



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 10:43 AM UTC

PDB ID : 8P8N / pdb_00008p8n
EMDB ID : EMD-17550
Title : Mouse RPL39 integrated into the yeast 60S ribosomal subunit
Authors : Rabl, J.; Banerjee, A.; Boehringer, D.; Zavolan, M.
Deposited on : 2023-06-02
Resolution : 2.15 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:

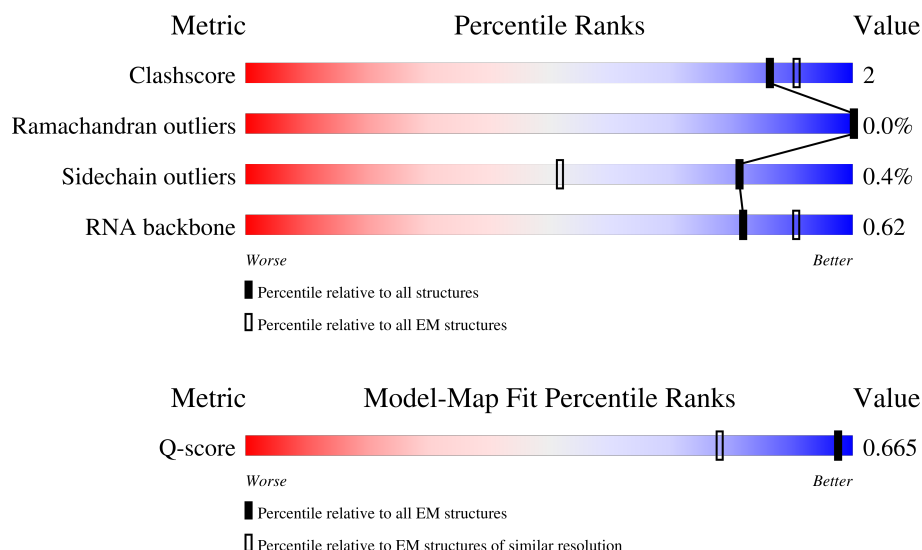
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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

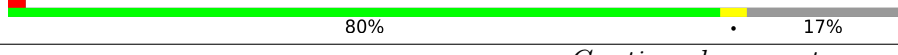
The reported resolution of this entry is 2.15 Å.

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	2551 (1.66 - 2.65)

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	2	51	
2	LK	244	
3	QX	142	

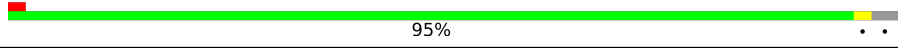
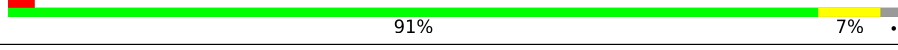
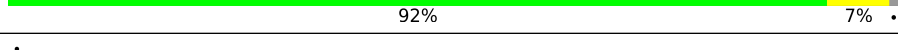
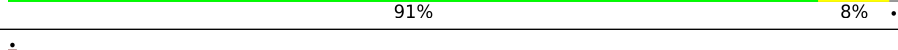
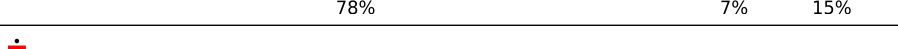
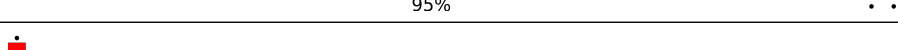
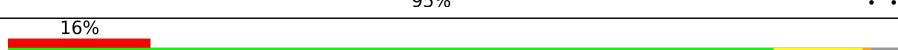
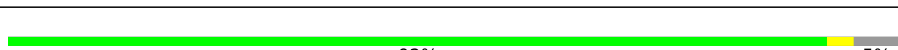
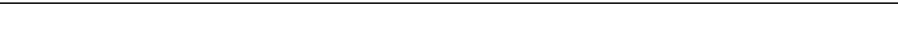
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Mol	Chain	Length	Quality of chain
4	RM	78	
5	A	3396	
6	LL	256	
7	QY	127	
8	RO	128	
9	JT	199	
10	LM	191	
11	QZ	136	
12	RQ	106	
13	JU	138	
14	LN	221	
15	RA	149	
16	RT	92	
17	JV	204	
18	LO	174	
19	RB	59	
20	QO	184	
21	JW	199	
22	QP	186	
23	RC	105	
24	QQ	189	
25	LD	158	
26	QS	172	
27	RD	113	
28	QT	160	

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Mol	Chain	Length	Quality of chain
29	LE	121	
30	QU	121	
31	RE	130	
32	QV	137	
33	LF	254	
34	QW	155	
35	RF	107	
36	LG	387	
37	RG	121	
38	LH	362	
39	RH	120	
40	LI	297	
41	RI	100	
42	LJ	176	
43	RJ	88	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	CL	A	3404	-	-	X	-

2 Entry composition

There are 49 unique types of molecules in this entry. The entry contains 119886 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 Large ribosomal subunit protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	50	Total	C	N	O	S	0	0
			443	281	98	63	1		

- Molecule 2 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	LK	220	Total	C	N	O	S	0	0
			1770	1143	322	304	1		

- Molecule 3 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	QX	118	Total	C	N	O	S	0	0
			946	608	166	170	2		

- Molecule 4 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	RM	77	Total	C	N	O	0	0
			612	391	115	106		

- Molecule 5 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	3043	Total	C	N	O	P	0	0
			65092	29075	11734	21240	3043		

- Molecule 6 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	LL	218	Total	C	N	O	S	0	0
			1719	1102	308	306	3		

- Molecule 7 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	QY	124	Total	C	N	O	0	0
			976	614	190	172		

- Molecule 8 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	RO	50	Total	C	N	O	S	0	0
			401	247	84	65	5		

- Molecule 9 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	JT	189	Total	C	N	O	0	0
			1515	946	311	258		

- Molecule 10 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LM	188	Total	C	N	O	S	0	0
			1493	948	271	270	4		

- Molecule 11 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	QZ	135	Total	C	N	O	0	0
			1092	710	202	180		

- Molecule 12 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	RQ	102	Total	C	N	O	S	0	0
			819	514	166	134	5		

- Molecule 13 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	JU	134	Total	C	N	O	S	0	0
			1039	666	196	175	2		

- Molecule 14 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LN	204	Total	C	N	O	S	0	0
			1664	1056	315	287	6		

- Molecule 15 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	RA	148	Total	C	N	O	S	0	0
			1173	749	231	190	3		

- Molecule 16 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	RT	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	JV	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 18 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LO	168	Total	C	N	O	S	0	0
			1344	841	251	248	4		

- Molecule 19 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	RB	55	Total	C	N	O	0	0
			439	274	95	70		

- Molecule 20 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	QO	168	Total	C	N	O	0	0
			1331	827	266	238		

- Molecule 21 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	JW	197	Total	C	N	O	S	0	0
			1555	1003	289	262	1		

- Molecule 22 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	QP	185	Total	C	N	O	S	0	0
			1441	908	290	241	2		

- Molecule 23 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	RC	95	Total	C	N	O	S	0	0
			729	470	122	136	1		

- Molecule 24 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	QQ	147	Total	C	N	O		0	0
			1185	738	250	197			

- Molecule 25 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LD	157	Total	C	N	O	P	0	0
			3333	1491	584	1101	157		

- Molecule 26 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	QS	171	Total	C	N	O	S	0	0
			1437	925	266	243	3		

- Molecule 27 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	RD	97	Total	C	N	O	S	0	0
			791	508	152	130	1		

- Molecule 28 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	QT	159	Total	C	N	O	S	0	0
			1276	805	246	221	4		

- Molecule 29 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LE	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 30 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	QU	97	Total	C	N	O	0	0
			766	496	126	144		

- Molecule 31 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	RE	126	Total	C	N	O	S	0	0
			1012	641	204	166	1		

- Molecule 32 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	QV	133	Total	C	N	O	S	0	0
			985	619	185	174	7		

- Molecule 33 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	LF	244	Total	C	N	O	S	0	0
			1855	1156	375	323	1		

- Molecule 34 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	QW	61	Total	C	N	O	S	0	0
			509	328	100	80	1		

