



Full wwPDB EM Validation Report ⓘ

Apr 7, 2025 – 01:23 PM EDT

PDB ID : 8UJC / pdb_00008ujc
EMDB ID : EMD-42318
Title : In situ human 60S ribosome
Authors : Wei, Z.; Yong, X.
Deposited on : 2023-10-11
Resolution : 2.87 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:

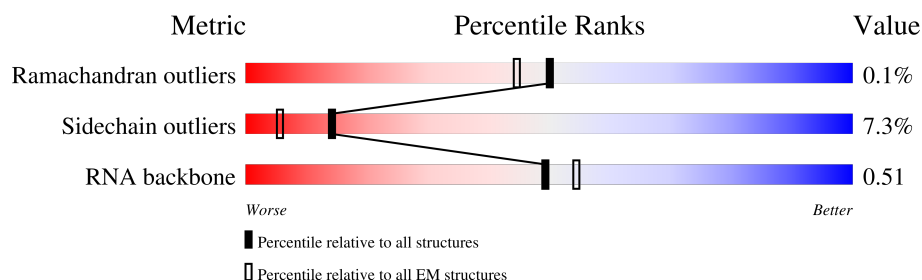
EMDB validation analysis : 0.0.1.dev117
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

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 2.87 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	LW	124	<div> <div>34%</div> <div>45%</div> <div>6%</div> <div>49%</div> </div>
2	L5	5070	<div> <div>8%</div> <div>56%</div> <div>16%</div> <div>28%</div> </div>
3	L7	120	<div> <div>88%</div> <div>12%</div> </div>
4	L8	156	<div> <div>6%</div> <div>83%</div> <div>17%</div> </div>
5	LA	248	<div> <div>92%</div> <div>8%</div> </div>
6	LB	402	<div> <div>94%</div> <div>6%</div> </div>
7	LC	368	<div> <div>94%</div> <div>6%</div> </div>
8	LD	293	<div> <div>6%</div> <div>95%</div> <div>5%</div> </div>






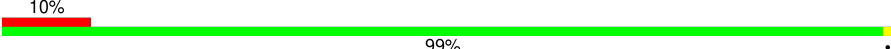
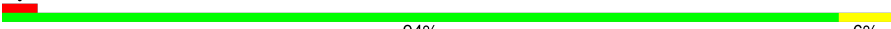

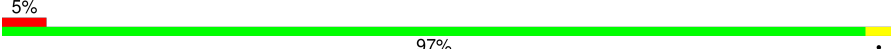



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Mol	Chain	Length	Quality of chain
9	LE	247	
10	LF	225	
11	LG	241	
12	LH	190	
13	LI	213	
14	LJ	176	
15	LL	210	
16	LM	139	
17	LN	203	
18	LO	201	
19	LP	153	
20	LQ	187	
21	LR	187	
22	LS	175	
23	LT	159	
24	LU	101	
25	LV	131	
26	LX	120	
27	LY	134	
28	LZ	135	
29	La	147	
30	Lb	121	
31	Lc	98	
32	Ld	107	
33	Le	128	

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Mol	Chain	Length	Quality of chain
34	Lf	109	 89% 11%
35	Lg	114	 7% 91% 9%
36	Lh	122	 93% 7%
37	Li	102	 6% 92% 8%
38	Lj	86	 91% 9%
39	Lk	69	 10% 99%
40	Ll	50	 94% 6%
41	Lm	52	 98%
42	Lo	105	 5% 97%
43	Lp	91	 92% 8%
44	Lr	125	 91% 9%
45	CA	356	 84% 90% 10%

2 Entry composition

There are 47 unique types of molecules in this entry. The entry contains 139414 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	LW	63	Total	C	N	O	S	0	0
			528	337	103	85	3		

- Molecule 2 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L5	3649	Total	C	N	O	P	0	0
			78229	34837	14317	25427	3648		

- Molecule 3 is a RNA chain called 5S rRNA [Homo sapiens].

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L7	120	Total	C	N	O	P	0	0
			2561	1141	456	844	120		

- Molecule 4 is a RNA chain called 5.8S rRNA [Homo sapiens].

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L8	156	Total	C	N	O	P	0	0
			3314	1480	585	1094	155		

- Molecule 5 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	LA	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 6 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	LB	402	Total	C	N	O	S	0	0
			3238	2060	608	556	14		

- Molecule 7 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	LC	368	Total	C	N	O	S	0	0
			2927	1840	583	489	15		

- Molecule 8 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LD	293	Total	C	N	O	S	0	0
			2382	1507	434	427	14		

- Molecule 9 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LE	236	Total	C	N	O	S	0	0
			1904	1222	361	317	4		

- Molecule 10 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LF	225	Total	C	N	O	S	0	0
			1870	1202	358	301	9		

- Molecule 11 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LG	241	Total	C	N	O	S	0	0
			1927	1228	371	324	4		

- Molecule 12 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LH	190	Total	C	N	O	S	0	0
			1518	956	284	272	6		

- Molecule 13 is a protein called Ribosomal protein uL16-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LI	202	Total	C	N	O	S	0	0
			1634	1037	314	269	14		

- Molecule 14 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LJ	176	Total	C	N	O	S	0	0
			1410	888	263	253	6		

- Molecule 15 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LL	210	Total	C	N	O	S	0	0
			1701	1064	352	281	4		

- Molecule 16 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LM	139	Total	C	N	O	S	0	0
			1138	730	218	183	7		

- Molecule 17 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LN	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 18 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LO	201	Total	C	N	O	S	0	0
			1650	1063	321	261	5		

- Molecule 19 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LP	153	Total	C	N	O	S	0	0
			1242	776	241	216	9		

- Molecule 20 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LQ	187	Total	C	N	O	S	0	0
			1513	944	314	250	5		

- Molecule 21 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LR	153	Total	C	N	O	S	0	0
			1281	799	276	197	9		

- Molecule 22 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LS	175	Total	C	N	O	S	0	0
			1453	925	283	235	10		

- Molecule 23 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LT	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 24 is a protein called Heparin-binding protein HBp15.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LU	101	Total	C	N	O	S	0	0
			825	529	144	150	2		

- Molecule 25 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LV	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 26 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LX	120	Total	C	N	O	S	0	0
			985	630	185	169	1		

- Molecule 27 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LY	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 28 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LZ	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 29 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	La	147	Total	C	N	O	S	0	0
			1162	736	237	186	3		

- Molecule 30 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Lb	109	Total	C	N	O	S	0	0
			876	546	189	137	4		

- Molecule 31 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Lc	98	Total	C	N	O	S	0	0
			764	485	135	138	6		

- Molecule 32 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Ld	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 33 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Le	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 34 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Lf	109	Total	C	N	O	S	0	0
			876	555	174	144	3		

- Molecule 35 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Lg	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 36 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Lh	122	Total	C	N	O	S	0	0
			1015	641	205	168	1		

- Molecule 37 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Li	102	Total	C	N	O	S	0	0
			832	521	177	129	5		

- Molecule 38 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Lj	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 39 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Lk	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 40 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Ll	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 41 is a protein called Large ribosomal subunit protein eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Lm	52	Total	C	N	O	S	0	0
			429	266	90	67	6		

- Molecule 42 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Lo	105	Total	C	N	O	S	0	0
			862	542	175	139	6		

- Molecule 43 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Lp	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 44 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Lr	125	Total	C	N	O	S	0	0
			1002	622	207	168	5		

- Molecule 45 is a protein called Proliferation-associated protein 2G4.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	CA	354	Total	C	N	O	S	4	0
			2764	1744	475	528	17		

- Molecule 46 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
46	L5	212	Total	Mg	0
			212	212	
46	L7	3	Total	Mg	0
			3	3	
46	L8	4	Total	Mg	0
			4	4	
46	LA	1	Total	Mg	0
			1	1	
46	LI	1	Total	Mg	0
			1	1	
46	LP	1	Total	Mg	0
			1	1	
46	LV	1	Total	Mg	0
			1	1	
46	Le	1	Total	Mg	0
			1	1	
46	Lg	1	Total	Mg	0
			1	1	

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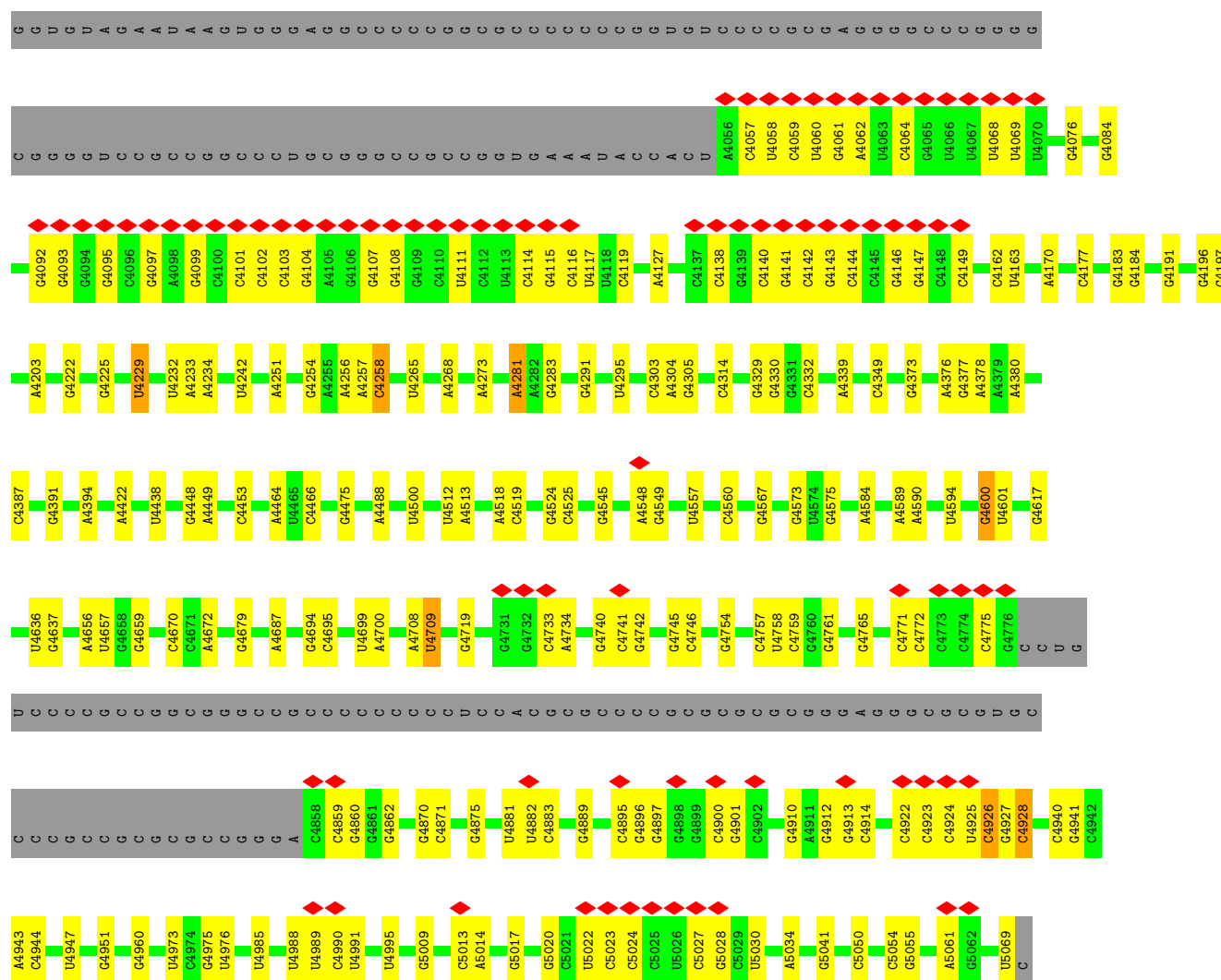
Mol	Chain	Residues	Atoms		AltConf
46	Lj	1	Total 1	Mg 1	0

- Molecule 47 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

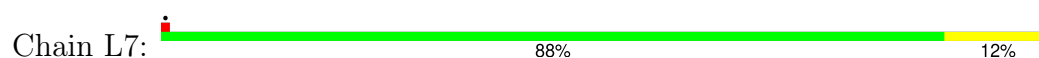
Mol	Chain	Residues	Atoms		AltConf
47	Lg	1	Total 1	Zn 1	0
47	Lj	1	Total 1	Zn 1	0
47	Lm	1	Total 1	Zn 1	0
47	Lo	1	Total 1	Zn 1	0
47	Lp	1	Total 1	Zn 1	0



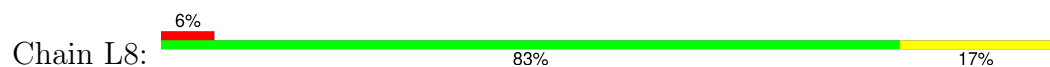




• Molecule 3: 5S rRNA [Homo sapiens]



• Molecule 4: 5.8S rRNA [Homo sapiens]



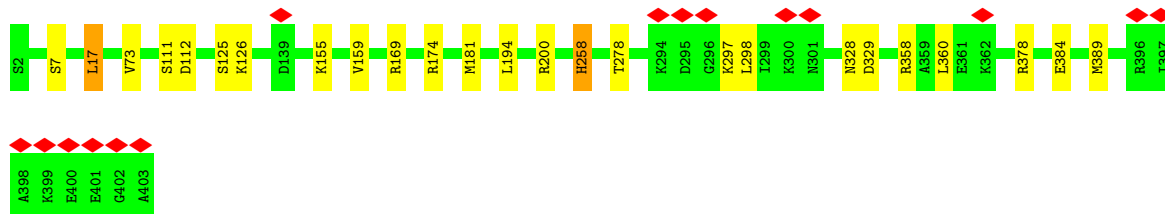
• Molecule 5: 60S ribosomal protein L8





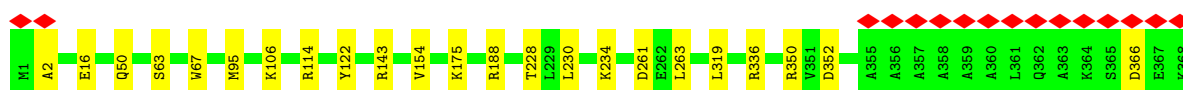
- Molecule 6: Large ribosomal subunit protein uL3

Chain LB: 94% 6%



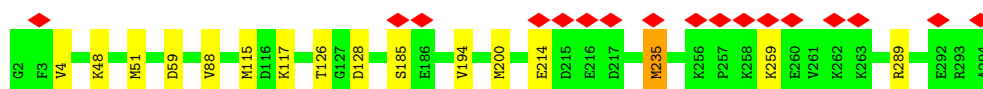
- Molecule 7: 60S ribosomal protein L4

Chain LC: 94% 6%



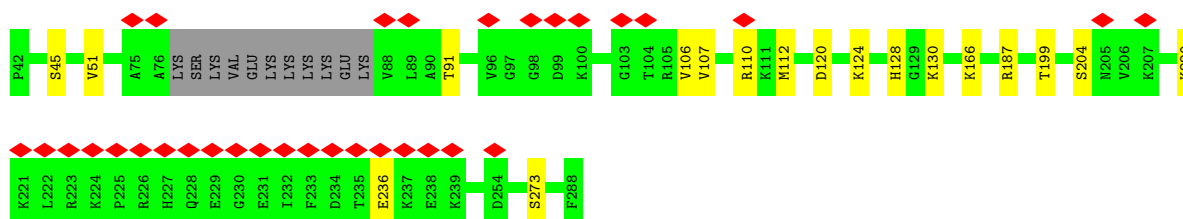
- Molecule 8: Large ribosomal subunit protein uL18

