



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 07:00 PM UTC

PDB ID : 9N7A / pdb_00009n7a
EMDB ID : EMD-49090
Title : SSU processome maturation and disassembly, State N
Authors : Buzovetsky, O.; Klinge, S.
Deposited on : 2025-02-05
Resolution : 3.84 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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) : 2.49

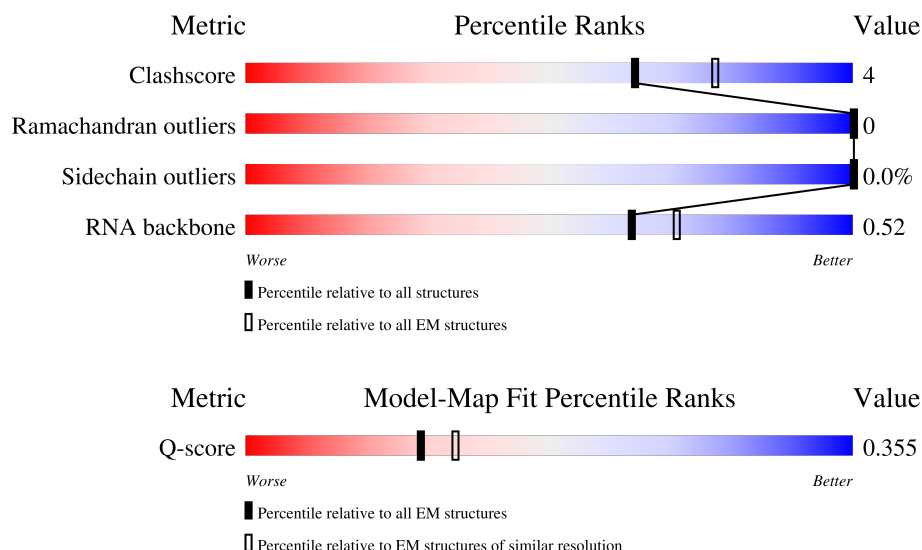
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.84 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.



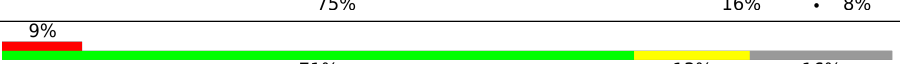
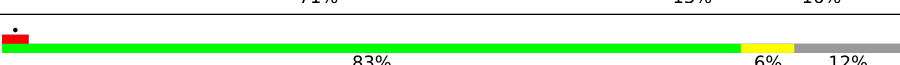
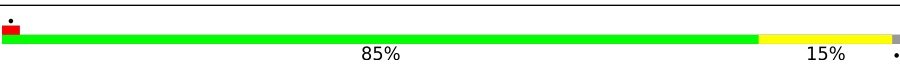
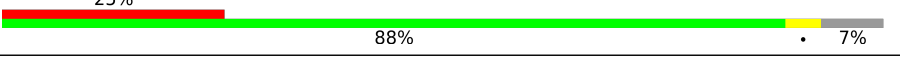
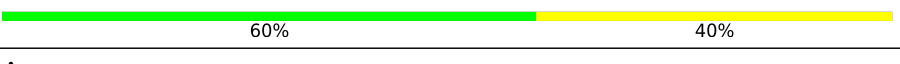
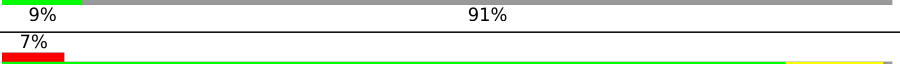
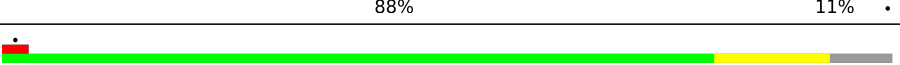
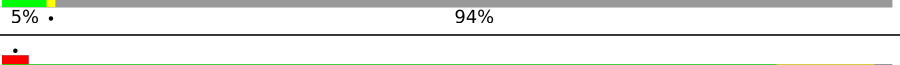
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	9033 (3.34 - 4.34)

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	9% 55% 20% • 22%
2	L2	334	• • • 93%
3	L3	146	18% 55% 14% 32%

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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	SG	573	
27	SH	367	
28	SI	1183	

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Mol	Chain	Length	Quality of chain
29	SJ	252	
29	SK	252	
30	SL	189	
31	SM	290	
32	SP	2493	
33	SR	145	
34	SS	899	
35	ST	810	
36	SU	552	
37	SW	274	
38	SZ	483	

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 93089 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	110	Total	C	N	O	S	0	0
			907	562	154	190	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	893	Total	C	N	O	S	0	0
			4947	3014	974	957	2		

- 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 Ribosomal RNA-processing protein 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	SG	33	Total	C	N	O	0	0
			271	166	52	53		

- Molecule 27 is a protein called RNA 3'-terminal phosphate cyclase-like protein.

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

- Molecule 28 is a protein called Ribosome biogenesis protein BMS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	SI	708	Total	C	N	O	S	0	0
			5748	3692	1018	1011	27		

- Molecule 29 is a protein called Ribosomal RNA small subunit methyltransferase NEP1.

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

- Molecule 30 is a protein called rRNA-processing protein FCF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	SL	142	Total	C	N	O	S	0	0
			1121	720	198	193	10		

- Molecule 31 is a protein called U3 small nucleolar ribonucleoprotein protein IMP4.

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

- Molecule 32 is a protein called U3 small nucleolar RNA-associated protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	SP	945	Total	C	N	O	S	0	0
			7764	5052	1269	1422	21		

- Molecule 33 is a protein called 40S ribosomal protein S23-A.

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

- Molecule 34 is a protein called U3 small nucleolar RNA-associated protein 14.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	SS	153	Total	C	N	O	P	S	0	0
			1186	723	231	221	1	10		

- Molecule 35 is a protein called Nucleolar complex protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	ST	573	Total	C	N	O	S	0	0
			3316	2025	651	635	5		

- Molecule 36 is a protein called Nucleolar complex protein 4.

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

- Molecule 37 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	SW	182	Total	C	N	O	S	0	0
			1444	923	262	255	4		

- Molecule 38 is a protein called Essential nuclear protein 1.

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

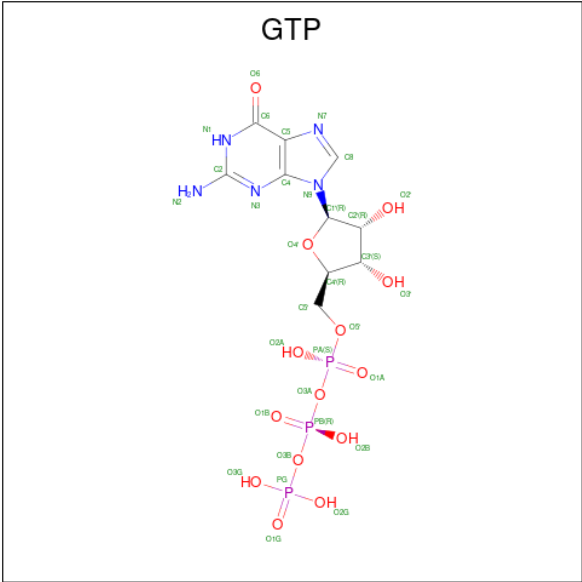
- Molecule 39 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 40 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

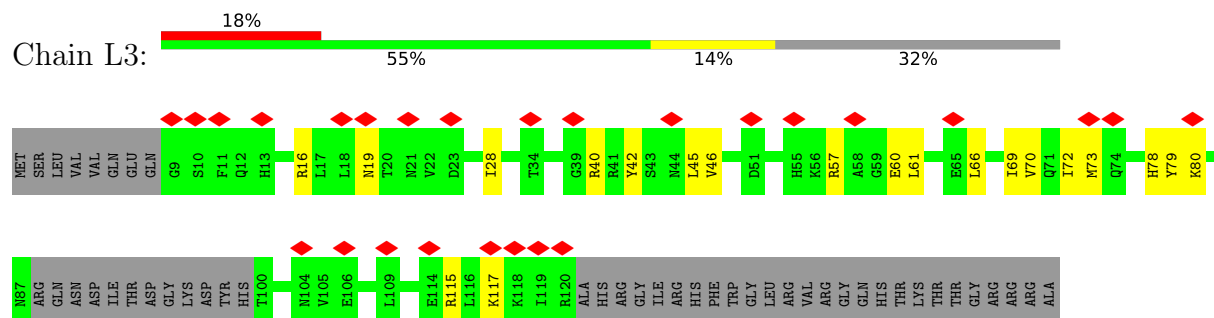
- Molecule 41 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



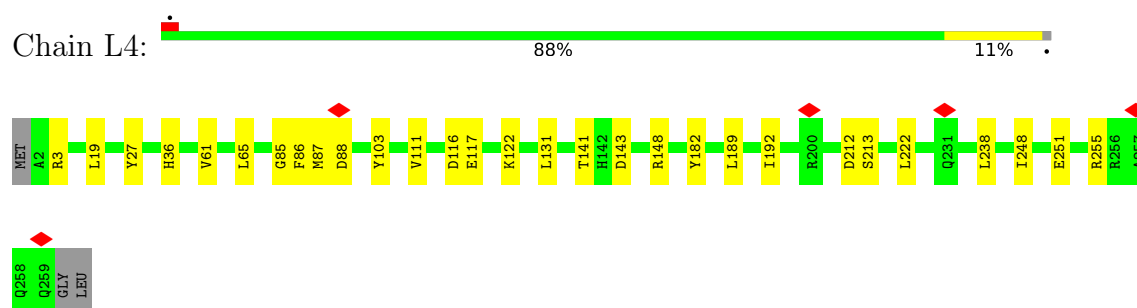
Mol	Chain	Residues	Atoms					AltConf
41	SI	1	Total	C	N	O	P	0
			32	10	5	14	3	

G
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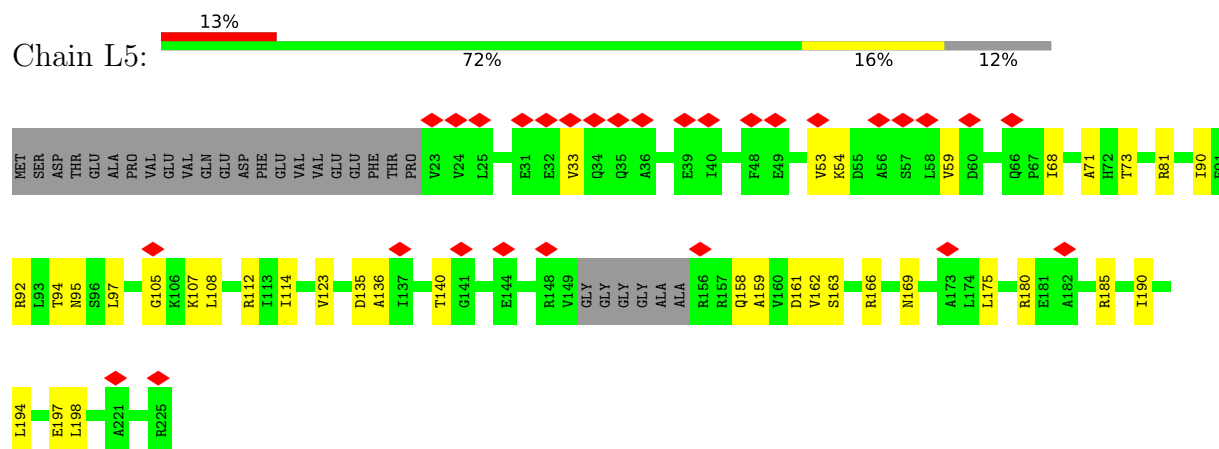
• Molecule 3: 40S ribosomal protein S18-A



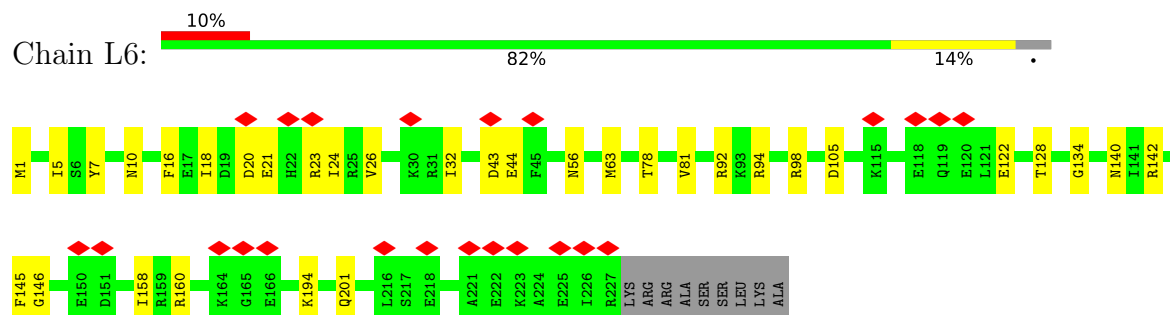
• Molecule 4: 40S ribosomal protein S4-A



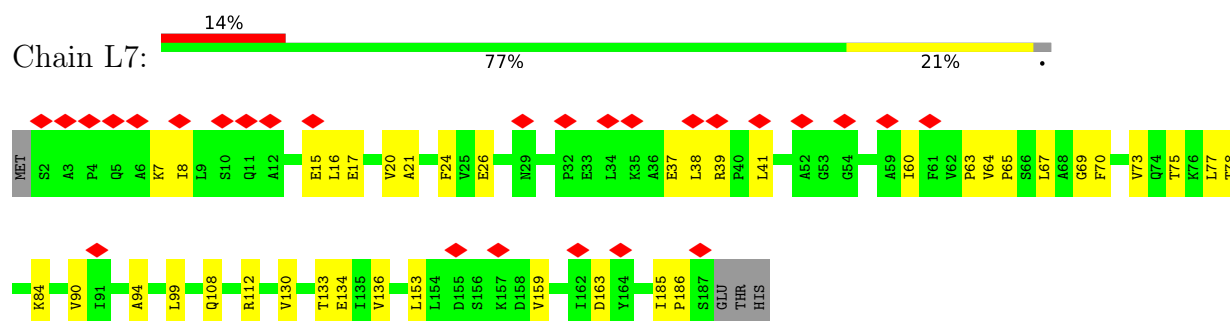
• Molecule 5: 40S ribosomal protein S5



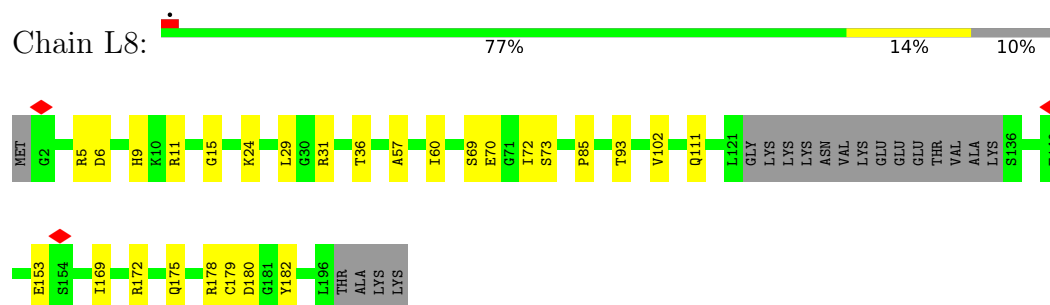
• Molecule 6: 40S ribosomal protein S6-A



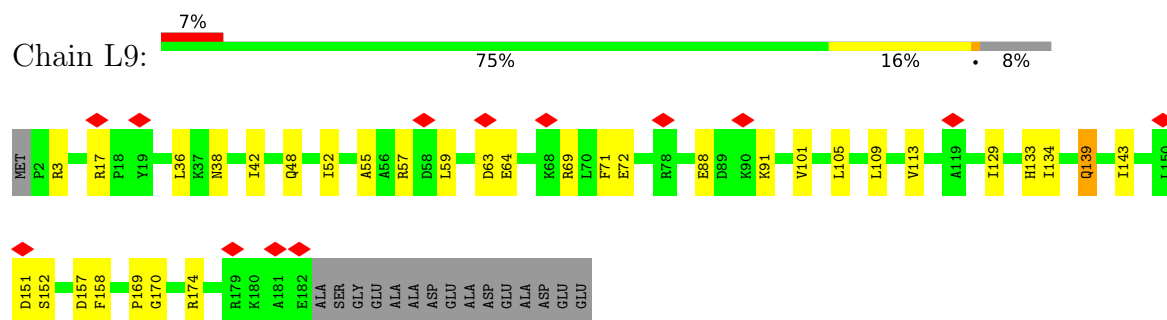
- Molecule 7: 40S ribosomal protein S7-A



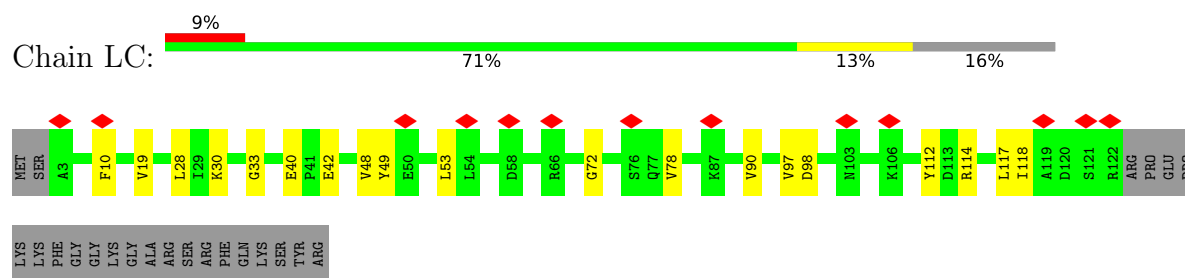
- Molecule 8: 40S ribosomal protein S8-A