- Molecule 35 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	RF	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 36 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	LG	385	Total	C	N	O	S	0	0
			3070	1947	583	532	8		

- Molecule 37 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	RG	103	Total	C	N	O	S	0	0
			811	503	167	137	4		

- Molecule 38 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	LH	360	Total	C	N	O	S	0	0
			2742	1726	521	492	3		

- Molecule 39 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	RH	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 40 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	LI	286	Total	C	N	O	S	0	0
			2301	1456	400	443	2		

- Molecule 41 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	RI	96	Total	C	N	O	S	0	0
			739	463	145	129	2		

- Molecule 42 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	LJ	156	Total	C	N	O	S	0	0
			1239	800	222	216	1		

- Molecule 43 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	RJ	84	Total	C	N	O	S	0	0
			665	405	145	110	5		

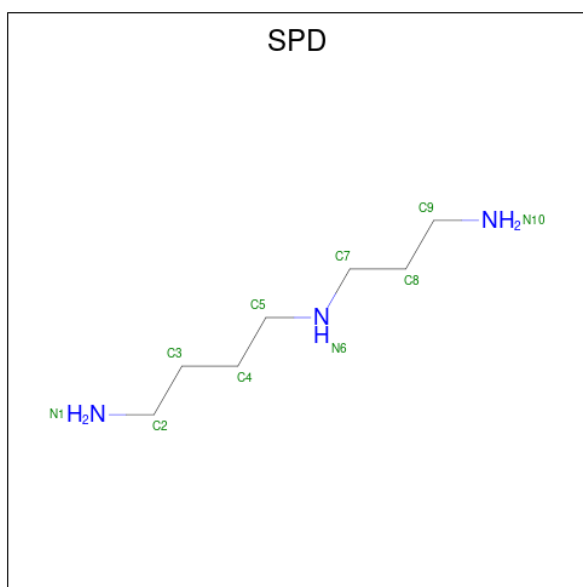
- Molecule 44 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
44	A	146	Total	Mg	0
			146	146	
44	QO	1	Total	Mg	0
			1	1	
44	LD	1	Total	Mg	0
			1	1	
44	LE	1	Total	Mg	0
			1	1	
44	RE	2	Total	Mg	0
			2	2	
44	RI	1	Total	Mg	0
			1	1	

- Molecule 45 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

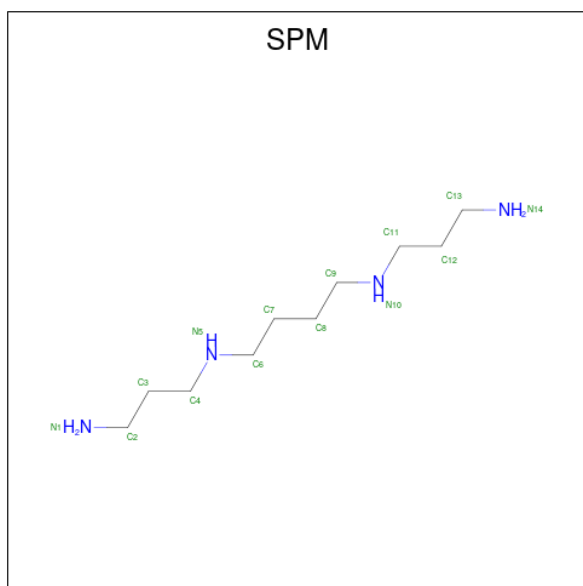
Mol	Chain	Residues	Atoms		AltConf
45	A	19	Total	Cl	0
			19	19	
45	QO	1	Total	Cl	0
			1	1	

- Molecule 46 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃).



Mol	Chain	Residues	Atoms			AltConf
46	A	1	Total	C	N	0
			10	7	3	

- Molecule 47 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms			AltConf
47	A	1	Total	C	N	0
			14	10	4	

- Molecule 48 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
48	RO	1	Total 1	Zn 1	0
48	RQ	1	Total 1	Zn 1	0
48	RT	1	Total 1	Zn 1	0
48	RG	1	Total 1	Zn 1	0
48	RJ	1	Total 1	Zn 1	0

- Molecule 49 is water.

Mol	Chain	Residues	Atoms		AltConf
49	LK	1	Total 1	O 1	0
49	QX	1	Total 1	O 1	0
49	A	532	Total 532	O 532	0
49	RQ	1	Total 1	O 1	0
49	RA	4	Total 4	O 4	0
49	JV	2	Total 2	O 2	0
49	RB	1	Total 1	O 1	0
49	QO	3	Total 3	O 3	0
49	JW	2	Total 2	O 2	0
49	QQ	1	Total 1	O 1	0
49	LD	4	Total 4	O 4	0
49	LE	3	Total 3	O 3	0
49	RE	2	Total 2	O 2	0
49	LF	5	Total 5	O 5	0
49	LH	1	Total 1	O 1	0

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Mol	Chain	Residues	Atoms		AltConf
49	LI	1	Total	O	0
			1	1	

3 Residue-property plots [i](#)

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

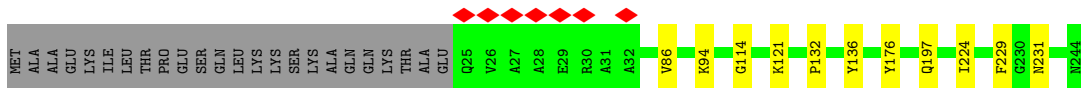
- Molecule 1: Large ribosomal subunit protein eL39

Chain 2: 



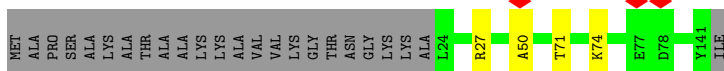
- Molecule 2: 60S ribosomal protein L7-A

Chain LK: 



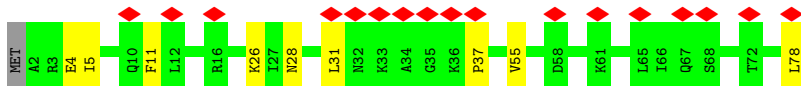
- Molecule 3: 60S ribosomal protein L25

Chain QX: 



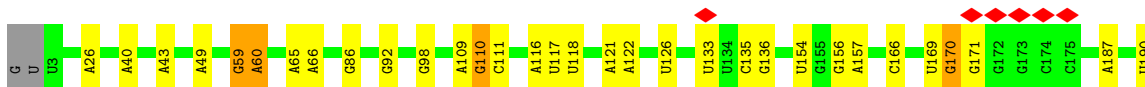
- Molecule 4: 60S ribosomal protein L38

Chain RM: 



- Molecule 5: 25S rRNA

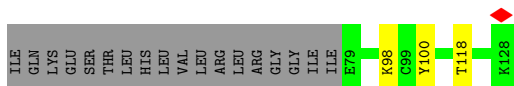
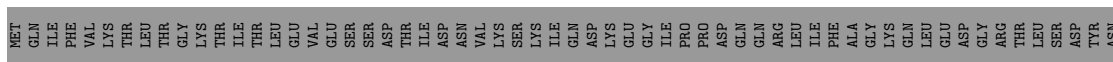
Chain A: 



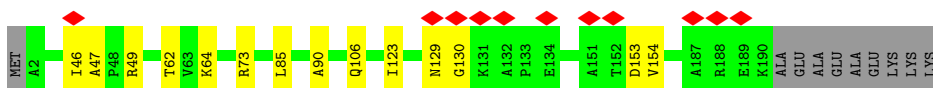
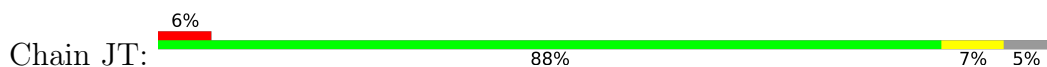




- Molecule 8: Ubiquitin-60S ribosomal protein L40



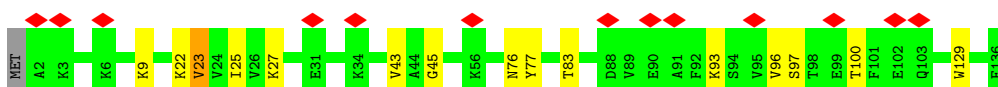
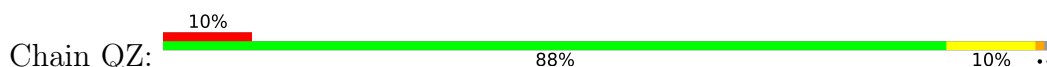
- Molecule 9: 60S ribosomal protein L13-A