Chain LD: 95% 6% 5%



- Molecule 9: Large ribosomal subunit protein eL6

Chain LE: 88% 13% 7%

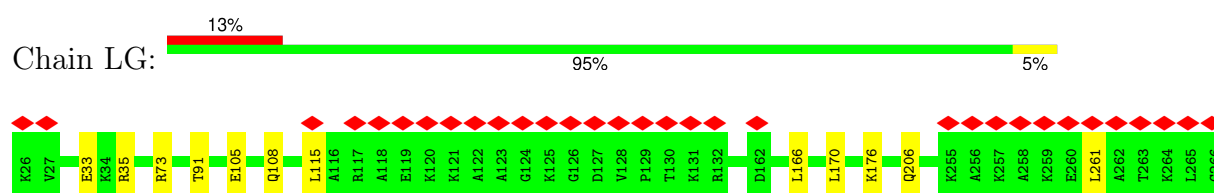


- Molecule 10: 60S ribosomal protein L7

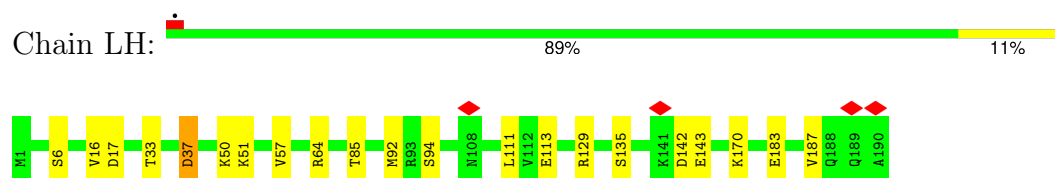
Chain LF: 95% 5%



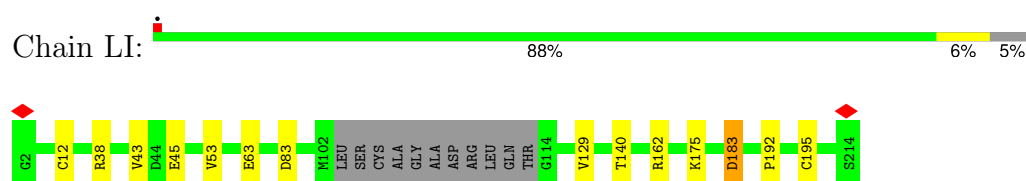
- Molecule 11: 60S ribosomal protein L7a



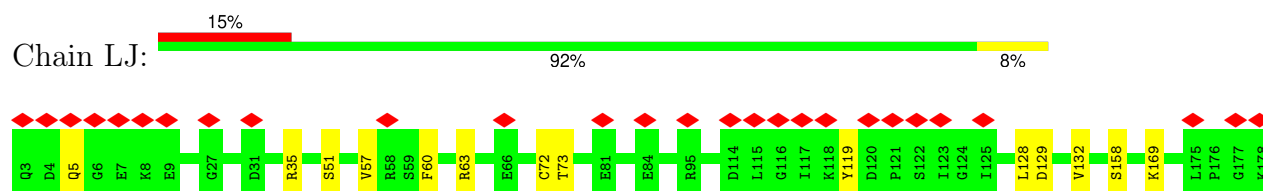
- Molecule 12: 60S ribosomal protein L9



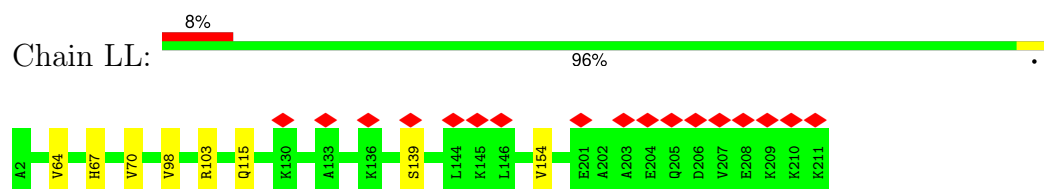
- Molecule 13: Ribosomal protein uL16-like



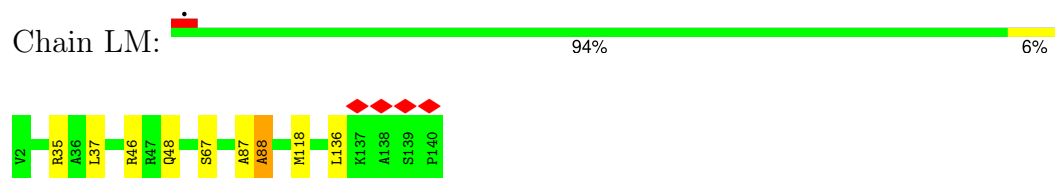
- Molecule 14: 60S ribosomal protein L11



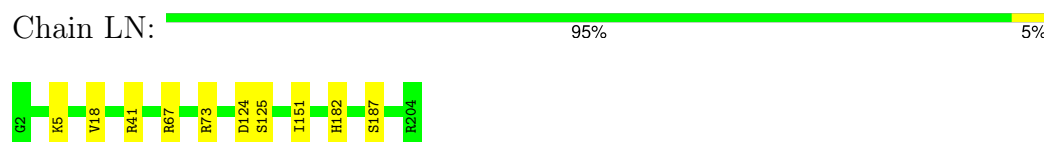
- Molecule 15: Large ribosomal subunit protein eL13



- Molecule 16: 60S ribosomal protein L14



- Molecule 17: 60S ribosomal protein L15



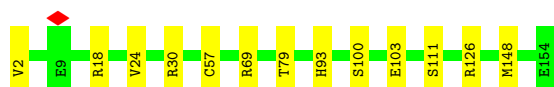
- Molecule 18: 60S ribosomal protein L13a

Chain LO:  95% 5%



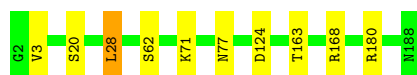
- Molecule 19: 60S ribosomal protein L17

Chain LP:  92% 8%




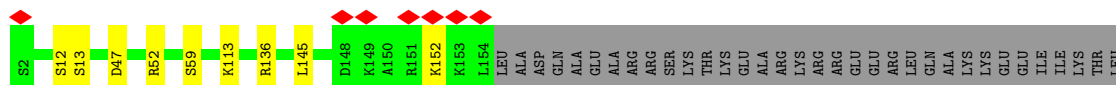
- Molecule 20: 60S ribosomal protein L18

Chain LQ:  95% 5%



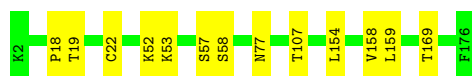
- Molecule 21: 60S ribosomal protein L19

Chain LR:  77% 5% 18%



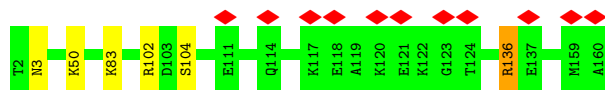
- Molecule 22: 60S ribosomal protein L18a

Chain LS:  93% 7%




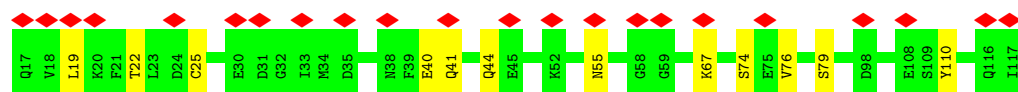
- Molecule 23: 60S ribosomal protein L21

Chain LT:  7% 96%



- Molecule 24: Heparin-binding protein HBp15

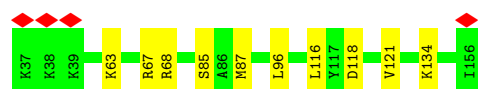
Chain LU:  22% 88% 12%



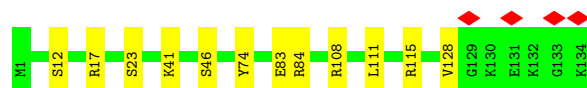
- Molecule 25: 60S ribosomal protein L23



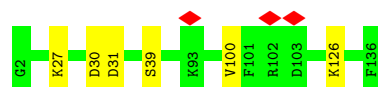
- Molecule 26: 60S ribosomal protein L23a



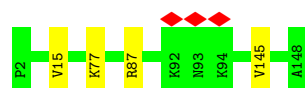
- Molecule 27: 60S ribosomal protein L26



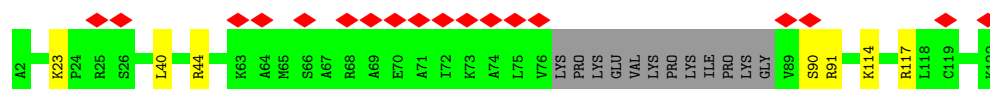
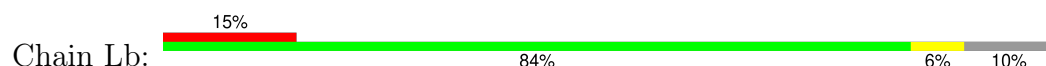
- Molecule 28: 60S ribosomal protein L27



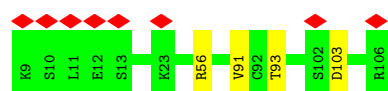
- Molecule 29: 60S ribosomal protein L27a



- Molecule 30: Large ribosomal subunit protein eL29



- Molecule 31: 60S ribosomal protein L30



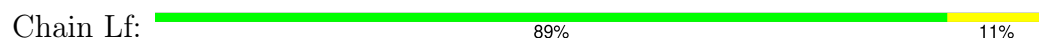
- Molecule 32: 60S ribosomal protein L31



- Molecule 33: 60S ribosomal protein L32



- Molecule 34: 60S ribosomal protein L35a



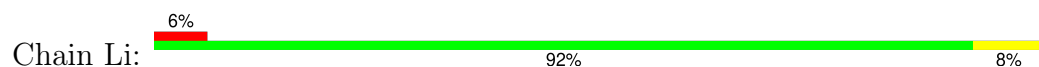
- Molecule 35: 60S ribosomal protein L34



- Molecule 36: 60S ribosomal protein L35

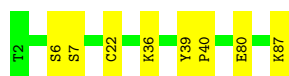


- Molecule 37: 60S ribosomal protein L36



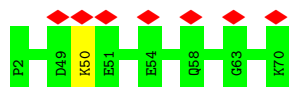
- Molecule 38: 60S ribosomal protein L37

Chain Lj:  91% 9%



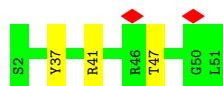
- Molecule 39: 60S ribosomal protein L38

Chain Lk:  10% 99%



- Molecule 40: 60S ribosomal protein L39

Chain Ll:  94% 6%



- Molecule 41: Large ribosomal subunit protein eL40

Chain Lm:  98%



- Molecule 42: 60S ribosomal protein L36a

Chain Lo:  5% 97%



- Molecule 43: 60S ribosomal protein L37a

Chain Lp:  92% 8%

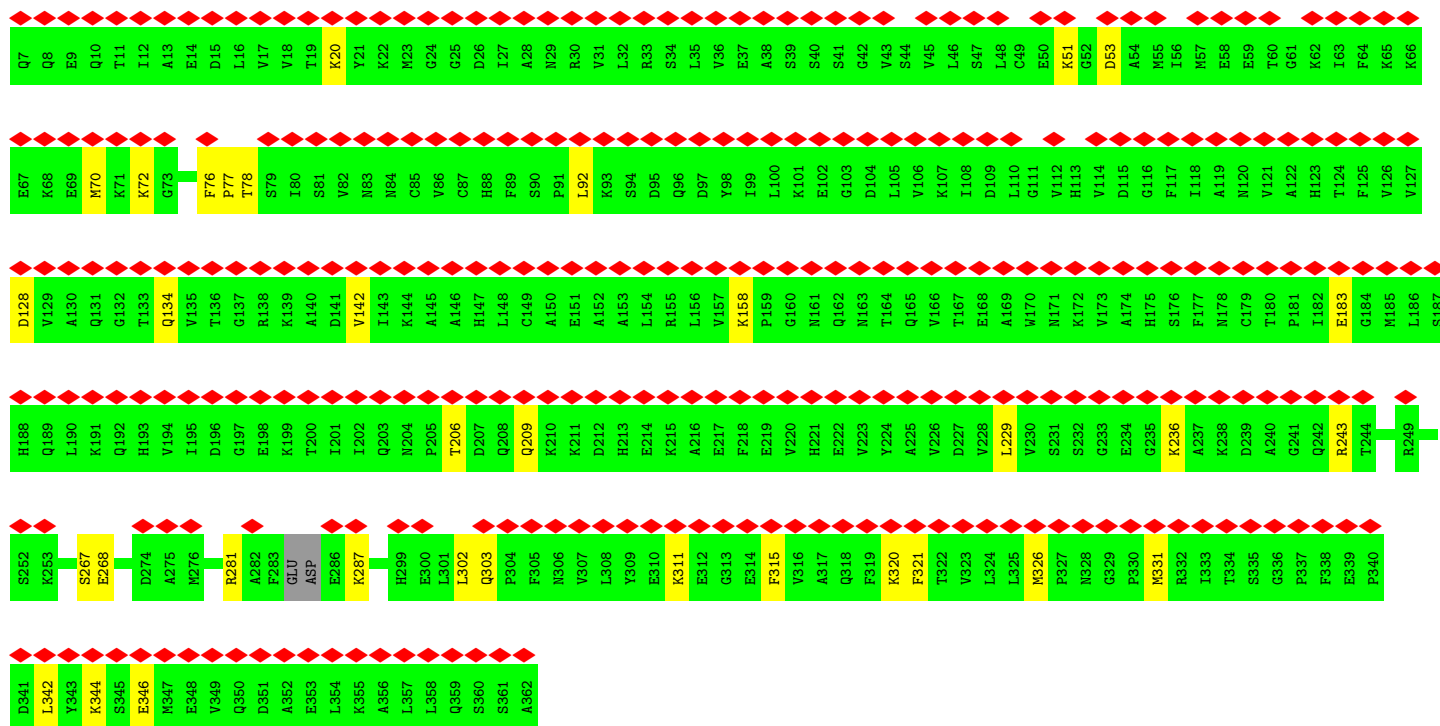
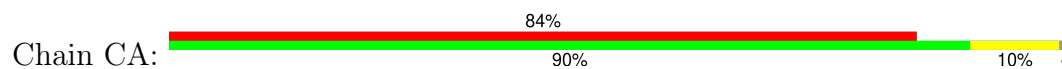


- Molecule 44: 60S ribosomal protein L28

Chain Lr:  91% 9%



- Molecule 45: Proliferation-associated protein 2G4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	220618	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.822	Depositor
Minimum map value	-0.439	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.0495	Depositor
Map size (\AA)	546.816, 546.816, 546.816	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.068, 1.068, 1.068	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	LW	0.32	0/541	0.61	0/720
2	L5	0.32	0/87512	0.92	117/136518 (0.1%)
3	L7	0.30	0/2861	0.87	1/4459 (0.0%)
4	L8	0.31	0/3701	0.88	4/5766 (0.1%)
5	LA	0.30	0/1936	0.63	0/2596
6	LB	0.29	0/3306	0.60	1/4424 (0.0%)
7	LC	0.29	0/2981	0.59	1/4002 (0.0%)
8	LD	0.29	0/2428	0.57	1/3252 (0.0%)
9	LE	0.28	0/1942	0.59	0/2606
10	LF	0.29	0/1905	0.56	0/2539
11	LG	0.29	0/1960	0.58	1/2637 (0.0%)
12	LH	0.31	0/1537	0.63	2/2066 (0.1%)
13	LI	0.28	0/1673	0.57	1/2233 (0.0%)
14	LJ	0.30	0/1433	0.65	0/1915
15	LL	0.29	0/1732	0.61	0/2315
16	LM	0.28	0/1161	0.57	0/1554
17	LN	0.27	0/1746	0.60	0/2338
18	LO	0.29	0/1682	0.55	0/2250
19	LP	0.28	0/1268	0.54	0/1701
20	LQ	0.28	0/1537	0.61	1/2052 (0.0%)
21	LR	0.28	0/1296	0.60	0/1713
22	LS	0.31	0/1493	0.60	1/2003 (0.0%)
23	LT	0.29	0/1326	0.59	0/1770
24	LU	0.36	0/839	0.66	0/1126
25	LV	0.28	0/993	0.55	0/1332
26	LX	0.28	0/1002	0.63	2/1345 (0.1%)
27	LY	0.28	0/1132	0.56	0/1504
28	LZ	0.30	0/1130	0.60	1/1507 (0.1%)
29	La	0.28	0/1191	0.56	0/1591
30	Lb	0.26	0/889	0.61	0/1175
31	Lc	0.32	0/774	0.58	1/1038 (0.1%)
32	Ld	0.27	0/903	0.59	1/1216 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Le	0.34	0/1071	0.60	0/1429
34	Lf	0.28	0/895	0.60	0/1198
35	Lg	0.26	0/916	0.57	0/1220
36	Lh	0.27	0/1023	0.57	0/1351
37	Li	0.26	0/843	0.58	0/1115
38	Lj	0.28	0/720	0.63	0/952
39	Lk	0.30	0/575	0.61	0/761
40	Ll	0.25	0/454	0.64	0/599
41	Lm	0.25	0/435	0.55	0/575
42	Lo	0.28	0/876	0.57	0/1156
43	Lp	0.28	0/718	0.59	0/953
44	Lr	0.27	0/1017	0.59	0/1364
45	CA	0.58	3/2810 (0.1%)	0.87	6/3780 (0.2%)
All	All	0.32	3/150163 (0.0%)	0.82	142/221716 (0.1%)