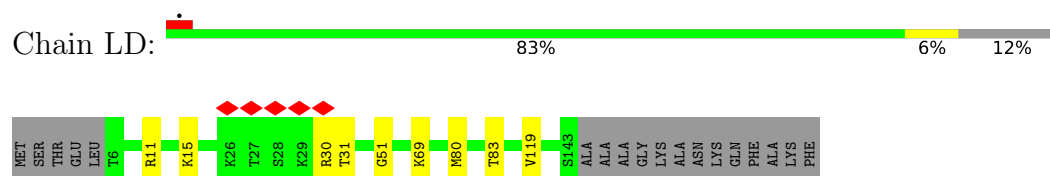
- Molecule 9: 40S ribosomal protein S9-A



- Molecule 10: 40S ribosomal protein S16-A



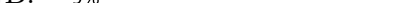
- Molecule 11: 40S ribosomal protein S11-A



-
- | Protein | Number of Amino Acids | Database |
|---------|-----------------------|----------------|
| E312 | 10 | UniProt |
| Q313 | 10 | UniProt |
| E317 | 10 | UniProt |
| K322 | 10 | UniProt |
| K327 | 10 | UniProt |
| R335 | 10 | UniProt |
| E344 | 10 | UniProt |
| L345 | 10 | UniProt |
| E346 | 10 | UniProt |
| F347 | 10 | UniProt |
| D348 | 10 | UniProt |
| R349 | 10 | UniProt |
| T358 | 10 | Not in UniProt |
| D367 | 10 | UniProt |
| M368 | 10 | UniProt |
| T369 | 10 | UniProt |
| R370 | 10 | UniProt |
| R371 | 10 | UniProt |
| R372 | 10 | UniProt |
| D375 | 10 | Not in UniProt |
| D380 | 10 | UniProt |
| R383 | 10 | UniProt |
| R384 | 10 | UniProt |
| THR | 10 | UniProt |
| LEU | 10 | UniProt |
| LEU | 10 | UniProt |
| ASP | 10 | UniProt |
| ASP | 10 | UniProt |
| ILE | 10 | UniProt |
| THR | 10 | UniProt |
| THR | 10 | UniProt |
| ARG | 10 | UniProt |
| ARG | 10 | UniProt |
| LYS | 10 | UniProt |
| LYS | 10 | UniProt |
| SER | 10 | UniProt |
| SER | 10 | UniProt |
| GLN | 10 | UniProt |
| ARG | 10 | UniProt |
| ARG | 10 | UniProt |
| PRO | 10 | UniProt |
| PRO | 10 | UniProt |
| GLN | 10 | UniProt |
| F398 | 10 | UniProt |
| E399 | 10 | UniProt |
| D402 | 10 | Not in UniProt |
| S408 | 10 | UniProt |
| E411 | 10 | UniProt |
| I412 | 10 | UniProt |
| D415 | 10 | UniProt |
| D416 | 10 | UniProt |
| Y417 | 10 | UniProt |
| D418 | 10 | UniProt |

[illegible]

- Molecule 17: Something about silencing protein 10

Chain NB:  9% 91%

[illegible]

K577 **S578** **V579** ARG ALA VAL TYR SER GLY GLY GLN SER SER GLY VAL TYR TYR GLU GLU GLU LYS THR GLY ILE LYS LYS GLY LEU THR ARG SER VAL LYS PHE LYS ASN

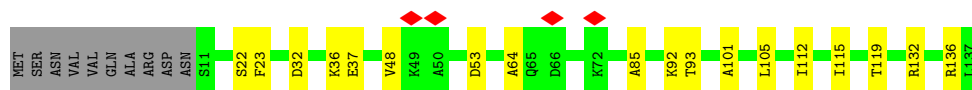
- Molecule 18: 40S ribosomal protein S13

Chain NF:

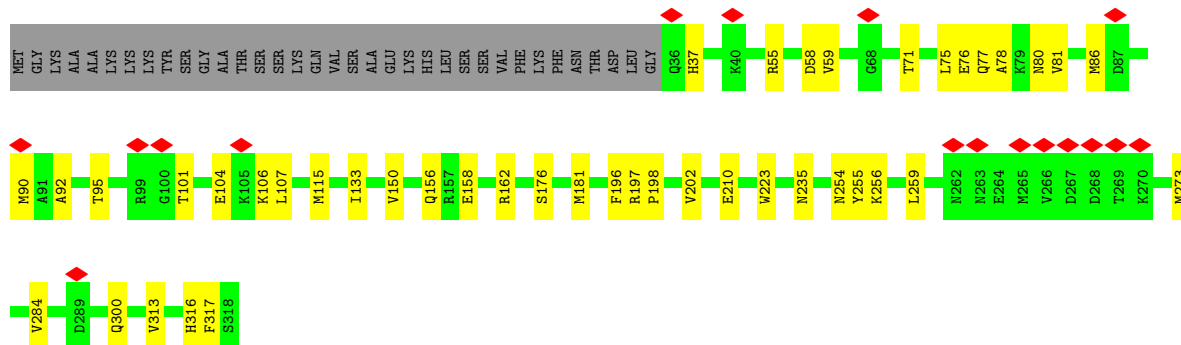
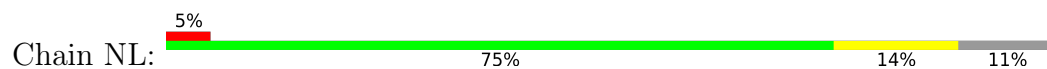
Amino Acid	Hits per Residue
MET	1
G2	1
R42	1
R55	2
D66	2
Q62	2
A63	2
R64	2
E83	2
I84	2
D87	2
R99	2
K107	2
D108	2
E119	2
R124	2
V132	2
L135	2
W139	2
F142	3
S143	3
A144	3
T145	3
A146	3
S147	3
L148	3
L149	3
V150	3
W151	3

- Molecule 19: 40S ribosomal protein S14-A

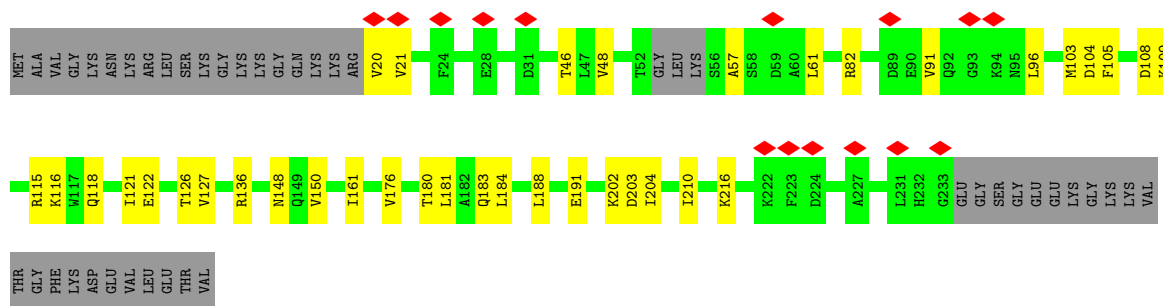
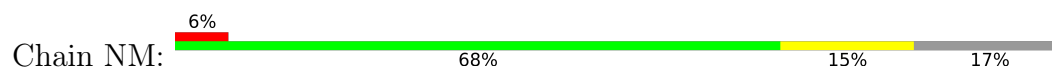
Chain NG: 



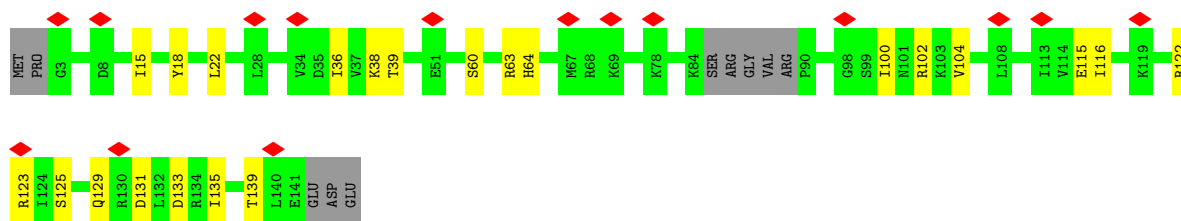
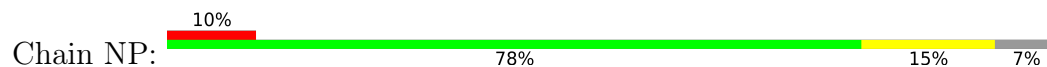
- Molecule 20: Dimethyladenosine transferase



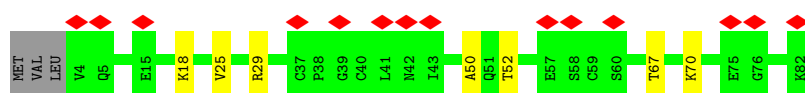
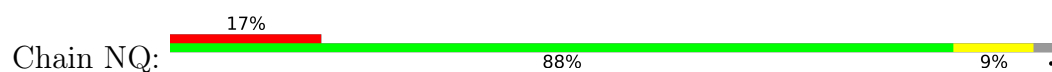
- Molecule 21: Small ribosomal subunit protein eS1A



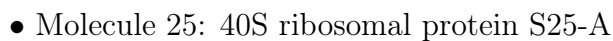
- Molecule 22: 40S ribosomal protein S19-A

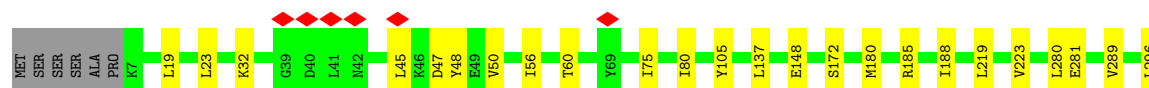


- Molecule 23: 40S ribosomal protein S27-A



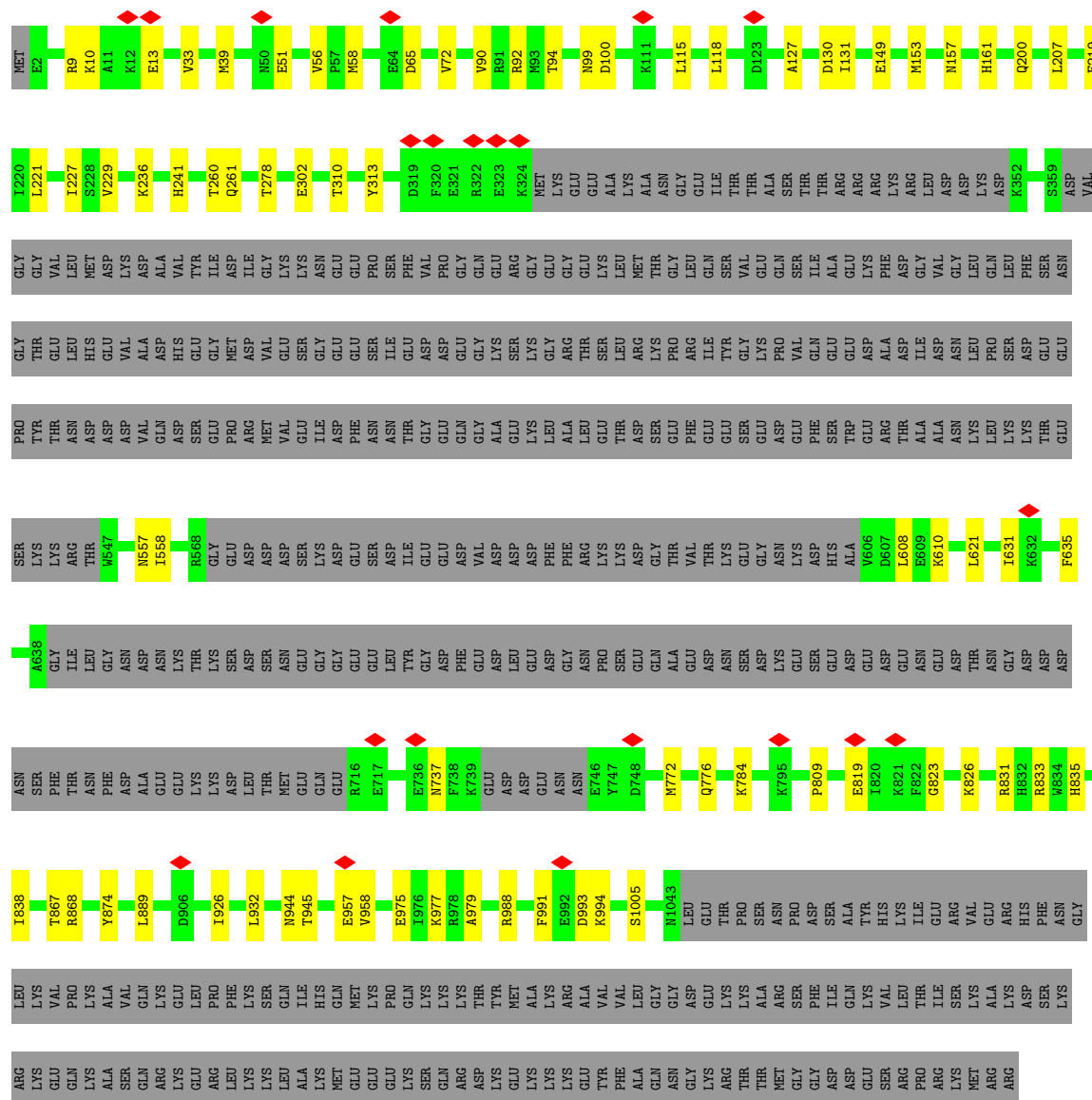
Chain NS:



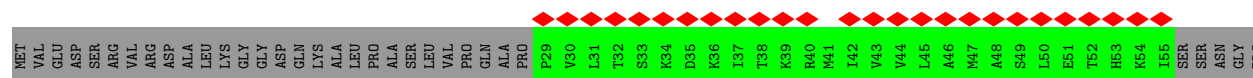
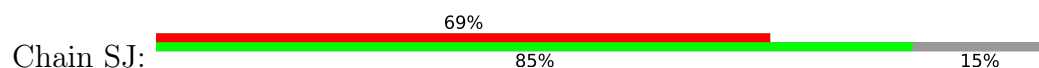


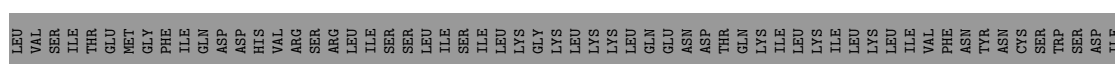


• Molecule 28: Ribosome biogenesis protein BMS1



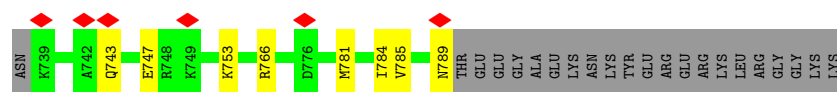
• Molecule 29: Ribosomal RNA small subunit methyltransferase NEP1











• Molecule 36: Nucleolar complex protein 4



• Molecule 37: Pre-rRNA-processing protein PNO1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14551	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	5.016	Depositor
Minimum map value	-0.472	Depositor
Average map value	0.084	Depositor
Map value standard deviation	0.148	Depositor
Recommended contour level	0.85	Depositor
Map size (Å)	535.75195, 535.75195, 535.75195	wwPDB
Map dimensions	504, 504, 504	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: SEP, M7G, GTP, MG, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	L1	0.15	0/33399	0.27	0/52011
2	L2	0.13	0/521	0.23	0/809
3	L3	0.14	0/825	0.38	0/1109
4	L4	0.17	0/2097	0.35	0/2823
5	L5	0.14	0/1575	0.33	0/2127
6	L6	0.15	0/1855	0.33	0/2478
7	L7	0.20	0/1517	0.45	1/2044 (0.0%)
8	L8	0.17	0/1462	0.33	0/1955
9	L9	0.17	0/1495	0.33	0/2003
10	LC	0.15	0/945	0.33	0/1274
11	LD	0.17	0/1145	0.33	0/1543
12	LE	0.22	0/1039	0.40	0/1395
13	LF	0.17	0/1060	0.36	0/1412
14	LG	0.12	0/492	0.31	0/659
15	N2	0.09	0/109	0.24	0/166
16	NA	0.17	0/916	0.39	0/1228
17	NB	0.15	0/464	0.33	0/608
18	NF	0.16	0/1215	0.33	0/1638
19	NG	0.18	0/952	0.36	0/1279
20	NL	0.18	0/2305	0.37	0/3116
21	NM	0.15	0/1713	0.33	0/2305
22	NP	0.17	0/1056	0.41	0/1416
23	NQ	0.14	0/605	0.34	0/817
24	NS	0.15	0/4994	0.36	0/6900
25	NW	0.16	0/564	0.38	0/758
26	SG	0.13	0/271	0.30	0/359
27	SH	0.16	0/2832	0.34	0/3825
28	SI	0.16	0/5879	0.33	0/7920
29	SJ	0.11	0/1080	0.30	0/1508
29	SK	0.12	0/1170	0.32	0/1639
30	SL	0.18	0/1142	0.37	0/1541
31	SM	0.15	0/1792	0.35	0/2425