- Molecule 10: 60S ribosomal protein L9-A



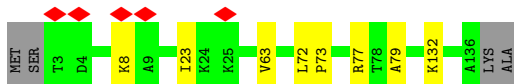
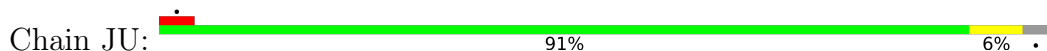
- Molecule 11: 60S ribosomal protein L27-A



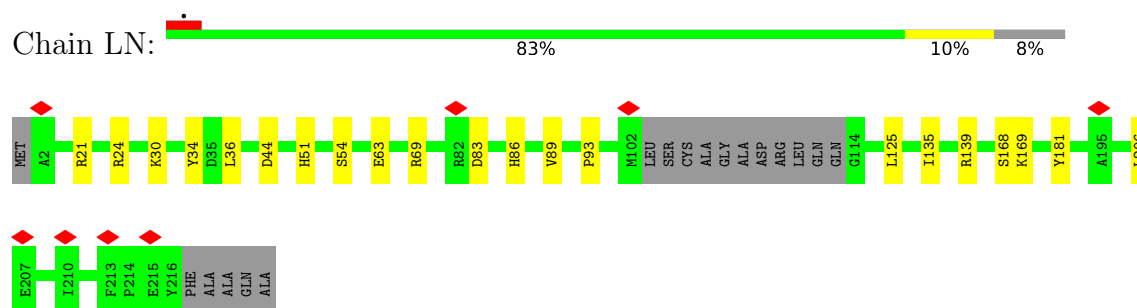
- Molecule 12: 60S ribosomal protein L42-A



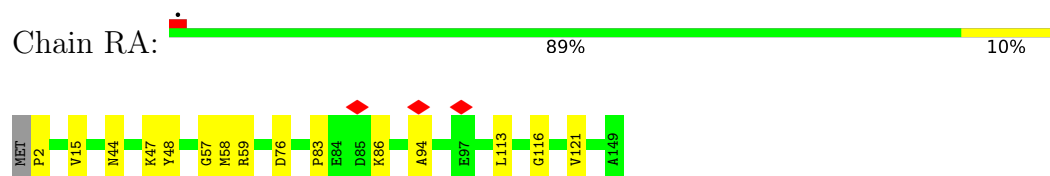
- Molecule 13: 60S ribosomal protein L14-A



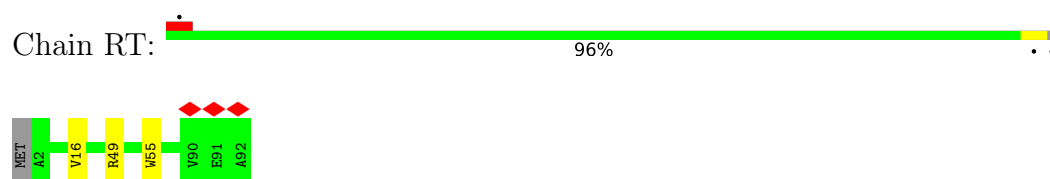
- Molecule 14: 60S ribosomal protein L10



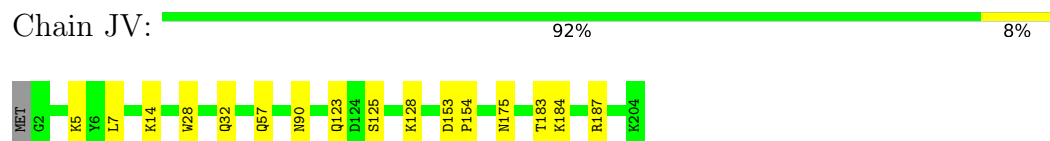
- Molecule 15: 60S ribosomal protein L28



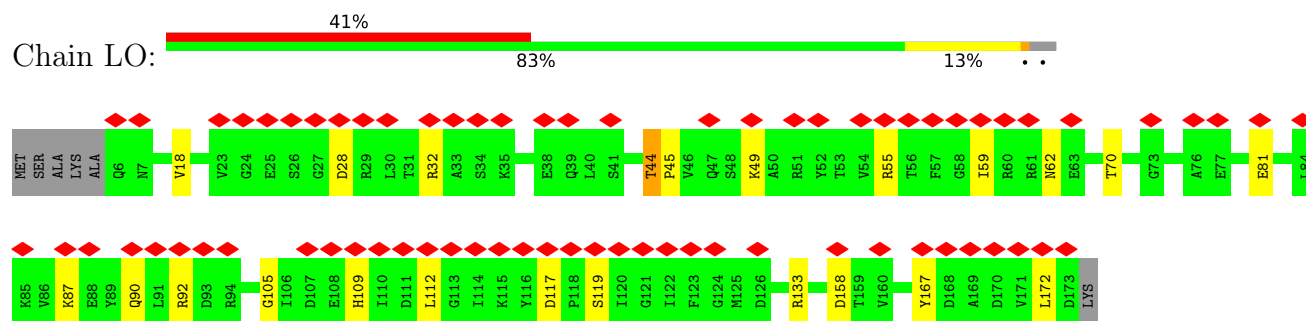
- Molecule 16: 60S ribosomal protein L43-A



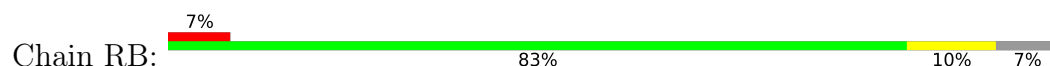
- Molecule 17: 60S ribosomal protein L15-A



- Molecule 18: 60S ribosomal protein L11-A

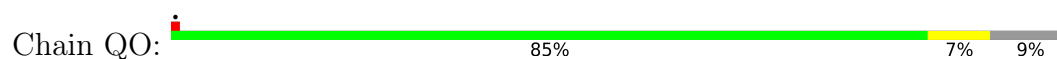


- Molecule 19: 60S ribosomal protein L29





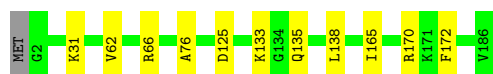
- Molecule 20: 60S ribosomal protein L17-A



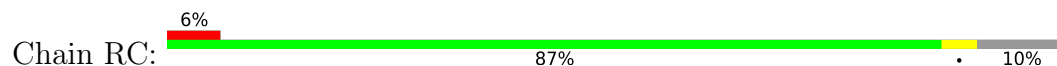
- Molecule 21: 60S ribosomal protein L16-A



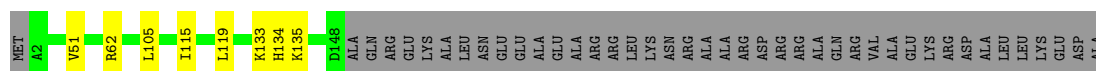
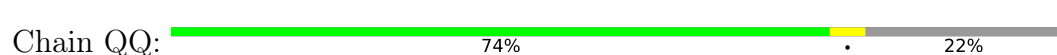
- Molecule 22: 60S ribosomal protein L18-A



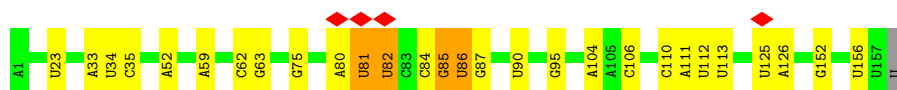
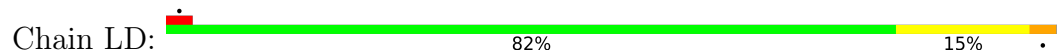
- Molecule 23: 60S ribosomal protein L30



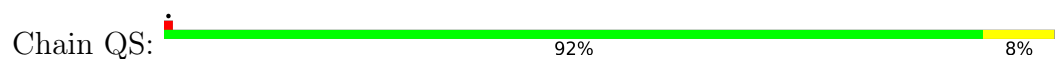
- Molecule 24: 60S ribosomal protein L19-A



