2.26	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:SH:57:GLU:OE1	26:SH:63:SER:OG	2.10	0.69
7:L7:141:ARG:NH1	12:LE:49:GLU:OE1	2.25	0.69
16:NA:319:VAL:HG13	27:SI:1042:MET:HE1	1.75	0.69
1:L1:207:U:O2	8:L8:178:ARG:NH2	2.25	0.69
1:L1:933:A:OP1	21:NM:116:LYS:NZ	2.27	0.68
21:NM:104:ASP:OD1	21:NM:105:PHE:N	2.27	0.68
1:L1:1778:G:OP2	20:NL:162:ARG:NH2	2.26	0.68
4:L4:171:ASP:OD1	4:L4:172:PHE:N	2.26	0.68
27:SI:956:MET:HA	27:SI:956:MET:HE2	1.76	0.67
1:L1:862:A:OP2	18:NF:64:ARG:NH2	2.28	0.67
30:SM:116:ARG:NH1	30:SM:118:ASN:OD1	2.28	0.67
19:NG:37:GLU:OE1	21:NM:27:LYS:NZ	2.28	0.66
13:LF:8:ARG:NH2	13:LF:26:ASP:OD2	2.29	0.66
20:NL:194:ASN:O	20:NL:197:ARG:NH1	2.28	0.66
21:NM:127:VAL:HG13	21:NM:176:VAL:HG11	1.78	0.66
2:L2:15:U:OP1	32:SS:466:ARG:NH2	2.29	0.66
16:NA:347:PHE:O	16:NA:349:ARG:NH1	2.29	0.65
27:SI:124:ASP:OD1	27:SI:126:ASN:N	2.30	0.65
1:L1:1497:U:O3'	22:NP:75:LYS:NZ	2.27	0.65
7:L7:123:ASP:OD1	7:L7:138:LYS:NZ	2.25	0.65
1:L1:578:U:OP2	27:SI:874:TYR:OH	2.08	0.65
7:L7:7:LYS:NZ	7:L7:39:ARG:O	2.30	0.64
25:NW:90:LYS:NZ	25:NW:103:ARG:O	2.22	0.64
1:L1:742:U:O2'	1:L1:743:U:OP1	2.15	0.64
24:NS:902:MET:CG	24:NS:916:LEU:HD11	2.27	0.64
1:L1:1610:G:OP1	5:L5:72:HIS:NE2	2.23	0.63
1:L1:1482:C:O2'	10:LC:72:GLY:O	2.15	0.63
22:NP:131:ASP:O	22:NP:135:ILE:HD12	1.98	0.63
1:L1:93:A:O4'	4:L4:3:ARG:NH1	2.31	0.63
24:NS:1137:PRO:O	24:NS:1142:ASN:ND2	2.32	0.63
1:L1:1555:A:O2'	1:L1:1556:A:O5'	2.17	0.62
1:L1:1163:A:O3'	5:L5:166:ARG:NH2	2.32	0.62
8:L8:85:PRO:O	11:LD:11:ARG:NH1	2.33	0.62
22:NP:38:LYS:O	22:NP:39:THR:OG1	2.17	0.62
1:L1:1090:C:OP1	32:SS:398:LYS:NZ	2.29	0.62
1:L1:447:U:O2'	4:L4:27:TYR:O	2.17	0.61
1:L1:277:U:O2'	1:L1:278:U:OP1	2.16	0.61
30:SM:260:GLU:OE2	30:SM:262:ARG:NH1	2.34	0.61
4:L4:148:ARG:NH2	6:L6:201:GLN:OE1	2.33	0.61
1:L1:1534:G:OP1	3:L3:57:ARG:NH1	2.33	0.61
9:L9:94:ASP:OD1	9:L9:95:TYR:N	2.35	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:NM:77:GLU:OE1	35:SW:98:LYS:NZ	2.34	0.60
1:L1:1119:G:OP1	24:NS:88:LYS:NZ	2.31	0.60
1:L1:557:G:O3'	27:SI:931:LYS:NZ	2.35	0.60
35:SW:258:LYS:O	35:SW:262:ASN:ND2	2.35	0.60
1:L1:433:C:N4	1:L1:436:A:OP1	2.34	0.60
1:L1:557:G:OP1	27:SI:1004:ARG:NH2	2.34	0.59
7:L7:48:GLU:OE2	7:L7:88:ARG:NE	2.35	0.59
3:L3:52:VAL:HG23	3:L3:65:GLU:OE1	2.02	0.59
24:NS:911:PHE:HB3	24:NS:931:VAL:HG13	1.84	0.59
1:L1:530:C:O2	13:LF:61:ARG:NH1	2.36	0.59
26:SH:289:VAL:O	26:SH:317:GLN:NE2	2.33	0.59
3:L3:27:LYS:NZ	3:L3:55:HIS:O	2.33	0.59
1:L1:1499:G:OP1	22:NP:122:ARG:NH1	2.36	0.59
6:L6:67:VAL:HG21	6:L6:73:ILE:HD11	1.84	0.59
30:SM:74:ASP:O	30:SM:78:ALA:N	2.35	0.59
1:L1:1531:G:OP2	25:NW:94:LYS:NZ	2.32	0.59
12:LE:11:LEU:HD12	12:LE:74:VAL:HG13	1.85	0.59
26:SH:181:HIS:NE2	27:SI:761:GLN:OE1	2.30	0.59
24:NS:114:ILE:HG22	24:NS:118:GLN:HE22	1.67	0.58
1:L1:331:A:OP1	8:L8:56:ARG:NH1	2.36	0.58
16:NA:345:LEU:HD21	27:SI:932:LEU:HD23	1.85	0.58
33:ST:615:PRO:HA	34:SU:551:ALA:HB3	1.86	0.58
1:L1:1616:G:O5'	5:L5:81:ARG:NH1	2.36	0.58
4:L4:103:TYR:O	4:L4:182:TYR:OH	2.20	0.58
24:NS:1147:MET:N	24:NS:1147:MET:HE2	2.19	0.58
29:SL:69:THR:HG22	32:SS:440:MET:SD	2.44	0.58
6:L6:21:GLU:OE1	6:L6:25:ARG:NH1	2.37	0.58
1:L1:705:U:HO2'	1:L1:706:A:H8	1.52	0.57
1:L1:706:A:N6	1:L1:732:G:O2'	2.37	0.57
5:L5:53:VAL:HG21	5:L5:59:VAL:HA	1.85	0.57
24:NS:22:GLU:OE2	24:NS:25:ARG:NH1	2.37	0.57
1:L1:66:U:O4	6:L6:134:GLY:N	2.36	0.57
16:NA:335:ARG:NH1	27:SI:957:GLU:OE2	2.37	0.57
21:NM:32:ILE:HG12	21:NM:96:LEU:HD12	1.86	0.57
1:L1:388:G:OP2	1:L1:423:G:O2'	2.22	0.57
27:SI:841:THR:HG21	27:SI:871:MET:HE3	1.85	0.57
12:LE:81:VAL:O	12:LE:122:SER:OG	2.21	0.57
27:SI:157:ASN:O	27:SI:161:HIS:ND1	2.38	0.56
32:SS:793:GLU:OE1	32:SS:793:GLU:N	2.38	0.56
30:SM:276:GLN:O	30:SM:278:ARG:NH1	2.39	0.56
20:NL:181:MET:SD	20:NL:300:GLN:NE2	2.79	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:LC:55:VAL:HG13	10:LC:109:PHE:HE2	1.71	0.56
1:L1:155:U:O4	13:LF:128:LYS:NZ	2.35	0.56
10:LC:10:PHE:CE2	10:LC:19:VAL:HG23	2.41	0.56
30:SM:144:GLU:OE1	30:SM:147:GLY:N	2.39	0.56
1:L1:1802:A:OP1	21:NM:115:ARG:NH1	2.40	0.55
24:NS:502:MET:CE	24:NS:857:MET:HE2	2.37	0.55
8:L8:67:TRP:NE1	8:L8:185:GLU:OE2	2.39	0.55
1:L1:594:A:OP1	9:L9:38:ASN:ND2	2.39	0.55
1:L1:1051:G:O2'	1:L1:1052:U:OP1	2.18	0.55
10:LC:89:LEU:HD21	10:LC:105:LEU:HD22	1.89	0.55
30:SM:100:LEU:HD22	30:SM:144:GLU:CG	2.37	0.55
1:L1:1131:A:N3	20:NL:146:ARG:NH1	2.55	0.54
1:L1:324:U:O2'	11:LD:80:MET:HE1	2.08	0.54
1:L1:1082:C:O2'	1:L1:1083:G:OP1	2.25	0.54
28:SJ:236:VAL:O	28:SJ:240:LYS:N	2.37	0.54
4:L4:54:TYR:O	13:LF:15:ASN:ND2	2.40	0.54
6:L6:18:ILE:HG23	6:L6:23:ARG:HD2	1.89	0.54
1:L1:1555:A:O2'	1:L1:1556:A:O4'	2.25	0.54
7:L7:159:VAL:HG22	7:L7:163:ASP:OD2	2.07	0.54
24:NS:555:LEU:HD21	24:NS:557:ILE:HD11	1.89	0.54
1:L1:976:G:N1	1:L1:1023:A:O2'	2.40	0.54
30:SM:241:THR:OG1	30:SM:244:GLY:O	2.24	0.54
32:SS:462:ASP:OD1	32:SS:463:ALA:N	2.41	0.54
10:LC:60:PHE:CE1	10:LC:89:LEU:HD12	2.43	0.53
12:LE:44:HIS:NE2	12:LE:112:ASP:OD2	2.36	0.53
23:NQ:55:THR:HG22	23:NQ:62:ILE:HD13	1.90	0.53
1:L1:1521:G:O2'	1:L1:1523:G:OP2	2.19	0.53
27:SI:952:PHE:HD2	27:SI:958:VAL:HG22	1.72	0.53
34:SU:137:GLU:O	34:SU:140:ALA:N	2.42	0.53
1:L1:162:A:H3'	1:L1:163:G:H21	1.74	0.53
22:NP:18:TYR:CE2	22:NP:22:LEU:HD11	2.43	0.53
24:NS:388:ARG:NH1	24:NS:426:GLN:OE1	2.41	0.53
35:SW:131:ASN:O	35:SW:135:LYS:N	2.41	0.53
1:L1:1594:G:O2'	1:L1:1600:A:N1	2.26	0.52
32:SS:718:ASP:OD1	32:SS:719:LEU:N	2.42	0.52
27:SI:549:ILE:HD13	27:SI:567:TRP:NE1	2.24	0.52
27:SI:993:ASP:OD1	27:SI:994:LYS:N	2.43	0.52
27:SI:83:THR:OG1	27:SI:119:GLU:OE1	2.28	0.52
1:L1:125:U:OP1	6:L6:201:GLN:NE2	2.42	0.52
5:L5:33:VAL:HG13	10:LC:53:LEU:HD11	1.92	0.52
24:NS:1118:ILE:HG21	24:NS:1227:ILE:HG21	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:1480:G:OP1	22:NP:64:HIS:NE2	2.43	0.52
24:NS:1204:LEU:HD11	24:NS:1210:TYR:CE2	2.45	0.52
1:L1:241:U:H5'	6:L6:216:LEU:HD21	1.92	0.51
7:L7:67:LEU:HD22	7:L7:94:ALA:HB2	1.93	0.51
29:SL:73:ASN:HB2	32:SS:440:MET:HE3	1.92	0.51
1:L1:738:G:O2'	1:L1:739:G:OP1	2.28	0.51
1:L1:1090:C:P	32:SS:398:LYS:HZ1	2.34	0.51
6:L6:18:ILE:HG21	6:L6:24:ILE:HD11	1.92	0.51
24:NS:1051:SER:HA	24:NS:1060:VAL:HG21	1.92	0.51
1:L1:326:G:OP1	11:LD:57:LYS:NZ	2.43	0.51
1:L1:802:G:H21	12:LE:107:SER:HB2	1.75	0.51
21:NM:108:ASP:OD1	21:NM:109:LYS:N	2.44	0.51
26:SH:337:VAL:N	27:SI:554:TYR:OH	2.43	0.51
30:SM:89:ILE:CD1	30:SM:136:THR:HG21	2.40	0.51
24:NS:501:MET:HE1	24:NS:535:CYS:SG	2.51	0.50
1:L1:32:U:O2'	1:L1:594:A:N1	2.42	0.50
18:NF:55:ARG:NH1	18:NF:56:ASP:OD1	2.44	0.50
24:NS:1152:MET:HA	24:NS:1152:MET:HE3	1.93	0.50
22:NP:39:THR:OG1	22:NP:43:ASN:ND2	2.45	0.50
27:SI:968:THR:HG22	27:SI:1001:VAL:HG12	1.93	0.50
1:L1:1190:C:N4	1:L1:1197:C:O2	2.44	0.50
12:LE:24:GLN:OE1	12:LE:64:GLN:NE2	2.40	0.50
7:L7:99:LEU:O	7:L7:112:ARG:NH1	2.44	0.50
1:L1:322:G:O2'	8:L8:10:LYS:NZ	2.45	0.50
5:L5:125:THR:HG21	5:L5:199:ILE:HD11	1.94	0.50
8:L8:113:PHE:CD1	8:L8:121:LEU:HD11	2.47	0.50
27:SI:127:ALA:O	27:SI:131:ILE:HD12	2.11	0.50
1:L1:334:G:O6	8:L8:5:ARG:NH2	2.44	0.50
27:SI:193:ARG:NH1	27:SI:197:GLU:OE2	2.43	0.50
1:L1:1126:G:N7	24:NS:107:ARG:NH1	2.60	0.49
5:L5:31:GLU:OE1	5:L5:31:GLU:N	2.45	0.49
35:SW:154:LYS:NZ	35:SW:177:LEU:O	2.45	0.49
4:L4:19:LEU:HD11	4:L4:108:ARG:HD2	1.92	0.49
5:L5:143:ARG:HB2	14:LG:57:MET:HE1	1.93	0.49
36:SZ:391:VAL:O	36:SZ:395:MET:N	2.45	0.49
1:L1:560:U:OP2	30:SM:282:ARG:NH2	2.45	0.49
1:L1:1473:U:O4	5:L5:180:ARG:NE	2.43	0.49
19:NG:112:ILE:N	35:SW:95:GLU:OE2	2.40	0.49
24:NS:114:ILE:O	24:NS:118:GLN:NE2	2.46	0.49
30:SM:123:VAL:HG12	30:SM:125:PRO:HD2	1.94	0.49
1:L1:619:A:N3	1:L1:1110:G:O2'	2.40	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:647:G:N2	1:L1:687:G:H22	2.09	0.49