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	SP	0.14	0/7933	0.33	2/10729 (0.0%)
33	SR	0.15	0/1069	0.31	0/1427
34	SS	0.14	0/1184	0.31	0/1567
35	ST	0.12	0/3338	0.30	0/4580
36	SU	0.19	1/2726 (0.0%)	0.38	2/3825 (0.1%)
37	SW	0.16	0/1470	0.35	0/1980
38	SZ	0.12	0/1326	0.30	0/1859
All	All	0.15	1/97532 (0.0%)	0.32	5/139057 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
32	SP	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	SU	241	PRO	CG-CD	-7.29	1.25	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	SU	241	PRO	N-CD-CG	-10.49	87.46	103.20
36	SU	241	PRO	CA-N-CD	-7.33	101.74	112.00
32	SP	2	ALA	CA-C-N	7.11	130.67	120.79
32	SP	2	ALA	C-N-CA	7.11	130.67	120.79
7	L7	186	PRO	CA-N-CD	-6.55	102.83	112.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
32	SP	203	CYS	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	L1	29868	0	15038	165	0
2	L2	496	0	253	8	0
3	L3	815	0	850	18	0
4	L4	2056	0	2140	25	0
5	L5	1558	0	1629	29	0
6	L6	1831	0	1931	29	0
7	L7	1492	0	1581	28	0
8	L8	1437	0	1458	21	0
9	L9	1470	0	1554	24	0
10	LC	930	0	983	17	0
11	LD	1119	0	1186	7	0
12	LE	1022	0	1060	16	0
13	LF	1046	0	1114	10	0
14	LG	490	0	529	3	0
15	N2	100	0	51	0	0
16	NA	907	0	893	16	0
17	NB	460	0	508	1	0
18	NF	1192	0	1255	15	0
19	NG	941	0	979	14	0
20	NL	2262	0	2330	28	0
21	NM	1688	0	1756	27	0
22	NP	1040	0	1057	17	0
23	NQ	595	0	613	5	0
24	NS	4947	0	3060	19	0
25	NW	556	0	596	8	0
26	SG	271	0	279	3	0
27	SH	2781	0	2878	33	0
28	SI	5748	0	5873	60	0
29	SJ	1074	0	514	0	0
29	SK	1160	0	570	1	0
30	SL	1121	0	1177	14	0
31	SM	1756	0	1765	23	0
32	SP	7764	0	7883	96	0
33	SR	1052	0	1120	12	0
34	SS	1186	0	1134	12	0
35	ST	3316	0	2190	17	0
36	SU	2703	0	1302	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	SW	1444	0	1526	13	0
38	SZ	1314	0	649	1	0
39	L1	46	0	0	0	0
39	SI	1	0	0	0	0
40	NQ	1	0	0	0	0
40	SL	1	0	0	0	0
41	SI	32	0	12	0	0
All	All	93089	0	73276	669	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (669) 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:L1:209:U:O2'	8:L8:180:ASP:OD2	1.86	0.92
1:L1:904:G:N2	1:L1:1000:C:O2	2.07	0.87
16:NA:367:ASP:OD2	16:NA:370:ARG:NH2	2.10	0.84
1:L1:1480:G:OP1	22:NP:63:ARG:NH2	2.11	0.84
5:L5:112:ARG:NH2	10:LC:42:GLU:OE2	2.11	0.83
2:L2:17:G:O2'	34:SS:470:GLU:OE2	1.95	0.82
1:L1:622:A:O2'	1:L1:1032:G:OP2	1.97	0.82
1:L1:318:U:OP2	24:NS:33:ARG:NH2	2.13	0.81
1:L1:1773:C:OP1	28:SI:10:LYS:NZ	2.13	0.81
1:L1:410:A:O3'	24:NS:11:LYS:NZ	2.13	0.80
32:SP:892:LEU:O	32:SP:932:ARG:NH2	2.14	0.80
34:SS:470:GLU:OE2	34:SS:474:ARG:NH2	2.14	0.80
1:L1:126:A:O2'	6:L6:194:LYS:NZ	2.14	0.80
3:L3:16:ARG:NH2	3:L3:19:ASN:OD1	2.15	0.79
32:SP:354:SER:OG	32:SP:356:ASP:OD1	2.00	0.79
5:L5:158:GLN:NE2	5:L5:159:ALA:O	2.15	0.79
1:L1:406:U:O2'	6:L6:94:ARG:NH2	2.16	0.79
1:L1:539:G:N2	1:L1:539:G:OP2	2.15	0.79
1:L1:787:G:O5'	4:L4:255:ARG:NH2	2.15	0.79
16:NA:372:ARG:NH2	31:SM:192:ASP:OD1	2.16	0.79
32:SP:149:GLU:OE2	32:SP:153:ASN:ND2	2.14	0.79
16:NA:322:LYS:O	16:NA:327:LYS:NZ	2.17	0.78
1:L1:976:G:H1	1:L1:1023:A:HO2'	1.28	0.78
13:LF:86:GLU:OE2	13:LF:90:ARG:NE	2.16	0.77
1:L1:330:G:OP2	8:L8:172:ARG:NH1	2.18	0.77
20:NL:162:ARG:O	20:NL:176:SER:OG	2.02	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:LD:80:MET:SD	11:LD:83:THR:OG1	2.42	0.77
32:SP:283:SER:O	32:SP:329:LYS:NZ	2.17	0.76
1:L1:594:A:OP1	9:L9:38:ASN:ND2	2.18	0.76
13:LF:76:TYR:OH	13:LF:86:GLU:OE1	2.03	0.76
18:NF:99:ARG:NH2	18:NF:119:GLU:OE2	2.18	0.75
8:L8:85:PRO:O	11:LD:11:ARG:NH1	2.20	0.75
1:L1:619:A:O5'	28:SI:9:ARG:NH1	2.19	0.75
3:L3:28:ILE:HD13	3:L3:61:LEU:HD11	1.69	0.75
1:L1:904:G:N1	1:L1:1000:C:N3	2.34	0.75
1:L1:1594:G:O2'	1:L1:1600:A:N1	2.18	0.74
32:SP:717:GLN:NE2	32:SP:718:PRO:O	2.21	0.74
1:L1:1533:C:OP2	25:NW:77:ARG:NH2	2.20	0.74
24:NS:138:GLN:NE2	24:NS:143:GLU:OE1	2.20	0.74
1:L1:1056:U:O2'	21:NM:202:LYS:NZ	2.17	0.73
27:SH:148:GLU:OE1	27:SH:172:SER:OG	2.06	0.73
1:L1:460:A:O2'	4:L4:27:TYR:OH	2.05	0.73
28:SI:772:MET:HE1	28:SI:776:GLN:HG3	1.69	0.73
1:L1:810:G:N2	7:L7:108:GLN:OE1	2.22	0.73
1:L1:706:A:N6	1:L1:732:G:O2'	2.22	0.73
1:L1:1540:G:OP2	3:L3:40:ARG:NH2	2.21	0.72
1:L1:392:G:OP2	8:L8:24:LYS:NZ	2.22	0.72
16:NA:335:ARG:NH2	28:SI:957:GLU:OE1	2.22	0.72
1:L1:1779:U:OP2	1:L1:1781:A:N6	2.22	0.72
6:L6:1:MET:HE3	6:L6:24:ILE:HG23	1.72	0.72
35:ST:388:LEU:O	35:ST:392:LYS:N	2.22	0.72
1:L1:862:A:OP2	18:NF:64:ARG:NH2	2.22	0.72
5:L5:54:LYS:NZ	5:L5:135:ASP:OD1	2.16	0.72
1:L1:895:G:O2'	19:NG:37:GLU:OE1	2.06	0.71
1:L1:99:C:OP2	1:L1:378:A:O2'	2.04	0.71
31:SM:241:THR:OG1	31:SM:244:GLY:O	2.02	0.71
37:SW:154:LYS:NZ	37:SW:177:LEU:O	2.23	0.71
31:SM:116:ARG:NH1	31:SM:118:ASN:OD1	2.24	0.71
1:L1:110:U:OP1	1:L1:753:A:O2'	2.08	0.70
10:LC:42:GLU:N	10:LC:42:GLU:OE1	2.24	0.70
32:SP:565:LEU:CD2	32:SP:571:LEU:HD11	2.20	0.70
32:SP:493:ASN:ND2	32:SP:525:ILE:O	2.24	0.70
6:L6:98:ARG:NH1	6:L6:105:ASP:OD1	2.24	0.70
1:L1:1609:U:O2'	5:L5:105:GLY:O	2.07	0.69
32:SP:583:LEU:O	32:SP:586:THR:OG1	2.10	0.69
1:L1:93:A:O4'	4:L4:3:ARG:NH1	2.24	0.69
7:L7:99:LEU:O	7:L7:112:ARG:NH2	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:742:U:O2'	1:L1:743:U:OP1	2.11	0.69
4:L4:148:ARG:NH2	6:L6:201:GLN:OE1	2.26	0.69
28:SI:51:GLU:OE1	33:SR:50:LYS:N	2.25	0.69
9:L9:88:GLU:OE1	9:L9:91:LYS:NZ	2.20	0.68
16:NA:347:PHE:O	16:NA:349:ARG:NH1	2.26	0.68
1:L1:1177:C:O3'	35:ST:88:LYS:NZ	2.27	0.68
16:NA:348:ASP:OD1	35:ST:766:ARG:NH2	2.26	0.68
1:L1:1190:C:N4	1:L1:1197:C:O2	2.26	0.68
1:L1:334:G:O6	8:L8:5:ARG:NH2	2.26	0.68
1:L1:863:A:OP1	12:LE:57:ARG:NH1	2.26	0.67
1:L1:619:A:O4'	28:SI:9:ARG:NH1	2.27	0.67
32:SP:668:GLY:O	32:SP:671:THR:OG1	2.13	0.67
6:L6:92:ARG:NH2	24:NS:59:ASN:OD1	2.27	0.67
1:L1:159:U:OP2	13:LF:117:LYS:NZ	2.27	0.67
1:L1:1555:A:O2'	1:L1:1556:A:O5'	2.13	0.67
28:SI:302:GLU:N	28:SI:302:GLU:OE2	2.28	0.67
32:SP:438:GLU:OE2	32:SP:750:TYR:OH	2.08	0.67
27:SH:137:LEU:HD11	27:SH:296:LEU:HD22	1.76	0.66
1:L1:1778:G:OP2	20:NL:162:ARG:NH2	2.29	0.66
1:L1:577:G:OP1	16:NA:322:LYS:NZ	2.25	0.66
1:L1:1521:G:O2'	1:L1:1523:G:OP2	2.05	0.66
2:L2:0:M7G:H81	2:L2:0:M7G:H5'1	1.78	0.66
4:L4:103:TYR:O	4:L4:182:TYR:OH	2.13	0.66
1:L1:1616:G:O5'	5:L5:81:ARG:NH1	2.28	0.65
9:L9:48:GLN:O	9:L9:52:ILE:HD12	1.96	0.65
28:SI:833:ARG:NH2	33:SR:141:GLU:OE1	2.28	0.65
32:SP:806:THR:OG1	32:SP:820:THR:OG1	2.13	0.65
1:L1:1482:C:O2'	10:LC:72:GLY:O	2.14	0.65
1:L1:1777:G:OP1	20:NL:235:ASN:ND2	2.29	0.65
37:SW:238:THR:HG22	37:SW:242:MET:HE1	1.79	0.65
1:L1:304:U:O2	11:LD:69:LYS:NZ	2.24	0.64
5:L5:53:VAL:HG21	5:L5:59:VAL:HA	1.78	0.64
27:SH:45:LEU:HD23	27:SH:50:VAL:HG22	1.78	0.64
1:L1:1471:A:OP1	5:L5:185:ARG:NH1	2.30	0.64
27:SH:321:ARG:NH1	28:SI:610:LYS:O	2.30	0.64
1:L1:1034:C:HO2'	12:LE:2:THR:N	1.95	0.64
5:L5:33:VAL:HG13	10:LC:53:LEU:HD11	1.79	0.64
8:L8:36:THR:OG1	8:L8:57:ALA:O	2.13	0.64
20:NL:156:GLN:NE2	20:NL:158:GLU:OE1	2.31	0.64
23:NQ:18:LYS:O	23:NQ:29:ARG:NH2	2.31	0.64
2:L2:15:U:OP1	34:SS:466:ARG:NH2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:NM:82:ARG:NH1	21:NM:191:GLU:OE2	2.31	0.64
1:L1:201:G:O3'	32:SP:946:LYS:NZ	2.29	0.64
20:NL:150:VAL:HG22	20:NL:210:GLU:OE2	1.98	0.63
21:NM:127:VAL:HG13	21:NM:176:VAL:HG11	1.79	0.63
1:L1:1051:G:O2'	1:L1:1052:U:OP1	2.12	0.63
34:SS:374:ARG:O	34:SS:377:THR:OG1	2.15	0.63
21:NM:108:ASP:OD1	21:NM:109:LYS:N	2.32	0.63
6:L6:7:TYR:CD2	6:L6:10:ASN:ND2	2.66	0.63
28:SI:831:ARG:NH1	28:SI:835:HIS:O	2.31	0.63
28:SI:833:ARG:NE	33:SR:141:GLU:OE2	2.32	0.63
32:SP:572:LYS:NZ	32:SP:611:GLN:O	2.29	0.63
22:NP:131:ASP:O	22:NP:135:ILE:HD12	1.99	0.63
1:L1:66:U:O4	6:L6:134:GLY:N	2.33	0.62
11:LD:30:ARG:NH1	11:LD:31:THR:OG1	2.31	0.62
1:L1:1163:A:O3'	5:L5:166:ARG:NH2	2.32	0.62
20:NL:101:THR:OG1	20:NL:104:GLU:OE2	2.18	0.62
32:SP:749:LYS:O	32:SP:756:SER:OG	2.18	0.62
1:L1:878:G:O2'	18:NF:108:ASP:OD1	2.17	0.62
1:L1:1499:G:OP1	22:NP:122:ARG:NH1	2.32	0.62
9:L9:63:ASP:OD1	9:L9:64:GLU:N	2.33	0.62
5:L5:94:THR:HG22	5:L5:114:ILE:HG13	1.82	0.61
1:L1:1528:U:H5''	5:L5:108:LEU:HD22	1.82	0.61
32:SP:860:SER:O	32:SP:866:GLN:NE2	2.32	0.61
10:LC:48:VAL:HG23	10:LC:78:VAL:HG13	1.81	0.61
19:NG:32:ASP:OD1	21:NM:46:THR:OG1	2.17	0.61
7:L7:38:LEU:HD13	7:L7:77:LEU:HD21	1.80	0.61
22:NP:115:GLU:OE2	22:NP:123:ARG:NH1	2.33	0.61
1:L1:162:A:H3'	1:L1:163:G:H21	1.64	0.61
27:SH:312:ARG:NH1	27:SH:349:ASP:OD2	2.34	0.60
30:SL:75:SER:OG	30:SL:80:VAL:O	2.19	0.60
32:SP:565:LEU:HD21	32:SP:571:LEU:HD11	1.82	0.60
1:L1:1555:A:O2'	1:L1:1556:A:O4'	2.19	0.60
7:L7:7:LYS:NZ	7:L7:39:ARG:O	2.34	0.60
22:NP:38:LYS:O	22:NP:39:THR:OG1	2.17	0.60
32:SP:316:LYS:O	32:SP:319:THR:OG1	2.19	0.60
8:L8:69:SER:OG	8:L8:70:GLU:OE1	2.17	0.60
30:SL:139:ASP:OD1	30:SL:140:CYS:N	2.34	0.60
1:L1:1788:G:OP2	19:NG:132:ARG:NH1	2.34	0.60
3:L3:115:ARG:NH2	16:NA:344:GLU:OE1	2.35	0.60
30:SL:100:ASP:OD1	30:SL:130:CYS:N	2.35	0.60
21:NM:122:GLU:OE1	21:NM:122:GLU:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:933:A:OP1	21:NM:116:LYS:NZ	2.33	0.59
19:NG:85:ALA:H	19:NG:119:THR:HG22	1.67	0.59
24:NS:22:GLU:OE2	24:NS:25:ARG:NH1	2.35	0.59
28:SI:819:GLU:OE1	28:SI:819:GLU:N	2.35	0.59
7:L7:8:ILE:HG23	7:L7:17:GLU:OE2	2.01	0.59
35:ST:785:VAL:O	35:ST:789:ASN:ND2	2.35	0.59
21:NM:104:ASP:OD1	21:NM:105:PHE:N	2.34	0.59
16:NA:335:ARG:NH1	28:SI:957:GLU:OE2	2.36	0.59
32:SP:793:PHE:CZ	32:SP:850:LEU:HD12	2.38	0.59
6:L6:43:ASP:OD1	6:L6:44:GLU:N	2.36	0.59
27:SH:219:LEU:HD22	28:SI:635:PHE:HE2	1.68	0.59
27:SH:137:LEU:CD1	27:SH:296:LEU:HD22	2.32	0.58
1:L1:935:U:OP2	1:L1:1075:C:O2'	2.20	0.58
32:SP:307:ASP:OD1	32:SP:308:ALA:N	2.36	0.58
1:L1:1082:C:O2'	1:L1:1083:G:OP1	2.19	0.58
5:L5:161:ASP:OD1	5:L5:162:VAL:N	2.36	0.58
32:SP:476:LEU:CD2	32:SP:515:THR:HG22	2.34	0.58
7:L7:8:ILE:HD11	7:L7:21:ALA:HB2	1.86	0.58
27:SH:56:ILE:O	27:SH:60:THR:HG22	2.04	0.58
1:L1:60:U:OP2	32:SP:12:LYS:NZ	2.24	0.58
3:L3:78:HIS:O	3:L3:80:LYS:NZ	2.37	0.57
27:SH:307:ASP:OD1	27:SH:308:ILE:N	2.37	0.57
32:SP:298:MET:HE2	32:SP:321:ILE:HD11	1.87	0.57
32:SP:200:VAL:HG21	32:SP:235:LEU:HD21	1.85	0.57
1:L1:277:U:O2'	1:L1:278:U:OP1	2.20	0.57
1:L1:1108:G:OP2	1:L1:1108:G:N2	2.31	0.57
7:L7:130:VAL:O	7:L7:133:THR:OG1	2.17	0.57
16:NA:408:SER:O	16:NA:411:GLU:N	2.38	0.56
7:L7:136:VAL:N	7:L7:153:LEU:O	2.38	0.56
24:NS:88:LYS:HA	24:NS:91:ARG:HE	1.70	0.56
1:L1:447:U:O2'	4:L4:27:TYR:O	2.23	0.56
1:L1:472:U:O2'	1:L1:769:A:N3	2.31	0.56
1:L1:705:U:O2'	1:L1:706:A:O4'	2.23	0.56
1:L1:802:G:H21	12:LE:107:SER:HB2	1.71	0.56
4:L4:36:HIS:NE2	4:L4:88:ASP:OD2	2.38	0.56
4:L4:192:ILE:HD11	4:L4:238:LEU:HD12	1.86	0.56
11:LD:30:ARG:NH2	11:LD:51:GLY:O	2.37	0.56
20:NL:55:ARG:N	20:NL:58:ASP:OD2	2.37	0.56
32:SP:949:VAL:O	32:SP:952:VAL:HG12	2.05	0.56
37:SW:137:VAL:HG11	37:SW:159:ILE:HG21	1.86	0.56
1:L1:1169:G:N1	1:L1:1575:G:OP2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:1473:U:O4	5:L5:180:ARG:NE	2.37	0.56
32:SP:137:ASP:O	32:SP:140:ILE:HG22	2.05	0.56
1:L1:207:U:O2	8:L8:178:ARG:NH2	2.39	0.56
3:L3:69:ILE:HG22	3:L3:73:MET:HE1	1.87	0.56
20:NL:156:GLN:HE21	20:NL:202:VAL:HG21	1.71	0.56
1:L1:861:U:O2'	12:LE:56:HIS:O	2.24	0.56
20:NL:115:MET:SD	20:NL:115:MET:N	2.78	0.56
9:L9:151:ASP:OD1	9:L9:152:SER:N	2.38	0.56
12:LE:106:THR:HG23	12:LE:108:ALA:H	1.71	0.56
1:L1:1528:U:C5'	5:L5:108:LEU:HD22	2.35	0.56
32:SP:339:LEU:O	32:SP:343:ILE:HD12	2.05	0.55
20:NL:92:ALA:O	20:NL:95:THR:OG1	2.19	0.55
32:SP:356:ASP:OD1	32:SP:357:LYS:N	2.39	0.55
1:L1:1147:A:N3	35:ST:21:GLN:NE2	2.54	0.55
16:NA:345:LEU:HD21	28:SI:932:LEU:HD23	1.88	0.55
28:SI:118:LEU:HD23	28:SI:131:ILE:HD13	1.87	0.55
1:L1:578:U:OP2	28:SI:874:TYR:OH	2.13	0.55
9:L9:55:ALA:O	9:L9:59:LEU:HD23	2.07	0.55
28:SI:65:ASP:OD1	28:SI:784:LYS:NZ	2.36	0.55
31:SM:288:ASP:OD1	31:SM:289:TYR:N	2.40	0.55
1:L1:151:G:OP2	13:LF:127:LYS:NZ	2.40	0.55
1:L1:1043:A:O3'	34:SS:384:ARG:NH2	2.40	0.55
1:L1:1502:G:N2	1:L1:1505:A:OP2	2.39	0.55
7:L7:41:LEU:HD21	7:L7:69:GLY:C	2.31	0.55
7:L7:134:GLU:N	7:L7:134:GLU:OE1	2.40	0.55
1:L1:39:A:OP1	9:L9:3:ARG:NH2	2.40	0.55
1:L1:1595:U:OP1	28:SI:945:THR:OG1	2.20	0.55
1:L1:560:U:OP2	31:SM:282:ARG:NH2	2.40	0.55
1:L1:934:C:O2	34:SS:399:LYS:NZ	2.28	0.55
4:L4:86:PHE:CE1	4:L4:87:MET:HE3	2.42	0.55
18:NF:56:ASP:OD2	23:NQ:52:THR:OG1	2.24	0.55
27:SH:305:LYS:O	27:SH:307:ASP:N	2.40	0.55
32:SP:513:ASN:ND2	32:SP:714:ASP:O	2.39	0.55
4:L4:122:LYS:NZ	4:L4:143:ASP:OD2	2.31	0.54
7:L7:159:VAL:HG23	7:L7:185:ILE:HD13	1.89	0.54
20:NL:75:LEU:HD12	20:NL:81:VAL:HG21	1.89	0.54
35:ST:743:GLN:NE2	35:ST:747:GLU:OE2	2.39	0.54
4:L4:248:ILE:HD12	9:L9:71:PHE:CD2	2.42	0.54
20:NL:78:ALA:O	20:NL:106:LYS:NZ	2.36	0.54
27:SH:289:VAL:O	27:SH:317:GLN:NE2	2.39	0.54
4:L4:103:TYR:CD2	4:L4:189:LEU:HD11	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:854:U:O4	1:L1:855:A:N6	2.41	0.54
1:L1:125:U:OP1	6:L6:201:GLN:NE2	2.37	0.54
28:SI:58:MET:HE1	28:SI:236:LYS:HG3	1.88	0.54
32:SP:864:ASP:OD1	32:SP:865:VAL:N	2.40	0.54
28:SI:975:GLU:OE1	31:SM:279:ARG:NH1	2.41	0.54
33:SR:130:VAL:HG11	33:SR:135:LEU:HD21	1.89	0.54
1:L1:31:C:OP1	33:SR:140:LYS:NZ	2.41	0.54
1:L1:221:A:OP2	1:L1:832:U:O2'	2.15	0.54
31:SM:106:GLU:O	31:SM:110:LEU:N	2.38	0.54
5:L5:71:ALA:O	5:L5:73:THR:HG23	2.08	0.54
9:L9:36:LEU:HD12	9:L9:42:ILE:HD11	1.90	0.53
32:SP:389:ILE:O	32:SP:393:PHE:N	2.41	0.53
33:SR:57:LEU:HB3	35:ST:784:ILE:HD11	1.88	0.53
28:SI:153:MET:HE2	28:SI:153:MET:HA	1.91	0.53
1:L1:358:U:OP2	24:NS:2:GLY:N	2.41	0.53
21:NM:121:ILE:HG22	21:NM:161:ILE:HG23	1.90	0.53
28:SI:867:THR:OG1	28:SI:868:ARG:NH1	2.41	0.53
6:L6:18:ILE:HG23	6:L6:23:ARG:HD2	1.90	0.53
25:NW:92:ILE:HD11	25:NW:102:THR:HG23	1.91	0.53
1:L1:960:U:O4'	18:NF:55:ARG:NH2	2.41	0.53
18:NF:83:GLU:OE1	18:NF:84:ILE:HG23	2.08	0.53
21:NM:126:THR:HG22	21:NM:136:ARG:HE	1.73	0.53
22:NP:100:ILE:O	22:NP:104:VAL:HG23	2.07	0.53
1:L1:129:U:OP1	32:SP:938:THR:HG23	2.09	0.53
10:LC:30:LYS:NZ	10:LC:33:GLY:O	2.34	0.53
24:NS:848:GLU:HA	24:NS:879:ALA:HB1	1.90	0.53
7:L7:8:ILE:HD12	7:L7:17:GLU:HG2	1.90	0.53
31:SM:123:VAL:HG12	31:SM:125:PRO:HD2	1.89	0.53
4:L4:141:THR:OG1	4:L4:143:ASP:OD1	2.27	0.53
32:SP:183:HIS:CD2	32:SP:188:LEU:HD12	2.44	0.53
8:L8:182:TYR:OH	11:LD:15:LYS:NZ	2.41	0.53
18:NF:62:GLN:N	18:NF:62:GLN:OE1	2.43	0.53
19:NG:64:ALA:HB1	19:NG:105:LEU:HD22	1.91	0.53
1:L1:1076:A:O3'	34:SS:395:ARG:NH1	2.42	0.52
12:LE:105:THR:HG23	12:LE:105:THR:O	2.08	0.52
22:NP:129:GLN:NE2	22:NP:133:ASP:OD2	2.39	0.52
13:LF:51:GLU:OE1	32:SP:36:LYS:N	2.38	0.52
23:NQ:25:VAL:O	23:NQ:25:VAL:HG13	2.10	0.52
27:SH:188:ILE:HD11	28:SI:635:PHE:HE1	1.75	0.52
6:L6:142:ARG:O	6:L6:146:GLY:N	2.43	0.52
33:SR:36:THR:O	33:SR:36:THR:HG22	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:NM:48:VAL:HG11	21:NM:61:LEU:HD21	1.92	0.52
28:SI:260:THR:HG1	28:SI:261:GLN:CD	2.16	0.52
31:SM:171:VAL:HG22	35:ST:86:ILE:HD11	1.92	0.52
1:L1:976:G:N1	1:L1:1023:A:O2'	2.33	0.51
3:L3:66:LEU:O	3:L3:70:VAL:HG23	2.10	0.51
7:L7:20:VAL:HG12	7:L7:24:PHE:HE2	1.75	0.51
20:NL:133:ILE:O	20:NL:133:ILE:HG22	2.10	0.51
3:L3:60:GLU:OE1	25:NW:41:ILE:HD13	2.10	0.51
5:L5:123:VAL:HG13	25:NW:102:THR:HG22	1.93	0.51
1:L1:1599:C:OP2	28:SI:988:ARG:NH2	2.43	0.51
7:L7:41:LEU:HD23	7:L7:70:PHE:CD2	2.46	0.51
12:LE:81:VAL:O	12:LE:122:SER:OG	2.23	0.51
16:NA:345:LEU:HD23	28:SI:1005:SER:OG	2.11	0.51
28:SI:130:ASP:OD1	28:SI:131:ILE:N	2.44	0.51
31:SM:239:VAL:CG2	35:ST:9:LEU:HD22	2.41	0.51
1:L1:2:A:N3	9:L9:17:ARG:NH2	2.59	0.51
10:LC:114:ARG:HD3	10:LC:118:ILE:HD11	1.93	0.51
30:SL:142:VAL:HG22	30:SL:164:ILE:HD11	1.93	0.51
31:SM:100:LEU:HD22	31:SM:144:GLU:CG	2.41	0.51
32:SP:562:VAL:HG23	32:SP:610:LEU:HD11	1.93	0.51
28:SI:737:ASN:O	28:SI:737:ASN:ND2	2.44	0.51
30:SL:138:ASP:OD1	30:SL:139:ASP:N	2.43	0.51
9:L9:157:ASP:OD1	9:L9:158:PHE:N	2.44	0.50
14:LG:57:MET:N	14:LG:57:MET:HE2	2.26	0.50
21:NM:82:ARG:HH21	21:NM:103:MET:HE1	1.77	0.50
18:NF:145:THR:HG22	18:NF:145:THR:O	2.10	0.50
27:SH:280:LEU:CD1	28:SI:631:ILE:HD13	2.41	0.50
4:L4:111:VAL:HG13	4:L4:111:VAL:O	2.11	0.50
23:NQ:67:THR:OG1	23:NQ:70:LYS:O	2.28	0.50
1:L1:75:U:H1'	32:SP:3:LYS:HA	1.94	0.50
1:L1:154:G:OP2	13:LF:131:ARG:NH1	2.43	0.50
2:L2:1:G:O2'	2:L2:2:U:O5'	2.21	0.50
28:SI:13:GLU:OE1	28:SI:13:GLU:N	2.45	0.50
1:L1:1473:U:C6	5:L5:190:ILE:HD11	2.46	0.50
1:L1:1096:C:OP2	12:LE:15:ASN:ND2	2.45	0.50
7:L7:159:VAL:HG22	7:L7:163:ASP:OD2	2.12	0.50
20:NL:90:MET:N	20:NL:90:MET:HE2	2.27	0.50
16:NA:408:SER:O	16:NA:412:ILE:HD12	2.12	0.50
32:SP:170:LEU:CD2	32:SP:199:LEU:HD23	2.42	0.50
32:SP:625:ILE:HD13	32:SP:642:ILE:HD13	1.94	0.50
32:SP:713:LEU:HD11	32:SP:765:ARG:NH1	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L8:11:ARG:NH1	8:L8:15:GLY:O	2.44	0.49
19:NG:136:ARG:O	37:SW:248:VAL:HG11	2.12	0.49
28:SI:33:VAL:HG11	28:SI:39:MET:CE	2.42	0.49
9:L9:109:LEU:O	9:L9:113:VAL:HG23	2.12	0.49
32:SP:113:PHE:O	32:SP:117:LEU:HD23	2.11	0.49
1:L1:113:U:O2'	1:L1:115:G:O2'	2.26	0.49
1:L1:886:U:OP2	21:NM:216:LYS:NZ	2.44	0.49
1:L1:1019:A:OP2	18:NF:107:LYS:NZ	2.38	0.49
1:L1:1480:G:OP1	22:NP:64:HIS:NE2	2.45	0.49
1:L1:1534:G:OP1	3:L3:57:ARG:NH1	2.42	0.49
12:LE:20:THR:HG22	12:LE:20:THR:O	2.11	0.49
28:SI:56:VAL:HG23	33:SR:101:GLU:HG2	1.94	0.49
1:L1:332:U:OP2	8:L8:175:GLN:NE2	2.43	0.49
1:L1:1066:C:O2'	21:NM:148:ASN:OD1	2.20	0.49
1:L1:1484:G:N2	1:L1:1606:C:O2	2.44	0.49
21:NM:180:THR:OG1	21:NM:183:GLN:OE1	2.21	0.49
27:SH:47:ASP:OD1	27:SH:48:TYR:N	2.46	0.49
27:SH:280:LEU:HD11	28:SI:631:ILE:HD13	1.94	0.49
28:SI:118:LEU:HD23	28:SI:131:ILE:CD1	2.42	0.49
30:SL:142:VAL:HG22	30:SL:164:ILE:CD1	2.42	0.49
32:SP:636:ARG:O	32:SP:640:ILE:HD12	2.12	0.49
37:SW:131:ASN:O	37:SW:135:LYS:N	2.45	0.49
1:L1:153:G:H21	6:L6:56:ASN:HD21	1.61	0.49
1:L1:909:U:H5''	24:NS:139:THR:HG21	1.95	0.49
19:NG:48:VAL:HG11	19:NG:53:ASP:HB2	1.94	0.49
30:SL:86:MET:HG2	30:SL:173:MET:HE1	1.93	0.49
13:LF:121:THR:HG21	13:LF:123:LYS:HE3	1.93	0.49
1:L1:738:G:O2'	1:L1:739:G:OP1	2.31	0.48
28:SI:993:ASP:OD1	28:SI:994:LYS:N	2.46	0.48
32:SP:240:MET:HE1	32:SP:254:ILE:HB	1.95	0.48
32:SP:358:VAL:HG12	32:SP:389:ILE:HD11	1.95	0.48
32:SP:374:LEU:O	32:SP:378:HIS:N	2.46	0.48
37:SW:111:ASN:O	37:SW:111:ASN:ND2	2.46	0.48
20:NL:254:ASN:ND2	20:NL:317:PHE:O	2.46	0.48