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
5	LA	0	1
6	LB	0	2
15	LL	0	1
16	LM	0	2
18	LO	0	1
23	LT	0	1
34	Lf	0	2
36	Lh	0	1
38	Lj	0	2
All	All	0	13

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	CA	77	PRO	CG-CD	-19.24	0.87	1.50
45	CA	77	PRO	CB-CG	13.34	2.16	1.50
45	CA	77	PRO	N-CD	9.43	1.61	1.47

All (142) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	CA	77	PRO	CB-CG-CD	-27.30	0.02	106.50
45	CA	77	PRO	N-CA-CB	-17.10	82.78	103.30
45	CA	77	PRO	CA-N-CD	-16.01	89.08	111.50
2	L5	485	C	C2-N1-C1'	11.29	131.22	118.80
2	L5	2710	C	N1-C2-O2	9.79	124.78	118.90
45	CA	76	PHE	C-N-CD	9.53	148.41	128.40
2	L5	2710	C	C2-N1-C1'	9.10	128.81	118.80
2	L5	4138	C	N3-C2-O2	-8.62	115.87	121.90
2	L5	485	C	C6-N1-C1'	-8.48	110.62	120.80
2	L5	456	C	O4'-C1'-N1	7.99	114.59	108.20
2	L5	2710	C	N3-C2-O2	-7.98	116.32	121.90
2	L5	1414	C	N3-C2-O2	-7.89	116.38	121.90
2	L5	1414	C	N1-C2-O2	7.87	123.62	118.90
2	L5	1252	C	N3-C2-O2	-7.86	116.40	121.90
2	L5	654	C	N1-C2-O2	7.59	123.45	118.90
2	L5	1082	C	O4'-C1'-N1	7.58	114.27	108.20
26	LX	116	LEU	CA-CB-CG	7.56	132.70	115.30
2	L5	100	C	C2-N1-C1'	7.51	127.07	118.80
2	L5	4928	C	C6-N1-C2	-7.39	117.34	120.30
2	L5	925	C	N3-C2-O2	-7.34	116.76	121.90
2	L5	456	C	N3-C2-O2	-7.32	116.78	121.90
2	L5	175	C	N3-C2-O2	-7.29	116.80	121.90
2	L5	490	C	N3-C2-O2	-7.24	116.83	121.90
28	LZ	30	ASP	CB-CG-OD2	7.08	124.67	118.30
2	L5	1082	C	N3-C2-O2	-7.01	117.00	121.90
2	L5	4928	C	C2-N1-C1'	7.01	126.51	118.80
2	L5	209	U	C2-N1-C1'	6.92	126.00	117.70
2	L5	925	C	N1-C2-O2	6.92	123.05	118.90
2	L5	753	C	N3-C2-O2	-6.87	117.09	121.90
2	L5	1216	C	C2-N1-C1'	6.85	126.34	118.80
2	L5	753	C	N1-C2-O2	6.84	123.00	118.90
2	L5	181	C	C2-N1-C1'	6.81	126.29	118.80
2	L5	3741	C	N3-C2-O2	-6.79	117.15	121.90
2	L5	4709	U	C2-N1-C1'	6.71	125.76	117.70
2	L5	2627	C	C2-N1-C1'	6.64	126.10	118.80
2	L5	255	C	N3-C2-O2	-6.64	117.25	121.90
2	L5	4926	C	C2-N1-C1'	6.58	126.03	118.80
2	L5	2710	C	C6-N1-C2	-6.57	117.67	120.30
4	L8	111	U	C2-N1-C1'	6.56	125.57	117.70
2	L5	4926	C	N1-C2-O2	6.53	122.82	118.90
2	L5	129	C	N3-C2-O2	-6.52	117.33	121.90
2	L5	3773	U	N3-C2-O2	-6.47	117.67	122.20
2	L5	181	C	N1-C2-O2	6.43	122.76	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L5	2410	C	C2-N1-C1'	6.43	125.87	118.80
2	L5	417	G	O4'-C1'-N9	6.42	113.33	108.20
3	L7	28	C	C6-N1-C2	-6.39	117.74	120.30
45	CA	77	PRO	N-CD-CG	-6.34	93.68	103.20
12	LH	142	ASP	CB-CG-OD2	6.32	123.99	118.30
12	LH	37	ASP	CB-CG-OD2	6.30	123.97	118.30
2	L5	485	C	N1-C2-O2	6.26	122.66	118.90
2	L5	654	C	C5-C6-N1	6.25	124.12	121.00
2	L5	485	C	C5-C6-N1	6.13	124.07	121.00
2	L5	2710	C	C6-N1-C1'	-6.07	113.51	120.80
2	L5	4147	G	C5-C6-O6	6.04	132.22	128.60
2	L5	3773	U	C2-N1-C1'	6.00	124.90	117.70
2	L5	100	C	C6-N1-C2	-5.99	117.90	120.30
2	L5	2627	C	N1-C2-O2	5.94	122.46	118.90
2	L5	4928	C	N1-C2-O2	5.92	122.45	118.90
2	L5	1191	C	N3-C2-O2	-5.90	117.77	121.90
8	LD	235	MET	CA-CB-CG	5.90	123.32	113.30
2	L5	1245	C	C2-N1-C1'	5.89	125.28	118.80
2	L5	4758	U	C2-N1-C1'	5.88	124.75	117.70
2	L5	1216	C	N1-C2-O2	5.87	122.42	118.90
11	LG	115	LEU	CA-CB-CG	5.87	128.80	115.30
7	LC	2	ALA	C-N-CA	5.87	136.37	121.70
2	L5	3773	U	N1-C2-O2	5.85	126.89	122.80
2	L5	1251	C	N1-C2-O2	5.82	122.39	118.90
26	LX	118	ASP	CB-CG-OD2	5.81	123.53	118.30
2	L5	4147	G	N1-C6-O6	-5.81	116.42	119.90
2	L5	1241	C	C2-N1-C1'	5.75	125.12	118.80
2	L5	2018	C	C5-C6-N1	5.74	123.87	121.00
2	L5	261	G	N3-C4-N9	5.67	129.40	126.00
2	L5	1241	C	N1-C2-O2	5.66	122.30	118.90
2	L5	2528	G	C4-N9-C1'	5.66	133.85	126.50
2	L5	4928	C	N3-C2-O2	-5.66	117.94	121.90
4	L8	111	U	N1-C2-O2	5.65	126.75	122.80
2	L5	1082	C	C6-N1-C2	-5.65	118.04	120.30
2	L5	914	U	C5-C4-O4	-5.62	122.53	125.90
2	L5	4107	G	N3-C4-C5	-5.61	125.79	128.60
2	L5	654	C	C2-N1-C1'	5.61	124.97	118.80
2	L5	4107	G	C4-N9-C1'	5.60	133.78	126.50
22	LS	18	PRO	C-N-CA	5.60	135.69	121.70
2	L5	985	C	C2-N1-C1'	5.57	124.93	118.80
2	L5	655	C	C6-N1-C2	-5.55	118.08	120.30
45	CA	302	LEU	CA-CB-CG	5.54	128.05	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L5	1340	C	C5-C6-N1	5.54	123.77	121.00
13	LI	183	ASP	CB-CG-OD1	5.53	123.27	118.30
2	L5	3773	U	O4'-C1'-N1	5.53	112.62	108.20
2	L5	4709	U	C5-C4-O4	-5.52	122.58	125.90
2	L5	3741	C	N1-C2-O2	5.49	122.19	118.90
2	L5	2760	G	P-O3'-C3'	5.47	126.27	119.70
2	L5	3911	C	C5-C6-N1	5.47	123.73	121.00
2	L5	1082	C	P-O3'-C3'	5.47	126.26	119.70
2	L5	485	C	C6-N1-C2	-5.46	118.12	120.30
2	L5	4258	C	C5-C6-N1	5.42	123.71	121.00
6	LB	17	LEU	CA-CB-CG	5.41	127.74	115.30
2	L5	115	C	C2-N1-C1'	5.40	124.74	118.80
2	L5	914	U	P-O3'-C3'	5.39	126.17	119.70
2	L5	664	G	C5-C6-O6	5.35	131.81	128.60
2	L5	4138	C	N1-C2-O2	5.33	122.10	118.90
4	L8	51	U	N1-C2-O2	5.33	126.53	122.80
2	L5	4107	G	N3-C4-N9	5.32	129.19	126.00
2	L5	4281	A	N1-C2-N3	5.30	131.95	129.30
2	L5	4600	G	P-O3'-C3'	5.27	126.03	119.70
2	L5	4229	U	N3-C2-O2	-5.25	118.52	122.20
2	L5	2018	C	C6-N1-C2	-5.25	118.20	120.30
2	L5	2262	G	C4-N9-C1'	5.23	133.30	126.50
4	L8	111	U	N3-C2-O2	-5.22	118.55	122.20
2	L5	181	C	N3-C2-O2	-5.20	118.26	121.90
2	L5	914	U	N3-C4-O4	5.19	123.04	119.40
2	L5	4281	A	O4'-C1'-N9	5.18	112.35	108.20
2	L5	4926	C	N3-C2-O2	-5.18	118.27	121.90
2	L5	4303	C	C6-N1-C2	-5.18	118.23	120.30
2	L5	4746	C	C2-N1-C1'	5.17	124.48	118.80
2	L5	489	C	N1-C2-O2	5.16	122.00	118.90
32	Ld	46	LEU	CA-CB-CG	-5.16	103.44	115.30
2	L5	1259	G	N1-C2-N2	-5.15	111.56	116.20
2	L5	263	G	N1-C2-N2	-5.14	111.57	116.20
2	L5	2867	C	C2-N1-C1'	5.14	124.46	118.80
2	L5	1686	C	N3-C2-O2	-5.13	118.31	121.90
31	Lc	103	ASP	CB-CG-OD2	5.13	122.92	118.30
2	L5	209	U	C6-N1-C1'	-5.13	114.02	121.20
2	L5	1252	C	C6-N1-C2	-5.11	118.25	120.30
2	L5	2033	A	P-O3'-C3'	5.10	125.82	119.70
2	L5	2710	C	C5-C6-N1	5.10	123.55	121.00
2	L5	2262	G	N3-C4-N9	5.09	129.05	126.00
2	L5	4758	U	N1-C2-O2	5.08	126.36	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L5	1853	G	C4-N9-C1'	5.08	133.11	126.50
2	L5	1216	C	N3-C2-O2	-5.08	118.35	121.90
2	L5	1081	C	N1-C2-O2	5.07	121.94	118.90
20	LQ	28	LEU	CA-CB-CG	5.06	126.95	115.30
2	L5	2257	C	N1-C2-O2	5.06	121.94	118.90
2	L5	2410	C	C5-C6-N1	5.05	123.52	121.00
2	L5	1182	C	C2-N1-C1'	5.05	124.35	118.80
2	L5	2262	G	N3-C4-C5	-5.05	126.08	128.60
2	L5	3909	C	C6-N1-C2	-5.05	118.28	120.30
2	L5	4924	C	N3-C2-O2	-5.04	118.37	121.90
2	L5	513	U	N1-C2-O2	5.04	126.32	122.80
2	L5	100	C	N1-C2-O2	5.02	121.91	118.90
2	L5	1367	C	C2-N1-C1'	5.02	124.32	118.80
2	L5	26	C	C6-N1-C2	-5.01	118.30	120.30
2	L5	181	C	C6-N1-C2	-5.01	118.30	120.30

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	LA	13	GLY	Peptide
6	LB	17	LEU	Peptide
6	LB	258	HIS	Peptide
15	LL	154	VAL	Peptide
16	LM	87	ALA	Peptide
16	LM	88	ALA	Peptide
18	LO	110	PRO	Peptide
23	LT	136	ARG	Peptide
34	Lf	106	TYR	Peptide
34	Lf	79	GLY	Peptide
36	Lh	86	LYS	Peptide
38	Lj	39	TYR	Peptide
38	Lj	40	PRO	Peptide

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	
1	LW	61/124 (49%)	55 (90%)	6 (10%)	0	100	100
5	LA	246/248 (99%)	223 (91%)	22 (9%)	1 (0%)	30	58
6	LB	400/402 (100%)	373 (93%)	27 (7%)	0	100	100
7	LC	366/368 (100%)	342 (93%)	24 (7%)	0	100	100
8	LD	291/293 (99%)	272 (94%)	19 (6%)	0	100	100
9	LE	232/247 (94%)	210 (90%)	22 (10%)	0	100	100
10	LF	223/225 (99%)	214 (96%)	9 (4%)	0	100	100
11	LG	239/241 (99%)	224 (94%)	15 (6%)	0	100	100
12	LH	188/190 (99%)	170 (90%)	18 (10%)	0	100	100
13	LI	198/213 (93%)	188 (95%)	10 (5%)	0	100	100
14	LJ	174/176 (99%)	158 (91%)	16 (9%)	0	100	100
15	LL	208/210 (99%)	191 (92%)	17 (8%)	0	100	100
16	LM	137/139 (99%)	129 (94%)	7 (5%)	1 (1%)	19	46
17	LN	201/203 (99%)	193 (96%)	7 (4%)	1 (0%)	25	53
18	LO	199/201 (99%)	191 (96%)	8 (4%)	0	100	100
19	LP	151/153 (99%)	141 (93%)	10 (7%)	0	100	100
20	LQ	185/187 (99%)	177 (96%)	8 (4%)	0	100	100
21	LR	149/187 (80%)	142 (95%)	7 (5%)	0	100	100
22	LS	173/175 (99%)	162 (94%)	11 (6%)	0	100	100
23	LT	157/159 (99%)	146 (93%)	11 (7%)	0	100	100
24	LU	99/101 (98%)	81 (82%)	18 (18%)	0	100	100
25	LV	129/131 (98%)	123 (95%)	6 (5%)	0	100	100
26	LX	118/120 (98%)	115 (98%)	3 (2%)	0	100	100
27	LY	132/134 (98%)	127 (96%)	5 (4%)	0	100	100
28	LZ	133/135 (98%)	125 (94%)	8 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	La	145/147 (99%)	137 (94%)	8 (6%)	0	100	100
30	Lb	105/121 (87%)	94 (90%)	11 (10%)	0	100	100
31	Lc	96/98 (98%)	86 (90%)	10 (10%)	0	100	100
32	Ld	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
33	Le	126/128 (98%)	118 (94%)	7 (6%)	1 (1%)	16	42
34	Lf	107/109 (98%)	98 (92%)	8 (8%)	1 (1%)	14	39
35	Lg	112/114 (98%)	111 (99%)	1 (1%)	0	100	100
36	Lh	120/122 (98%)	119 (99%)	1 (1%)	0	100	100
37	Li	100/102 (98%)	97 (97%)	3 (3%)	0	100	100
38	Lj	84/86 (98%)	79 (94%)	5 (6%)	0	100	100
39	Lk	67/69 (97%)	62 (92%)	5 (8%)	0	100	100
40	Ll	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
41	Lm	50/52 (96%)	50 (100%)	0	0	100	100
42	Lo	103/105 (98%)	99 (96%)	4 (4%)	0	100	100
43	Lp	89/91 (98%)	84 (94%)	5 (6%)	0	100	100
44	Lr	123/125 (98%)	114 (93%)	9 (7%)	0	100	100
45	CA	350/356 (98%)	328 (94%)	20 (6%)	2 (1%)	22	49
All	All	6719/6944 (97%)	6293 (94%)	419 (6%)	7 (0%)	50	75