24:NS:507:LEU:HD12	24:NS:510:TYR:CD2	2.47	0.49
24:NS:902:MET:HG3	24:NS:916:LEU:HD11	1.94	0.49
24:NS:398:HIS:O	24:NS:402:GLU:HG2	2.12	0.49
24:NS:1080:LEU:HA	24:NS:1083:MET:HE2	1.93	0.49
27:SI:841:THR:HG23	27:SI:859:ILE:HA	1.95	0.49
30:SM:134:SER:OG	30:SM:136:THR:HG23	2.13	0.49
18:NF:101:HIS:NE2	18:NF:108:ASP:OD2	2.34	0.49
2:L2:0:M7G:O2'	27:SI:734:GLU:OE1	2.13	0.49
12:LE:105:THR:HG23	12:LE:105:THR:O	2.11	0.49
6:L6:78:THR:O	6:L6:81:VAL:HG22	2.13	0.49
18:NF:31:GLU:OE1	18:NF:31:GLU:N	2.45	0.49
19:NG:30:VAL:HG11	19:NG:71:CYS:SG	2.53	0.49
8:L8:69:SER:OG	8:L8:185:GLU:OE1	2.29	0.48
7:L7:63:PRO:O	7:L7:67:LEU:N	2.46	0.48
4:L4:212:ASP:OD1	4:L4:216:ASN:N	2.47	0.48
17:NB:555:ASN:OD1	17:NB:556:LYS:N	2.46	0.48
27:SI:126:ASN:OD1	27:SI:1020:SER:OG	2.27	0.48
32:SS:464:GLU:OE1	32:SS:464:GLU:N	2.47	0.48
5:L5:133:VAL:HG22	5:L5:198:LEU:HD21	1.96	0.48
24:NS:502:MET:HE2	24:NS:857:MET:HE2	1.95	0.48
1:L1:854:U:O4	1:L1:855:A:N6	2.47	0.48
1:L1:1169:G:N1	1:L1:1575:G:OP2	2.44	0.48
30:SM:100:LEU:HD22	30:SM:144:GLU:HG2	1.95	0.48
30:SM:192:ASP:OD1	30:SM:193:ASN:N	2.47	0.48
7:L7:38:LEU:HD22	7:L7:77:LEU:HD21	1.96	0.48
9:L9:157:ASP:OD1	9:L9:158:PHE:N	2.47	0.48
10:LC:55:VAL:CG1	10:LC:105:LEU:HD23	2.42	0.48
19:NG:48:VAL:HG21	19:NG:59:ALA:HB2	1.96	0.48
19:NG:136:ARG:O	35:SW:248:VAL:HG11	2.13	0.48
35:SW:102:PRO:HD2	35:SW:163:THR:HG23	1.96	0.48
6:L6:1:MET:HE3	6:L6:24:ILE:HG23	1.95	0.47
12:LE:15:ASN:ND2	12:LE:72:CYS:O	2.44	0.47
29:SL:98:ILE:CD1	29:SL:125:ILE:HG21	2.44	0.47
1:L1:886:U:OP2	21:NM:216:LYS:NZ	2.36	0.47
18:NF:130:ARG:NH1	18:NF:139:TRP:O	2.48	0.47
27:SI:831:ARG:NH1	27:SI:835:HIS:O	2.46	0.47
29:SL:138:ASP:OD1	29:SL:139:ASP:N	2.47	0.47
35:SW:183:GLU:HB2	35:SW:240:ILE:HD12	1.96	0.47
1:L1:789:A:OP1	4:L4:108:ARG:NH1	2.47	0.47
21:NM:180:THR:HG1	21:NM:183:GLN:CD	2.19	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:SI:833:ARG:NH2	31:SR:141:GLU:OE2	2.45	0.47
4:L4:87:MET:HE1	4:L4:236:ILE:HD13	1.96	0.47
4:L4:163:ASP:O	4:L4:167:GLY:N	2.47	0.47
1:L1:258:C:O2	8:L8:178:ARG:NH1	2.46	0.47
1:L1:982:U:O4	1:L1:983:A:N6	2.47	0.47
15:N2:9:U:O3'	24:NS:493:THR:HG21	2.15	0.47
30:SM:246:GLU:N	30:SM:246:GLU:OE1	2.47	0.47
1:L1:284:G:N7	6:L6:188:ARG:NH1	2.61	0.47
1:L1:1502:G:N7	22:NP:102:ARG:NH2	2.63	0.47
1:L1:1515:A:O2'	1:L1:1517:U:OP2	2.32	0.47
2:L2:0:M7G:H82	2:L2:1:G:O4'	2.15	0.47
7:L7:27:LEU:HD21	7:L7:80:GLU:CB	2.44	0.47
24:NS:914:MET:HE3	24:NS:1084:ILE:HA	1.97	0.47
27:SI:736:GLU:OE1	27:SI:736:GLU:N	2.39	0.47
1:L1:1595:U:OP1	27:SI:945:THR:OG1	2.25	0.47
6:L6:5:ILE:HD12	6:L6:16:PHE:CD2	2.50	0.47
11:LD:76:VAL:HG21	11:LD:87:ARG:HB2	1.97	0.47
1:L1:1230:A:N3	1:L1:1258:U:N3	2.63	0.47
7:L7:159:VAL:HG23	7:L7:185:ILE:HG21	1.96	0.47
27:SI:249:PHE:CE2	27:SI:269:VAL:HG21	2.49	0.47
1:L1:58:U:OP1	1:L1:456:A:O2'	2.32	0.47
1:L1:632:U:O2'	1:L1:1103:U:OP1	2.31	0.47
4:L4:230:GLU:N	4:L4:230:GLU:OE1	2.48	0.47
27:SI:927:GLU:N	27:SI:927:GLU:OE1	2.47	0.47
1:L1:1231:U:O2'	1:L1:1258:U:O2'	2.28	0.46
6:L6:141:ILE:HG21	6:L6:153:VAL:HG13	1.97	0.46
21:NM:61:LEU:HD13	21:NM:96:LEU:HD21	1.97	0.46
23:NQ:56:CYS:O	23:NQ:60:SER:N	2.47	0.46
24:NS:493:THR:HG22	24:NS:494:ASP:OD1	2.15	0.46
1:L1:871:G:H2'	1:L1:872:G:C8	2.51	0.46
16:NA:297:LEU:O	16:NA:302:LYS:NZ	2.49	0.46
16:NA:338:ASP:OD1	27:SI:954:SER:OG	2.33	0.46
27:SI:252:LEU:HD11	27:SI:270:ALA:HB2	1.97	0.46
20:NL:165:ALA:O	20:NL:180:GLN:NE2	2.49	0.46
24:NS:494:ASP:OD1	24:NS:495:GLY:N	2.48	0.46
27:SI:849:LEU:HD23	27:SI:896:PHE:HB3	1.97	0.46
24:NS:907:LEU:HD13	24:NS:931:VAL:CG1	2.45	0.46
1:L1:1534:G:O6	25:NW:77:ARG:NH1	2.49	0.46
18:NF:87:ASP:OD1	18:NF:88:LEU:N	2.49	0.46
19:NG:48:VAL:HG11	19:NG:53:ASP:HB2	1.98	0.46
24:NS:515:ILE:HD11	24:NS:532:LEU:HD12	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:NS:924:LEU:HD21	24:NS:1049:ILE:HD13	1.98	0.46
1:L1:909:U:H5''	24:NS:139:THR:HG21	1.98	0.46
7:L7:8:ILE:HD13	7:L7:13:PRO:HB3	1.99	0.45
26:SH:47:ASP:OD1	26:SH:48:TYR:N	2.49	0.45
10:LC:55:VAL:HG11	10:LC:105:LEU:CD2	2.39	0.45
16:NA:380:ASP:O	16:NA:382:GLN:NE2	2.49	0.45
10:LC:10:PHE:HE2	10:LC:19:VAL:HG23	1.80	0.45
1:L1:358:U:O2'	1:L1:360:A:OP1	2.34	0.45
3:L3:65:GLU:HG2	3:L3:68:ARG:HH21	1.80	0.45
4:L4:87:MET:HE1	4:L4:236:ILE:CD1	2.47	0.45
4:L4:122:LYS:NZ	4:L4:143:ASP:OD2	2.36	0.45
27:SI:849:LEU:HD12	27:SI:854:PHE:HZ	1.82	0.45
14:LG:11:LYS:NZ	14:LG:51:ASN:O	2.44	0.45
22:NP:76:LEU:CD1	22:NP:105:LEU:HD21	2.47	0.45
24:NS:902:MET:HG2	24:NS:916:LEU:HD11	1.99	0.45
24:NS:913:LYS:HD2	24:NS:916:LEU:HD12	1.99	0.45
25:NW:49:ARG:NE	25:NW:53:GLU:OE2	2.50	0.45
26:SH:59:VAL:HG23	26:SH:60:THR:HG23	1.98	0.45
1:L1:522:U:O2'	13:LF:60:PHE:O	2.34	0.45
1:L1:1178:G:N7	33:ST:753:LYS:NZ	2.50	0.45
21:NM:32:ILE:CG1	21:NM:96:LEU:HD12	2.47	0.45
25:NW:53:GLU:O	25:NW:56:THR:OG1	2.31	0.45
30:SM:173:ARG:HE	30:SM:179:ALA:HB1	1.80	0.45
1:L1:1082:C:HO2'	1:L1:1083:G:P	2.38	0.45
1:L1:1220:C:O2'	36:SZ:379:LYS:O	2.30	0.45
24:NS:534:ARG:HH21	32:SS:759:PHE:CB	2.30	0.45
24:NS:1204:LEU:HD11	24:NS:1210:TYR:HE2	1.80	0.45
27:SI:616:ASP:OD1	27:SI:617:THR:N	2.49	0.45
1:L1:277:U:HO2'	1:L1:278:U:P	2.39	0.45
24:NS:101:ILE:O	24:NS:105:LEU:HD23	2.17	0.45
26:SH:134:LYS:HA	26:SH:138:MET:HE2	1.99	0.45
27:SI:952:PHE:CD2	27:SI:958:VAL:HG22	2.51	0.45
1:L1:68:A:OP1	6:L6:160:ARG:NH2	2.47	0.45
1:L1:428:A:N3	1:L1:440:U:O2'	2.45	0.45
7:L7:27:LEU:HD21	7:L7:80:GLU:HB2	1.98	0.45
20:NL:59:VAL:HG23	20:NL:80:ASN:OD1	2.17	0.45
1:L1:501:U:O2'	1:L1:502:U:OP2	2.22	0.45
8:L8:11:ARG:NH1	8:L8:15:GLY:O	2.48	0.45
24:NS:527:ILE:HD13	24:NS:850:ILE:HD12	1.98	0.44
29:SL:65:VAL:HG11	29:SL:86:MET:CE	2.47	0.44
16:NA:373:ILE:HG21	30:SM:245:VAL:HG11	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L7:168:SER:O	7:L7:172:VAL:HG23	2.18	0.44
20:NL:39:LEU:HD13	20:NL:196:PHE:HE1	1.83	0.44
1:L1:358:U:OP2	24:NS:2:GLY:N	2.51	0.44
24:NS:917:VAL:HG12	24:NS:917:VAL:O	2.17	0.44
33:ST:388:LEU:O	33:ST:392:LYS:N	2.51	0.44
11:LD:30:ARG:NH2	11:LD:51:GLY:O	2.50	0.44
24:NS:538:LEU:HD22	32:SS:755:ILE:HG23	2.00	0.44
26:SH:312:ARG:NH2	26:SH:347:ASN:OD1	2.51	0.44
2:L2:0:M7G:H82	2:L2:1:G:C1'	2.48	0.44
6:L6:102:VAL:HG13	6:L6:106:LEU:HD12	1.99	0.44
1:L1:9:U:O2'	1:L1:11:A:OP2	2.31	0.44
10:LC:89:LEU:HD21	10:LC:105:LEU:HD13	2.00	0.44
26:SH:16:ASN:N	27:SI:607:ASP:OD1	2.51	0.44
1:L1:1524:A:N3	1:L1:1590:G:O2'	2.35	0.44
7:L7:64:VAL:HG23	7:L7:65:PRO:HD3	2.00	0.44
7:L7:77:LEU:O	7:L7:81:LEU:HD13	2.18	0.44
19:NG:22:SER:OG	19:NG:23:PHE:N	2.50	0.44
1:L1:447:U:H2'	1:L1:448:C:O4'	2.17	0.44
27:SI:99:ASN:OD1	27:SI:100:ASP:N	2.50	0.44
27:SI:819:GLU:OE1	27:SI:819:GLU:N	2.50	0.44
30:SM:288:ASP:OD1	30:SM:289:TYR:N	2.51	0.44
1:L1:85:A:N3	1:L1:148:A:O2'	2.47	0.43
5:L5:94:THR:HG22	5:L5:114:ILE:HG13	1.99	0.43
1:L1:545:A:H61	1:L1:594:A:H5''	1.84	0.43
8:L8:46:VAL:N	8:L8:54:LYS:O	2.47	0.43
15:N2:10:U:P	24:NS:493:THR:HG21	2.58	0.43
20:NL:39:LEU:HD11	20:NL:44:VAL:HG21	1.99	0.43
21:NM:52:THR:O	21:NM:52:THR:OG1	2.30	0.43
20:NL:178:ASN:OD1	20:NL:182:TRP:NE1	2.51	0.43
29:SL:65:VAL:HG21	29:SL:86:MET:HE2	2.01	0.43
29:SL:81:ASP:OD1	29:SL:82:ILE:N	2.51	0.43
1:L1:1059:U:OP2	1:L1:1059:U:H4'	2.18	0.43
1:L1:1107:G:OP1	27:SI:16:THR:HG21	2.18	0.43
5:L5:123:VAL:HG11	25:NW:59:TYR:HD1	1.84	0.43
26:SH:224:ASN:OD1	26:SH:224:ASN:O	2.37	0.43
27:SI:941:ILE:HD12	27:SI:997:MET:HE2	1.99	0.43
10:LC:107:LYS:HA	10:LC:110:THR:HG22	2.01	0.43
21:NM:71:ALA:O	21:NM:75:GLY:N	2.51	0.43
21:NM:171:ILE:O	21:NM:175:GLU:OE1	2.37	0.43
35:SW:102:PRO:CD	35:SW:163:THR:HG23	2.49	0.43
7:L7:22:GLN:HA	7:L7:25:VAL:HG22	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:NS:398:HIS:O	24:NS:401:MET:HG3	2.19	0.43