22:NP:18:TYR:O	22:NP:22:LEU:HD23	2.13	0.48
1:L1:332:U:OP1	8:L8:31:ARG:NH1	2.41	0.48
32:SP:725:ASN:OD1	32:SP:726:LYS:N	2.45	0.48
35:ST:25:LYS:O	35:ST:26:SER:OG	2.23	0.48
3:L3:72:ILE:HD13	3:L3:79:TYR:CD2	2.48	0.48
17:NB:538:ARG:N	28:SI:149:GLU:OE2	2.45	0.48
10:LC:49:TYR:HB3	10:LC:53:LEU:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:1584:G:H22	1:L1:1611:A:P	2.37	0.48
4:L4:248:ILE:HD12	9:L9:71:PHE:HD2	1.79	0.48
6:L6:78:THR:O	6:L6:81:VAL:HG22	2.13	0.48
20:NL:76:GLU:OE1	20:NL:77:GLN:NE2	2.47	0.48
32:SP:311:ILE:HD11	32:SP:343:ILE:HG23	1.95	0.48
32:SP:394:LEU:HD21	32:SP:435:PHE:CB	2.44	0.48
35:ST:105:MET:HE2	35:ST:105:MET:HA	1.95	0.48
1:L1:1230:A:N3	1:L1:1258:U:N3	2.61	0.48
8:L8:153:GLU:OE1	8:L8:153:GLU:N	2.45	0.48
10:LC:90:VAL:HG21	10:LC:117:LEU:HD11	1.96	0.48
32:SP:701:LEU:HD21	32:SP:795:ASP:HB3	1.95	0.48
3:L3:70:VAL:HA	3:L3:73:MET:SD	2.54	0.48
9:L9:139:GLN:HE21	9:L9:139:GLN:HB3	1.50	0.48
20:NL:71:THR:O	20:NL:75:LEU:HD13	2.13	0.48
20:NL:196:PHE:O	20:NL:197:ARG:NE	2.43	0.48
32:SP:476:LEU:CB	32:SP:518:MET:HE1	2.44	0.48
5:L5:123:VAL:HG21	25:NW:100:ILE:HD11	1.94	0.48
6:L6:7:TYR:HD2	6:L6:10:ASN:HD22	1.61	0.48
8:L8:6:ASP:OD1	8:L8:9:HIS:ND1	2.41	0.48
35:ST:615:PRO:HA	36:SU:551:ALA:HB3	1.96	0.48
3:L3:46:VAL:HG13	3:L3:72:ILE:HG21	1.95	0.48
4:L4:61:VAL:O	4:L4:65:LEU:HD23	2.14	0.48
5:L5:68:ILE:HD12	10:LC:112:TYR:OH	2.14	0.48
5:L5:194:LEU:O	5:L5:198:LEU:HD23	2.14	0.48
27:SH:348:GLU:N	27:SH:348:GLU:OE1	2.47	0.48
7:L7:185:ILE:HG23	7:L7:185:ILE:O	2.14	0.47
30:SL:68:ASP:OD1	30:SL:69:THR:N	2.47	0.47
32:SP:641:ARG:O	32:SP:645:VAL:HG22	2.14	0.47
20:NL:284:VAL:CG1	20:NL:313:VAL:HG21	2.44	0.47
32:SP:165:PHE:O	32:SP:169:LYS:NZ	2.33	0.47
21:NM:181:LEU:HD23	21:NM:181:LEU:C	2.39	0.47
1:L1:512:A:O2'	9:L9:133:HIS:NE2	2.36	0.47
1:L1:1584:G:O2'	1:L1:1585:U:OP2	2.30	0.47
2:L2:0:M7G:H82	2:L2:1:G:O4'	2.14	0.47
1:L1:129:U:O4'	1:L1:264:G:N1	2.48	0.47
27:SH:312:ARG:HG3	27:SH:351:ILE:HD13	1.96	0.47
1:L1:1126:G:N7	24:NS:107:ARG:NH1	2.63	0.47
1:L1:1492:A:O2'	1:L1:1493:A:O5'	2.32	0.47
4:L4:85:GLY:N	4:L4:88:ASP:OD2	2.45	0.47
7:L7:75:THR:O	7:L7:78:THR:HG22	2.15	0.47
24:NS:1033:LYS:O	24:NS:1036:GLU:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:SH:223:VAL:HG23	27:SH:223:VAL:O	2.14	0.47
33:SR:90:ASP:OD1	33:SR:91:GLY:N	2.48	0.47
1:L1:522:U:O2'	13:LF:60:PHE:O	2.33	0.47
28:SI:557:ASN:OD1	28:SI:558:ILE:N	2.48	0.47
1:L1:705:U:HO2'	1:L1:706:A:H8	1.62	0.47
9:L9:101:VAL:HG12	9:L9:105:LEU:HD23	1.97	0.47
27:SH:19:LEU:HD22	28:SI:608:LEU:HD22	1.96	0.47
30:SL:142:VAL:HG11	30:SL:163:ARG:NH1	2.30	0.47
31:SM:134:SER:OG	31:SM:136:THR:HG23	2.15	0.47
32:SP:938:THR:O	32:SP:943:ARG:NH1	2.48	0.47
37:SW:168:LEU:O	37:SW:171:SER:OG	2.29	0.47
4:L4:116:ASP:OD1	4:L4:117:GLU:N	2.48	0.47
7:L7:64:VAL:HG23	7:L7:65:PRO:HD3	1.97	0.47
28:SI:229:VAL:O	28:SI:229:VAL:HG22	2.15	0.47
18:NF:87:ASP:OD1	18:NF:87:ASP:N	2.47	0.46
20:NL:59:VAL:HG23	20:NL:80:ASN:OD1	2.13	0.46
20:NL:75:LEU:HD21	20:NL:107:LEU:HB2	1.97	0.46
32:SP:793:PHE:HA	32:SP:796:ILE:HG22	1.97	0.46
32:SP:919:LYS:HD3	32:SP:919:LYS:N	2.30	0.46
1:L1:168:A:OP1	6:L6:140:ASN:ND2	2.43	0.46
1:L1:501:U:O2'	1:L1:502:U:OP2	2.25	0.46
28:SI:310:THR:HG23	28:SI:313:TYR:H	1.80	0.46
5:L5:163:SER:OG	14:LG:47:PRO:O	2.26	0.46
12:LE:83:ILE:HD12	12:LE:83:ILE:H	1.80	0.46
27:SH:45:LEU:CD2	27:SH:50:VAL:HG22	2.45	0.46
32:SP:870:LEU:HD13	32:SP:892:LEU:HD11	1.97	0.46
34:SS:383:MET:N	34:SS:383:MET:HE2	2.30	0.46
1:L1:1082:C:HO2'	1:L1:1083:G:P	2.36	0.46
1:L1:1801:A:OP1	21:NM:115:ARG:NH2	2.49	0.46
9:L9:59:LEU:HD11	9:L9:72:GLU:HB2	1.97	0.46
19:NG:92:LYS:O	19:NG:119:THR:HG21	2.16	0.46
31:SM:260:GLU:OE2	31:SM:262:ARG:HG3	2.15	0.46
1:L1:75:U:O2'	32:SP:3:LYS:O	2.33	0.46
1:L1:1488:G:H3'	1:L1:1515:A:H61	1.81	0.46
16:NA:313:GLN:NE2	16:NA:317:GLU:OE2	2.43	0.46
18:NF:56:ASP:OD1	23:NQ:50:ALA:HB1	2.15	0.46
1:L1:628:G:OP1	18:NF:124:ARG:NH1	2.49	0.46
9:L9:59:LEU:HD12	9:L9:69:ARG:HA	1.98	0.46
32:SP:496:ILE:HD12	32:SP:496:ILE:H	1.81	0.46
34:SS:440:MET:HE3	34:SS:440:MET:O	2.16	0.46
1:L1:1502:G:N7	22:NP:102:ARG:NH2	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:SP:308:ALA:O	32:SP:311:ILE:HG22	2.15	0.46
32:SP:512:ASP:OD1	32:SP:515:THR:HG23	2.15	0.46
12:LE:83:ILE:O	12:LE:86:ILE:HG22	2.16	0.46
28:SI:72:VAL:HG21	28:SI:115:LEU:HD23	1.98	0.46
32:SP:370:ASP:OD1	32:SP:370:ASP:N	2.47	0.46
32:SP:651:LYS:HG3	32:SP:652:THR:HG23	1.98	0.46
1:L1:1096:C:O4'	12:LE:19:LYS:HE3	2.16	0.46
31:SM:238:TYR:O	31:SM:239:VAL:HG23	2.16	0.46
18:NF:99:ARG:NH2	18:NF:143:SER:OG	2.49	0.46
27:SH:301:MET:HE1	27:SH:311:LEU:HD13	1.98	0.46
3:L3:117:LYS:O	3:L3:117:LYS:NZ	2.45	0.45
21:NM:210:ILE:HD12	21:NM:210:ILE:H	1.81	0.45
32:SP:464:PHE:O	32:SP:468:ALA:HB2	2.15	0.45
5:L5:123:VAL:HG13	25:NW:102:THR:CG2	2.46	0.45
21:NM:184:LEU:O	21:NM:188:LEU:HD23	2.16	0.45
32:SP:512:ASP:O	32:SP:515:THR:OG1	2.33	0.45
6:L6:145:PHE:HZ	6:L6:158:ILE:HD11	1.82	0.45
28:SI:90:VAL:O	28:SI:94:THR:OG1	2.32	0.45
28:SI:200:GLN:OE1	28:SI:200:GLN:N	2.46	0.45
32:SP:323:PHE:HB2	32:SP:364:LEU:HD13	1.97	0.45
32:SP:476:LEU:HB3	32:SP:518:MET:HE1	1.98	0.45
4:L4:222:LEU:O	4:L4:222:LEU:HD23	2.16	0.45
4:L4:251:GLU:OE2	4:L4:255:ARG:NH1	2.49	0.45
13:LF:40:LEU:HD12	13:LF:60:PHE:CE2	2.51	0.45
32:SP:84:ASP:OD1	32:SP:85:LYS:N	2.49	0.45
32:SP:517:ASP:OD1	32:SP:553:ASN:ND2	2.49	0.45
4:L4:86:PHE:CZ	4:L4:87:MET:HE3	2.52	0.45
22:NP:125:SER:O	22:NP:129:GLN:N	2.44	0.45
26:SG:77:GLU:OE2	26:SG:120:ARG:NE	2.50	0.45
30:SL:172:LEU:HD23	30:SL:173:MET:N	2.31	0.45
32:SP:446:GLN:OE1	32:SP:449:ARG:NH2	2.46	0.45
8:L8:111:GLN:NE2	32:SP:955:ASN:OD1	2.43	0.45
28:SI:118:LEU:HD21	28:SI:809:PRO:HB3	1.97	0.45
1:L1:1057:U:C4'	21:NM:202:LYS:HZ1	2.30	0.45
7:L7:63:PRO:O	7:L7:67:LEU:N	2.49	0.45
8:L8:70:GLU:OE1	8:L8:70:GLU:N	2.50	0.45
21:NM:57:ALA:O	21:NM:61:LEU:HD23	2.17	0.45
28:SI:127:ALA:O	28:SI:131:ILE:HG22	2.17	0.45
32:SP:229:TYR:OH	32:SP:277:ASP:OD2	2.24	0.45
10:LC:10:PHE:CE2	10:LC:19:VAL:HG13	2.51	0.45
1:L1:392:G:H21	24:NS:59:ASN:HD21	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:647:G:N2	1:L1:687:G:H22	2.15	0.45
9:L9:42:ILE:HD12	9:L9:42:ILE:H	1.82	0.45
12:LE:106:THR:HG21	12:LE:121:VAL:HG21	1.98	0.45
32:SP:375:THR:O	32:SP:378:HIS:ND1	2.48	0.45
1:L1:68:A:OP1	6:L6:160:ARG:NH2	2.48	0.44
6:L6:23:ARG:O	6:L6:26:VAL:HG12	2.17	0.44
26:SG:70:TYR:CZ	26:SG:74:LEU:HD11	2.52	0.44
28:SI:99:ASN:OD1	28:SI:100:ASP:N	2.50	0.44
30:SL:68:ASP:OD1	34:SS:439:ARG:NH2	2.50	0.44
31:SM:272:ASP:OD2	31:SM:273:VAL:N	2.50	0.44
1:L1:512:A:OP1	9:L9:170:GLY:N	2.42	0.44
1:L1:1192:C:O2'	1:L1:1194:A:N6	2.49	0.44
31:SM:132:LYS:NZ	31:SM:158:PRO:O	2.49	0.44
37:SW:204:ARG:NH1	37:SW:250:LEU:O	2.50	0.44
6:L6:18:ILE:HG21	6:L6:24:ILE:HD11	1.99	0.44
8:L8:60:ILE:HD12	8:L8:179:CYS:HB2	2.00	0.44
8:L8:72:ILE:HG22	8:L8:73:SER:N	2.32	0.44
1:L1:126:A:C2'	6:L6:194:LYS:HZ3	2.25	0.44
1:L1:1802:A:OP1	21:NM:115:ARG:NH1	2.50	0.44
6:L6:32:ILE:HD11	6:L6:63:MET:HE2	1.99	0.44
7:L7:73:VAL:HG13	7:L7:77:LEU:CD1	2.47	0.44
27:SH:313:ILE:HD11	27:SH:339:LEU:HD22	1.99	0.44
1:L1:1463:C:O3'	35:ST:83:LYS:NZ	2.51	0.44
19:NG:22:SER:OG	19:NG:23:PHE:N	2.51	0.44
27:SH:105:TYR:CE2	27:SH:296:LEU:HD12	2.52	0.44
1:L1:768:C:C2	9:L9:143:ILE:HD13	2.52	0.44
3:L3:28:ILE:CD1	3:L3:61:LEU:HD11	2.44	0.44
9:L9:169:PRO:O	9:L9:174:ARG:NH1	2.50	0.44
12:LE:106:THR:HG21	12:LE:121:VAL:CG2	2.48	0.44
20:NL:256:LYS:HG2	20:NL:273:MET:HE1	1.99	0.44
32:SP:537:LEU:HD23	32:SP:561:LEU:CD1	2.48	0.44
14:LG:60:GLU:N	14:LG:60:GLU:OE2	2.50	0.44
19:NG:93:THR:HG21	37:SW:184:THR:HB	2.00	0.44
19:NG:112:ILE:CG2	19:NG:115:ILE:HD11	2.48	0.44
32:SP:255:MET:HE3	32:SP:259:LEU:HB2	2.00	0.44
3:L3:46:VAL:HG13	3:L3:72:ILE:CG2	2.48	0.44
7:L7:90:VAL:O	7:L7:90:VAL:HG13	2.17	0.44
31:SM:273:VAL:HG13	31:SM:273:VAL:O	2.17	0.44
32:SP:55:LYS:NZ	32:SP:71:GLU:OE2	2.36	0.44
8:L8:29:LEU:C	8:L8:29:LEU:HD12	2.43	0.43
20:NL:255:TYR:CZ	20:NL:259:LEU:HD11	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:SI:241:HIS:C	28:SI:278:THR:HG22	2.42	0.43
6:L6:32:ILE:HD12	6:L6:32:ILE:H	1.84	0.43
24:NS:83:THR:HG23	24:NS:83:THR:O	2.18	0.43
1:L1:65:A:N6	1:L1:84:A:OP2	2.51	0.43
5:L5:33:VAL:CG1	10:LC:53:LEU:HD11	2.48	0.43
6:L6:122:GLU:OE2	6:L6:122:GLU:N	2.48	0.43
27:SH:23:LEU:HD11	27:SH:329:ILE:HD13	1.99	0.43
28:SI:260:THR:OG1	28:SI:261:GLN:OE1	2.29	0.43
28:SI:958:VAL:CG1	28:SI:979:ALA:HB2	2.49	0.43
31:SM:224:PHE:HE1	31:SM:233:VAL:HG13	1.82	0.43
32:SP:913:ILE:HD12	32:SP:913:ILE:H	1.82	0.43
35:ST:781:MET:HE2	35:ST:781:MET:HA	1.99	0.43
1:L1:612:U:OP2	1:L1:613:G:O2'	2.32	0.43
1:L1:1801:A:N7	37:SW:107:THR:OG1	2.51	0.43
5:L5:175:LEU:HD23	5:L5:197:GLU:OE2	2.18	0.43
20:NL:37:HIS:ND1	20:NL:198:PRO:O	2.51	0.43
28:SI:944:ASN:ND2	28:SI:991:PHE:O	2.51	0.43
1:L1:68:A:OP1	6:L6:160:ARG:NH1	2.48	0.43
1:L1:610:G:HO2'	1:L1:613:G:HO2'	1.63	0.43
1:L1:820:U:O2'	1:L1:821:U:O5'	2.37	0.43
4:L4:36:HIS:HE2	4:L4:88:ASP:CG	2.26	0.43
31:SM:100:LEU:HD22	31:SM:144:GLU:HG2	1.99	0.43
21:NM:150:VAL:O	34:SS:384:ARG:NH1	2.52	0.43
31:SM:162:THR:OG1	31:SM:264:GLY:O	2.26	0.43
32:SP:70:ILE:O	32:SP:70:ILE:HG22	2.17	0.43
32:SP:146:ASN:OD1	32:SP:150:TRP:NE1	2.52	0.43
7:L7:60:ILE:HD11	7:L7:90:VAL:HG23	2.00	0.43
9:L9:57:ARG:NH2	30:SL:88:ASP:OD2	2.50	0.43
10:LC:48:VAL:CG2	10:LC:78:VAL:HG13	2.49	0.43
32:SP:360:PHE:CE2	32:SP:364:LEU:HD11	2.54	0.43
32:SP:562:VAL:HG21	32:SP:607:LEU:HD23	2.01	0.43
32:SP:728:LEU:HB2	32:SP:740:ILE:HG23	2.00	0.43
22:NP:18:TYR:CZ	22:NP:22:LEU:HD21	2.54	0.43
22:NP:116:ILE:HD12	22:NP:116:ILE:H	1.83	0.43
32:SP:56:GLU:OE1	32:SP:56:GLU:HA	2.19	0.43
1:L1:1598:U:OP2	28:SI:977:LYS:NZ	2.49	0.43
4:L4:212:ASP:OD1	4:L4:213:SER:N	2.49	0.43
5:L5:136:ALA:O	5:L5:140:THR:HG22	2.19	0.43
1:L1:919:A:N3	19:NG:36:LYS:NZ	2.67	0.42
7:L7:26:GLU:OE1	7:L7:84:LYS:NZ	2.52	0.42
7:L7:73:VAL:HG13	7:L7:77:LEU:HD13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:NA:308:ARG:HA	16:NA:311:ILE:HG22	2.01	0.42
12:LE:30:SER:OG	12:LE:58:SER:O	2.36	0.42
21:NM:203:ASP:OD1	21:NM:204:ILE:N	2.52	0.42
27:SH:301:MET:HE1	27:SH:311:LEU:HB2	2.01	0.42
28:SI:157:ASN:O	28:SI:161:HIS:ND1	2.53	0.42
2:L2:0:M7G:HN22	24:NS:96:ARG:HH12	1.66	0.42
7:L7:38:LEU:CD1	7:L7:77:LEU:HD21	2.49	0.42
10:LC:28:LEU:HD21	10:LC:30:LYS:CD	2.49	0.42
20:NL:181:MET:HG3	20:NL:223:TRP:NE1	2.34	0.42
24:NS:98:ASP:O	24:NS:102:GLU:OE1	2.37	0.42
27:SH:32:LYS:HD2	27:SH:75:ILE:HD11	2.01	0.42
20:NL:86:MET:SD	20:NL:86:MET:N	2.87	0.42
5:L5:97:LEU:O	5:L5:180:ARG:NH2	2.53	0.42
19:NG:101:ALA:O	19:NG:105:LEU:HD23	2.20	0.42
24:NS:57:ASN:OD1	24:NS:57:ASN:O	2.38	0.42
27:SH:19:LEU:HD21	27:SH:325:LEU:HD12	2.02	0.42
27:SH:281:GLU:CG	28:SI:621:LEU:HD22	2.49	0.42
27:SH:312:ARG:NH2	27:SH:347:ASN:OD1	2.51	0.42
1:L1:1530:C:O5'	25:NW:96:SER:OG	2.37	0.42
5:L5:92:ARG:NH2	5:L5:169:ASN:OD1	2.46	0.42
6:L6:128:THR:HG21	32:SP:637:ASP:OD1	2.19	0.42
3:L3:45:LEU:HD13	22:NP:36:ILE:HG22	2.02	0.42
13:LF:72:PHE:CE2	13:LF:74:LEU:HD21	2.54	0.42
27:SH:60:THR:OG1	27:SH:80:ILE:O	2.18	0.42
37:SW:117:TYR:N	37:SW:118:PRO:CD	2.83	0.42
1:L1:352:A:P	33:SR:13:ARG:HH22	2.43	0.42
32:SP:360:PHE:CD1	32:SP:728:LEU:HD13	2.54	0.42
32:SP:585:LEU:HB3	32:SP:604:MET:HE1	2.01	0.42
28:SI:823:GLY:CA	28:SI:889:LEU:HD21	2.49	0.42
35:ST:283:ALA:HB3	38:SZ:382:LEU:O	2.19	0.42
1:L1:1178:G:N7	35:ST:753:LYS:NZ	2.64	0.42
1:L1:1480:G:H5''	22:NP:63:ARG:HH22	1.85	0.42
3:L3:42:TYR:O	3:L3:46:VAL:HG23	2.20	0.42
11:LD:119:VAL:O	11:LD:119:VAL:HG13	2.20	0.42
16:NA:369:ILE:HD11	31:SM:223:THR:HG21	2.02	0.42
18:NF:135:LEU:HD21	18:NF:139:TRP:CD2	2.55	0.42
1:L1:9:U:O2'	1:L1:11:A:OP2	2.24	0.41
1:L1:1524:A:N3	1:L1:1590:G:O2'	2.48	0.41
5:L5:90:ILE:O	5:L5:94:THR:HG23	2.20	0.41
28:SI:826:LYS:HZ2	28:SI:926:ILE:HD13	1.85	0.41
32:SP:640:ILE:HD12	32:SP:640:ILE:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:SP:897:PHE:CZ	32:SP:901:ILE:HD11	2.54	0.41
8:L8:93:THR:HG22	8:L8:93:THR:O	2.19	0.41
32:SP:550:GLU:OE1	32:SP:591:LEU:HD21	2.20	0.41
7:L7:15:GLU:HG2	7:L7:16:LEU:HD12	2.02	0.41
10:LC:40:GLU:N	10:LC:40:GLU:OE1	2.53	0.41
22:NP:135:ILE:O	22:NP:139:THR:HG23	2.20	0.41
6:L6:20:ASP:OD2	6:L6:21:GLU:N	2.52	0.41
20:NL:316:HIS:NE2	24:NS:120:TYR:OH	2.44	0.41
32:SP:728:LEU:HD12	32:SP:740:ILE:HG12	2.02	0.41
6:L6:5:ILE:HD12	6:L6:16:PHE:CD2	2.55	0.41
10:LC:97:VAL:HG12	10:LC:98:ASP:N	2.36	0.41
1:L1:1568:C:O2'	1:L1:1569:A:P	2.78	0.41
18:NF:132:VAL:HG12	18:NF:132:VAL:O	2.21	0.41
27:SH:180:MET:CB	27:SH:301:MET:HE2	2.51	0.41
30:SL:73:ASN:HB2	34:SS:440:MET:HE2	2.02	0.41
37:SW:106:MET:O	37:SW:109:LEU:HB3	2.20	0.41
1:L1:251:A:C2	4:L4:131:LEU:HD12	2.56	0.41
2:L2:0:M7G:H82	2:L2:1:G:C1'	2.51	0.41
10:LC:10:PHE:HE2	10:LC:19:VAL:HG13	1.86	0.41
32:SP:233:LEU:O	32:SP:237:THR:HG22	2.21	0.41
32:SP:264:THR:HG22	32:SP:266:SER:H	1.85	0.41
32:SP:461:ILE:HG13	32:SP:486:PHE:CE1	2.55	0.41
32:SP:567:PRO:HA	32:SP:571:LEU:HD12	2.01	0.41
35:ST:104:MET:C	35:ST:105:MET:HE2	2.46	0.41
1:L1:351:C:OP1	1:L1:630:A:O2'	2.29	0.41
1:L1:609:U:O2	33:SR:19:ARG:NH1	2.54	0.41
1:L1:788:A:C4	4:L4:19:LEU:HD23	2.55	0.41
8:L8:102:VAL:HG21	8:L8:169:ILE:HD11	2.02	0.41
19:NG:112:ILE:HG21	19:NG:115:ILE:HD11	2.03	0.41
32:SP:628:ILE:HB	32:SP:638:LEU:HD21	2.03	0.41
1:L1:1057:U:H3'	1:L1:1058:U:H5''	2.03	0.41
1:L1:1124:A:N1	2:L2:0:M7G:HM72	2.35	0.41
1:L1:1801:A:C2	37:SW:106:MET:HE1	2.56	0.41
21:NM:20:VAL:HG23	21:NM:21:VAL:HG23	2.02	0.41
22:NP:15:ILE:HD12	22:NP:60:SER:HA	2.02	0.41
24:NS:114:ILE:HG22	24:NS:118:GLN:HE22	1.86	0.41
28:SI:115:LEU:HD21	28:SI:227:ILE:HG21	2.02	0.41
28:SI:838:ILE:HD12	28:SI:874:TYR:HB3	2.03	0.41
29:SK:46:ALA:N	29:SK:206:VAL:O	2.54	0.41
31:SM:89:ILE:CD1	31:SM:136:THR:HG21	2.51	0.41
32:SP:369:SER:O	32:SP:407:ARG:NH2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:241:U:H2'	1:L1:242:U:C6	2.56	0.41
7:L7:37:GLU:O	7:L7:41:LEU:HD13	2.21	0.41
7:L7:67:LEU:HD22	7:L7:94:ALA:HB2	2.02	0.41
20:NL:181:MET:HE1	20:NL:300:GLN:CG	2.50	0.41
25:NW:54:VAL:HG12	25:NW:55:PRO:HD3	2.02	0.41
32:SP:353:LEU:O	32:SP:355:GLN:NE2	2.54	0.41
1:L1:931:C:O2'	21:NM:118:GLN:O	2.36	0.40
27:SH:185:ARG:HG3	27:SH:312:ARG:NH1	2.35	0.40
30:SL:82:ILE:HG23	30:SL:83:VAL:N	2.37	0.40
32:SP:394:LEU:HD21	32:SP:435:PHE:HB3	2.02	0.40
1:L1:277:U:HO2'	1:L1:278:U:P	2.40	0.40
1:L1:738:G:O2'	1:L1:739:G:P	2.79	0.40
1:L1:1080:U:O2'	1:L1:1082:C:OP1	2.20	0.40
1:L1:1525:A:H2'	1:L1:1526:A:O4'	2.21	0.40
5:L5:95:ASN:OD1	5:L5:107:LYS:NZ	2.48	0.40
6:L6:23:ARG:HA	6:L6:26:VAL:HG12	2.03	0.40
28:SI:92:ARG:HD3	28:SI:221:LEU:HD23	2.03	0.40
3:L3:69:ILE:HG22	3:L3:73:MET:CE	2.51	0.40
9:L9:129:ILE:HD13	9:L9:134:ILE:HB	2.03	0.40
12:LE:112:ASP:OD2	12:LE:114:GLU:HG2	2.22	0.40
24:NS:1117:TYR:O	24:NS:1133:VAL:N	2.51	0.40
21:NM:91:VAL:HG12	21:NM:96:LEU:HD23	2.03	0.40
26:SG:70:TYR:O	26:SG:74:LEU:HD13	2.22	0.40
27:SH:180:MET:HB3	27:SH:301:MET:HE2	2.03	0.40
28:SI:207:LEU:HD23	28:SI:219:GLU:HG3	2.02	0.40
31:SM:173:ARG:HE	31:SM:179:ALA:HB1	1.86	0.40
32:SP:850:LEU:HD23	32:SP:854:LEU:HD13	2.04	0.40
33:SR:68:ILE:HD12	33:SR:68:ILE:H	1.86	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	L3	96/146 (66%)	93 (97%)	3 (3%)	0	100	100
4	L4	256/261 (98%)	252 (98%)	4 (2%)	0	100	100
5	L5	193/225 (86%)	189 (98%)	4 (2%)	0	100	100
6	L6	225/236 (95%)	223 (99%)	2 (1%)	0	100	100
7	L7	184/190 (97%)	177 (96%)	7 (4%)	0	100	100
8	L8	177/200 (88%)	175 (99%)	2 (1%)	0	100	100
9	L9	179/197 (91%)	177 (99%)	2 (1%)	0	100	100
10	LC	118/143 (82%)	117 (99%)	1 (1%)	0	100	100
11	LD	136/156 (87%)	132 (97%)	4 (3%)	0	100	100
12	LE	127/130 (98%)	124 (98%)	3 (2%)	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	106/593 (18%)	106 (100%)	0	0	100	100
17	NB	50/610 (8%)	50 (100%)	0	0	100	100
18	NF	148/151 (98%)	145 (98%)	3 (2%)	0	100	100
19	NG	125/137 (91%)	121 (97%)	4 (3%)	0	100	100
20	NL	281/318 (88%)	277 (99%)	4 (1%)	0	100	100
21	NM	207/255 (81%)	204 (99%)	3 (1%)	0	100	100
22	NP	130/144 (90%)	128 (98%)	2 (2%)	0	100	100
23	NQ	77/82 (94%)	76 (99%)	1 (1%)	0	100	100
24	NS	877/1267 (69%)	869 (99%)	8 (1%)	0	100	100
25	NW	67/108 (62%)	66 (98%)	1 (2%)	0	100	100
26	SG	29/573 (5%)	29 (100%)	0	0	100	100
27	SH	358/367 (98%)	352 (98%)	6 (2%)	0	100	100
28	SI	696/1183 (59%)	680 (98%)	16 (2%)	0	100	100
29	SJ	207/252 (82%)	204 (99%)	3 (1%)	0	100	100
29	SK	225/252 (89%)	220 (98%)	5 (2%)	0	100	100
30	SL	140/189 (74%)	134 (96%)	6 (4%)	0	100	100
31	SM	217/290 (75%)	212 (98%)	5 (2%)	0	100	100
32	SP	935/2493 (38%)	918 (98%)	17 (2%)	0	100	100
33	SR	130/145 (90%)	129 (99%)	1 (1%)	0	100	100
34	SS	142/899 (16%)	137 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	ST	555/810 (68%)	551 (99%)	4 (1%)	0	100	100
36	SU	524/552 (95%)	522 (100%)	2 (0%)	0	100	100
37	SW	180/274 (66%)	177 (98%)	3 (2%)	0	100	100
38	SZ	255/483 (53%)	250 (98%)	5 (2%)	0	100	100
All	All	8540/14513 (59%)	8401 (98%)	139 (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%)	155 (99%)	1 (1%)	78	80
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%)	108 (99%)	1 (1%)	70	75
14	LG	55/60 (92%)	55 (100%)	0	100	100
16	NA	103/535 (19%)	103 (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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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	160/1140 (14%)	160 (100%)	0	100	100
25	NW	60/89 (67%)	60 (100%)	0	100	100
26	SG	29/503 (6%)	29 (100%)	0	100	100
27	SH	307/312 (98%)	307 (100%)	0	100	100
28	SI	621/1039 (60%)	621 (100%)	0	100	100
29	SJ	9/222 (4%)	9 (100%)	0	100	100
29	SK	12/222 (5%)	12 (100%)	0	100	100
30	SL	125/169 (74%)	125 (100%)	0	100	100
31	SM	194/258 (75%)	194 (100%)	0	100	100
32	SP	881/2307 (38%)	881 (100%)	0	100	100
33	SR	113/120 (94%)	113 (100%)	0	100	100
34	SS	108/807 (13%)	108 (100%)	0	100	100
35	ST	132/732 (18%)	132 (100%)	0	100	100
36	SU	27/506 (5%)	27 (100%)	0	100	100
37	SW	159/238 (67%)	159 (100%)	0	100	100
38	SZ	14/424 (3%)	14 (100%)	0	100	100
All	All	5586/12868 (43%)	5584 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	L9	139	GLN
13	LF	34	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
4	L4	69	HIS
4	L4	142	HIS
4	L4	197	HIS
5	L5	224	ASN