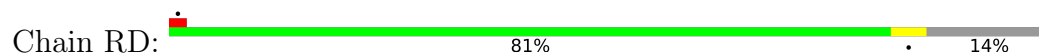
- Molecule 25: 5.8S rRNA



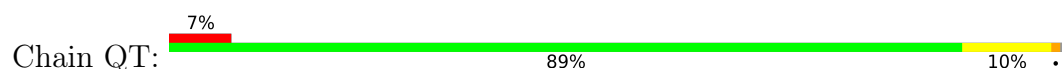
- Molecule 26: 60S ribosomal protein L20-A



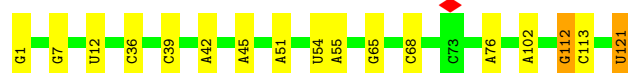
- Molecule 27: 60S ribosomal protein L31-A



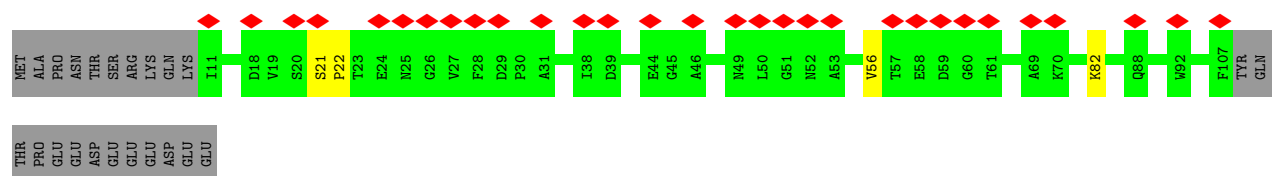
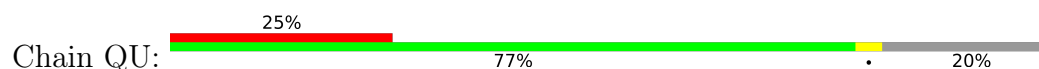
- Molecule 28: 60S ribosomal protein L21-A



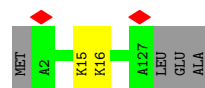
- Molecule 29: 5S rRNA



- Molecule 30: 60S ribosomal protein L22-A



- Molecule 31: 60S ribosomal protein L32



- Molecule 32: 60S ribosomal protein L23-A

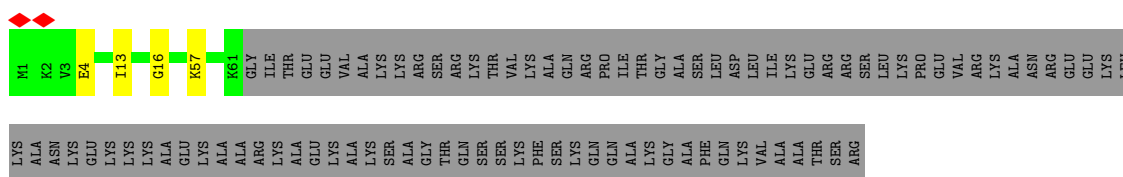




- Molecule 33: 60S ribosomal protein L2-A



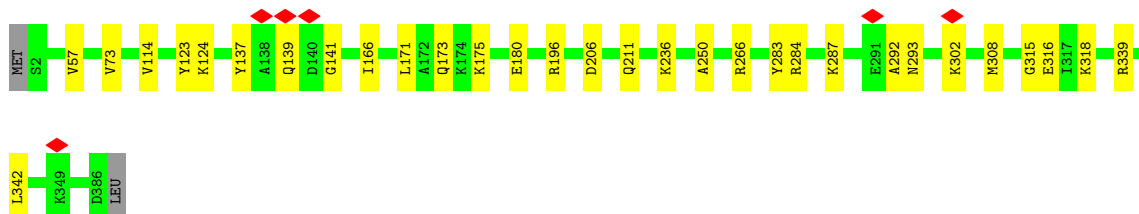
- Molecule 34: 60S ribosomal protein L24-A



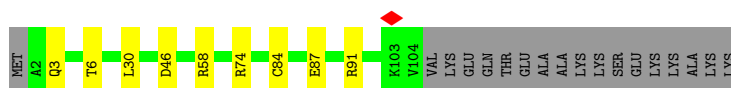
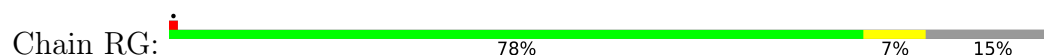
- Molecule 35: 60S ribosomal protein L33-A



- Molecule 36: 60S ribosomal protein L3



- Molecule 37: 60S ribosomal protein L34-A



- Molecule 38: 60S ribosomal protein L4-A





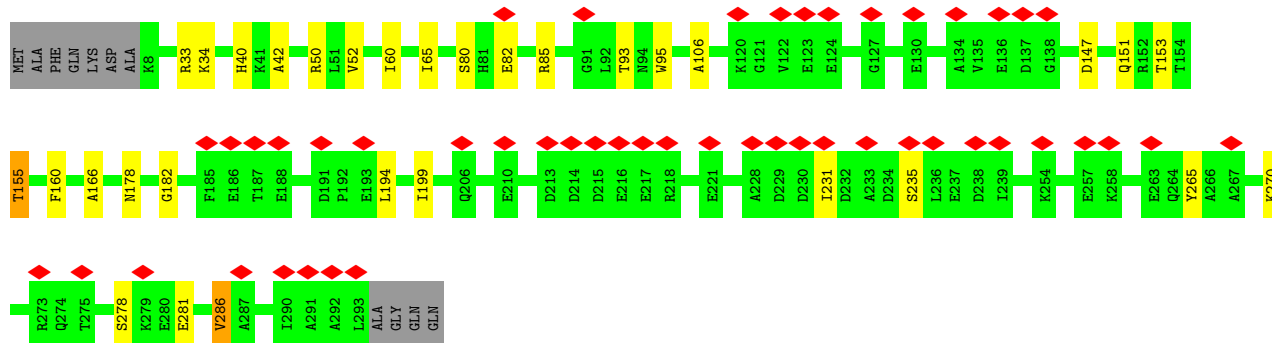
- Molecule 39: 60S ribosomal protein L35-A

Chain RH: 95%



- Molecule 40: 60S ribosomal protein L5

Chain LI: 16% 86% 10%



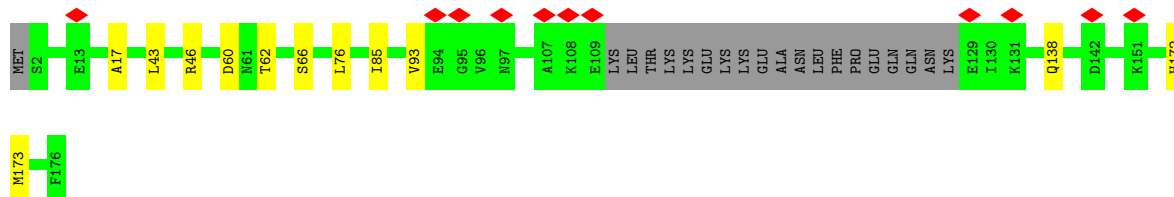
- Molecule 41: 60S ribosomal protein L36-A