1:L1:865:A:OP1	12:LE:28:ARG:NH1	2.44	0.43
1:L1:931:C:O2'	21:NM:118:GLN:O	2.36	0.43
10:LC:54:LEU:HD11	10:LC:112:TYR:CD2	2.54	0.42
16:NA:408:SER:O	16:NA:411:GLU:N	2.49	0.42
1:L1:188:A:N6	1:L1:197:A:O2'	2.51	0.42
10:LC:89:LEU:CD2	10:LC:105:LEU:HD13	2.48	0.42
16:NA:361:VAL:O	16:NA:365:LEU:HD23	2.19	0.42
6:L6:24:ILE:HG22	6:L6:28:PHE:CE1	2.54	0.42
21:NM:98:THR:O	21:NM:232:HIS:NE2	2.43	0.42
3:L3:78:HIS:O	3:L3:80:LYS:NZ	2.51	0.42
11:LD:121:ASP:OD2	11:LD:121:ASP:N	2.53	0.42
20:NL:157:ARG:NH2	20:NL:203:GLU:OE1	2.51	0.42
26:SH:219:LEU:HD23	27:SI:628:VAL:HG11	2.02	0.42
27:SI:219:GLU:OE1	27:SI:219:GLU:N	2.49	0.42
30:SM:77:TYR:O	30:SM:81:SER:N	2.53	0.42
1:L1:1130:G:N1	26:SH:225:ILE:O	2.47	0.42
7:L7:38:LEU:CD2	7:L7:77:LEU:HD21	2.50	0.42
16:NA:368:MET:HE1	30:SM:192:ASP:HB3	2.01	0.42
25:NW:40:VAL:O	25:NW:40:VAL:HG12	2.19	0.42
10:LC:60:PHE:CZ	10:LC:89:LEU:HD12	2.55	0.42
24:NS:409:VAL:HG12	24:NS:555:LEU:HB3	2.02	0.42
1:L1:1529:C:OP1	5:L5:112:ARG:NE	2.52	0.42
1:L1:1605:G:OP1	30:SM:119:ARG:NH1	2.53	0.42
26:SH:301:MET:HE1	26:SH:311:LEU:HB2	2.02	0.42
27:SI:179:SER:HB3	27:SI:182:THR:HG22	2.01	0.42
1:L1:861:U:O2'	12:LE:56:HIS:O	2.36	0.41
1:L1:924:A:H2'	1:L1:925:G:C8	2.55	0.41
5:L5:118:LEU:HD22	5:L5:129:PRO:HB2	2.02	0.41
24:NS:1146:GLU:C	24:NS:1147:MET:HE2	2.45	0.41
1:L1:513:U:O2'	1:L1:514:G:O4'	2.31	0.41
1:L1:1803:G:OP2	32:SS:381:ARG:NH1	2.47	0.41
4:L4:251:GLU:OE2	4:L4:255:ARG:NH2	2.52	0.41
8:L8:29:LEU:C	8:L8:29:LEU:HD12	2.45	0.41
24:NS:534:ARG:HH21	32:SS:759:PHE:HB3	1.84	0.41
6:L6:78:THR:OG1	6:L6:79:LYS:N	2.54	0.41
16:NA:329:GLU:HB3	27:SI:935:VAL:HG21	2.02	0.41
19:NG:77:THR:C	19:NG:110:LEU:HD12	2.45	0.41
6:L6:23:ARG:O	6:L6:26:VAL:HG12	2.20	0.41
16:NA:379:ASP:OD1	16:NA:379:ASP:N	2.50	0.41
21:NM:43:VAL:HG22	21:NM:43:VAL:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:SI:253:THR:HG21	27:SI:258:ILE:HD11	2.03	0.41
35:SW:117:TYR:N	35:SW:118:PRO:CD	2.83	0.41
16:NA:307:ILE:O	16:NA:311:ILE:HG13	2.21	0.41
16:NA:408:SER:O	16:NA:412:ILE:HD12	2.19	0.41
24:NS:1052:ASN:O	32:SS:732:VAL:HG22	2.21	0.41
29:SL:98:ILE:HG23	29:SL:102:VAL:HG23	2.02	0.41
1:L1:123:G:OP1	4:L4:75:LYS:NZ	2.38	0.41
2:L2:22:A:O2'	24:NS:1109:ARG:NH1	2.54	0.41
3:L3:68:ARG:HA	3:L3:71:GLN:HG2	2.02	0.41
9:L9:27:GLU:OE1	9:L9:42:ILE:HG21	2.20	0.41
20:NL:179:VAL:O	20:NL:183:ALA:N	2.54	0.41
22:NP:125:SER:O	22:NP:129:GLN:N	2.45	0.41
24:NS:1023:ILE:H	24:NS:1023:ILE:HD12	1.86	0.41
27:SI:866:ARG:NH2	31:SR:61:SER:O	2.47	0.41
27:SI:958:VAL:CG1	27:SI:979:ALA:HB2	2.51	0.41
6:L6:208:TYR:CE2	6:L6:212:LEU:HD11	2.56	0.41
10:LC:99:GLU:OE1	10:LC:99:GLU:N	2.47	0.41
27:SI:556:ASP:OD2	27:SI:557:ASN:N	2.54	0.41
35:SW:262:ASN:HD22	35:SW:262:ASN:H	1.69	0.41
1:L1:1568:C:O2'	1:L1:1569:A:P	2.79	0.40
18:NF:132:VAL:O	18:NF:132:VAL:HG12	2.21	0.40
27:SI:130:ASP:OD1	27:SI:131:ILE:N	2.54	0.40
1:L1:738:G:O2'	1:L1:739:G:P	2.79	0.40
1:L1:1085:G:N2	1:L1:1088:A:OP2	2.46	0.40
26:SH:32:LYS:HD2	26:SH:75:ILE:HD11	2.02	0.40
21:NM:119:THR:HG21	21:NM:161:ILE:HD11	2.01	0.40
24:NS:384:ILE:HG23	24:NS:465:GLU:OE2	2.22	0.40
3:L3:116:LEU:HD11	33:ST:758:ASP:OD2	2.21	0.40
10:LC:60:PHE:HE1	10:LC:89:LEU:HD12	1.84	0.40
24:NS:409:VAL:HG11	24:NS:574:PHE:HE1	1.87	0.40
24:NS:516:ASP:OD1	24:NS:517:GLU:N	2.54	0.40
7:L7:78:THR:HA	7:L7:90:VAL:HG11	2.04	0.40
10:LC:8:GLN:O	10:LC:9:THR:HG23	2.21	0.40
16:NA:319:VAL:CG1	27:SI:1042:MET:HE1	2.49	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	L3	96/146 (66%)	95 (99%)	1 (1%)	0	100	100
4	L4	256/261 (98%)	253 (99%)	3 (1%)	0	100	100
5	L5	193/225 (86%)	187 (97%)	6 (3%)	0	100	100
6	L6	225/236 (95%)	222 (99%)	3 (1%)	0	100	100
7	L7	184/190 (97%)	178 (97%)	6 (3%)	0	100	100
8	L8	177/200 (88%)	176 (99%)	1 (1%)	0	100	100
9	L9	179/197 (91%)	177 (99%)	2 (1%)	0	100	100
10	LC	118/143 (82%)	116 (98%)	2 (2%)	0	100	100
11	LD	136/156 (87%)	132 (97%)	4 (3%)	0	100	100
12	LE	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
13	LF	128/135 (95%)	125 (98%)	3 (2%)	0	100	100
14	LG	60/67 (90%)	60 (100%)	0	0	100	100
16	NA	99/593 (17%)	99 (100%)	0	0	100	100
17	NB	50/610 (8%)	49 (98%)	1 (2%)	0	100	100
18	NF	148/151 (98%)	145 (98%)	3 (2%)	0	100	100
19	NG	125/137 (91%)	120 (96%)	5 (4%)	0	100	100
20	NL	281/318 (88%)	274 (98%)	7 (2%)	0	100	100
21	NM	207/255 (81%)	202 (98%)	5 (2%)	0	100	100
22	NP	130/144 (90%)	128 (98%)	2 (2%)	0	100	100
23	NQ	77/82 (94%)	75 (97%)	2 (3%)	0	100	100
24	NS	852/1267 (67%)	841 (99%)	11 (1%)	0	100	100
25	NW	67/108 (62%)	67 (100%)	0	0	100	100
26	SH	358/367 (98%)	352 (98%)	6 (2%)	0	100	100
27	SI	695/1183 (59%)	680 (98%)	15 (2%)	0	100	100
28	SJ	207/252 (82%)	205 (99%)	2 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	SK	225/252 (89%)	221 (98%)	4 (2%)	0	100	100
29	SL	138/189 (73%)	130 (94%)	8 (6%)	0	100	100
30	SM	217/290 (75%)	215 (99%)	2 (1%)	0	100	100
31	SR	130/145 (90%)	129 (99%)	1 (1%)	0	100	100
32	SS	142/899 (16%)	139 (98%)	3 (2%)	0	100	100
33	ST	480/810 (59%)	476 (99%)	4 (1%)	0	100	100
34	SU	524/552 (95%)	517 (99%)	7 (1%)	0	100	100
35	SW	177/274 (65%)	173 (98%)	4 (2%)	0	100	100
36	SZ	255/483 (53%)	251 (98%)	4 (2%)	0	100	100
All	All	7463/11447 (65%)	7335 (98%)	128 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	L3	90/129 (70%)	90 (100%)	0	100	100
4	L4	220/222 (99%)	220 (100%)	0	100	100
5	L5	170/191 (89%)	170 (100%)	0	100	100
6	L6	194/201 (96%)	194 (100%)	0	100	100
7	L7	166/170 (98%)	166 (100%)	0	100	100
8	L8	145/161 (90%)	145 (100%)	0	100	100
9	L9	156/166 (94%)	156 (100%)	0	100	100
10	LC	100/119 (84%)	100 (100%)	0	100	100
11	LD	125/137 (91%)	125 (100%)	0	100	100
12	LE	110/111 (99%)	110 (100%)	0	100	100
13	LF	109/113 (96%)	109 (100%)	0	100	100
14	LG	55/60 (92%)	55 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	NA	96/535 (18%)	96 (100%)	0	100	100
17	NB	50/538 (9%)	50 (100%)	0	100	100
18	NF	127/128 (99%)	127 (100%)	0	100	100
19	NG	96/105 (91%)	96 (100%)	0	100	100
20	NL	255/283 (90%)	255 (100%)	0	100	100
21	NM	189/224 (84%)	189 (100%)	0	100	100
22	NP	107/116 (92%)	107 (100%)	0	100	100
23	NQ	68/71 (96%)	68 (100%)	0	100	100
24	NS	634/1140 (56%)	634 (100%)	0	100	100
25	NW	60/89 (67%)	60 (100%)	0	100	100
26	SH	307/312 (98%)	307 (100%)	0	100	100
27	SI	620/1039 (60%)	620 (100%)	0	100	100
28	SJ	9/222 (4%)	9 (100%)	0	100	100
28	SK	12/222 (5%)	12 (100%)	0	100	100
29	SL	123/169 (73%)	123 (100%)	0	100	100
30	SM	194/258 (75%)	194 (100%)	0	100	100
31	SR	113/120 (94%)	113 (100%)	0	100	100
32	SS	134/807 (17%)	134 (100%)	0	100	100
33	ST	66/732 (9%)	66 (100%)	0	100	100
34	SU	27/506 (5%)	27 (100%)	0	100	100
35	SW	156/238 (66%)	156 (100%)	0	100	100
36	SZ	14/424 (3%)	14 (100%)	0	100	100
All	All	5097/10058 (51%)	5097 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
3	L3	13	HIS
4	L4	67	GLN
4	L4	69	HIS
4	L4	112	HIS
5	L5	128	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	L5	200	ASN
11	LD	16	GLN
11	LD	92	HIS
11	LD	104	HIS
11	LD	110	HIS
12	LE	12	ASN
13	LF	29	HIS
18	NF	49	GLN
18	NF	58	HIS
18	NF	123	HIS
20	NL	53	GLN
20	NL	201	GLN
20	NL	300	GLN
21	NM	101	HIS
21	NM	211	HIS
22	NP	43	ASN
22	NP	93	HIS
23	NQ	19	HIS
24	NS	104	GLN
24	NS	118	GLN
24	NS	398	HIS
24	NS	861	ASN
24	NS	1044	GLN
24	NS	1091	HIS
24	NS	1203	ASN
27	SI	55	HIS
27	SI	162	HIS
27	SI	737	ASN
27	SI	835	HIS
27	SI	878	HIS
27	SI	882	ASN
29	SL	147	GLN
29	SL	148	HIS
30	SM	102	GLN
31	SR	94	ASN
32	SS	416	ASN
32	SS	444	HIS
32	SS	475	GLN
33	ST	786	ASN
35	SW	262	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L1	1385/1803 (76%)	268 (19%)	9 (0%)
15	N2	4/5 (80%)	2 (50%)	0
2	L2	21/334 (6%)	5 (23%)	0
All	All	1410/2142 (65%)	275 (19%)	9 (0%)