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
45	CA	142[A]	VAL
17	LN	124	ASP
45	CA	78	THR
16	LM	88	ALA
34	Lf	107	PRO
5	LA	55	GLY
33	Le	73	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	LW	55/103 (53%)	48 (87%)	7 (13%)	3	10
5	LA	190/190 (100%)	172 (90%)	18 (10%)	7	20
6	LB	348/348 (100%)	324 (93%)	24 (7%)	13	34
7	LC	306/306 (100%)	284 (93%)	22 (7%)	12	32
8	LD	246/247 (100%)	230 (94%)	16 (6%)	14	37
9	LE	209/220 (95%)	191 (91%)	18 (9%)	8	25
10	LF	194/194 (100%)	182 (94%)	12 (6%)	15	39
11	LG	203/205 (99%)	192 (95%)	11 (5%)	18	46
12	LH	169/169 (100%)	149 (88%)	20 (12%)	4	12
13	LI	172/180 (96%)	158 (92%)	14 (8%)	9	27
14	LJ	148/148 (100%)	134 (90%)	14 (10%)	7	20
15	LL	176/176 (100%)	169 (96%)	7 (4%)	27	58
16	LM	118/118 (100%)	111 (94%)	7 (6%)	16	42
17	LN	171/171 (100%)	162 (95%)	9 (5%)	19	46
18	LO	173/173 (100%)	164 (95%)	9 (5%)	19	47
19	LP	134/134 (100%)	121 (90%)	13 (10%)	6	19
20	LQ	164/164 (100%)	154 (94%)	10 (6%)	15	40
21	LR	137/166 (82%)	128 (93%)	9 (7%)	14	36
22	LS	156/156 (100%)	144 (92%)	12 (8%)	10	29
23	LT	139/139 (100%)	133 (96%)	6 (4%)	25	55
24	LU	91/91 (100%)	79 (87%)	12 (13%)	3	9
25	LV	101/101 (100%)	95 (94%)	6 (6%)	16	42
26	LX	108/108 (100%)	100 (93%)	8 (7%)	11	31
27	LY	124/124 (100%)	112 (90%)	12 (10%)	6	19
28	LZ	117/117 (100%)	112 (96%)	5 (4%)	25	55
29	La	120/120 (100%)	116 (97%)	4 (3%)	33	65
30	Lb	88/101 (87%)	81 (92%)	7 (8%)	10	27
31	Lc	83/83 (100%)	80 (96%)	3 (4%)	30	62
32	Ld	98/98 (100%)	90 (92%)	8 (8%)	9	26
33	Le	114/114 (100%)	107 (94%)	7 (6%)	15	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	Lf	88/88 (100%)	79 (90%)	9 (10%)	6	17
35	Lg	98/98 (100%)	88 (90%)	10 (10%)	6	17
36	Lh	109/109 (100%)	102 (94%)	7 (6%)	14	38
37	Li	86/86 (100%)	78 (91%)	8 (9%)	7	21
38	Lj	73/73 (100%)	67 (92%)	6 (8%)	9	26
39	Lk	64/64 (100%)	63 (98%)	1 (2%)	58	82
40	Ll	47/47 (100%)	44 (94%)	3 (6%)	14	38
41	Lm	48/48 (100%)	47 (98%)	1 (2%)	48	76
42	Lo	93/93 (100%)	90 (97%)	3 (3%)	34	66
43	Lp	74/74 (100%)	67 (90%)	7 (10%)	7	20
44	Lr	109/109 (100%)	98 (90%)	11 (10%)	6	18
45	CA	303/305 (99%)	274 (90%)	29 (10%)	7	20
All	All	5844/5958 (98%)	5419 (93%)	425 (7%)	14	32

All (425) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	LW	19	ARG
1	LW	23	ARG
1	LW	30	GLN
1	LW	32	LEU
1	LW	38	SER
1	LW	55	TYR
1	LW	60	LYS
5	LA	3	ARG
5	LA	15	VAL
5	LA	30	ARG
5	LA	47	ASP
5	LA	54	ARG
5	LA	65	ASP
5	LA	68	ARG
5	LA	75	LEU
5	LA	77	ILE
5	LA	102	LEU
5	LA	111	THR
5	LA	146	THR
5	LA	154	SER
5	LA	169	VAL

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Mol	Chain	Res	Type
5	LA	207	VAL
5	LA	208	GLU
5	LA	221	LYS
5	LA	223	SER
6	LB	7	SER
6	LB	73	VAL
6	LB	111	SER
6	LB	112	ASP
6	LB	125	SER
6	LB	126	LYS
6	LB	155	LYS
6	LB	159	VAL
6	LB	169	ARG
6	LB	174	ARG
6	LB	181	MET
6	LB	194	LEU
6	LB	200	ARG
6	LB	258	HIS
6	LB	278	THR
6	LB	297	LYS
6	LB	298	LEU
6	LB	328	ASN
6	LB	329	ASP
6	LB	358	ARG
6	LB	360	LEU
6	LB	378	ARG
6	LB	384	GLU
6	LB	389	MET
7	LC	16	GLU
7	LC	50	GLN
7	LC	63	SER
7	LC	67	TRP
7	LC	95	MET
7	LC	106	LYS
7	LC	114	ARG
7	LC	122	TYR
7	LC	143	ARG
7	LC	154	VAL
7	LC	175	LYS
7	LC	188	ARG
7	LC	228	THR
7	LC	230	LEU

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Mol	Chain	Res	Type
7	LC	234	LYS
7	LC	261	ASP
7	LC	263	LEU
7	LC	319	LEU
7	LC	336	ARG
7	LC	350	ARG
7	LC	352	ASP
7	LC	366	ASP
8	LD	4	VAL
8	LD	48	LYS
8	LD	51	MET
8	LD	59	ASP
8	LD	88	VAL
8	LD	115	MET
8	LD	117	LYS
8	LD	126	THR
8	LD	128	ASP
8	LD	185	SER
8	LD	194	VAL
8	LD	200	MET
8	LD	214	GLU
8	LD	235	MET
8	LD	259	LYS
8	LD	289	ARG
9	LE	45	SER
9	LE	51	VAL
9	LE	91	THR
9	LE	106	VAL
9	LE	107	VAL
9	LE	110	ARG
9	LE	112	MET
9	LE	120	ASP
9	LE	124	LYS
9	LE	128	HIS
9	LE	130	LYS
9	LE	166	LYS
9	LE	187	ARG
9	LE	199	THR
9	LE	204	SER
9	LE	220	LYS
9	LE	236	GLU
9	LE	273	SER

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Mol	Chain	Res	Type
10	LF	36	LYS
10	LF	40	LYS
10	LF	44	LYS
10	LF	74	MET
10	LF	96	ARG
10	LF	102	SER
10	LF	178	SER
10	LF	189	ASP
10	LF	196	THR
10	LF	212	LYS
10	LF	221	LYS
10	LF	248	ASN
11	LG	33	GLU
11	LG	35	ARG
11	LG	73	ARG
11	LG	91	THR
11	LG	105	GLU
11	LG	108	GLN
11	LG	166	LEU
11	LG	170	LEU
11	LG	176	LYS
11	LG	206	GLN
11	LG	261	LEU
12	LH	6	SER
12	LH	16	VAL
12	LH	17	ASP
12	LH	33	THR
12	LH	37	ASP
12	LH	50	LYS
12	LH	51	LYS
12	LH	57	VAL
12	LH	64	ARG
12	LH	85	THR
12	LH	92	MET
12	LH	94	SER
12	LH	111	LEU
12	LH	113	GLU
12	LH	129	ARG
12	LH	135	SER
12	LH	143	GLU
12	LH	170	LYS
12	LH	183	GLU

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Mol	Chain	Res	Type
12	LH	187	VAL
13	LI	12	CYS
13	LI	38	ARG
13	LI	43	VAL
13	LI	45	GLU
13	LI	53	VAL
13	LI	63	GLU
13	LI	83	ASP
13	LI	129	VAL
13	LI	140	THR
13	LI	162	ARG
13	LI	175	LYS
13	LI	183	ASP
13	LI	192	PRO
13	LI	195	CYS
14	LJ	5	GLN
14	LJ	35	ARG
14	LJ	51	SER
14	LJ	57	VAL
14	LJ	60	PHE
14	LJ	63	ARG
14	LJ	72	CYS
14	LJ	73	THR
14	LJ	119	TYR
14	LJ	128	LEU
14	LJ	129	ASP
14	LJ	132	VAL
14	LJ	158	SER
14	LJ	169	LYS
15	LL	64	VAL
15	LL	67	HIS
15	LL	70	VAL
15	LL	98	VAL
15	LL	103	ARG
15	LL	115	GLN
15	LL	139	SER
16	LM	35	ARG
16	LM	37	LEU
16	LM	46	ARG
16	LM	48	GLN
16	LM	67	SER
16	LM	118	MET

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Mol	Chain	Res	Type
16	LM	136	LEU
17	LN	5	LYS
17	LN	18	VAL
17	LN	41	ARG
17	LN	67	ARG
17	LN	73	ARG
17	LN	125	SER
17	LN	151	ILE
17	LN	182	HIS
17	LN	187	SER
18	LO	18	ARG
18	LO	27	VAL
18	LO	63	ASN
18	LO	67	SER
18	LO	87	MET
18	LO	100	ASP
18	LO	145	VAL
18	LO	175	MET
18	LO	202	LEU
19	LP	2	VAL
19	LP	18	ARG
19	LP	24	VAL
19	LP	30	ARG
19	LP	57	CYS
19	LP	69	ARG
19	LP	79	THR
19	LP	93	HIS
19	LP	100	SER
19	LP	103	GLU
19	LP	111	SER
19	LP	126	ARG
19	LP	148	MET
20	LQ	3	VAL
20	LQ	20	SER
20	LQ	28	LEU
20	LQ	62	SER
20	LQ	71	LYS
20	LQ	77	ASN
20	LQ	124	ASP
20	LQ	163	THR
20	LQ	168	ARG
20	LQ	180	ARG

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Mol	Chain	Res	Type
21	LR	12	SER
21	LR	13	SER
21	LR	47	ASP
21	LR	52	ARG
21	LR	59	SER
21	LR	113	LYS
21	LR	136	ARG
21	LR	145	LEU
21	LR	152	LYS
22	LS	19	THR
22	LS	22	CYS
22	LS	52	LYS
22	LS	53	LYS
22	LS	57	SER
22	LS	58	SER
22	LS	77	ASN
22	LS	107	THR
22	LS	154	LEU
22	LS	158	VAL
22	LS	159	LEU
22	LS	169	THR
23	LT	3	ASN
23	LT	50	LYS
23	LT	83	LYS
23	LT	102	ARG
23	LT	104	SER
23	LT	136	ARG
24	LU	19	LEU
24	LU	22	THR
24	LU	25	CYS
24	LU	40	GLU
24	LU	41	GLN
24	LU	44	GLN
24	LU	55	ASN
24	LU	67	LYS
24	LU	74	SER
24	LU	76	VAL
24	LU	79	SER
24	LU	110	TYR
25	LV	36	ASN
25	LV	43	LYS
25	LV	48	ARG

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Mol	Chain	Res	Type
25	LV	59	ASP
25	LV	90	ARG
25	LV	115	SER
26	LX	63	LYS
26	LX	67	ARG
26	LX	68	ARG
26	LX	85	SER
26	LX	87	MET
26	LX	96	LEU
26	LX	121	VAL
26	LX	134	LYS
27	LY	12	SER
27	LY	17	ARG
27	LY	23	SER
27	LY	41	LYS
27	LY	46	SER
27	LY	74	TYR
27	LY	83	GLU
27	LY	84	ARG
27	LY	108	ARG
27	LY	111	LEU
27	LY	115	ARG
27	LY	128	VAL
28	LZ	27	LYS
28	LZ	31	ASP
28	LZ	39	SER
28	LZ	100	VAL
28	LZ	126	LYS
29	La	15	VAL
29	La	77	LYS
29	La	87	ARG
29	La	145	VAL
30	Lb	23	LYS
30	Lb	40	LEU
30	Lb	44	ARG
30	Lb	90	SER
30	Lb	91	ARG
30	Lb	114	LYS
30	Lb	117	ARG
31	Lc	56	ARG
31	Lc	91	VAL
31	Lc	93	THR

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Mol	Chain	Res	Type
32	Ld	26	THR
32	Ld	67	ARG
32	Ld	87	ARG
32	Ld	92	ARG
32	Ld	95	ASP
32	Ld	104	THR
32	Ld	106	VAL
32	Ld	118	GLN
33	Le	33	ARG
33	Le	45	VAL
33	Le	62	SER
33	Le	102	ASN
33	Le	123	THR
33	Le	126	ASN
33	Le	129	LEU
34	Lf	19	ARG
34	Lf	25	THR
34	Lf	33	VAL
34	Lf	37	ASP
34	Lf	40	GLU
34	Lf	63	LYS
34	Lf	73	LYS
34	Lf	83	MET
34	Lf	90	SER
35	Lg	19	LYS
35	Lg	20	THR
35	Lg	21	ARG
35	Lg	28	ASN
35	Lg	29	ARG
35	Lg	32	TYR
35	Lg	49	CYS
35	Lg	63	VAL
35	Lg	73	HIS
35	Lg	83	CYS
36	Lh	13	LYS
36	Lh	19	LYS
36	Lh	30	GLN
36	Lh	65	GLN
36	Lh	87	LYS
36	Lh	94	ARG
36	Lh	109	ARG
37	Li	3	LEU

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Mol	Chain	Res	Type
37	Li	4	ARG
37	Li	32	ARG
37	Li	34	THR
37	Li	45	ARG
37	Li	68	ARG
37	Li	98	ARG
37	Li	99	LYS
38	Lj	6	SER
38	Lj	7	SER
38	Lj	22	CYS
38	Lj	36	LYS
38	Lj	80	GLU
38	Lj	87	LYS
39	Lk	50	LYS
40	Ll	37	TYR
40	Ll	41	ARG
40	Ll	47	THR
41	Lm	127	VAL
42	Lo	22	LYS
42	Lo	27	LYS
42	Lo	77	CYS
43	Lp	3	LYS
43	Lp	6	LYS
43	Lp	24	LYS
43	Lp	28	LYS
43	Lp	36	LYS
43	Lp	63	THR
43	Lp	83	ILE
44	Lr	14	SER
44	Lr	20	ARG
44	Lr	21	ASN
44	Lr	58	LYS
44	Lr	61	VAL
44	Lr	66	ARG
44	Lr	67	ARG
44	Lr	76	SER
44	Lr	80	THR
44	Lr	84	LYS
44	Lr	125	MET
45	CA	20	LYS
45	CA	51	LYS
45	CA	53	ASP

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Mol	Chain	Res	Type
45	CA	70	MET
45	CA	72	LYS
45	CA	92	LEU
45	CA	128	ASP
45	CA	134	GLN
45	CA	158	LYS
45	CA	183	GLU
45	CA	206	THR
45	CA	209	GLN
45	CA	229	LEU
45	CA	236	LYS
45	CA	243	ARG
45	CA	267	SER
45	CA	268	GLU
45	CA	281	ARG
45	CA	287	LYS
45	CA	303	GLN
45	CA	311	LYS
45	CA	315	PHE
45	CA	320	LYS
45	CA	321	PHE
45	CA	326	MET
45	CA	331	MET
45	CA	342	LEU
45	CA	344	LYS
45	CA	346	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
5	LA	132	ASN
9	LE	227	HIS
11	LG	206	GLN
17	LN	8	GLN
29	La	93	ASN
33	Le	57	ASN
45	CA	88	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	L5	3638/5070 (71%)	785 (21%)	18 (0%)
3	L7	119/120 (99%)	13 (10%)	0
4	L8	155/156 (99%)	26 (16%)	0
All	All	3912/5346 (73%)	824 (21%)	18 (0%)