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Mol	Chain	Res	Type
6	L6	22	HIS
12	LE	12	ASN
13	LF	29	HIS
13	LF	63	GLN
17	NB	573	GLN
18	NF	123	HIS
20	NL	46	GLN
21	NM	124	ASN
21	NM	232	HIS
22	NP	25	GLN
22	NP	43	ASN
22	NP	93	HIS
23	NQ	9	HIS
23	NQ	51	GLN
24	NS	16	HIS
24	NS	104	GLN
24	NS	138	GLN
27	SH	88	HIS
28	SI	24	GLN
28	SI	112	HIS
28	SI	157	ASN
28	SI	776	GLN
28	SI	882	ASN
28	SI	904	ASN
28	SI	986	HIS
28	SI	1037	GLN
31	SM	102	GLN
31	SM	174	HIS
32	SP	46	HIS
32	SP	89	ASN
32	SP	183	HIS
32	SP	577	HIS
32	SP	614	GLN
32	SP	745	HIS
32	SP	802	ASN
32	SP	840	ASN
32	SP	887	ASN
33	SR	94	ASN
34	SS	416	ASN
34	SS	444	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L1	1385/1803 (76%)	280 (20%)	9 (0%)
15	N2	4/5 (80%)	2 (50%)	0
2	L2	21/334 (6%)	6 (28%)	0
All	All	1410/2142 (65%)	288 (20%)	9 (0%)