All (275) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L1	9	U
1	L1	10	G
1	L1	15	U
1	L1	21	U
1	L1	24	U
1	L1	34	G
1	L1	42	G
1	L1	46	A
1	L1	47	A
1	L1	63	G
1	L1	65	A
1	L1	68	A
1	L1	73	U
1	L1	74	U
1	L1	75	U
1	L1	76	A
1	L1	77	U
1	L1	78	A
1	L1	104	A
1	L1	114	C
1	L1	116	U
1	L1	127	G
1	L1	140	A
1	L1	142	G
1	L1	144	U
1	L1	145	A
1	L1	159	U
1	L1	166	C
1	L1	178	U
1	L1	179	A
1	L1	192	U
1	L1	194	U
1	L1	195	G
1	L1	215	A
1	L1	216	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L1	217	A
1	L1	232	U
1	L1	233	C
1	L1	235	G
1	L1	240	U
1	L1	241	U
1	L1	250	C
1	L1	260	U
1	L1	261	U
1	L1	265	A
1	L1	275	C
1	L1	276	C
1	L1	278	U
1	L1	279	G
1	L1	280	U
1	L1	299	A
1	L1	304	U
1	L1	314	C
1	L1	316	A
1	L1	322	G
1	L1	337	G
1	L1	338	C
1	L1	344	A
1	L1	352	A
1	L1	359	A
1	L1	360	A
1	L1	361	C
1	L1	400	A
1	L1	401	A
1	L1	402	C
1	L1	404	G
1	L1	423	G
1	L1	424	C
1	L1	425	A
1	L1	426	G
1	L1	437	A
1	L1	438	A
1	L1	439	U
1	L1	444	C
1	L1	448	C
1	L1	454	U
1	L1	467	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L1	477	A
1	L1	486	G
1	L1	502	U
1	L1	505	A
1	L1	507	U
1	L1	511	A
1	L1	515	A
1	L1	519	C
1	L1	532	U
1	L1	534	A
1	L1	542	A
1	L1	545	A
1	L1	563	U
1	L1	564	G
1	L1	565	C
1	L1	570	A
1	L1	575	C
1	L1	578	U
1	L1	594	A
1	L1	595	G
1	L1	611	U
1	L1	619	A
1	L1	623	A
1	L1	624	G
1	L1	639	U
1	L1	640	U
1	L1	649	U
1	L1	650	U
1	L1	685	A
1	L1	687	G
1	L1	689	G
1	L1	690	G
1	L1	691	C
1	L1	696	C
1	L1	710	U
1	L1	711	U
1	L1	739	G
1	L1	743	U
1	L1	745	U
1	L1	765	G
1	L1	766	U
1	L1	774	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L1	775	G
1	L1	783	G
1	L1	784	C
1	L1	789	A
1	L1	794	U
1	L1	803	A
1	L1	811	A
1	L1	812	A
1	L1	815	G
1	L1	821	U
1	L1	824	G
1	L1	830	U
1	L1	833	U
1	L1	834	G
1	L1	835	U
1	L1	863	A
1	L1	876	G
1	L1	881	A
1	L1	886	U
1	L1	898	A
1	L1	904	G
1	L1	907	A
1	L1	913	G
1	L1	921	U
1	L1	926	A
1	L1	934	C
1	L1	935	U
1	L1	944	A
1	L1	945	U
1	L1	951	A
1	L1	960	U
1	L1	966	A
1	L1	969	C
1	L1	992	A
1	L1	993	A
1	L1	1005	A
1	L1	1007	C
1	L1	1011	G
1	L1	1026	A
1	L1	1028	C
1	L1	1029	U
1	L1	1030	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L1	1032	G
1	L1	1051	G
1	L1	1052	U
1	L1	1053	G
1	L1	1054	U
1	L1	1058	U
1	L1	1059	U
1	L1	1060	U
1	L1	1062	A
1	L1	1076	A
1	L1	1078	C
1	L1	1081	A
1	L1	1083	G
1	L1	1092	A
1	L1	1098	U
1	L1	1099	U
1	L1	1100	G
1	L1	1109	G
1	L1	1110	G
1	L1	1119	G
1	L1	1128	C
1	L1	1129	U
1	L1	1130	G
1	L1	1131	A
1	L1	1158	C
1	L1	1167	G
1	L1	1189	A
1	L1	1190	C
1	L1	1191	U
1	L1	1192	C
1	L1	1193	A
1	L1	1197	C
1	L1	1200	G
1	L1	1202	A
1	L1	1207	C
1	L1	1208	A
1	L1	1218	G
1	L1	1220	C
1	L1	1227	A
1	L1	1228	G
1	L1	1230	A
1	L1	1232	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L1	1256	A
1	L1	1267	G
1	L1	1268	G
1	L1	1269	U
1	L1	1270	G
1	L1	1437	U
1	L1	1438	G
1	L1	1440	C
1	L1	1465	C
1	L1	1471	A
1	L1	1481	C
1	L1	1483	A
1	L1	1490	C
1	L1	1491	U
1	L1	1492	A
1	L1	1493	A
1	L1	1496	U
1	L1	1506	G
1	L1	1514	U
1	L1	1515	A
1	L1	1516	A
1	L1	1521	G
1	L1	1523	G
1	L1	1524	A
1	L1	1535	U
1	L1	1537	C
1	L1	1542	G
1	L1	1548	G
1	L1	1553	G
1	L1	1554	U
1	L1	1555	A
1	L1	1556	A
1	L1	1557	U
1	L1	1559	A
1	L1	1569	A
1	L1	1570	A
1	L1	1579	U
1	L1	1584	G
1	L1	1590	G
1	L1	1599	C
1	L1	1600	A
1	L1	1601	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L1	1617	U
1	L1	1618	C
1	L1	1619	C
1	L1	1624	C
1	L1	1628	U
1	L1	1645	G
1	L1	1651	A
1	L1	1653	C
1	L1	1755	A
1	L1	1772	C
1	L1	1777	G
1	L1	1780	G
1	L1	1781	A
1	L1	1782	A
1	L1	1783	C
1	L1	1784	C
1	L1	1792	G
1	L1	1794	A
1	L1	1795	U
1	L1	1800	A
1	L1	1801	A
1	L1	1802	A
1	L1	1803	G
2	L2	2	U
2	L2	10	C
2	L2	13	C
2	L2	15	U
2	L2	16	A
15	N2	7	U
15	N2	10	U