All (824) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	L5	2	G
2	L5	17	A
2	L5	25	A
2	L5	26	C
2	L5	30	C
2	L5	39	A
2	L5	42	A
2	L5	48	G
2	L5	56	A
2	L5	59	A
2	L5	64	A
2	L5	65	A
2	L5	66	A
2	L5	69	A
2	L5	73	A
2	L5	91	G
2	L5	104	G
2	L5	108	A
2	L5	109	G
2	L5	110	C
2	L5	119	G
2	L5	120	A
2	L5	132	G
2	L5	133	C
2	L5	134	G
2	L5	135	G
2	L5	136	C
2	L5	152	U
2	L5	158	A
2	L5	159	C
2	L5	165	A
2	L5	172	C
2	L5	182	G
2	L5	183	C
2	L5	184	U

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Mol	Chain	Res	Type
2	L5	185	C
2	L5	187	U
2	L5	188	G
2	L5	189	G
2	L5	200	U
2	L5	209	U
2	L5	210	C
2	L5	216	C
2	L5	218	A
2	L5	220	C
2	L5	234	G
2	L5	253	G
2	L5	255	C
2	L5	256	G
2	L5	261	G
2	L5	264	C
2	L5	265	C
2	L5	266	C
2	L5	267	G
2	L5	269	G
2	L5	276	C
2	L5	278	G
2	L5	280	G
2	L5	297	U
2	L5	306	A
2	L5	315	G
2	L5	316	U
2	L5	340	C
2	L5	347	A
2	L5	350	C
2	L5	373	G
2	L5	387	G
2	L5	388	A
2	L5	407	A
2	L5	409	G
2	L5	410	A
2	L5	411	G
2	L5	412	G
2	L5	413	G
2	L5	415	G
2	L5	431	G
2	L5	432	U

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Mol	Chain	Res	Type
2	L5	449	C
2	L5	450	G
2	L5	452	A
2	L5	453	G
2	L5	454	U
2	L5	456	C
2	L5	457	G
2	L5	467	U
2	L5	486	C
2	L5	489	C
2	L5	493	G
2	L5	494	U
2	L5	497	G
2	L5	498	C
2	L5	499	G
2	L5	500	G
2	L5	501	C
2	L5	502	C
2	L5	503	C
2	L5	504	G
2	L5	505	G
2	L5	509	A
2	L5	510	U
2	L5	512	U
2	L5	513	U
2	L5	514	U
2	L5	515	C
2	L5	517	C
2	L5	518	G
2	L5	643	C
2	L5	644	G
2	L5	646	G
2	L5	653	U
2	L5	654	C
2	L5	656	C
2	L5	657	C
2	L5	659	G
2	L5	666	G
2	L5	667	A
2	L5	668	C
2	L5	669	C
2	L5	673	C

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Mol	Chain	Res	Type
2	L5	685	C
2	L5	686	A
2	L5	687	U
2	L5	696	C
2	L5	703	G
2	L5	704	C
2	L5	706	C
2	L5	708	G
2	L5	730	G
2	L5	731	G
2	L5	738	C
2	L5	739	G
2	L5	742	G
2	L5	746	A
2	L5	747	A
2	L5	759	G
2	L5	904	C
2	L5	905	C
2	L5	906	C
2	L5	910	G
2	L5	913	U
2	L5	914	U
2	L5	915	A
2	L5	917	A
2	L5	918	G
2	L5	923	C
2	L5	924	C
2	L5	926	G
2	L5	932	A
2	L5	933	G
2	L5	936	C
2	L5	943	A
2	L5	944	A
2	L5	945	U
2	L5	958	G
2	L5	959	G
2	L5	960	A
2	L5	961	G
2	L5	962	C
2	L5	963	G
2	L5	965	G
2	L5	966	A

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Mol	Chain	Res	Type
2	L5	967	C
2	L5	969	C
2	L5	970	G
2	L5	971	U
2	L5	977	C
2	L5	982	U
2	L5	985	C
2	L5	988	C
2	L5	989	U
2	L5	990	C
2	L5	1070	G
2	L5	1072	C
2	L5	1075	G
2	L5	1082	C
2	L5	1083	U
2	L5	1095	A
2	L5	1168	G
2	L5	1171	G
2	L5	1172	C
2	L5	1173	G
2	L5	1179	U
2	L5	1180	C
2	L5	1181	C
2	L5	1182	C
2	L5	1183	C
2	L5	1202	C
2	L5	1203	G
2	L5	1210	C
2	L5	1211	G
2	L5	1214	C
2	L5	1215	C
2	L5	1218	G
2	L5	1219	G
2	L5	1222	A
2	L5	1235	G
2	L5	1241	C
2	L5	1242	G
2	L5	1253	G
2	L5	1254	A
2	L5	1257	A
2	L5	1258	G
2	L5	1266	G

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Mol	Chain	Res	Type
2	L5	1267	C
2	L5	1269	G
2	L5	1270	A
2	L5	1271	G
2	L5	1272	C
2	L5	1273	G
2	L5	1275	G
2	L5	1277	G
2	L5	1280	C
2	L5	1284	G
2	L5	1287	G
2	L5	1293	G
2	L5	1294	A
2	L5	1295	C
2	L5	1296	G
2	L5	1301	C
2	L5	1302	U
2	L5	1312	A
2	L5	1326	A
2	L5	1354	A
2	L5	1358	G
2	L5	1359	G
2	L5	1365	C
2	L5	1367	C
2	L5	1387	A
2	L5	1394	G
2	L5	1397	A
2	L5	1404	G
2	L5	1407	C
2	L5	1409	C
2	L5	1410	U
2	L5	1415	G
2	L5	1417	C
2	L5	1420	A
2	L5	1437	C
2	L5	1439	C
2	L5	1442	C
2	L5	1443	A
2	L5	1444	G
2	L5	1446	C
2	L5	1447	C
2	L5	1457	G

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Mol	Chain	Res	Type
2	L5	1465	G
2	L5	1480	C
2	L5	1482	G
2	L5	1483	C
2	L5	1493	G
2	L5	1497	A
2	L5	1498	G
2	L5	1502	G
2	L5	1517	G
2	L5	1518	A
2	L5	1525	A
2	L5	1534	A
2	L5	1535	C
2	L5	1562	G
2	L5	1566	C
2	L5	1574	G
2	L5	1578	U
2	L5	1582	U
2	L5	1591	U
2	L5	1596	U
2	L5	1612	G
2	L5	1621	A
2	L5	1624	G
2	L5	1625	G
2	L5	1631	A
2	L5	1633	G
2	L5	1634	A
2	L5	1638	A
2	L5	1640	C
2	L5	1641	G
2	L5	1642	A
2	L5	1654	G
2	L5	1661	C
2	L5	1663	C
2	L5	1676	C
2	L5	1677	U
2	L5	1678	C
2	L5	1694	C
2	L5	1699	A
2	L5	1700	G
2	L5	1703	C
2	L5	1704	C

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Mol	Chain	Res	Type
2	L5	1705	G
2	L5	1726	U
2	L5	1731	C
2	L5	1733	G
2	L5	1734	G
2	L5	1741	G
2	L5	1742	A
2	L5	1750	G
2	L5	1757	U
2	L5	1758	G
2	L5	1760	G
2	L5	1761	G
2	L5	1762	C
2	L5	1763	C
2	L5	1764	G
2	L5	1765	A
2	L5	1766	A
2	L5	1767	A
2	L5	1768	C
2	L5	1769	G
2	L5	1770	A
2	L5	1787	A
2	L5	1803	G
2	L5	1804	A
2	L5	1806	G
2	L5	1810	G
2	L5	1820	C
2	L5	1821	G
2	L5	1822	U
2	L5	1836	G
2	L5	1837	A
2	L5	1842	G
2	L5	1855	G
2	L5	1869	G
2	L5	1882	U
2	L5	1897	A
2	L5	1917	A
2	L5	1918	U
2	L5	1919	G
2	L5	1920	C
2	L5	1921	C
2	L5	1922	G

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Mol	Chain	Res	Type
2	L5	1925	G
2	L5	1931	C
2	L5	1932	A
2	L5	1936	C
2	L5	1940	G
2	L5	1948	G
2	L5	1949	U
2	L5	1961	G
2	L5	1962	A
2	L5	1971	C
2	L5	1974	U
2	L5	1975	G
2	L5	1978	C
2	L5	1980	U
2	L5	1981	G
2	L5	1982	G
2	L5	1984	A
2	L5	1985	G
2	L5	1986	U
2	L5	1987	C
2	L5	1991	A
2	L5	1992	U
2	L5	1993	C
2	L5	1997	U
2	L5	1998	A
2	L5	1999	A
2	L5	2001	G
2	L5	2002	A
2	L5	2003	G
2	L5	2011	C
2	L5	2017	A
2	L5	2018	C
2	L5	2024	G
2	L5	2026	A
2	L5	2033	A
2	L5	2034	G
2	L5	2046	G
2	L5	2048	U
2	L5	2055	G
2	L5	2056	G
2	L5	2069	A
2	L5	2084	C

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Mol	Chain	Res	Type
2	L5	2092	G
2	L5	2093	A
2	L5	2095	A
2	L5	2096	G
2	L5	2097	U
2	L5	2098	G
2	L5	2101	C
2	L5	2102	G
2	L5	2103	G
2	L5	2105	A
2	L5	2107	C
2	L5	2108	G
2	L5	2110	C
2	L5	2111	G
2	L5	2112	G
2	L5	2250	C
2	L5	2252	G
2	L5	2253	A
2	L5	2256	C
2	L5	2258	C
2	L5	2259	G
2	L5	2260	C
2	L5	2261	G
2	L5	2289	C
2	L5	2300	A
2	L5	2301	G
2	L5	2306	G
2	L5	2313	A
2	L5	2331	G
2	L5	2332	A
2	L5	2333	G
2	L5	2345	G
2	L5	2348	G
2	L5	2351	C
2	L5	2360	A
2	L5	2382	A
2	L5	2395	A
2	L5	2397	G
2	L5	2398	U
2	L5	2402	G
2	L5	2404	A
2	L5	2412	A

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Mol	Chain	Res	Type
2	L5	2417	A
2	L5	2421	G
2	L5	2425	U
2	L5	2441	C
2	L5	2450	G
2	L5	2453	A
2	L5	2464	C
2	L5	2465	C
2	L5	2469	C
2	L5	2471	G
2	L5	2474	G
2	L5	2475	G
2	L5	2478	C
2	L5	2479	G
2	L5	2483	G
2	L5	2484	A
2	L5	2485	U
2	L5	2486	G
2	L5	2487	G
2	L5	2488	C
2	L5	2489	C
2	L5	2490	U
2	L5	2503	G
2	L5	2504	C
2	L5	2505	C
2	L5	2506	G
2	L5	2513	A
2	L5	2519	U
2	L5	2520	C
2	L5	2536	A
2	L5	2537	A
2	L5	2544	G
2	L5	2546	G
2	L5	2547	G
2	L5	2554	U
2	L5	2555	G
2	L5	2560	C
2	L5	2565	A
2	L5	2567	G
2	L5	2573	A
2	L5	2583	C
2	L5	2587	A

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Mol	Chain	Res	Type
2	L5	2589	C
2	L5	2606	G
2	L5	2618	G
2	L5	2627	C
2	L5	2640	G
2	L5	2652	G
2	L5	2653	C
2	L5	2662	G
2	L5	2664	G
2	L5	2669	C
2	L5	2675	G
2	L5	2676	A
2	L5	2687	U
2	L5	2694	G
2	L5	2695	A
2	L5	2696	A
2	L5	2703	G
2	L5	2707	U
2	L5	2708	U
2	L5	2710	C
2	L5	2711	G
2	L5	2721	G
2	L5	2724	G
2	L5	2726	G
2	L5	2738	C
2	L5	2739	C
2	L5	2742	G
2	L5	2743	A
2	L5	2746	A
2	L5	2761	U
2	L5	2763	U
2	L5	2769	U
2	L5	2770	C
2	L5	2787	A
2	L5	2788	U
2	L5	2790	U
2	L5	2826	U
2	L5	2827	G
2	L5	2829	U
2	L5	2835	A
2	L5	2838	G
2	L5	2848	G

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Mol	Chain	Res	Type
2	L5	2855	G
2	L5	2875	C
2	L5	2892	C
2	L5	2897	G
2	L5	2900	U
2	L5	2902	G
2	L5	2903	G
2	L5	2904	U
2	L5	2905	C
2	L5	2906	G
2	L5	2908	U
2	L5	3588	C
2	L5	3590	G
2	L5	3591	C
2	L5	3594	C
2	L5	3595	U
2	L5	3596	A
2	L5	3597	G
2	L5	3599	A
2	L5	3604	A
2	L5	3605	C
2	L5	3615	G
2	L5	3617	G
2	L5	3626	G
2	L5	3630	A
2	L5	3635	A
2	L5	3644	U
2	L5	3646	A
2	L5	3648	A
2	L5	3662	A
2	L5	3664	G
2	L5	3670	C
2	L5	3673	C
2	L5	3674	G
2	L5	3680	U
2	L5	3710	G
2	L5	3711	A
2	L5	3713	U
2	L5	3714	G
2	L5	3727	A
2	L5	3748	A
2	L5	3750	G

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Mol	Chain	Res	Type
2	L5	3753	G
2	L5	3756	A
2	L5	3759	A
2	L5	3760	A
2	L5	3761	C
2	L5	3773	U
2	L5	3774	A
2	L5	3776	G
2	L5	3777	G
2	L5	3778	U
2	L5	3783	A
2	L5	3784	A
2	L5	3786	U
2	L5	3802	U
2	L5	3811	G
2	L5	3812	C
2	L5	3813	A
2	L5	3814	U
2	L5	3817	A
2	L5	3818	U
2	L5	3819	G
2	L5	3823	G
2	L5	3824	A
2	L5	3838	U
2	L5	3839	G
2	L5	3840	U
2	L5	3867	A
2	L5	3877	A
2	L5	3878	C
2	L5	3879	G
2	L5	3885	G
2	L5	3887	C
2	L5	3890	A
2	L5	3892	U
2	L5	3897	G
2	L5	3901	A
2	L5	3906	A
2	L5	3907	G
2	L5	3908	A
2	L5	3915	U
2	L5	3938	G
2	L5	3939	G

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Mol	Chain	Res	Type
2	L5	3942	A
2	L5	3943	A
2	L5	3947	A
2	L5	3949	A
2	L5	3950	U
2	L5	3953	G
2	L5	4057	C
2	L5	4058	U
2	L5	4059	C
2	L5	4060	U
2	L5	4061	G
2	L5	4062	A
2	L5	4064	C
2	L5	4068	U
2	L5	4069	U
2	L5	4076	G
2	L5	4084	G
2	L5	4092	G
2	L5	4093	G
2	L5	4095	G
2	L5	4097	G
2	L5	4099	G
2	L5	4101	C
2	L5	4102	C
2	L5	4103	C
2	L5	4104	G
2	L5	4108	G
2	L5	4111	U
2	L5	4114	C
2	L5	4115	G
2	L5	4116	C
2	L5	4117	U
2	L5	4119	C
2	L5	4127	A
2	L5	4140	C
2	L5	4141	G
2	L5	4142	C
2	L5	4143	G
2	L5	4144	C
2	L5	4146	G
2	L5	4149	C
2	L5	4162	C

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Mol	Chain	Res	Type
2	L5	4163	U
2	L5	4170	A
2	L5	4177	C
2	L5	4183	G
2	L5	4184	G
2	L5	4191	G
2	L5	4196	G
2	L5	4197	G
2	L5	4203	A
2	L5	4222	G
2	L5	4225	G
2	L5	4229	U
2	L5	4232	U
2	L5	4233	A
2	L5	4234	A
2	L5	4242	U
2	L5	4251	A
2	L5	4254	G
2	L5	4256	A
2	L5	4257	A
2	L5	4258	C
2	L5	4265	U
2	L5	4268	A
2	L5	4273	A
2	L5	4281	A
2	L5	4283	G
2	L5	4291	G
2	L5	4295	U
2	L5	4304	A
2	L5	4305	G
2	L5	4314	C
2	L5	4329	G
2	L5	4330	G
2	L5	4332	C
2	L5	4339	A
2	L5	4349	C
2	L5	4373	G
2	L5	4376	A
2	L5	4377	G
2	L5	4378	A
2	L5	4380	A
2	L5	4387	C