Chain RI: 87% 9%



- Molecule 42: 60S ribosomal protein L6-A

Chain LJ: 6% 82% 7% 11%



- Molecule 43: 60S ribosomal protein L37-A

Chain RJ: 92% 5%

MET	G2	K3	M64	L87	K85	ALA	SER	ALA
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	522193	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.792	Depositor
Minimum map value	-1.240	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.066	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	503.99997, 503.99997, 503.99997	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SPD, CL, SPM, 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	2	0.08	0/453	0.20	0/599
2	LK	0.10	0/1807	0.26	0/2432
3	QX	0.08	0/961	0.24	0/1296
4	RM	0.09	0/618	0.26	0/826
5	A	0.09	0/72859	0.21	0/113586
6	LL	0.09	0/1750	0.27	0/2361
7	QY	0.09	0/987	0.24	0/1318
8	RO	0.08	0/407	0.24	0/540
9	JT	0.09	0/1540	0.27	0/2068
10	LM	0.09	0/1514	0.25	0/2039
11	QZ	0.09	0/1118	0.29	0/1497
12	RQ	0.08	0/831	0.25	0/1097
13	JU	0.07	0/1054	0.22	0/1420
14	LN	0.09	0/1699	0.23	0/2277
15	RA	0.09	0/1204	0.27	0/1612
16	RT	0.09	0/701	0.28	0/934
17	JV	0.09	0/1757	0.25	0/2354
18	LO	0.09	0/1365	0.26	0/1831
19	RB	0.09	0/450	0.27	0/600
20	QO	0.08	0/1353	0.27	0/1817
21	JW	0.09	0/1585	0.24	0/2128
22	QP	0.09	0/1465	0.26	0/1965
23	RC	0.08	0/737	0.24	0/990
24	QQ	0.07	0/1202	0.19	0/1605
25	LD	0.09	0/3724	0.18	0/5798
26	QS	0.09	0/1473	0.27	0/1980
27	RD	0.08	0/804	0.21	0/1077
28	QT	0.09	0/1300	0.25	0/1743
29	LE	0.07	0/2883	0.14	0/4491
30	QU	0.08	0/781	0.23	0/1058
31	RE	0.08	0/1033	0.25	0/1383
32	QV	0.08	0/1000	0.25	0/1345

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	LF	0.09	0/1889	0.27	0/2539
34	QW	0.08	0/521	0.25	0/691
35	RF	0.09	0/868	0.26	0/1168
36	LG	0.09	0/3141	0.27	0/4222
37	RG	0.09	0/821	0.27	0/1097
38	LH	0.10	0/2794	0.29	0/3782
39	RH	0.08	0/978	0.20	0/1301
40	LI	0.08	0/2350	0.25	0/3171
41	RI	0.08	0/745	0.23	0/991
42	LJ	0.09	0/1260	0.25	0/1694
43	RJ	0.10	0/680	0.28	0/901
All	All	0.09	0/128462	0.22	0/189624

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2	443	0	483	3	0
2	LK	1770	0	1851	6	0
3	QX	946	0	1007	3	0
4	RM	612	0	682	4	0
5	A	65092	0	32707	197	0
6	LL	1719	0	1811	10	0
7	QY	976	0	1064	5	0
8	RO	401	0	433	2	0
9	JT	1515	0	1586	10	0
10	LM	1493	0	1566	7	0
11	QZ	1092	0	1155	8	0
12	RQ	819	0	886	7	0
13	JU	1039	0	1131	7	0
14	LN	1664	0	1706	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	RA	1173	0	1215	10	0
16	RT	694	0	734	2	0
17	JV	1720	0	1779	12	0
18	LO	1344	0	1370	14	0
19	RB	439	0	460	7	0
20	QO	1331	0	1362	8	0
21	JW	1555	0	1659	3	0
22	QP	1441	0	1543	7	0
23	RC	729	0	781	2	0
24	QQ	1185	0	1269	4	0
25	LD	3333	0	1685	7	0
26	QS	1437	0	1475	8	0
27	RD	791	0	852	3	0
28	QT	1276	0	1323	14	0
29	LE	2579	0	1304	8	0
30	QU	766	0	782	2	0
31	RE	1012	0	1079	2	0
32	QV	985	0	1034	6	0
33	LF	1855	0	1919	14	0
34	QW	509	0	537	3	0
35	RF	850	0	880	5	0
36	LG	3070	0	3142	20	0
37	RG	811	0	869	5	0
38	LH	2742	0	2854	13	0
39	RH	969	0	1078	4	0
40	LI	2301	0	2257	21	0
41	RI	739	0	816	5	0
42	LJ	1239	0	1326	8	0
43	RJ	665	0	668	2	0
44	A	146	0	0	0	0
44	LD	1	0	0	0	0
44	LE	1	0	0	0	0
44	QO	1	0	0	0	0
44	RE	2	0	0	0	0
44	RI	1	0	0	0	0
45	A	19	0	0	4	0
45	QO	1	0	0	0	0
46	A	10	0	19	1	0
47	A	14	0	26	0	0
48	RG	1	0	0	0	0
48	RJ	1	0	0	0	0
48	RO	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	RQ	1	0	0	0	0
48	RT	1	0	0	0	0
49	A	532	0	0	1	0
49	JV	2	0	0	0	0
49	JW	2	0	0	0	0
49	LD	4	0	0	0	0
49	LE	3	0	0	0	0
49	LF	5	0	0	0	0
49	LH	1	0	0	0	0
49	LI	1	0	0	0	0
49	LK	1	0	0	0	0
49	QO	3	0	0	0	0
49	QQ	1	0	0	0	0
49	QX	1	0	0	0	0
49	RA	4	0	0	0	0
49	RB	1	0	0	0	0
49	RE	2	0	0	0	0
49	RQ	1	0	0	0	0
All	All	119886	0	86165	405	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 2.