All (9) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	L1	240	U
1	L1	277	U
1	L1	278	U
1	L1	738	G
1	L1	1051	G
1	L1	1082	C
1	L1	1491	U
1	L1	1555	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L1	1568	C

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

1 non-standard protein/DNA/RNA residue is 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
32	SEP	SS	423	32	8,9,10	1.62	1 (12%)	7,12,14	1.53	1 (14%)

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
32	SEP	SS	423	32	-	4/6/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	SS	423	SEP	P-O1P	3.51	1.61	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	SS	423	SEP	OG-CB-CA	3.49	111.54	108.14

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	SS	423	SEP	CB-OG-P-O1P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	SS	423	SEP	CB-OG-P-O2P
32	SS	423	SEP	CB-OG-P-O3P
32	SS	423	SEP	N-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 50 ligands modelled in this entry, 49 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
39	GTP	SI	2001	37	29,34,34	0.92	0	35,54,54	0.74	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
39	GTP	SI	2001	37	-	1/18/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

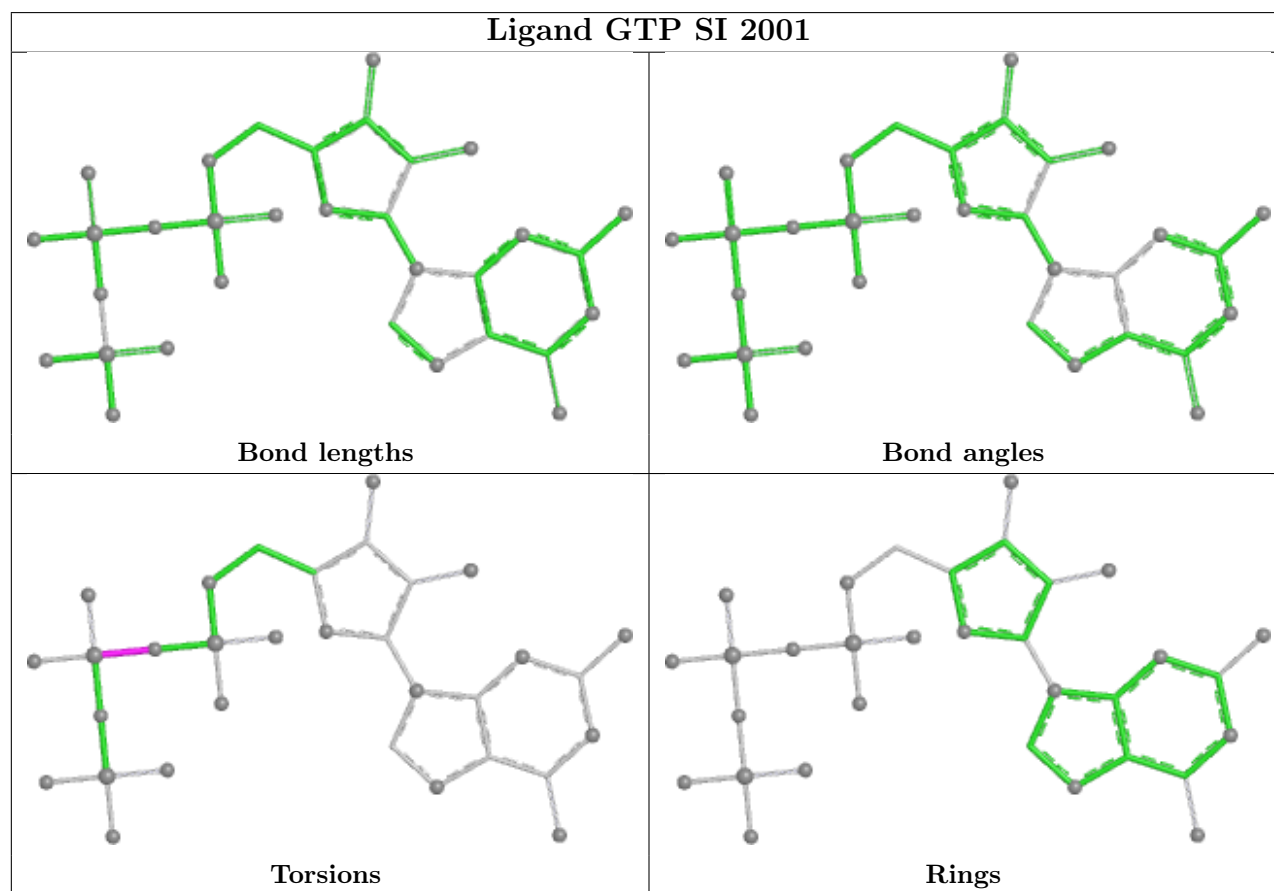
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
39	SI	2001	GTP	PA-O3A-PB-O1B