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Mol	Chain	Res	Type
2	L5	4391	G
2	L5	4394	A
2	L5	4422	A
2	L5	4438	U
2	L5	4448	G
2	L5	4449	A
2	L5	4453	C
2	L5	4464	A
2	L5	4466	C
2	L5	4475	G
2	L5	4488	A
2	L5	4500	U
2	L5	4512	U
2	L5	4513	A
2	L5	4518	A
2	L5	4519	C
2	L5	4524	G
2	L5	4525	C
2	L5	4545	G
2	L5	4548	A
2	L5	4549	G
2	L5	4557	U
2	L5	4560	C
2	L5	4567	G
2	L5	4573	G
2	L5	4575	G
2	L5	4584	A
2	L5	4589	A
2	L5	4590	A
2	L5	4594	U
2	L5	4600	G
2	L5	4601	U
2	L5	4617	G
2	L5	4636	U
2	L5	4637	G
2	L5	4656	A
2	L5	4657	U
2	L5	4659	G
2	L5	4670	C
2	L5	4672	A
2	L5	4679	G
2	L5	4687	A

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Mol	Chain	Res	Type
2	L5	4694	G
2	L5	4695	C
2	L5	4700	A
2	L5	4708	A
2	L5	4709	U
2	L5	4719	G
2	L5	4733	C
2	L5	4734	A
2	L5	4740	G
2	L5	4741	C
2	L5	4742	G
2	L5	4745	G
2	L5	4754	G
2	L5	4757	C
2	L5	4759	C
2	L5	4761	G
2	L5	4765	G
2	L5	4771	C
2	L5	4772	C
2	L5	4775	C
2	L5	4859	C
2	L5	4860	G
2	L5	4862	G
2	L5	4870	G
2	L5	4871	C
2	L5	4875	G
2	L5	4881	U
2	L5	4882	U
2	L5	4883	C
2	L5	4889	G
2	L5	4895	C
2	L5	4896	G
2	L5	4897	G
2	L5	4900	C
2	L5	4901	G
2	L5	4910	G
2	L5	4912	G
2	L5	4914	C
2	L5	4922	C
2	L5	4923	C
2	L5	4925	U
2	L5	4926	C

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Mol	Chain	Res	Type
2	L5	4927	G
2	L5	4928	C
2	L5	4940	C
2	L5	4941	G
2	L5	4943	A
2	L5	4944	C
2	L5	4947	U
2	L5	4951	G
2	L5	4960	G
2	L5	4973	U
2	L5	4975	G
2	L5	4976	U
2	L5	4985	U
2	L5	4988	U
2	L5	4989	U
2	L5	4990	C
2	L5	4991	U
2	L5	4995	U
2	L5	5009	G
2	L5	5013	C
2	L5	5014	A
2	L5	5017	G
2	L5	5020	G
2	L5	5022	U
2	L5	5023	C
2	L5	5024	C
2	L5	5027	C
2	L5	5028	G
2	L5	5030	U
2	L5	5034	A
2	L5	5041	G
2	L5	5050	C
2	L5	5054	C
2	L5	5055	G
2	L5	5061	A
2	L5	5069	U
3	L7	7	G
3	L7	22	A
3	L7	23	A
3	L7	33	U
3	L7	38	U
3	L7	53	U

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Mol	Chain	Res	Type
3	L7	54	A
3	L7	63	C
3	L7	64	G
3	L7	66	G
3	L7	100	A
3	L7	110	G
3	L7	111	C
4	L8	25	G
4	L8	34	U
4	L8	35	C
4	L8	48	A
4	L8	52	A
4	L8	59	A
4	L8	62	A
4	L8	63	U
4	L8	80	A
4	L8	82	A
4	L8	84	A
4	L8	85	U
4	L8	86	U
4	L8	87	G
4	L8	94	G
4	L8	103	A
4	L8	105	C
4	L8	108	A
4	L8	110	U
4	L8	111	U
4	L8	114	G
4	L8	123	U
4	L8	124	U
4	L8	125	C
4	L8	126	C
4	L8	127	U

All (18) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	L5	265	C
2	L5	406	C
2	L5	914	U
2	L5	1071	C
2	L5	1082	C

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Mol	Chain	Res	Type
2	L5	1633	G
2	L5	1977	C
2	L5	2033	A
2	L5	2416	G
2	L5	2485	U
2	L5	2675	G
2	L5	2760	G
2	L5	2786	C
2	L5	3614	G
2	L5	3673	C
2	L5	4600	G
2	L5	4699	U
2	L5	4913	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 231 ligands modelled in this entry, 231 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
21	LR	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	LR	134:ASN	C	135:LYS	N	2.94

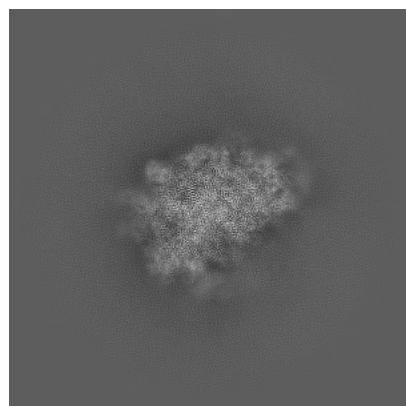
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42318. These allow visual inspection of the internal detail of the map and identification of artifacts.

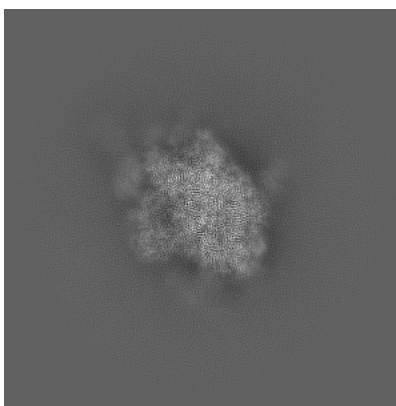
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

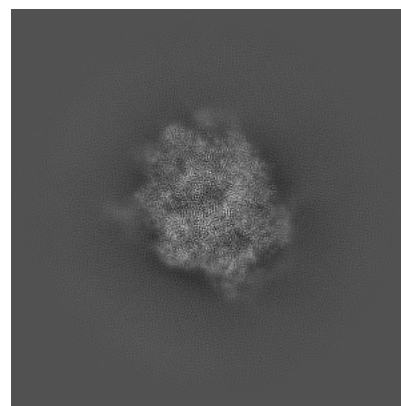
6.1.1 Primary map



X

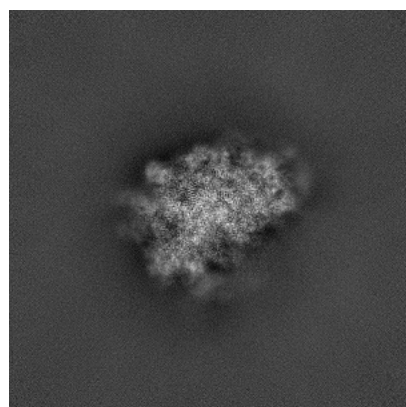


Y

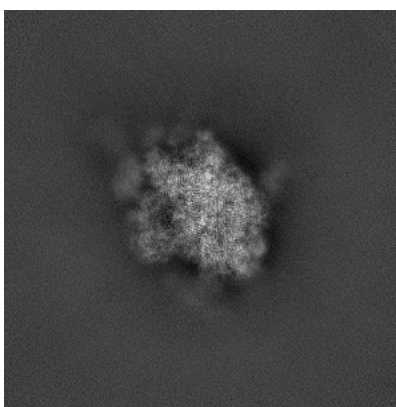


Z

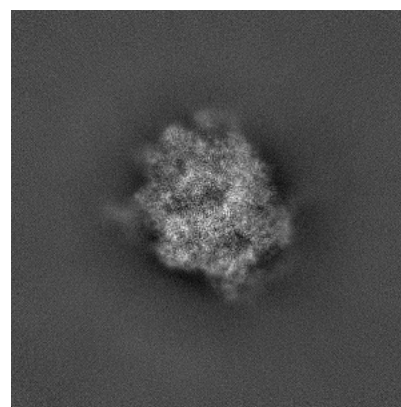
6.1.2 Raw map



X



Y

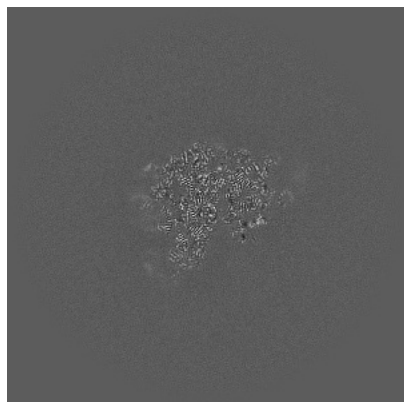


Z

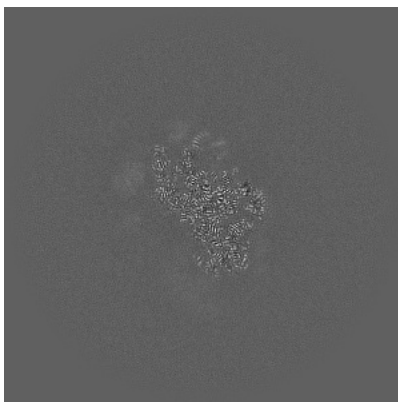
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

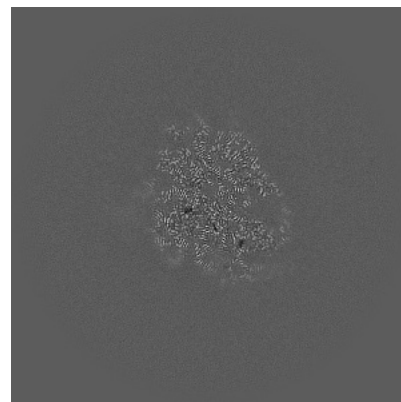
6.2.1 Primary map



X Index: 256

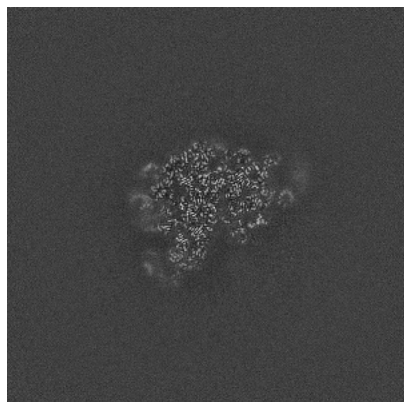


Y Index: 256

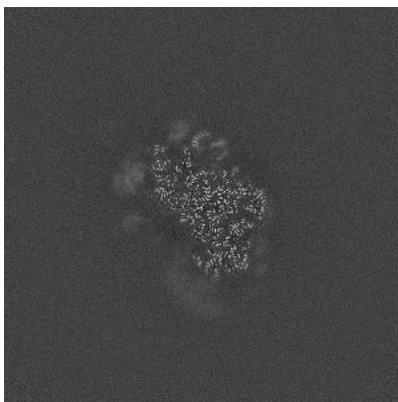


Z Index: 256

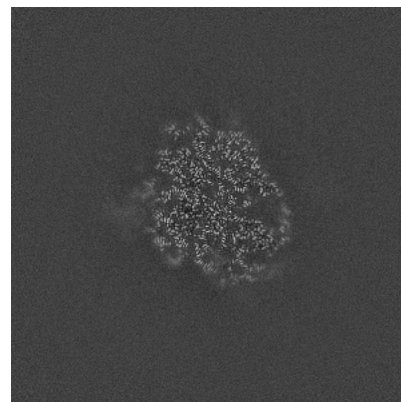
6.2.2 Raw map



X Index: 256



Y Index: 256

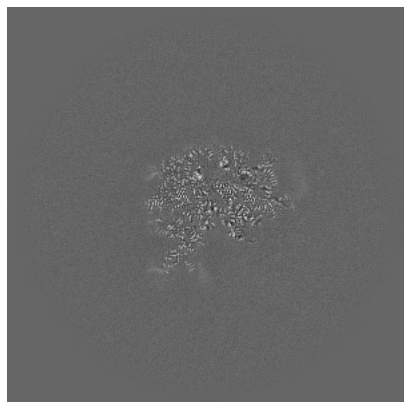


Z Index: 256

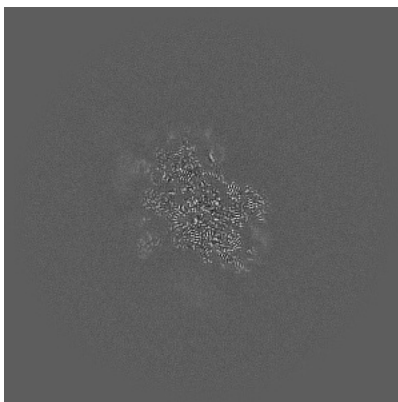
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

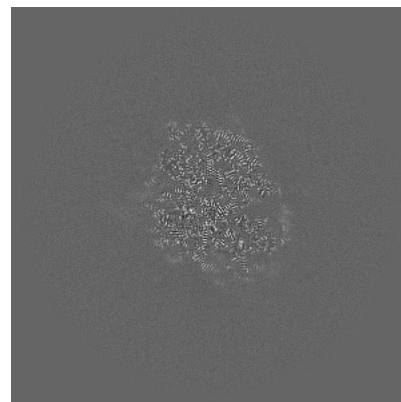
6.3.1 Primary map



X Index: 244

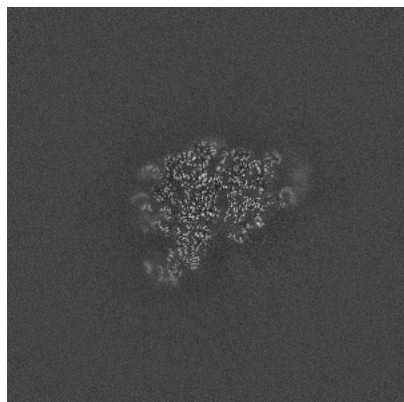


Y Index: 243

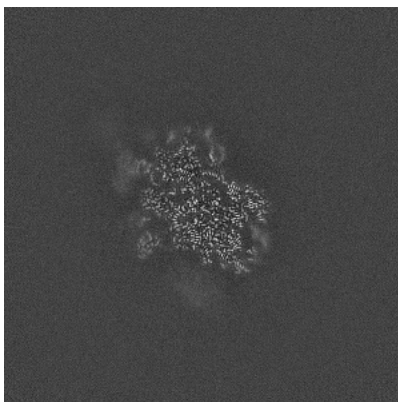


Z Index: 258

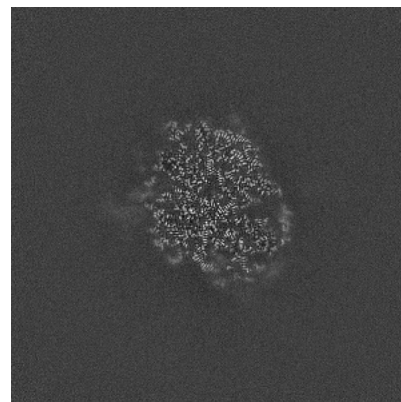
6.3.2 Raw map



X Index: 253



Y Index: 243

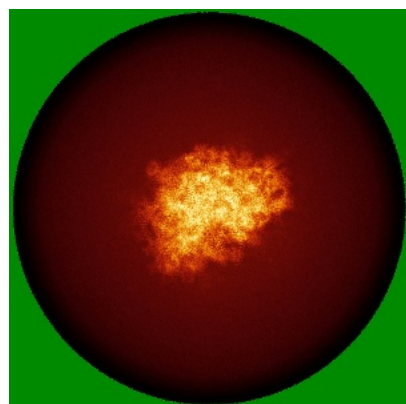


Z Index: 258

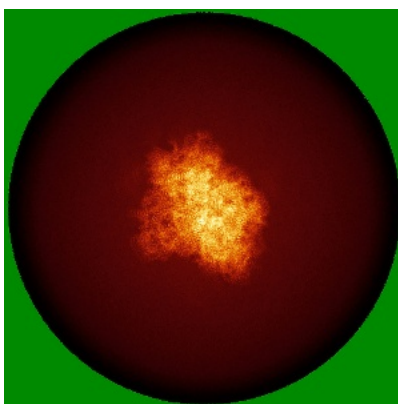
The images above show the largest variance slices of the map in three orthogonal directions.