All (405) 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)
5:A:888:A:N6	45:A:3404:CL:CL	2.55	0.76
3:QX:50:ALA:HB1	39:RH:66:VAL:HG11	1.67	0.75
5:A:1103:A:N6	5:A:1363:A:O2'	2.20	0.75
12:RQ:38:GLN:HE21	15:RA:59:ARG:HH22	1.35	0.73
15:RA:57:GLY:HA3	22:QP:170:ARG:HD2	1.71	0.71
40:LI:40:HIS:HD2	40:LI:42:ALA:H	1.38	0.70
5:A:3351:U:O2'	5:A:3353:G:N2	2.26	0.69
9:JT:62:THR:HG22	9:JT:64:LYS:H	1.56	0.69
5:A:2437:G:H1	5:A:2510:U:H3	1.41	0.68
5:A:3268:A:OP1	42:LJ:46:ARG:NH2	2.26	0.68
5:A:2969:A:N7	33:LF:215:ASN:ND2	2.41	0.68
10:LM:21:LYS:HG3	13:JU:8:LYS:HD2	1.75	0.68
22:QP:31:LYS:HE3	38:LH:286:VAL:HG21	1.76	0.67
5:A:3042:U:OP2	5:A:3092:C:N4	2.28	0.67
18:LO:92:ARG:HA	18:LO:172:LEU:HB2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:LJ:76:LEU:H	42:LJ:138:GLN:HE22	1.41	0.66
5:A:2185:G:O2'	5:A:2314:U:OP2	2.12	0.66
32:QV:63:LYS:O	32:QV:70:ARG:NH1	2.29	0.66
5:A:1213:G:H4'	26:QS:90:MET:HG3	1.78	0.65
5:A:3218:A:O2'	5:A:3219:G:OP2	2.11	0.65
5:A:1019:G:H1	5:A:1033:U:H3	1.45	0.65
14:LN:206:LEU:HD11	40:LI:286:VAL:HG23	1.78	0.64
36:LG:206:ASP:OD2	36:LG:287:LYS:NZ	2.29	0.63
5:A:1152:G:OP2	5:A:1152:G:N2	2.30	0.63
20:QO:122:ALA:HB3	20:QO:143:PRO:HB2	1.79	0.63
22:QP:62:VAL:HG13	22:QP:66:ARG:HD2	1.81	0.63
5:A:674:G:OP1	38:LH:31:ARG:NH1	2.32	0.62
5:A:3275:U:O2'	35:RF:99:ARG:NH1	2.32	0.62
5:A:3092:C:O2'	5:A:3094:A:OP2	2.17	0.62
5:A:824:C:H5''	33:LF:21:ARG:HD3	1.81	0.62
15:RA:76:ASP:HB3	15:RA:116:GLY:HA3	1.81	0.62
5:A:2794:G:OP1	12:RQ:61:LYS:NZ	2.33	0.62
27:RD:41:LYS:HE2	27:RD:47:ASP:HA	1.81	0.61
5:A:2282:U:OP1	5:A:2973:G:O2'	2.15	0.61
28:QT:116:ARG:HA	28:QT:126:VAL:HG21	1.82	0.61
11:QZ:25:ILE:HA	11:QZ:43:VAL:HG12	1.82	0.60
5:A:2964:G:N2	5:A:2967:A:OP2	2.30	0.60
26:QS:130:GLU:HG2	26:QS:131:LYS:HG2	1.83	0.60
5:A:2945:G:O2'	5:A:2948:C:OP2	2.19	0.60
41:RI:5:THR:HG23	41:RI:12:ASN:HB2	1.84	0.60
3:QX:27:ARG:HD3	6:LL:50:VAL:HG21	1.83	0.60
14:LN:36:LEU:HD21	14:LN:69:ARG:HD2	1.84	0.60
17:JV:123:GLN:OE1	17:JV:128:LYS:NZ	2.35	0.60
5:A:110:G:OP2	9:JT:73:ARG:NH2	2.31	0.59
5:A:2712:U:HO2'	5:A:2743:A:HO2'	1.49	0.59
36:LG:292:ALA:HB2	36:LG:302:LYS:HD2	1.83	0.59
5:A:979:U:O2'	5:A:980:A:OP2	2.18	0.58
5:A:2538:U:O2'	5:A:2541:U:O4	2.20	0.58
5:A:2895:G:O2'	8:RO:100:TYR:O	2.20	0.58
5:A:1639:C:OP2	37:RG:74:ARG:NH1	2.36	0.58
2:LK:94:LYS:NZ	5:A:1156:C:OP2	2.35	0.58
5:A:1504:A:H5''	20:QO:125:GLN:HE22	1.67	0.57
5:A:1635:G:N2	5:A:1638:A:OP2	2.32	0.57
19:RB:20:GLY:HA3	28:QT:82:ASN:HB2	1.86	0.57
36:LG:316:GLU:OE1	36:LG:318:LYS:NZ	2.37	0.57
6:LL:83:ASP:OD1	6:LL:86:THR:OG1	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:LI:50:ARG:NH1	40:LI:147:ASP:OD2	2.36	0.57
5:A:394:G:N1	5:A:397:A:OP2	2.38	0.57
10:LM:5:GLN:HE22	10:LM:7:GLU:HB2	1.70	0.57
5:A:2674:A:H5''	18:LO:105:GLY:HA3	1.86	0.56
9:JT:123:ILE:HG22	39:RH:118:ILE:HG12	1.87	0.56
28:QT:39:ILE:HD12	28:QT:102:ARG:HD3	1.86	0.56
5:A:966:U:OP1	15:RA:44:ASN:ND2	2.39	0.56
17:JV:183:THR:HG22	17:JV:187:ARG:HB2	1.87	0.56
5:A:216:G:OP1	7:QY:16:ARG:NH1	2.38	0.56
26:QS:8:GLN:HB3	26:QS:64:ILE:HD11	1.87	0.56
38:LH:3:ARG:NH1	38:LH:22:LEU:O	2.38	0.56
5:A:2112:U:H4'	5:A:2113:A:O5'	2.06	0.56
18:LO:90:GLN:HE21	18:LO:172:LEU:HG	1.71	0.56
40:LI:231:ILE:HG23	40:LI:235:SER:HB3	1.88	0.56
5:A:3346:U:H3	5:A:3359:A:H61	1.54	0.55
5:A:627:U:H4'	5:A:1399:A:H1'	1.89	0.55
24:QQ:105:LEU:HD12	24:QQ:135:LYS:HE3	1.88	0.55
5:A:1493:G:OP2	5:A:1493:G:N2	2.37	0.55
28:QT:115:LYS:HD3	28:QT:128:LEU:HD11	1.89	0.55
14:LN:21:ARG:O	14:LN:24:ARG:NH1	2.39	0.55
5:A:1814:A:H4'	5:A:1815:U:H5'	1.88	0.55
5:A:3218:A:H2'	5:A:3278:C:H5	1.72	0.55
18:LO:49:LYS:HB3	18:LO:62:ASN:HA	1.89	0.55
5:A:3207:U:O2	26:QS:166:LYS:NZ	2.39	0.54
5:A:2307:G:O2'	5:A:2310:U:OP2	2.24	0.54
5:A:2745:G:N2	5:A:2748:A:OP2	2.39	0.54
5:A:2526:C:OP1	33:LF:37:ARG:NH1	2.40	0.54
9:JT:85:LEU:HD13	9:JT:90:ALA:HB2	1.89	0.54
5:A:1094:U:H4'	5:A:1096:U:H5''	1.88	0.54
5:A:1419:A:N6	45:A:3489:CL:CL	2.75	0.54
4:RM:31:LEU:HA	4:RM:37:PRO:HA	1.90	0.54
5:A:2150:G:O2'	5:A:2189:U:OP1	2.25	0.53
29:LE:7:G:OP1	40:LI:33:ARG:NH1	2.41	0.53
38:LH:156:LEU:HD12	38:LH:159:ILE:HD12	1.88	0.53
5:A:3043:C:OP1	32:QV:45:ARG:NH1	2.41	0.53
10:LM:92:TYR:HB2	10:LM:142:ASP:HB3	1.90	0.53
5:A:518:G:OP2	5:A:518:G:N2	2.30	0.53
38:LH:159:ILE:HG23	38:LH:164:GLU:HG3	1.90	0.53
36:LG:284:ARG:NH1	36:LG:293:ASN:O	2.41	0.53
5:A:1686:U:O4	30:QU:82:LYS:NZ	2.41	0.53
5:A:269:G:H5''	17:JV:14:LYS:HE2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:3317:U:H4'	5:A:3318:G:H5'	1.91	0.53
33:LF:104:LEU:HD22	33:LF:136:ILE:HD11	1.90	0.53
12:RQ:71:ARG:HD2	12:RQ:80:ARG:HD3	1.91	0.52
14:LN:44:ASP:OD1	14:LN:181:TYR:OH	2.23	0.52
18:LO:18:VAL:HG22	18:LO:70:THR:HG22	1.89	0.52
19:RB:33:LYS:O	28:QT:88:ARG:NH1	2.42	0.52
5:A:591:G:O2'	42:LJ:17:ALA:O	2.25	0.52
5:A:900:G:H1'	5:A:1589:A:N6	2.25	0.52