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

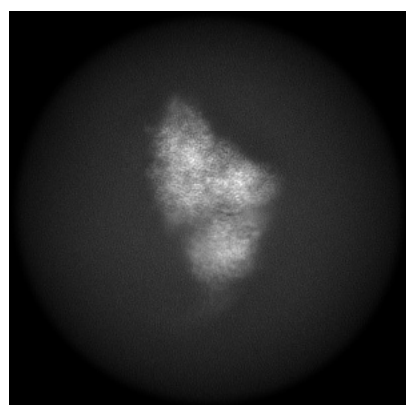
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49091. These allow visual inspection of the internal detail of the map and identification of artifacts.

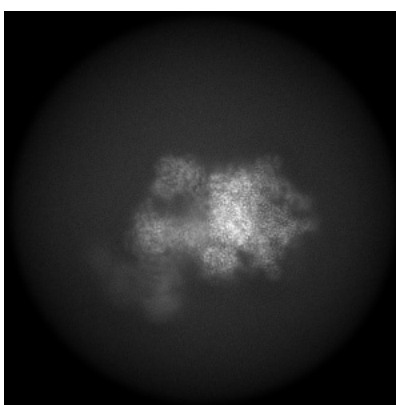
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

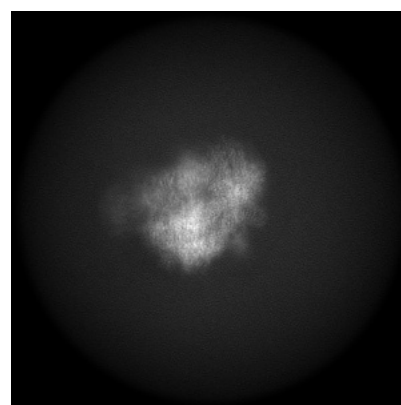
6.1.1 Primary map



X



Y

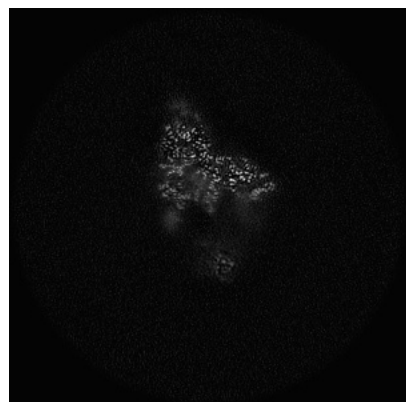


Z

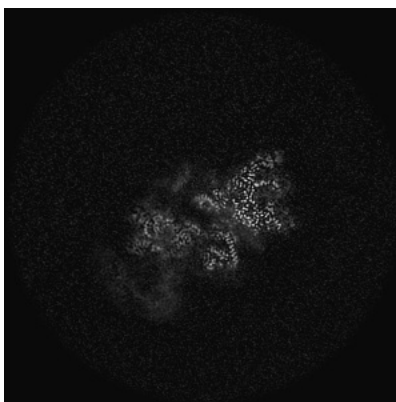
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

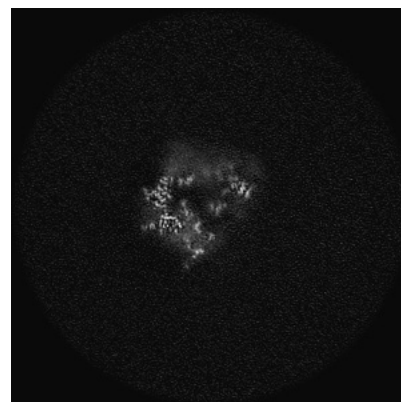
6.2.1 Primary map



X Index: 252



Y Index: 252

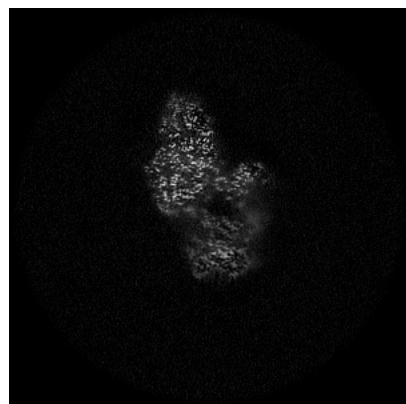


Z Index: 252

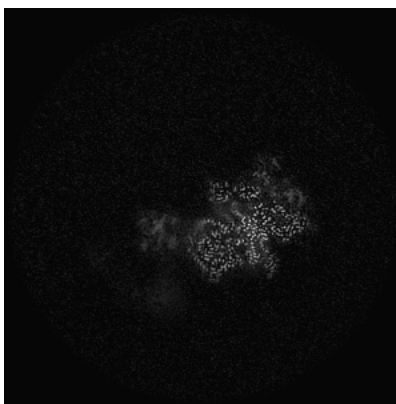
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

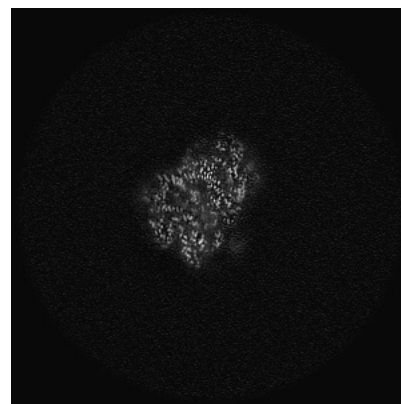
6.3.1 Primary map



X Index: 231



Y Index: 231

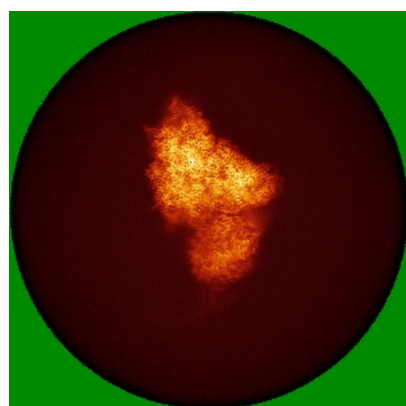


Z Index: 288

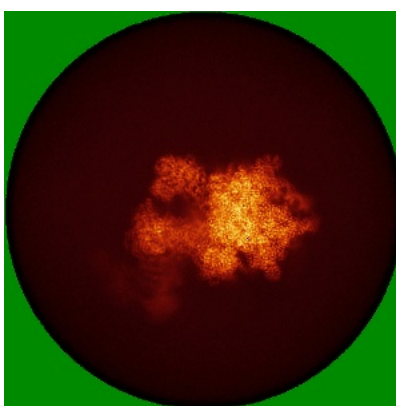
The images above show the largest variance slices of the map in three orthogonal directions.

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

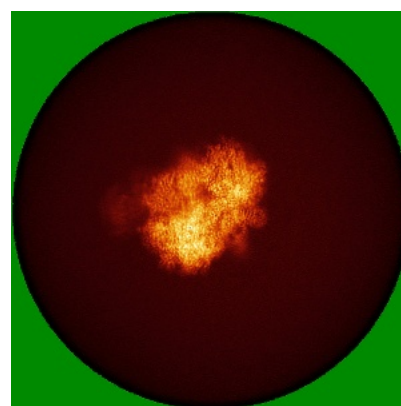
6.4.1 Primary map



X



Y

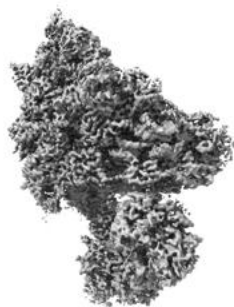


Z

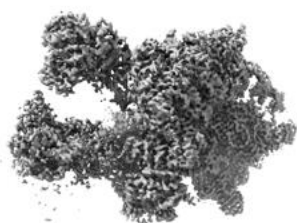
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

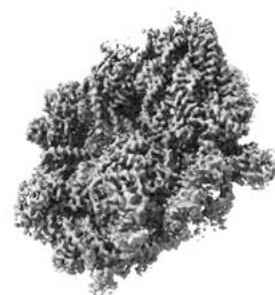
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.85. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