All (288) 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	60	U
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	179	A
1	L1	194	U
1	L1	195	G
1	L1	199	G
1	L1	205	U
1	L1	215	A
1	L1	216	U

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Mol	Chain	Res	Type
1	L1	217	A
1	L1	232	U
1	L1	233	C
1	L1	234	G
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	314	C
1	L1	316	A
1	L1	322	G
1	L1	333	A
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	411	C
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

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Mol	Chain	Res	Type
1	L1	459	G
1	L1	460	A
1	L1	467	G
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	520	A
1	L1	532	U
1	L1	534	A
1	L1	542	A
1	L1	545	A
1	L1	562	G
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	629	U
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

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Mol	Chain	Res	Type
1	L1	743	U
1	L1	765	G
1	L1	766	U
1	L1	767	U
1	L1	774	A
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	903	U
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	960	U
1	L1	962	C
1	L1	966	A
1	L1	969	C
1	L1	973	A
1	L1	992	A
1	L1	1005	A

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Mol	Chain	Res	Type
1	L1	1007	C
1	L1	1011	G
1	L1	1020	A
1	L1	1026	A
1	L1	1028	C
1	L1	1029	U
1	L1	1030	A
1	L1	1032	G
1	L1	1043	A
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	1081	A
1	L1	1083	G
1	L1	1092	A
1	L1	1096	C
1	L1	1097	U
1	L1	1098	U
1	L1	1099	U
1	L1	1100	G
1	L1	1109	G
1	L1	1114	G
1	L1	1119	G
1	L1	1122	G
1	L1	1128	C
1	L1	1129	U
1	L1	1131	A
1	L1	1158	C
1	L1	1159	C
1	L1	1160	A
1	L1	1166	A
1	L1	1167	G
1	L1	1179	G
1	L1	1189	A
1	L1	1191	U
1	L1	1192	C

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Mol	Chain	Res	Type
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
1	L1	1256	A
1	L1	1267	G
1	L1	1268	G
1	L1	1269	U
1	L1	1270	G
1	L1	1436	A
1	L1	1437	U
1	L1	1438	G
1	L1	1440	C
1	L1	1465	C
1	L1	1471	A
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	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

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Mol	Chain	Res	Type
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
1	L1	1602	C
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	14	A
2	L2	15	U
2	L2	16	A
15	N2	7	U

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Mol	Chain	Res	Type
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
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	$\# Z > 2$
34	SEP	SS	423	34	8,9,10	1.62	1 (12%)	7,12,14	1.45	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
34	SEP	SS	423	34	-	4/6/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	SS	423	SEP	P-O1P	3.53	1.61	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	SS	423	SEP	OG-CB-CA	3.23	111.28	108.14

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	SS	423	SEP	CB-OG-P-O1P
34	SS	423	SEP	CB-OG-P-O2P
34	SS	423	SEP	CB-OG-P-O3P
34	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	$\# Z > 2$
41	GTP	SI	2001	39	33,34,34	1.82	4 (12%)	50,54,54	1.47	7 (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
41	GTP	SI	2001	39	-	4/22/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	SI	2001	GTP	C5-N7	6.64	1.52	1.39
41	SI	2001	GTP	C8-N9	-4.23	1.28	1.37
41	SI	2001	GTP	C4-N9	-3.90	1.28	1.38
41	SI	2001	GTP	C4-N3	2.15	1.39	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	SI	2001	GTP	C8-N9-C4	7.18	119.49	106.03
41	SI	2001	GTP	N9-C4-N3	2.71	131.38	125.95
41	SI	2001	GTP	C1'-N9-C8	-2.39	119.94	126.73
41	SI	2001	GTP	C6-C5-N7	2.38	134.63	130.29
41	SI	2001	GTP	C8-N7-C5	-2.18	100.37	104.26
41	SI	2001	GTP	C5-C4-N9	-2.14	101.82	105.66
41	SI	2001	GTP	C1'-N9-C4	-2.01	120.56	126.49

There are no chirality outliers.