40:LI:60:ILE:HB	40:LI:80:SER:HB2	1.90	0.52
36:LG:139:GLN:HG3	36:LG:141:GLY:H	1.73	0.52
42:LJ:43:LEU:HD11	42:LJ:85:ILE:HG13	1.91	0.52
41:RI:70:ARG:HG2	41:RI:87:VAL:HG21	1.92	0.52
5:A:1579:C:H42	5:A:1580:A:H62	1.58	0.52
5:A:2433:U:H1'	17:JV:125:SER:HB2	1.91	0.52
33:LF:101:VAL:HG22	33:LF:165:VAL:HG22	1.91	0.52
5:A:2631:U:OP2	28:QT:4:SER:OG	2.26	0.52
12:RQ:35:LEU:HA	12:RQ:40:LYS:HG2	1.92	0.52
5:A:358:G:N2	5:A:361:A:OP2	2.43	0.51
35:RF:14:LEU:HD11	35:RF:31:LYS:HB2	1.91	0.51
6:LL:158:ASP:HB3	6:LL:159:PRO:HD3	1.92	0.51
43:RJ:64:MET:HE3	43:RJ:67:LEU:HD23	1.92	0.51
5:A:870:G:N2	45:A:3404:CL:CL	2.81	0.51
5:A:3218:A:HO2'	5:A:3219:G:P	2.32	0.51
14:LN:30:LYS:HG3	14:LN:63:GLU:HG3	1.93	0.51
14:LN:54:SER:HB2	14:LN:135:ILE:HD11	1.92	0.51
5:A:371:G:N1	5:A:374:A:OP2	2.39	0.51
7:QY:74:TYR:OH	25:LD:75:G:OP2	2.26	0.51
5:A:627:U:H2'	5:A:628:A:C8	2.47	0.50
5:A:3329:U:H5''	36:LG:308:MET:HE2	1.93	0.50
29:LE:45:A:OP1	40:LI:151:GLN:NE2	2.40	0.50
33:LF:117:GLU:HG2	33:LF:124:GLY:H	1.75	0.50
6:LL:84:ARG:NH1	25:LD:156:U:OP2	2.44	0.50
29:LE:12:U:OP2	29:LE:68:C:O2'	2.29	0.50
5:A:1717:U:H2'	5:A:1718:G:C8	2.47	0.50
26:QS:77:VAL:HG11	26:QS:106:LEU:HD22	1.94	0.50
5:A:2514:U:O2	5:A:2593:A:N6	2.43	0.50
5:A:3121:U:H1'	5:A:3122:A:H5''	1.92	0.50
5:A:3217:C:H6	5:A:3266:G:H21	1.60	0.50
5:A:609:G:OP2	38:LH:315:LYS:NZ	2.29	0.50
5:A:1404:G:O6	31:RE:16:LYS:NZ	2.43	0.50
5:A:1940:G:H21	5:A:3362:A:H8	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2103:U:H2'	5:A:2104:A:H8	1.77	0.50
4:RM:4:GLU:OE1	5:A:1746:U:O2'	2.30	0.50
5:A:1913:A:N3	5:A:2120:A:H2'	2.27	0.49
5:A:3348:G:H22	5:A:3357:U:H3	1.60	0.49
33:LF:113:VAL:HG12	33:LF:166:ILE:HD13	1.94	0.49
1:2:25:GLN:OE1	1:2:28:ARG:NH2	2.45	0.49
24:QQ:115:ILE:HD12	24:QQ:119:LEU:HD23	1.92	0.49
40:LI:106:ALA:HB2	40:LI:166:ALA:HA	1.93	0.49
5:A:170:G:H1	5:A:248:U:H3	1.61	0.49
10:LM:57:VAL:HG23	10:LM:68:LEU:HD13	1.94	0.49
20:QO:67:ILE:HD11	20:QO:80:LYS:HB3	1.95	0.49
5:A:655:C:H2'	5:A:656:A:C8	2.48	0.49
5:A:1054:A:H5''	5:A:2637:A:H61	1.78	0.49
5:A:1740:U:H1'	5:A:1741:A:H2	1.78	0.49
12:RQ:35:LEU:H	12:RQ:35:LEU:HD23	1.77	0.49
5:A:1134:G:O2'	5:A:2642:A:N3	2.43	0.49
5:A:2592:G:H4'	5:A:2594:C:C2	2.47	0.49
5:A:1064:A:H4'	5:A:1065:A:O5'	2.13	0.49
5:A:3379:C:H4'	36:LG:315:GLY:HA2	1.95	0.49
40:LI:278:SER:OG	40:LI:281:GLU:OE1	2.30	0.49
41:RI:66:GLU:OE2	41:RI:91:ASN:ND2	2.42	0.49
5:A:3067:C:H3'	24:QQ:62:ARG:HH22	1.78	0.49
6:LL:162:LEU:HD23	17:JV:7:LEU:HD11	1.95	0.49
40:LI:153:THR:HG23	40:LI:160:PHE:HZ	1.78	0.49
5:A:2890:A:O2'	5:A:2933:A:N3	2.45	0.48
40:LI:278:SER:N	40:LI:281:GLU:OE2	2.45	0.48
5:A:1404:G:N2	5:A:1407:A:OP2	2.39	0.48
5:A:3350:C:H42	5:A:3353:G:H1	1.60	0.48
26:QS:12:ARG:HH21	26:QS:22:PRO:HD2	1.77	0.48
4:RM:26:LYS:NZ	4:RM:28:ASN:OD1	2.43	0.48
5:A:1390:A:N6	5:A:1418:A:O2'	2.46	0.48
9:JT:129:ASN:OD1	9:JT:130:GLY:N	2.46	0.48
5:A:266:A:OP1	17:JV:5:LYS:NZ	2.45	0.48
5:A:340:C:OP2	38:LH:195:ARG:NH1	2.36	0.48
5:A:1108:U:H2'	5:A:1109:U:C6	2.48	0.48
5:A:1863:G:N1	5:A:1866:C:OP2	2.42	0.48
5:A:1191:U:H4'	5:A:1192:C:H5''	1.96	0.48
9:JT:47:ALA:C	9:JT:49:ARG:H	2.22	0.48
36:LG:339:ARG:HH12	36:LG:342:LEU:HG	1.79	0.48
5:A:3350:C:H2'	5:A:3351:U:H2'	1.96	0.48
18:LO:81:GLU:HG2	18:LO:167:TYR:HE1	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:LL:24:ASN:HB3	6:LL:25:PRO:HD3	1.96	0.48
36:LG:137:TYR:HE2	36:LG:196:ARG:HH22	1.60	0.48
3:QX:71:THR:HA	3:QX:74:LYS:HE2	1.96	0.47
5:A:1497:C:O2'	5:A:1602:A:N3	2.43	0.47
9:JT:153:ASP:OD1	9:JT:154:VAL:N	2.46	0.47
5:A:1643:A:O2'	5:A:1644:C:O4'	2.30	0.47
18:LO:28:ASP:OD2	18:LO:32:ARG:NH1	2.48	0.47
5:A:981:U:H2'	5:A:982:C:C6	2.50	0.47
5:A:916:G:H5'	5:A:917:A:OP1	2.14	0.47
5:A:412:G:OP1	20:QO:62:ARG:NH1	2.46	0.47
5:A:1597:C:H5'	5:A:1696:A:H1'	1.96	0.47
5:A:2787:G:H1'	15:RA:58:MET:HE2	1.95	0.47
5:A:2960:C:H2'	5:A:2961:G:C8	2.49	0.47
5:A:3231:U:H2'	5:A:3232:G:H8	1.80	0.47
15:RA:94:ALA:HB2	15:RA:121:VAL:HG22	1.95	0.47
1:2:9:ILE:HD12	1:2:51:LEU:HD13	1.97	0.47
5:A:2138:A:C4	43:RJ:3:LYS:HB3	2.49	0.47
21:JW:61:ALA:HA	21:JW:70:PRO:HD2	1.97	0.47
23:RC:100:ILE:HG23	23:RC:101:LEU:HD12	1.97	0.47
5:A:198:A:N3	5:A:218:G:O2'	2.48	0.47
5:A:3228:C:H4'	5:A:3229:G:O5'	2.15	0.47
7:QY:5:SER:HB3	7:QY:8:VAL:HG12	1.97	0.47
22:QP:165:ILE:HD11	22:QP:172:PHE:HB3	1.97	0.47
40:LI:52:VAL:HG21	40:LI:65:ILE:HD12	1.97	0.47
5:A:1097:G:H4'	5:A:1098:A:O5'	2.14	0.46
34:QW:4:GLU:HB2	34:QW:13:ILE:HB	1.97	0.46
5:A:681:U:O4	38:LH:118:LYS:NZ	2.41	0.46
5:A:1355:A:H4'	5:A:1356:U:O5'	2.14	0.46
45:A:3506:CL:CL	33:LF:6:ARG:HB2	2.52	0.46
20:QO:126:ARG:HA	20:QO:140:GLU:HG2	1.97	0.46
36:LG:57:VAL:HG22	36:LG:73:VAL:HG22	1.97	0.46
1:2:21:ARG:NH1	25:LD:52:A:OP1	2.41	0.46
33:LF:2:GLY:HA2	33:LF:207:VAL:HG23	1.96	0.46
19:RB:21:ILE:N	28:QT:82:ASN:O	2.46	0.46
5:A:2513:U:O2'	5:A:2514:U:O5'	2.33	0.46