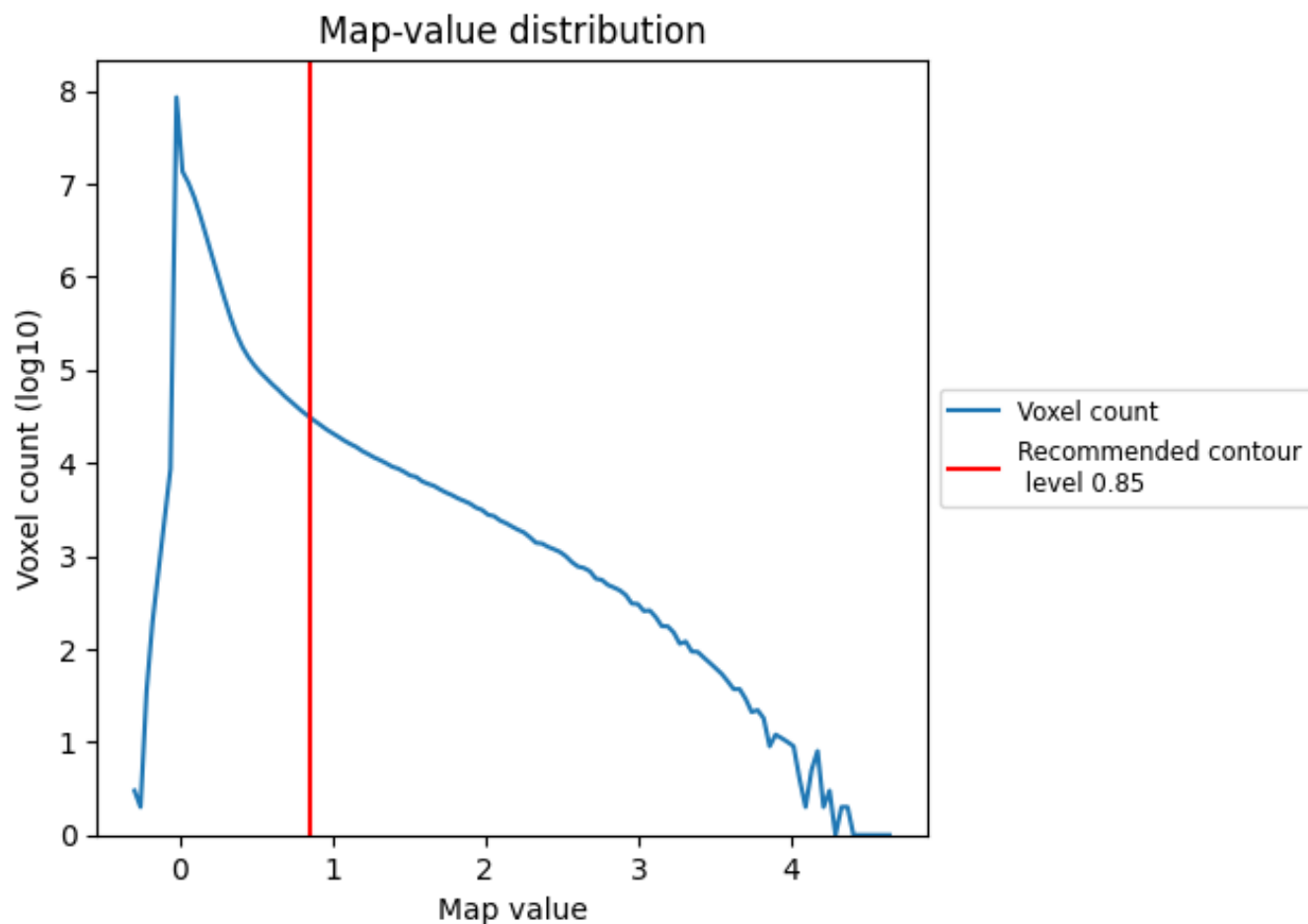
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

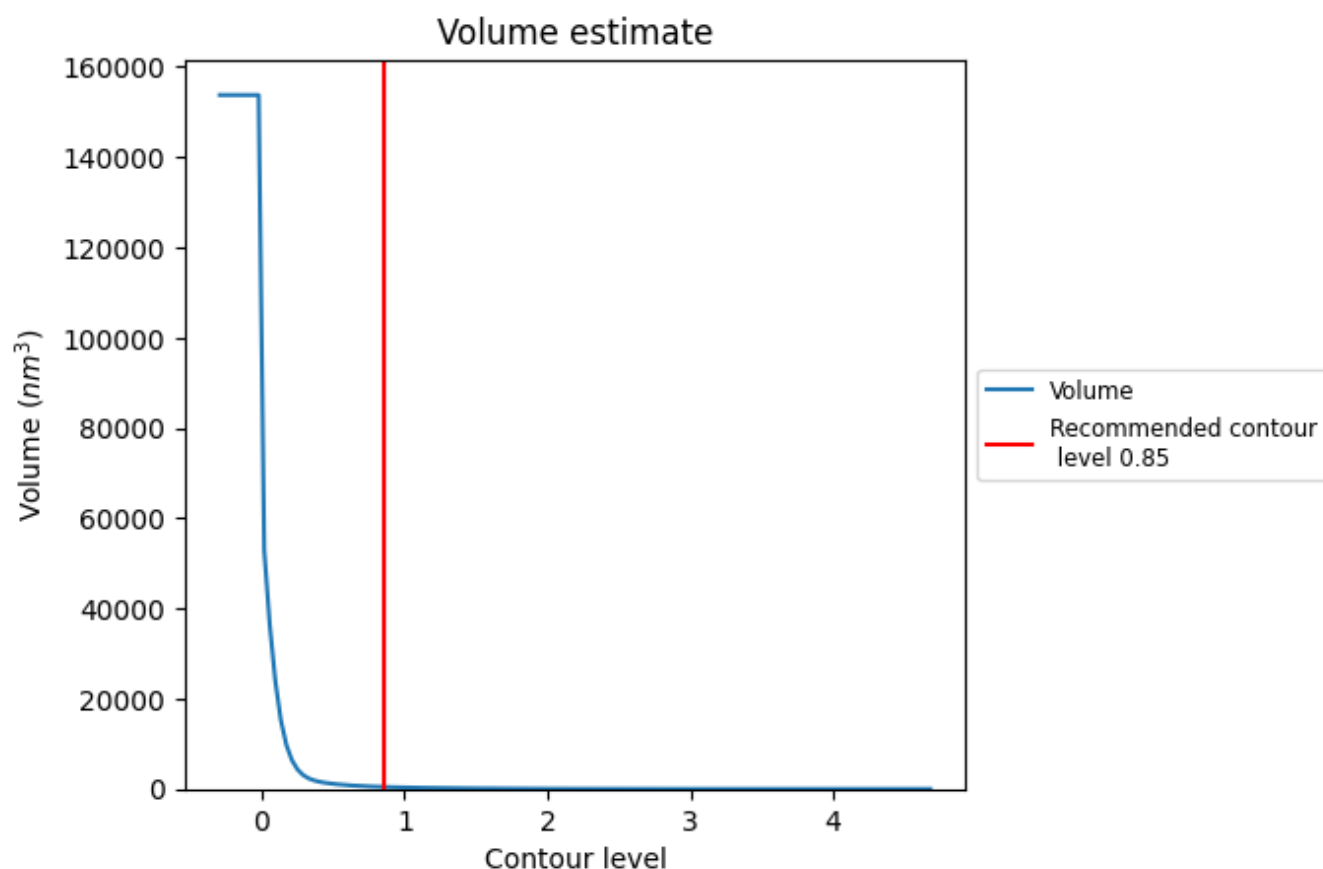
This section contains the results of statistical analysis of the map.

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.

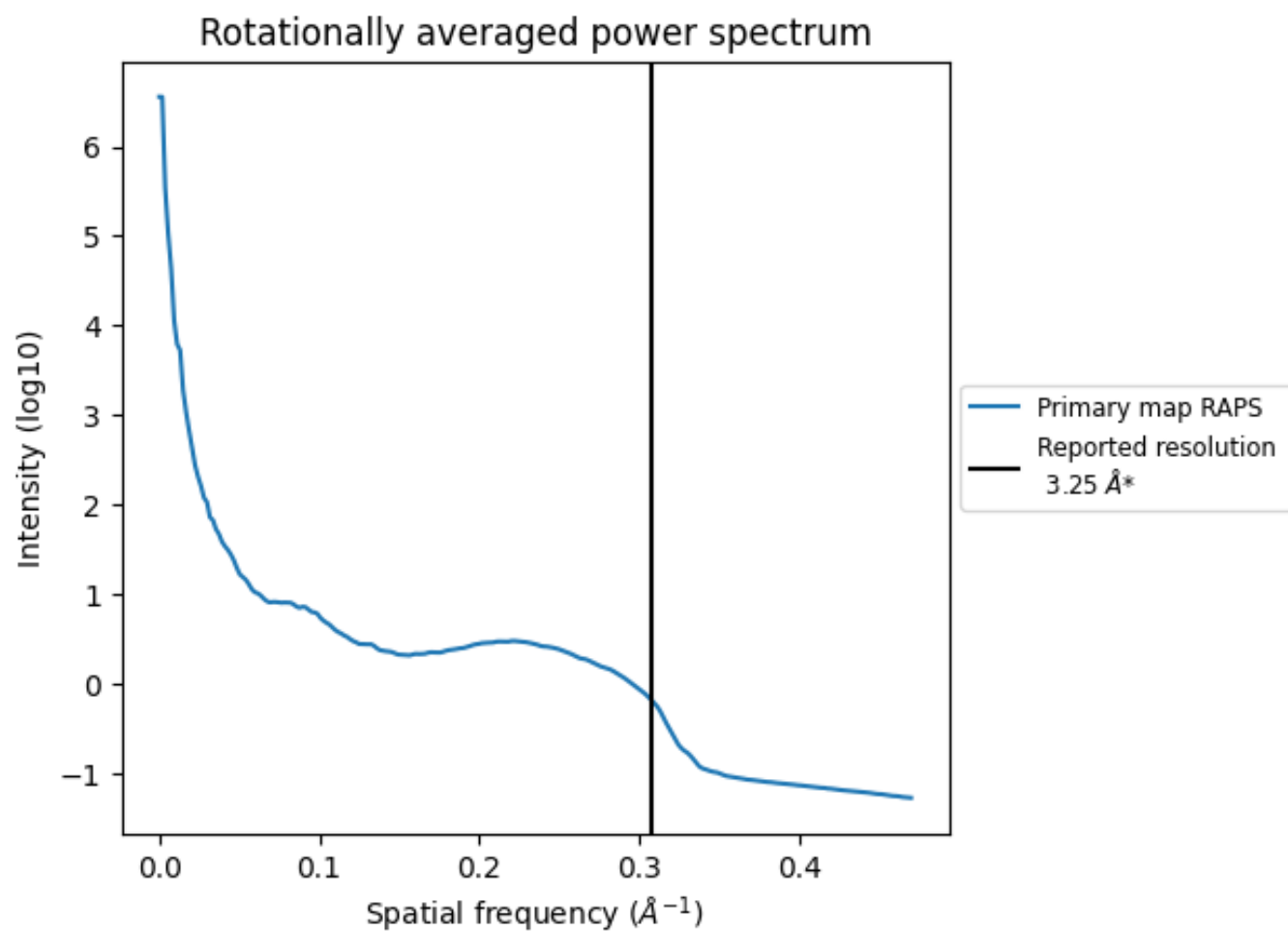
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 449 nm³; this corresponds to an approximate mass of 405 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 0.308 Å⁻¹