All (4) torsion outliers are listed below:

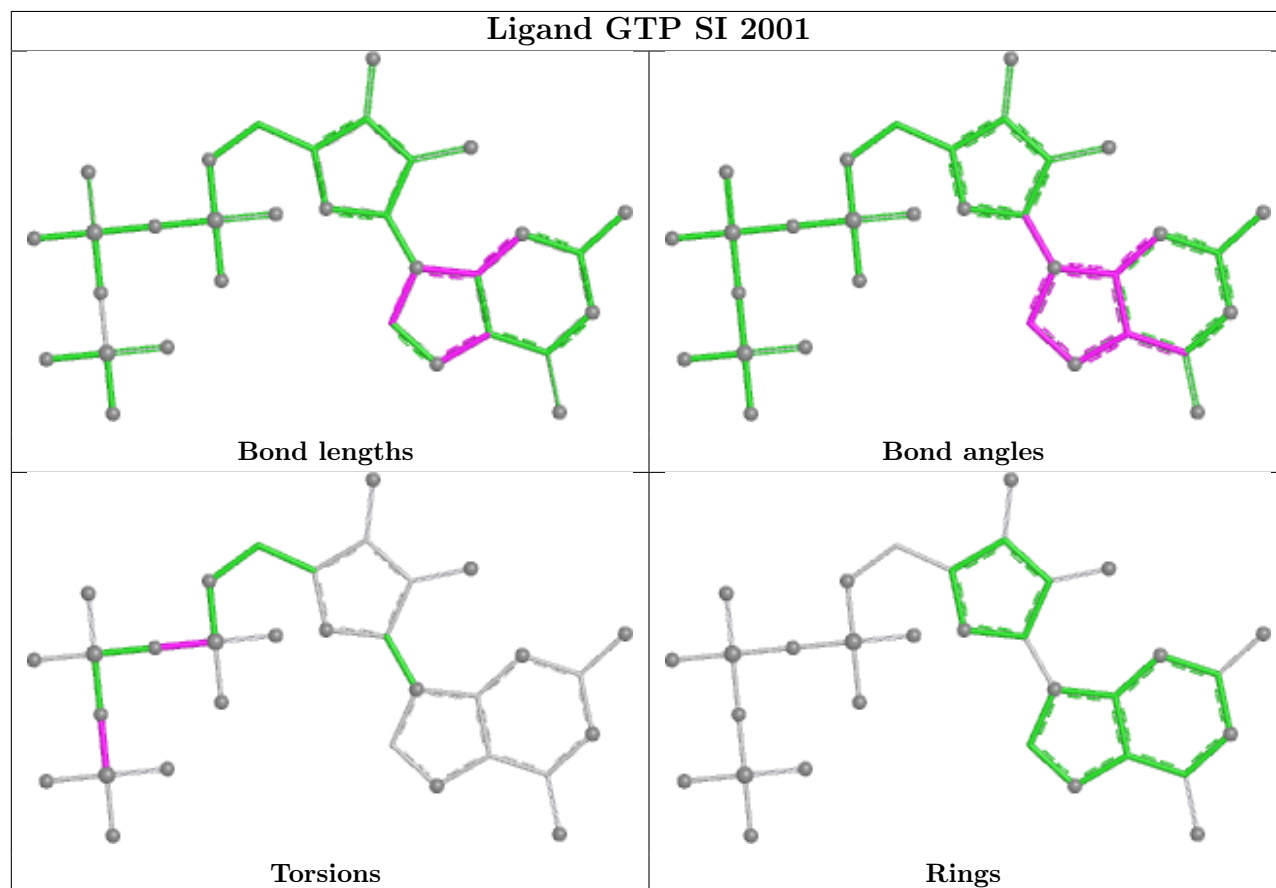
Mol	Chain	Res	Type	Atoms
41	SI	2001	GTP	PB-O3B-PG-O3G
41	SI	2001	GTP	PB-O3B-PG-O2G
41	SI	2001	GTP	PB-O3B-PG-O1G
41	SI	2001	GTP	PB-O3A-PA-O2A

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

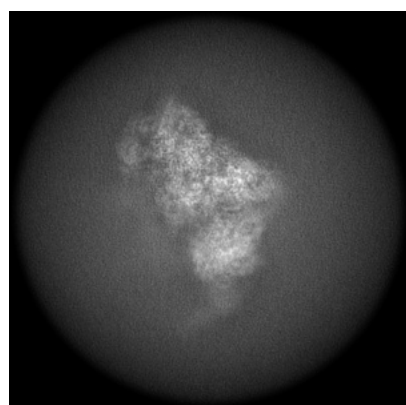
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49090. These allow visual inspection of the internal detail of the map and identification of artifacts.

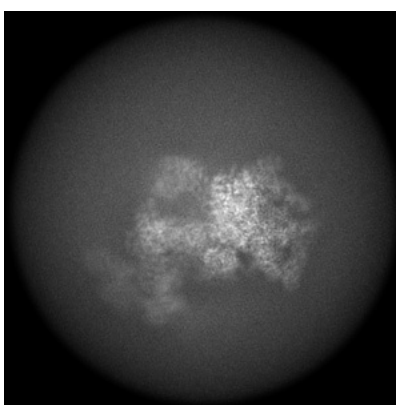
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

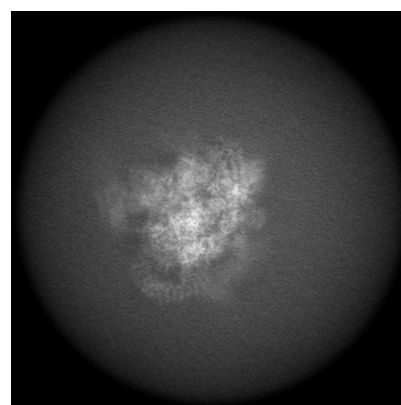
6.1.1 Primary map



X



Y

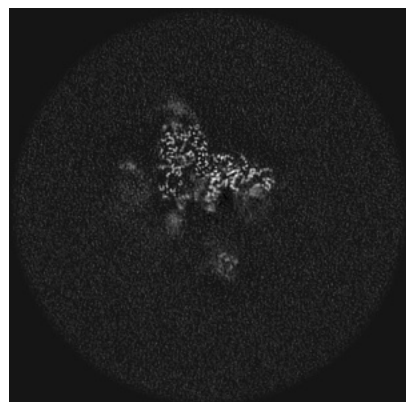


Z

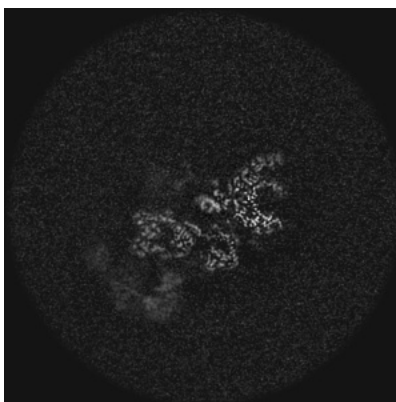
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

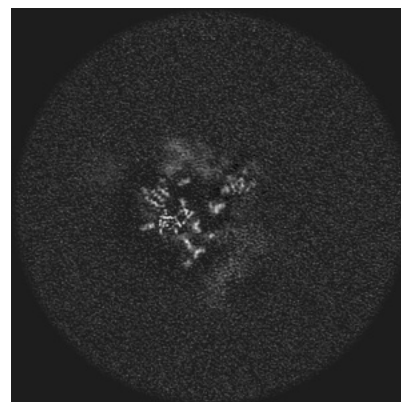
6.2.1 Primary map



X Index: 252



Y Index: 252

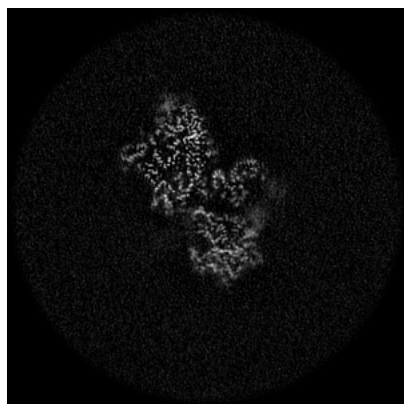


Z Index: 252

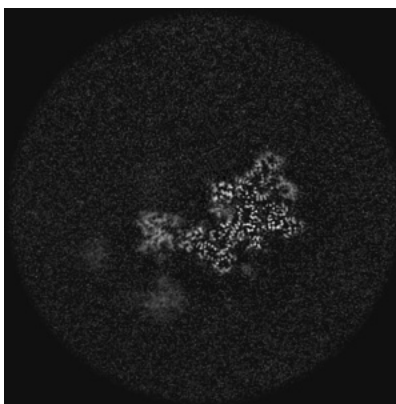
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

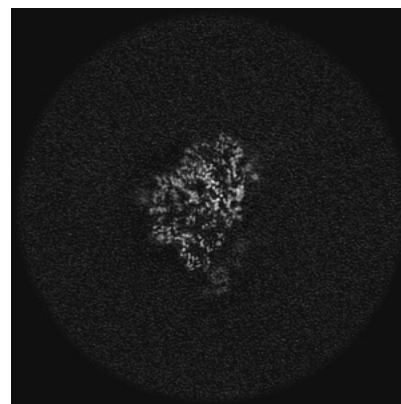
6.3.1 Primary map



X Index: 226



Y Index: 238

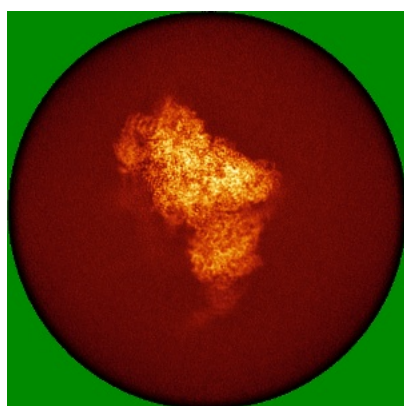


Z Index: 291

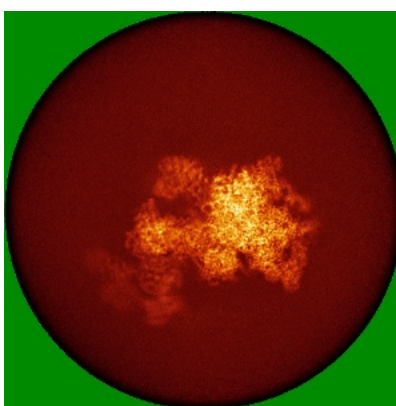
The images above show the largest variance slices of the map in three orthogonal directions.

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

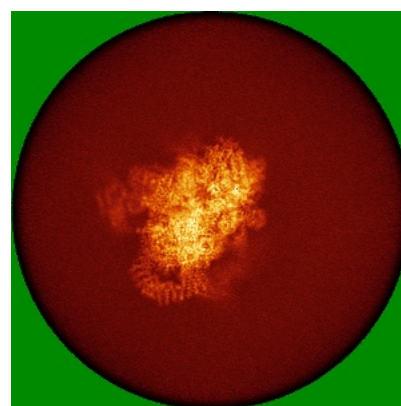
6.4.1 Primary map



X



Y

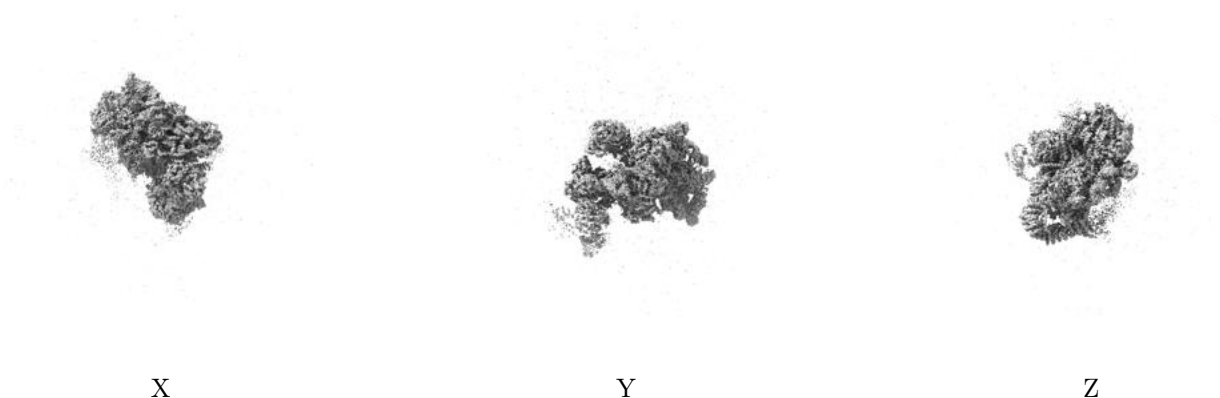


Z

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 0.85. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

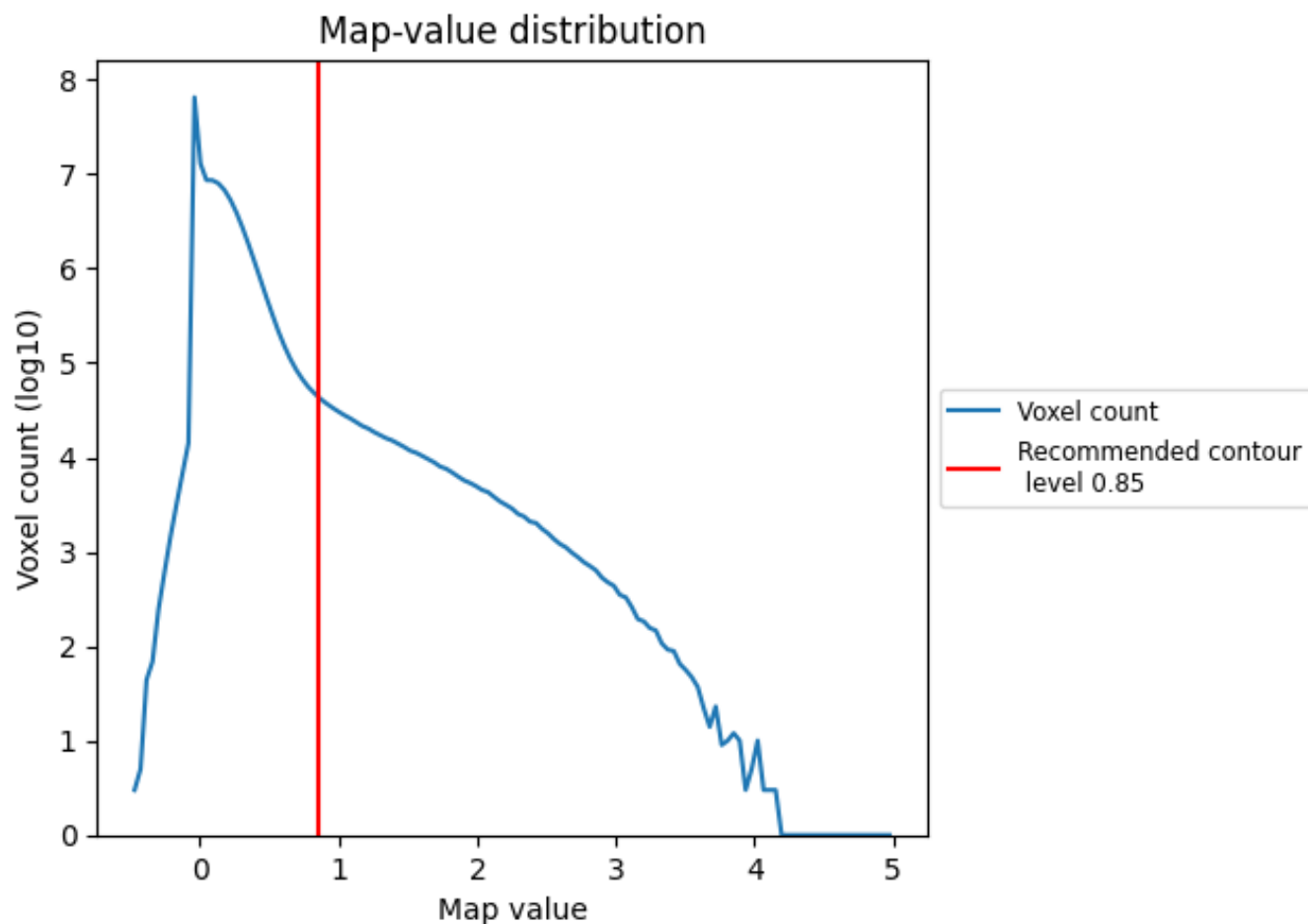
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