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

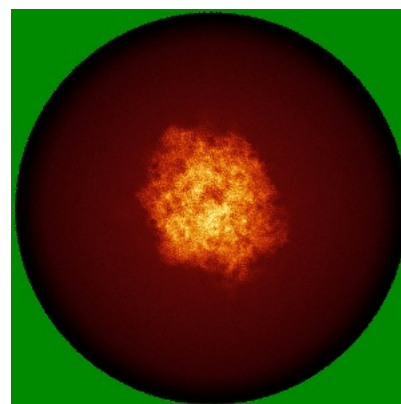
6.4.1 Primary map



X

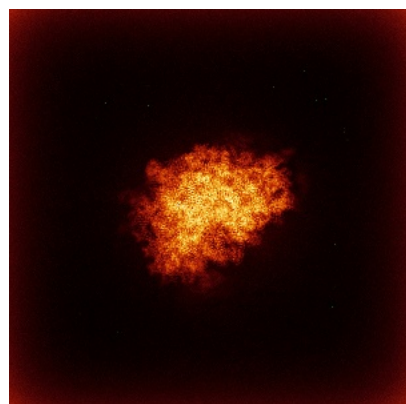


Y

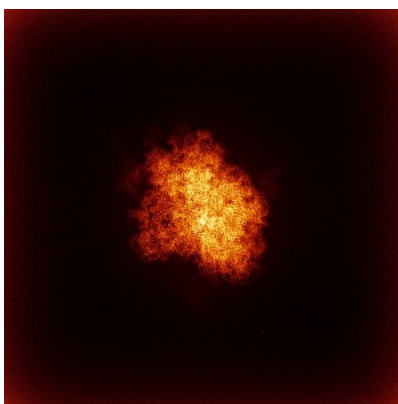


Z

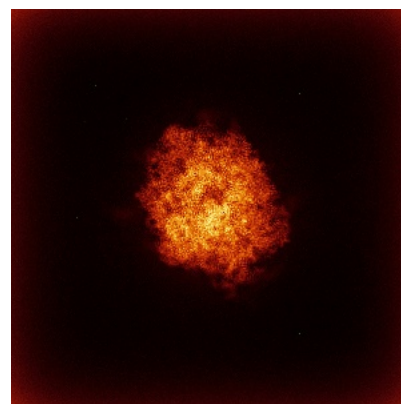
6.4.2 Raw map



X



Y

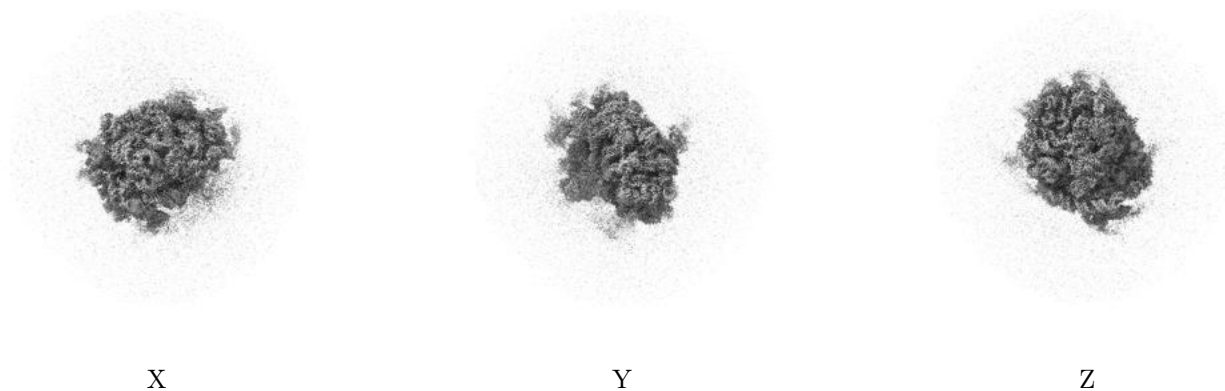


Z

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.

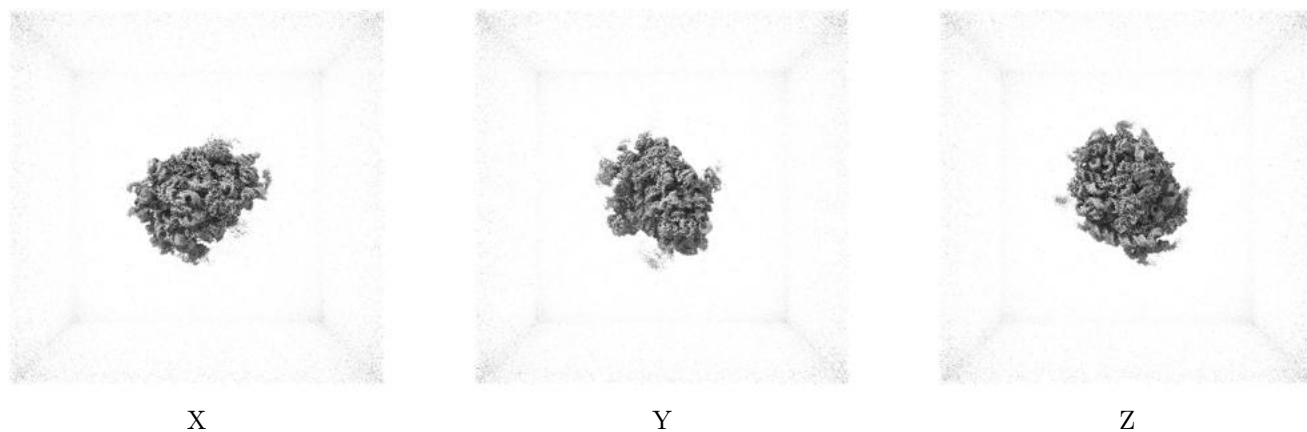
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0495. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

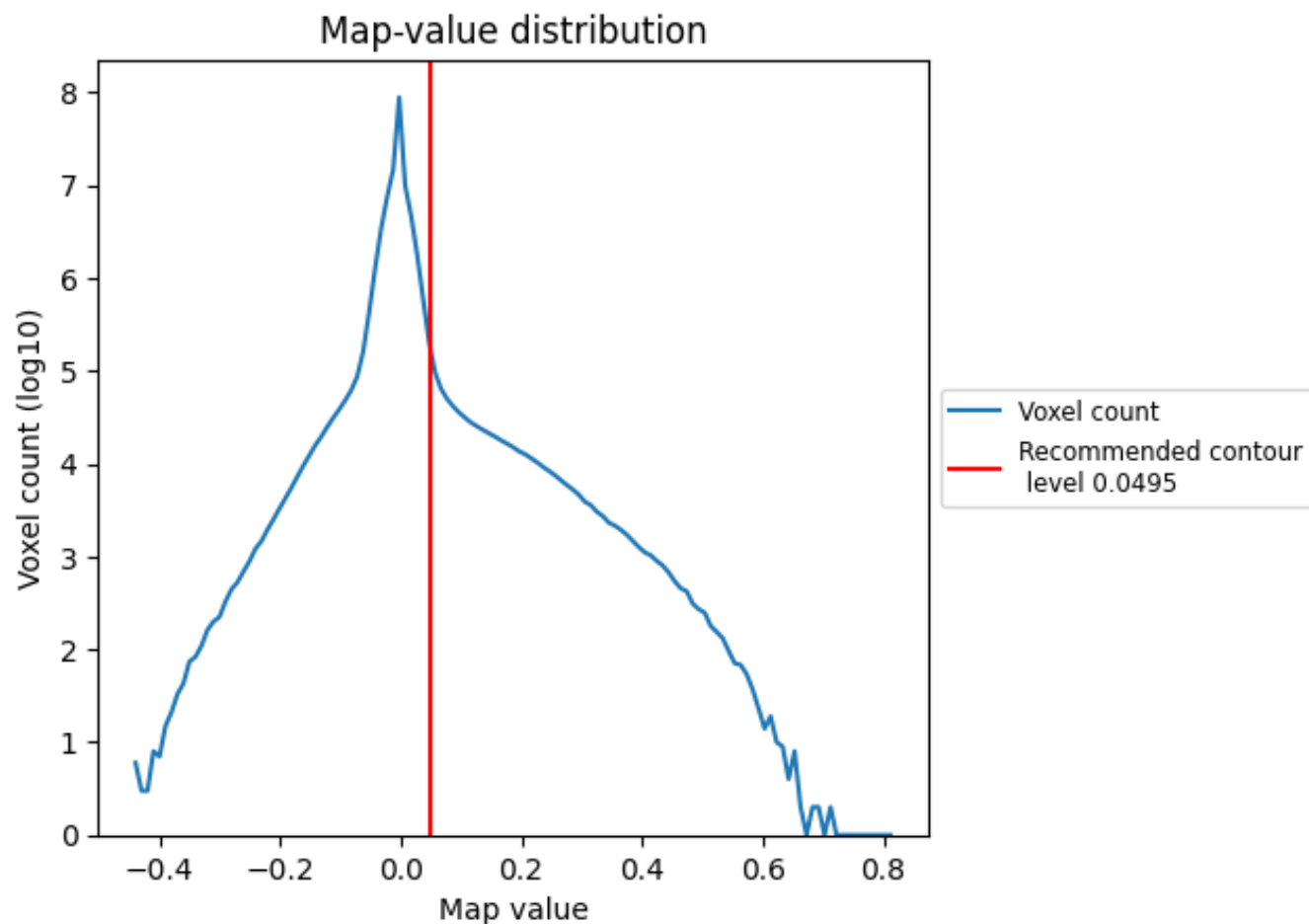
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

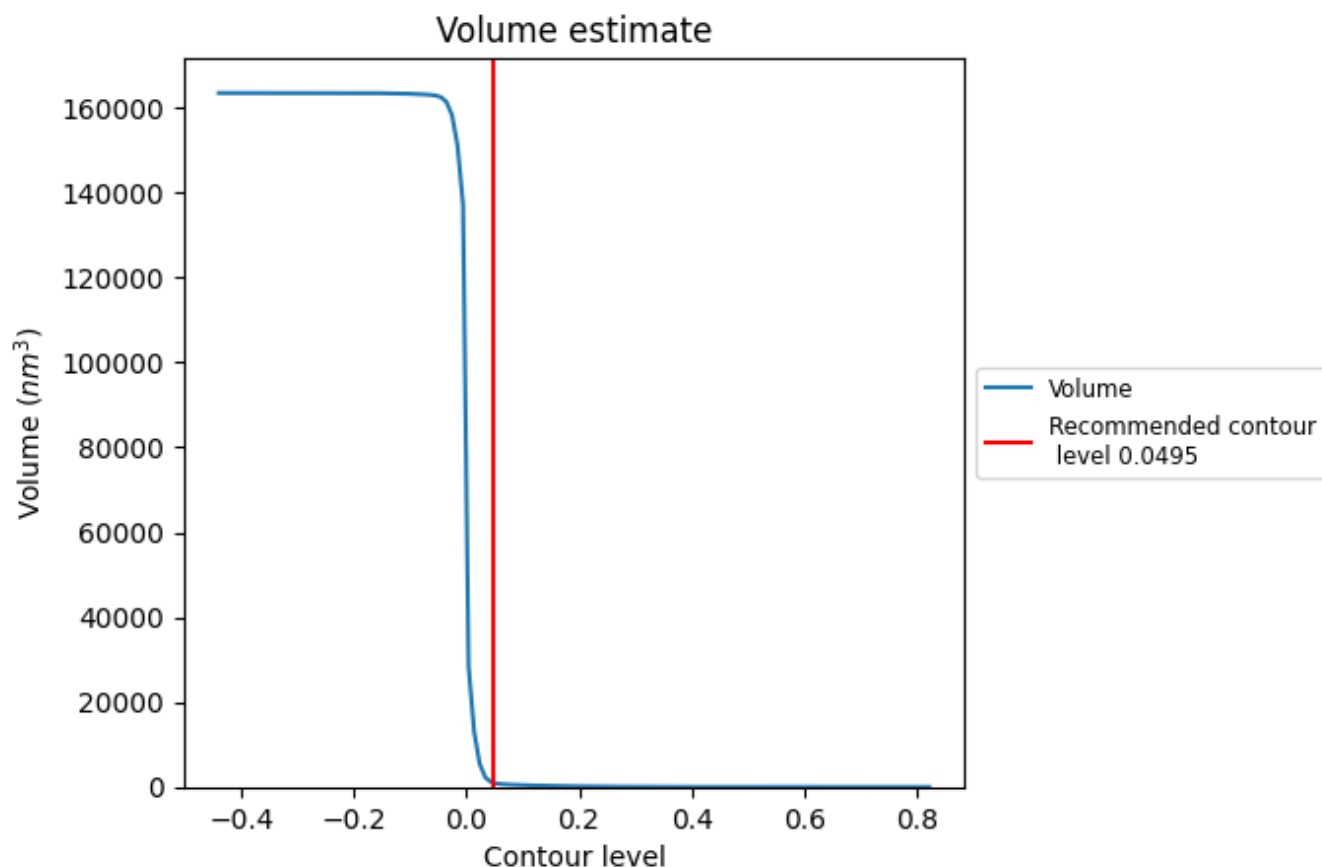
This section contains the results of statistical analysis of the map.

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.

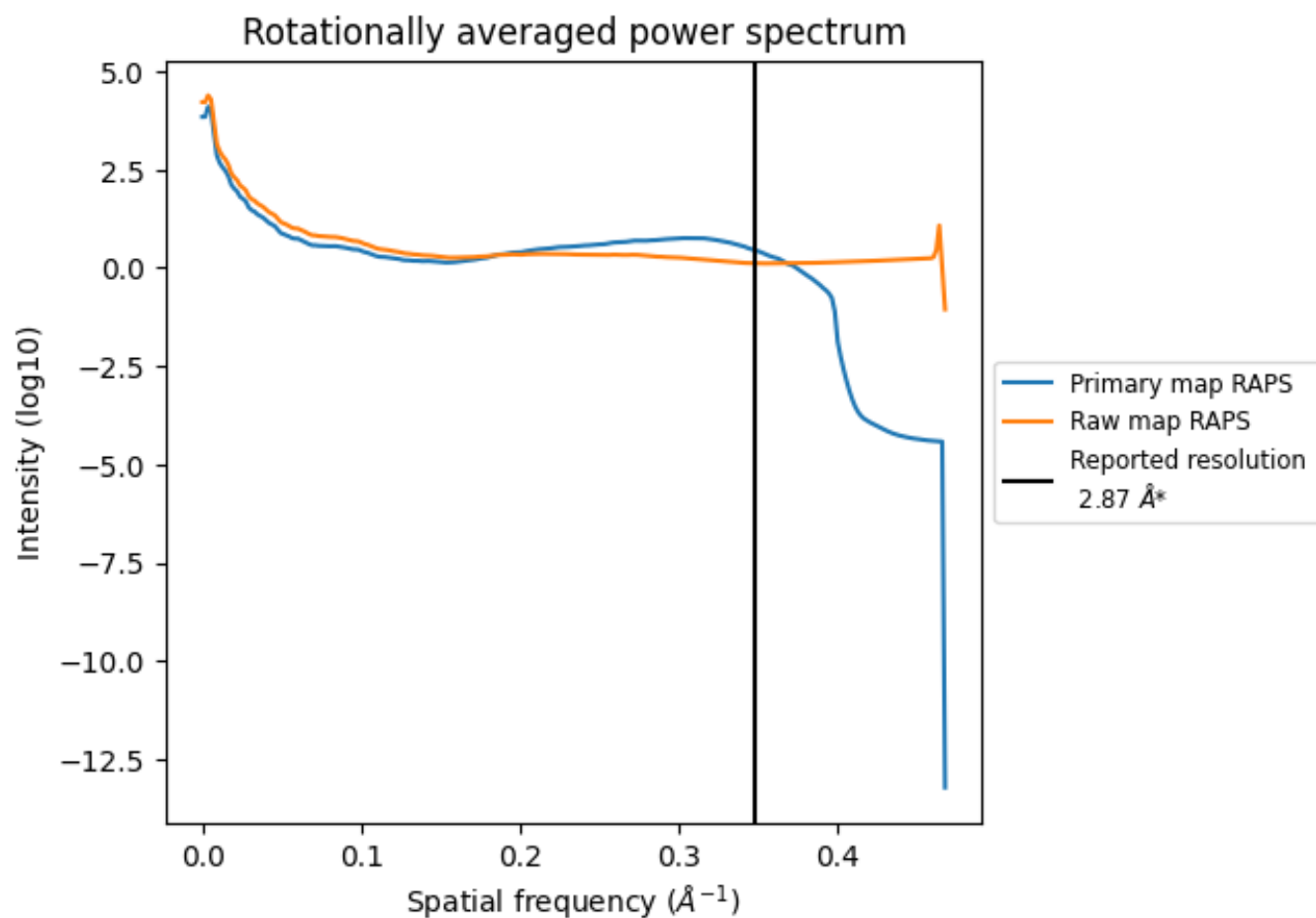
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 954 nm³; this corresponds to an approximate mass of 862 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 ⓘ