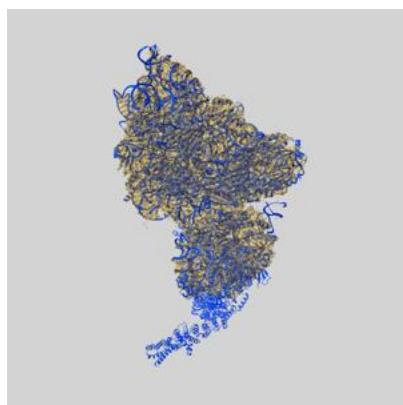
8 Fourier-Shell correlation ⓘ

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

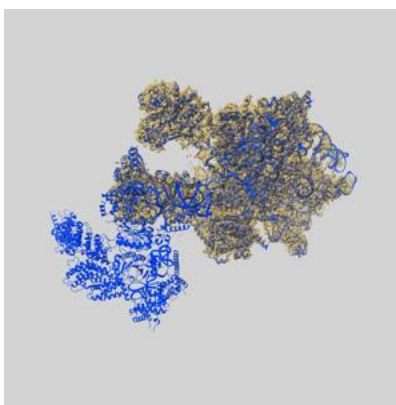
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-49091 and PDB model 9N7B. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

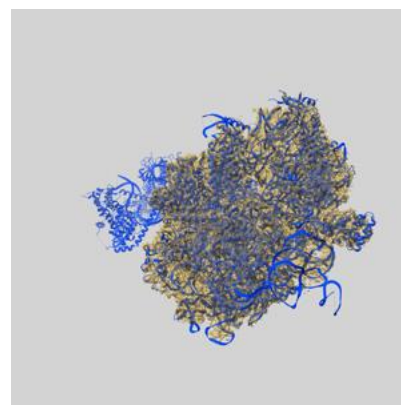
9.1 Map-model overlay [i](#)



X



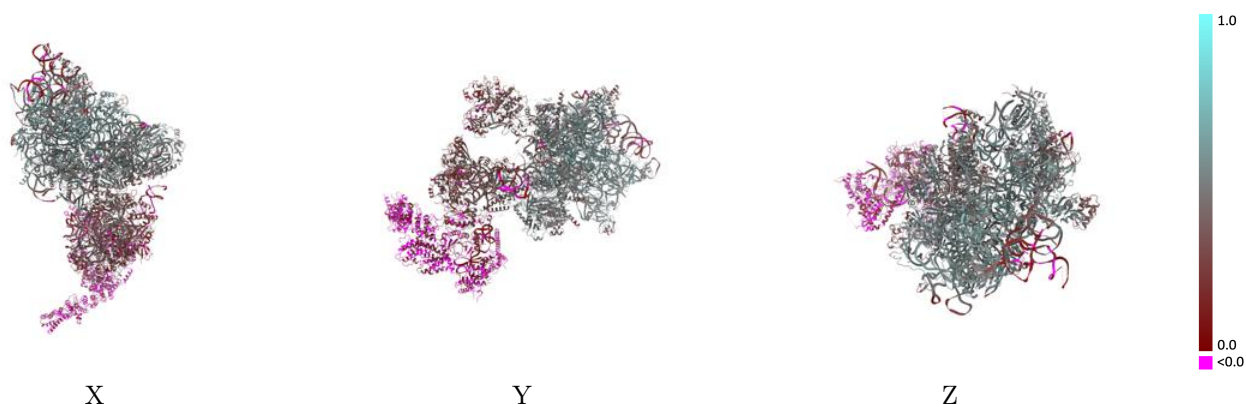
Y



Z

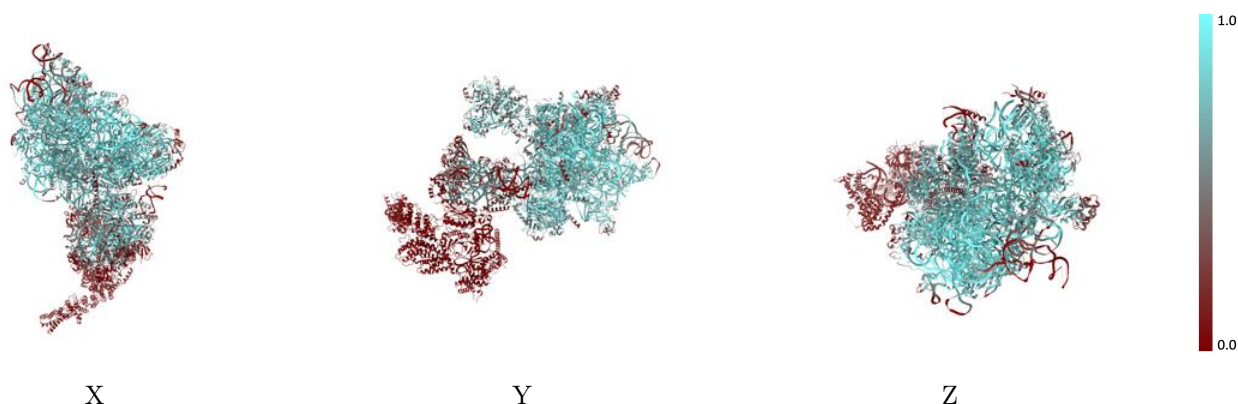
The images above show the 3D surface view of the map at the recommended contour level 0.85 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



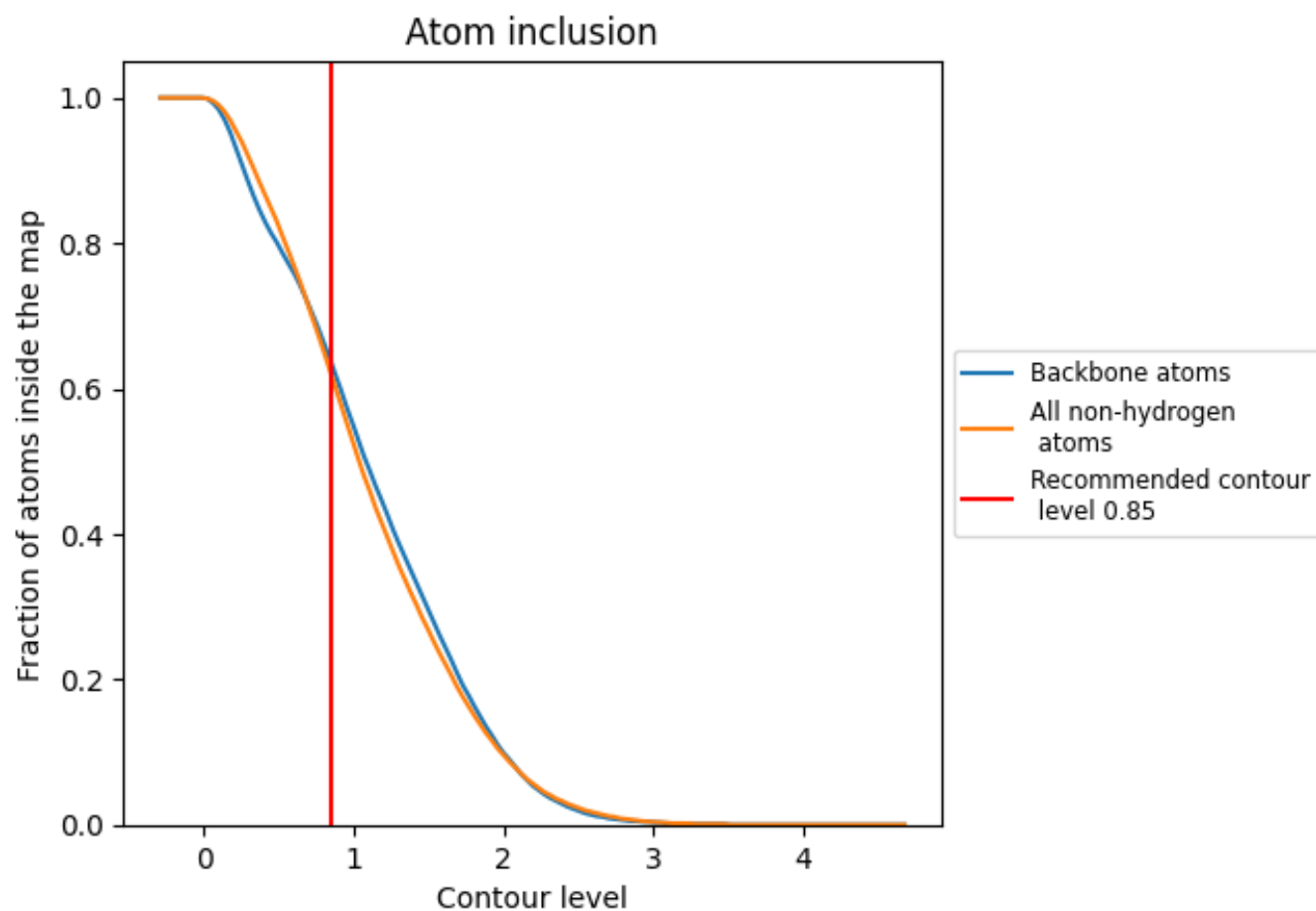
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.85).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 62% 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 (0.85) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6180	 0.4030
L1	 0.7420	 0.4290
L2	 0.8890	 0.4780
L3	 0.1530	 0.2860
L4	 0.8250	 0.5580
L5	 0.3660	 0.3110
L6	 0.6420	 0.4760
L7	 0.5680	 0.4450
L8	 0.8160	 0.5520
L9	 0.7670	 0.4980
LC	 0.3410	 0.3310
LD	 0.8470	 0.5570
LE	 0.8310	 0.5650
LF	 0.7640	 0.5200
LG	 0.0600	 0.1790
N2	 0.8700	 0.4820
NA	 0.4500	 0.4000
NB	 0.6160	 0.3850
NF	 0.7820	 0.5390
NG	 0.7450	 0.4700
NL	 0.7190	 0.4890
NM	 0.6210	 0.4960
NP	 0.3890	 0.3320
NQ	 0.6590	 0.5120
NS	 0.6250	 0.3500
NW	 0.0780	 0.3110
SH	 0.7440	 0.4950
SI	 0.7640	 0.4880
SJ	 0.0010	 0.1190
SK	 0.0150	 0.1850
SL	 0.6540	 0.5010
SM	 0.4340	 0.3850
SR	 0.7940	 0.5100
SS	 0.7030	 0.4510
ST	 0.0310	 0.0840



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
SU	 0.0000	 0.0110
SW	 0.7870	 0.4700
SZ	 0.0000	 0.0210