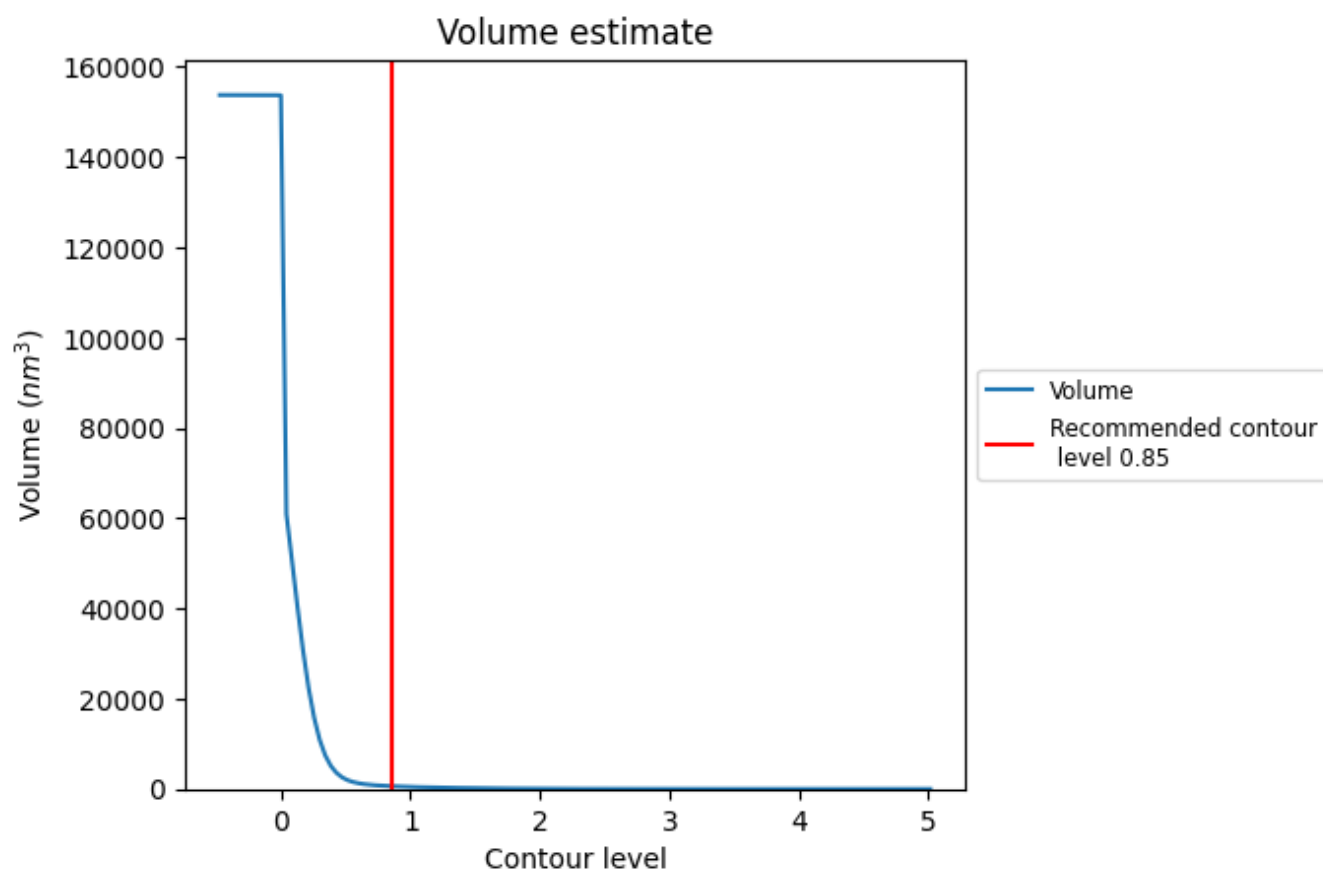
This section contains the results of statistical analysis of the map.

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.

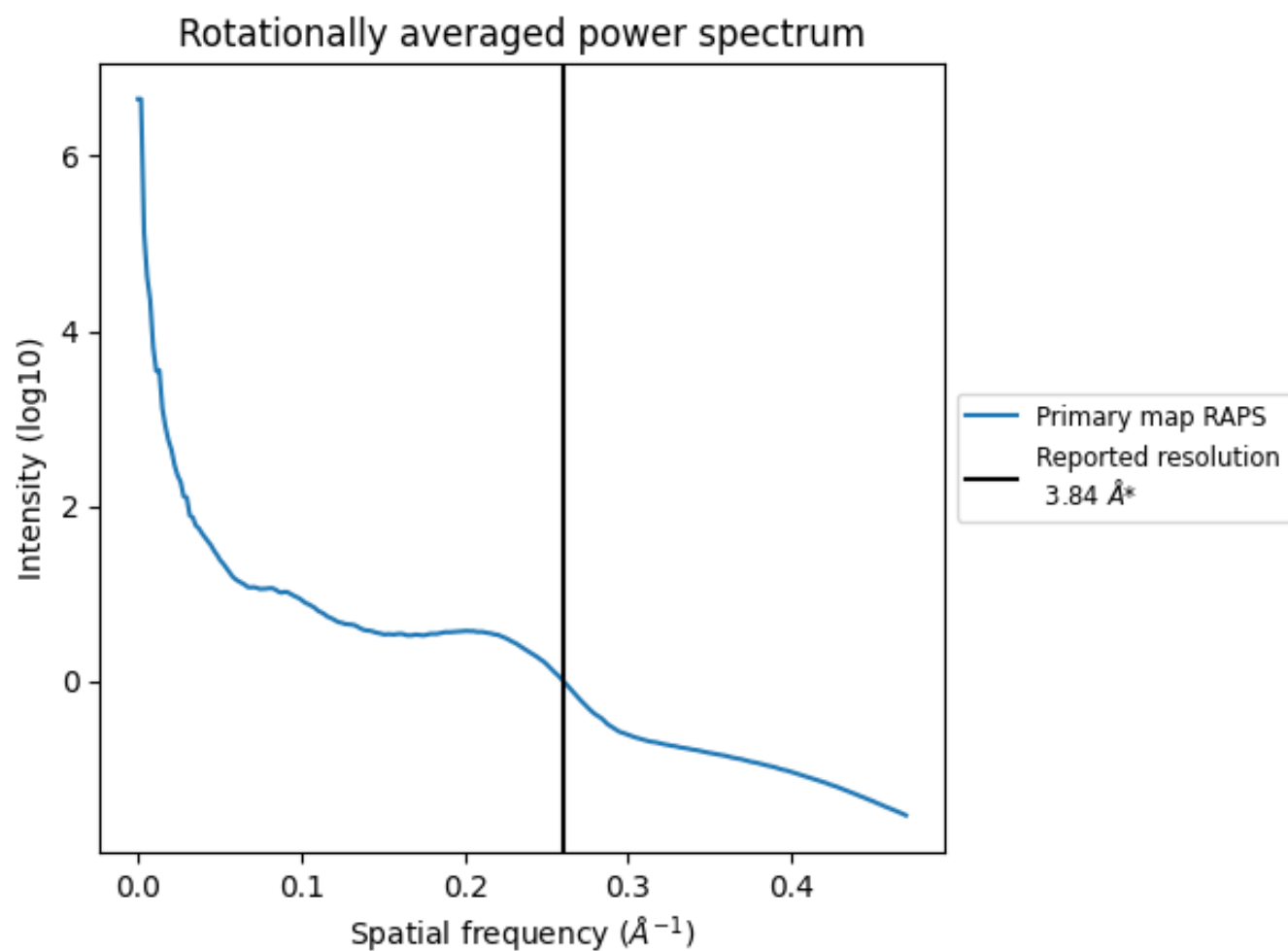
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 622 nm^3 ; this corresponds to an approximate mass of 562 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 $0.260 \text{ \AA}^{-1}$

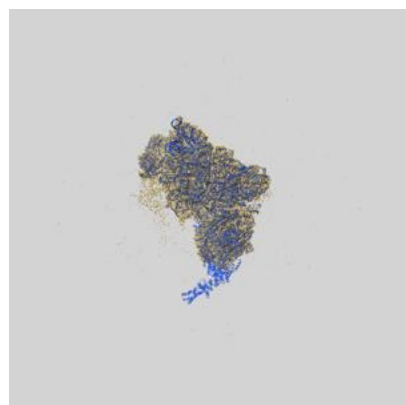
8 Fourier-Shell correlation

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

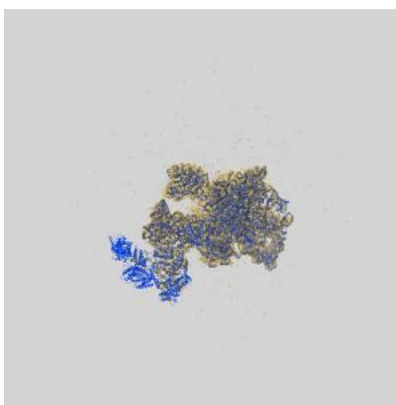
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-49090 and PDB model 9N7A. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

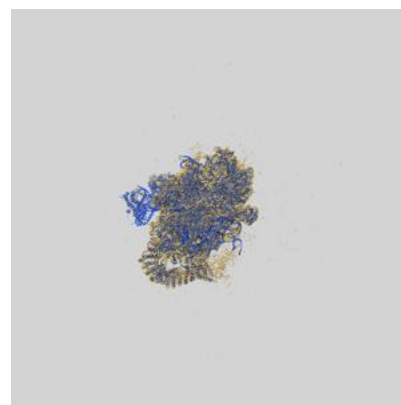
9.1 Map-model overlay [i](#)



X



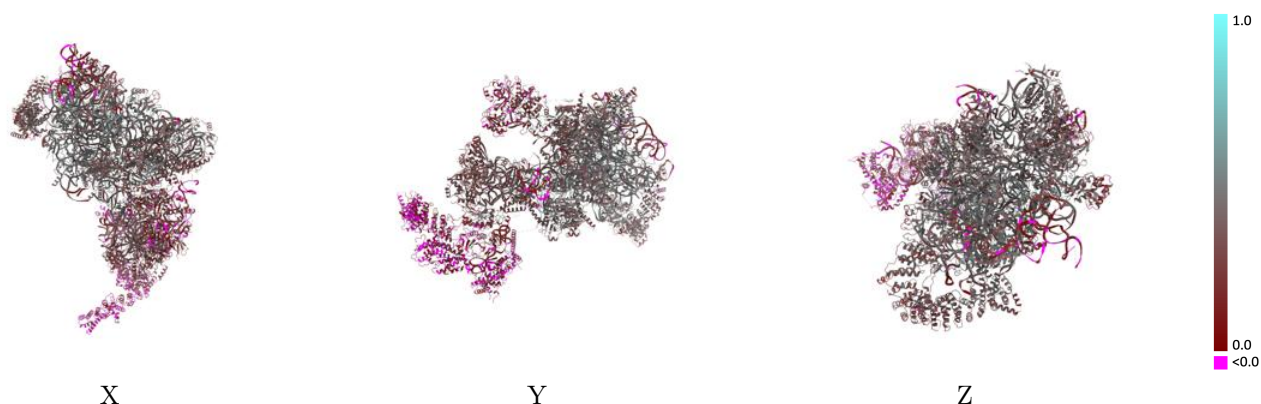
Y



Z

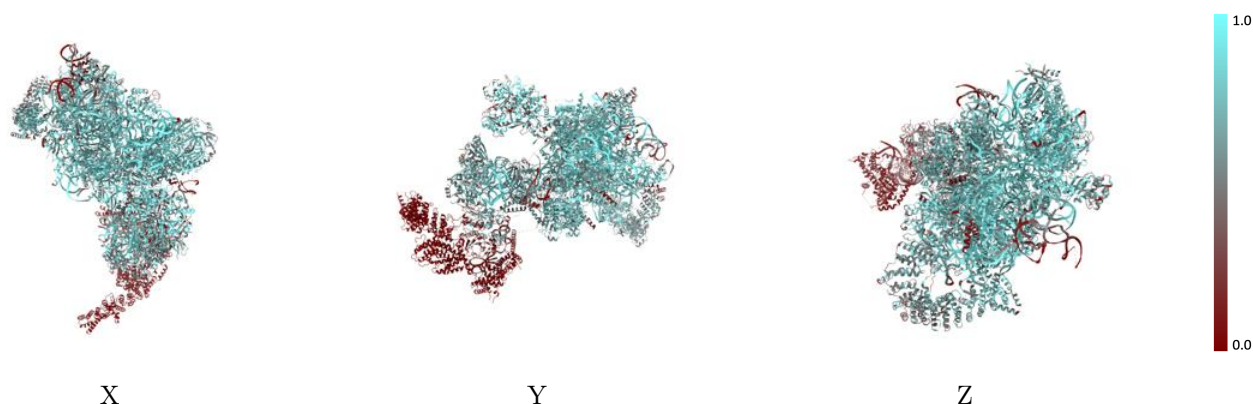
The images above show the 3D surface view of the map at the recommended contour level 0.85 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



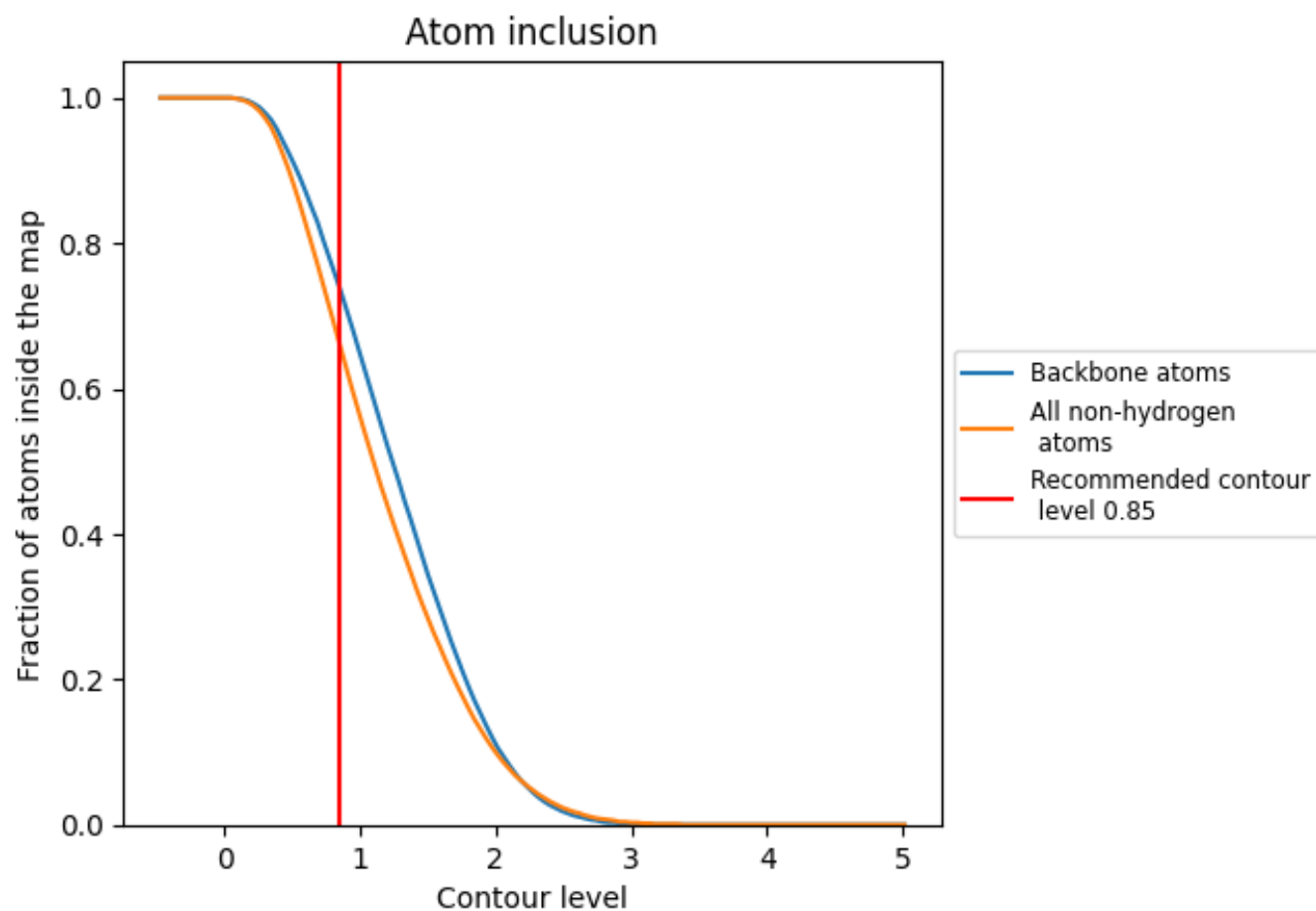
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 74% of all backbone atoms, 66% 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	 0.6600	 0.3550
L1	 0.7970	 0.3680
L2	 0.9350	 0.4040
L3	 0.5120	 0.2820
L4	 0.7530	 0.4820
L5	 0.6000	 0.3080
L6	 0.6960	 0.4180
L7	 0.6300	 0.3570
L8	 0.7860	 0.4630
L9	 0.7080	 0.4540
LC	 0.6170	 0.3270
LD	 0.7710	 0.4740
LE	 0.7600	 0.4540
LF	 0.7100	 0.4620
LG	 0.5210	 0.3070
N2	 0.6000	 0.2100
NA	 0.5910	 0.3660
NB	 0.5750	 0.3490
NF	 0.7280	 0.4470
NG	 0.7520	 0.3870
NL	 0.6900	 0.4120
NM	 0.6920	 0.4050
NP	 0.6580	 0.3160
NQ	 0.6540	 0.4170
NS	 0.6610	 0.2780
NW	 0.5040	 0.3280
SG	 0.5920	 0.3190
SH	 0.7330	 0.4220
SI	 0.7410	 0.4310
SJ	 0.2280	 0.1980
SK	 0.4030	 0.3030
SL	 0.7260	 0.3910
SM	 0.6190	 0.3900
SP	 0.5680	 0.3470
SR	 0.7390	 0.4630



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Chain	Atom inclusion	Q-score
SS	 0.7140	 0.3460
ST	 0.1620	 0.1570
SU	 0.0170	 0.0790
SW	 0.7470	 0.3640
SZ	 0.0370	 0.0830