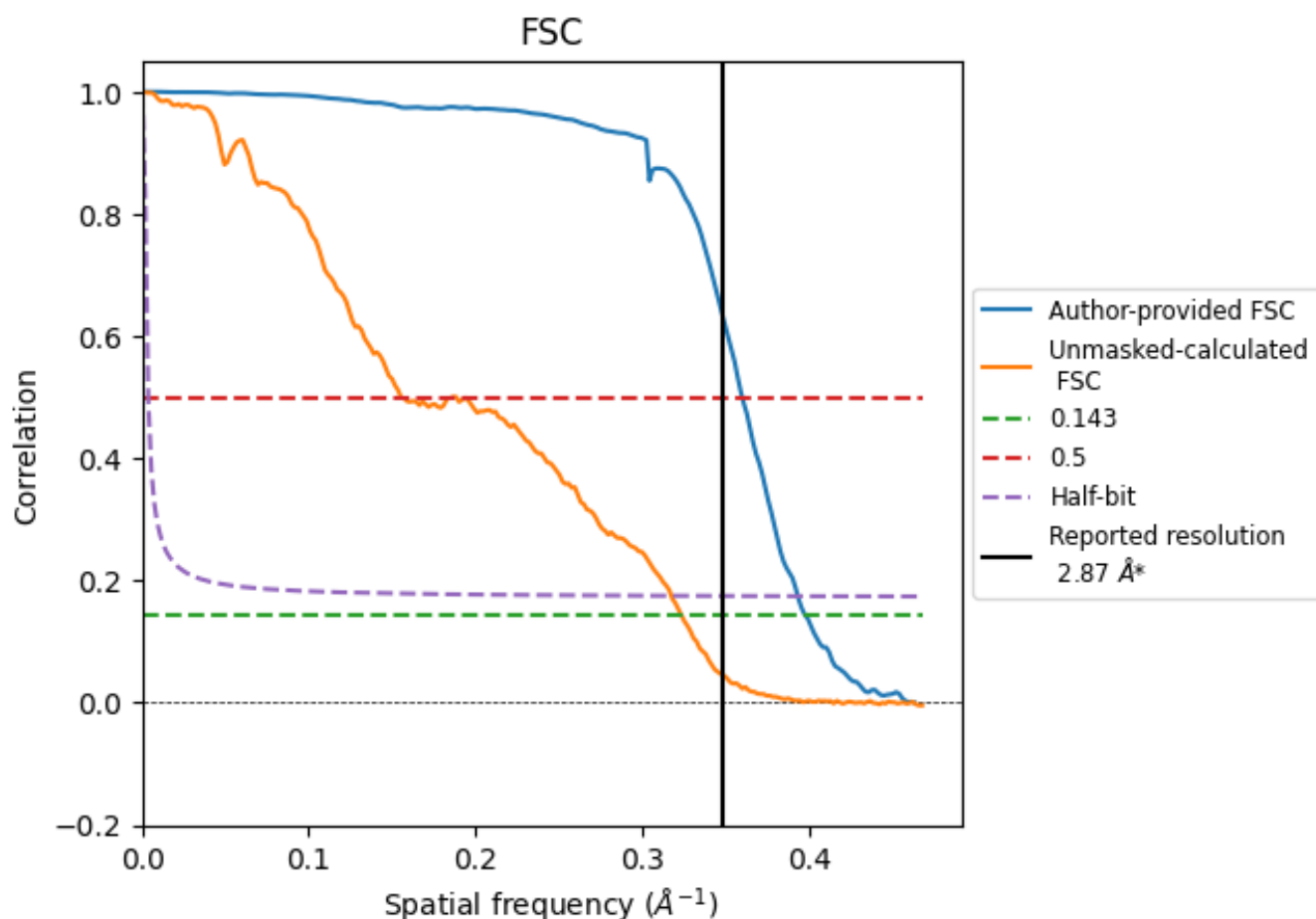


*Reported resolution corresponds to spatial frequency of 0.348 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.348 \AA^{-1}

8.2 Resolution estimates [i](#)

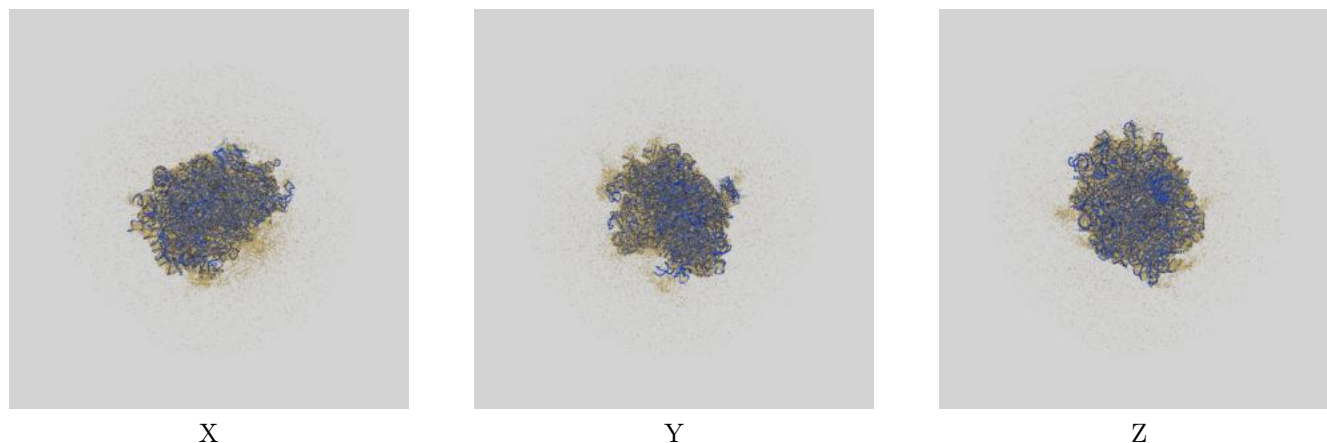
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.87	-	-
Author-provided FSC curve	2.51	2.78	2.54
Unmasked-calculated*	3.09	6.44	3.15

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 2.51 differs from the reported value 2.87 by more than 10 %

9 Map-model fit [i](#)

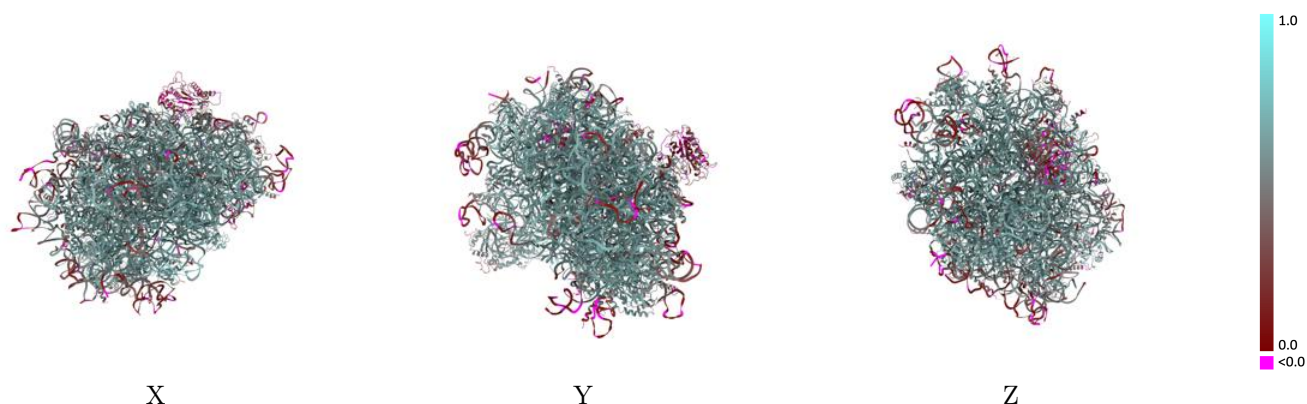
This section contains information regarding the fit between EMDB map EMD-42318 and PDB model 8UJC. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



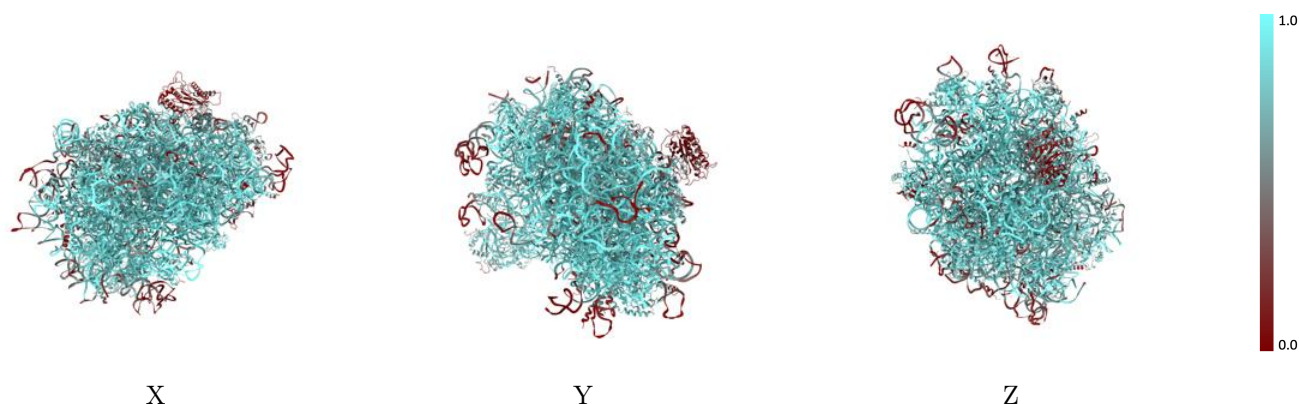
The images above show the 3D surface view of the map at the recommended contour level 0.0495 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



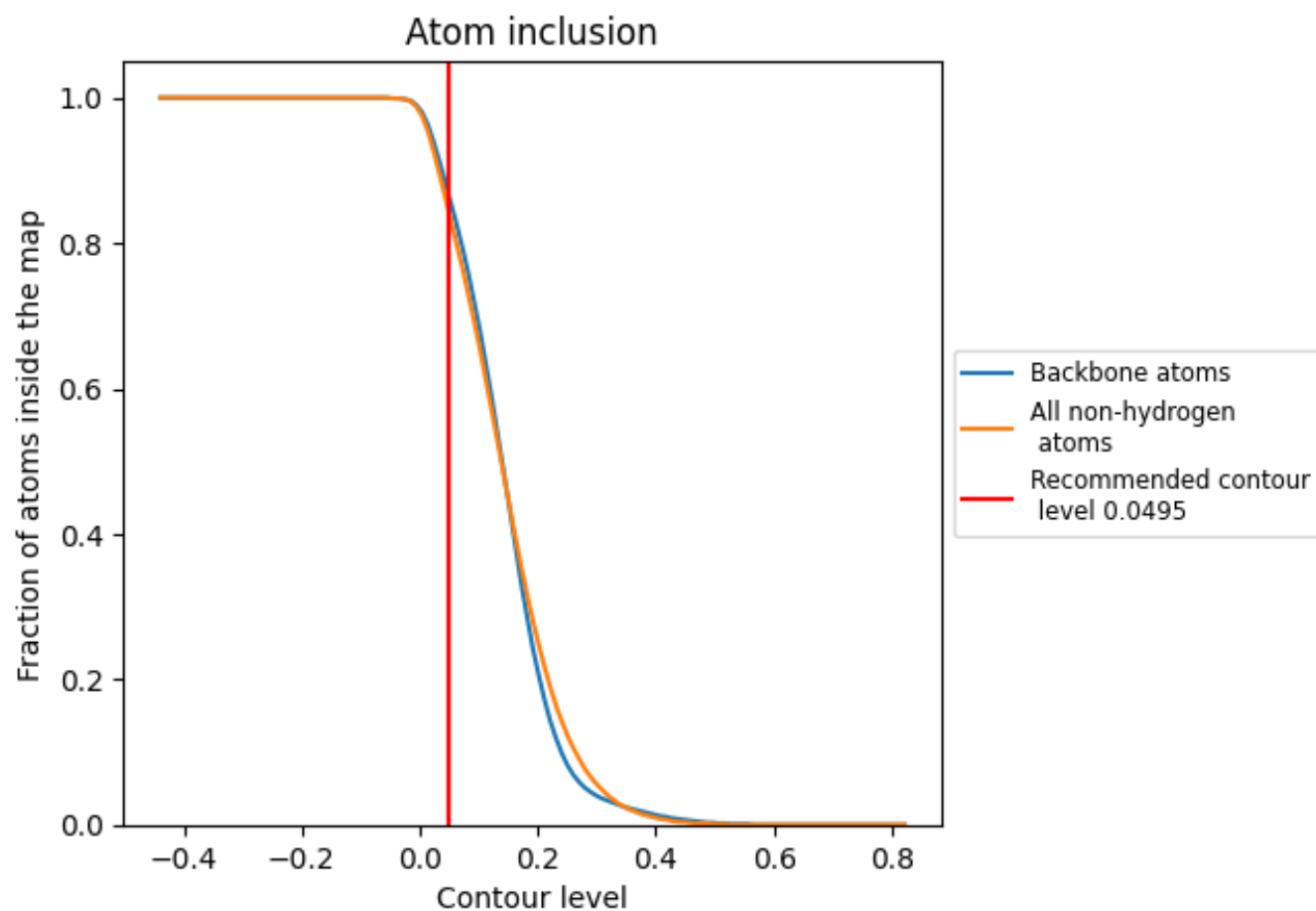
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0495).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 84% 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 (0.0495) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8430	 0.5650
CA	 0.1730	 0.1950
L5	 0.8450	 0.5560
L7	 0.9700	 0.6330
L8	 0.9060	 0.5950
LA	 0.9400	 0.6320
LB	 0.8900	 0.6080
LC	 0.9010	 0.6180
LD	 0.8360	 0.5710
LE	 0.7780	 0.5410
LF	 0.9250	 0.6270
LG	 0.7770	 0.5410
LH	 0.8760	 0.5950
LI	 0.8850	 0.6110
LJ	 0.6720	 0.4560
LL	 0.8320	 0.5700
LM	 0.8890	 0.5990
LN	 0.9610	 0.6520
LO	 0.9180	 0.6260
LP	 0.9100	 0.6300
LQ	 0.9320	 0.6430
LR	 0.8800	 0.6010
LS	 0.9390	 0.6400
LT	 0.8540	 0.5880
LU	 0.6150	 0.4380
LV	 0.9110	 0.6140
LW	 0.3200	 0.1330
LX	 0.8690	 0.6030
LY	 0.8740	 0.6070
LZ	 0.8440	 0.5850
La	 0.9310	 0.6410
Lb	 0.7500	 0.5200
Lc	 0.8430	 0.5460
Ld	 0.8470	 0.5800
Le	 0.9400	 0.6410



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Chain	Atom inclusion	Q-score
Lf	 0.9430	 0.6380
Lg	 0.8790	 0.6070
Lh	 0.8560	 0.5850
Li	 0.8370	 0.5830
Lj	 0.9420	 0.6380
Lk	 0.7040	 0.5130
Ll	 0.8910	 0.6050
Lm	 0.8770	 0.6140
Lo	 0.8710	 0.6010
Lp	 0.8970	 0.6160
Lr	 0.9180	 0.6200