5:A:3217:C:C5	5:A:3220:G:H1'	2.50	0.46
23:RC:42:ILE:HD11	23:RC:67:VAL:HG22	1.97	0.46
42:LJ:172:HIS:CD2	42:LJ:173:MET:HG3	2.50	0.46
6:LL:185:ARG:O	6:LL:188:THR:HG22	2.16	0.46
9:JT:46:ILE:HG23	9:JT:47:ALA:N	2.31	0.46
36:LG:166:ILE:HD11	36:LG:171:LEU:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2352:A:H5''	20:QO:83:TRP:O	2.16	0.46
38:LH:271:LYS:HB2	38:LH:274:TYR:HB3	1.97	0.46
5:A:2763:U:O2	46:A:3426:SPD:N1	2.49	0.46
5:A:3230:G:H4'	13:JU:132:LYS:HD3	1.98	0.45
6:LL:146:LYS:HE3	6:LL:173:MET:HE3	1.98	0.45
5:A:1833:G:N7	49:A:3626:HOH:O	2.35	0.45
36:LG:123:TYR:CZ	36:LG:124:LYS:HG3	2.51	0.45
5:A:528:U:H2'	5:A:529:A:C8	2.52	0.45
11:QZ:22:LYS:NZ	11:QZ:129:TRP:O	2.38	0.45
14:LN:169:LYS:HD2	28:QT:159:PHE:HA	1.99	0.45
38:LH:161:LYS:HB2	38:LH:164:GLU:HG2	1.97	0.45
5:A:427:C:OP2	31:RE:15:LYS:NZ	2.42	0.45
5:A:1554:U:H4'	5:A:1555:U:OP1	2.14	0.45
5:A:2193:U:H5'	5:A:2194:G:H5'	1.98	0.45
13:JU:23:ILE:HG13	13:JU:63:VAL:HG12	1.99	0.45
35:RF:37:THR:HG22	35:RF:39:GLN:H	1.82	0.45
5:A:792:G:H5''	15:RA:2:PRO:HD3	1.98	0.45
25:LD:81:U:H4'	25:LD:82:U:H5'	1.98	0.45
40:LI:82:GLU:O	40:LI:85:ARG:HG2	2.16	0.45
32:QV:13:ILE:HD11	32:QV:121:GLU:HG2	1.99	0.45
5:A:1098:A:OP2	28:QT:129:LYS:HA	2.17	0.45
5:A:2392:C:O2'	36:LG:266:ARG:NH1	2.47	0.45
13:JU:72:LEU:HD12	13:JU:73:PRO:HD2	1.98	0.45
5:A:283:G:OP2	5:A:285:A:O2'	2.31	0.44
2:LK:121:LYS:HB2	28:QT:133:ALA:HB3	1.99	0.44
5:A:2202:C:H5''	33:LF:226:SER:HB3	1.99	0.44
21:JW:136:THR:OG1	21:JW:140:LYS:NZ	2.50	0.44
2:LK:176:TYR:CZ	2:LK:197:GLN:HG2	2.52	0.44
4:RM:5:ILE:HD11	4:RM:11:PHE:HD2	1.83	0.44
5:A:1877:U:H5''	5:A:1878:G:O4'	2.17	0.44
5:A:3002:C:O2'	36:LG:180:GLU:OE2	2.28	0.44
14:LN:51:HIS:CD2	14:LN:168:SER:HB2	2.52	0.44
5:A:59:G:H4'	5:A:60:A:H4'	2.00	0.44
5:A:1486:G:H21	37:RG:6:THR:HG22	1.82	0.44
5:A:1895:A:O2'	5:A:3053:G:H4'	2.16	0.44
5:A:1927:G:C8	16:RT:16:VAL:HG12	2.53	0.44
5:A:3252:G:H2'	5:A:3253:G:C8	2.52	0.44
18:LO:87:LYS:NZ	18:LO:105:GLY:O	2.44	0.44
5:A:3188:G:OP2	13:JU:8:LYS:NZ	2.51	0.44
14:LN:93:PRO:HB2	14:LN:125:LEU:HB3	1.99	0.44
5:A:2585:G:H2'	5:A:2585:G:N3	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:JV:153:ASP:OD1	17:JV:154:PRO:HD2	2.18	0.44
14:LN:86:HIS:HB3	14:LN:139:ARG:HG2	1.99	0.43
5:A:525:C:H5''	13:JU:79:ALA:HB2	2.01	0.43
32:QV:6:ALA:HB1	32:QV:125:LEU:HD11	2.01	0.43
40:LI:182:GLY:HA2	40:LI:194:LEU:HD23	2.01	0.43
5:A:842:G:H1	5:A:851:C:H42	1.66	0.43
5:A:1110:U:H2'	5:A:1111:U:C6	2.53	0.43
5:A:2103:U:H2'	5:A:2104:A:C8	2.51	0.43
17:JV:28:TRP:O	17:JV:32:GLN:HG2	2.19	0.43
18:LO:92:ARG:HG2	18:LO:172:LEU:HD12	1.99	0.43
5:A:993:G:N3	5:A:2637:A:H2'	2.34	0.43
11:QZ:97:SER:O	11:QZ:100:THR:HG22	2.19	0.43
37:RG:87:GLU:OE2	37:RG:91:ARG:NH2	2.44	0.43
5:A:1095:U:H4'	5:A:1096:U:H5'	2.00	0.43
5:A:1192:C:N4	5:A:1302:A:OP2	2.40	0.43
21:JW:96:LYS:O	21:JW:100:GLU:HG2	2.19	0.43
5:A:715:A:OP2	15:RA:113:LEU:HB3	2.19	0.43
18:LO:44:THR:HG23	29:LE:39:C:H4'	2.00	0.43
29:LE:112:G:H2'	29:LE:113:C:C6	2.53	0.43
2:LK:132:PRO:HA	2:LK:229:PHE:CG	2.53	0.43
5:A:3050:U:O2'	34:QW:16:GLY:O	2.35	0.43
5:A:3218:A:H2'	5:A:3278:C:C5	2.52	0.43
7:QY:35:LEU:HD23	7:QY:39:LEU:HB3	1.99	0.43
22:QP:125:ASP:OD2	38:LH:282:SER:OG	2.25	0.43
29:LE:1:G:O4'	40:LI:270:LYS:NZ	2.51	0.43
42:LJ:66:SER:HB3	42:LJ:76:LEU:HD23	2.00	0.43
5:A:1621:A:H2'	5:A:1622:U:C6	2.53	0.43
33:LF:80:GLU:HG2	33:LF:170:ALA:HA	2.01	0.43
15:RA:83:PRO:HG2	15:RA:86:LYS:HE2	2.00	0.43
42:LJ:76:LEU:N	42:LJ:138:GLN:HE22	2.14	0.43
5:A:1176:C:H2'	5:A:1177:G:N2	2.33	0.42
5:A:1579:C:N4	5:A:1580:A:H62	2.16	0.42
5:A:2244:A:H5''	33:LF:243:THR:HB	2.01	0.42
18:LO:117:ASP:OD1	18:LO:119:SER:OG	2.34	0.42
22:QP:133:LYS:HB2	22:QP:135:GLN:NE2	2.34	0.42
5:A:524:U:OP1	13:JU:77:ARG:NH2	2.41	0.42
5:A:1039:U:H2'	5:A:1040:A:C8	2.55	0.42
5:A:3288:G:HO2'	5:A:3289:G:H8	1.64	0.42
10:LM:87:LYS:HE3	10:LM:187:ILE:HA	2.00	0.42
5:A:2356:A:H61	5:A:2983:C:H5	1.65	0.42
32:QV:27:ASP:OD1	32:QV:27:ASP:N	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:595:G:H1	5:A:609:G:H5''	1.84	0.42
5:A:2213:A:H2'	5:A:2214:A:C8	2.55	0.42
11:QZ:27:LYS:NZ	11:QZ:93:LYS:O	2.52	0.42
5:A:3274:A:H5''	5:A:3276:G:OP2	2.18	0.42
8:RO:98:LYS:HD3	8:RO:118:THR:HG21	2.01	0.42
25:LD:110:C:O2'	25:LD:112:U:OP2	2.33	0.42
5:A:2611:U:H2'	5:A:2612:U:C6	2.55	0.42
12:RQ:46:LYS:HE3	12:RQ:54:THR:HB	2.00	0.42
27:RD:55:LEU:HB2	27:RD:95:PRO:HD3	2.01	0.42
5:A:86:G:O2'	5:A:98:G:O6	2.35	0.42
5:A:170:G:H2'	5:A:171:G:C8	2.55	0.42
5:A:1458:U:O2'	27:RD:56:ASN:ND2	2.52	0.42
5:A:2794:G:O2'	5:A:2795:U:OP2	2.35	0.42
20:QO:56:ARG:NH2	20:QO:75:GLU:OE2	2.44	0.42
39:RH:102:GLU:HG3	39:RH:106:LYS:HE3	2.00	0.42
5:A:2880:U:H1'	36:LG:250:ALA:HB3	2.01	0.42
5:A:3233:C:H2'	5:A:3234:A:C8	2.55	0.42
25:LD:85:G:H4'	25:LD:86:U:OP1	2.20	0.42
40:LI:95:TRP:HZ3	40:LI:199:ILE:HD13	1.85	0.42
41:RI:34:SER:H	41:RI:37:THR:HG22	1.84	0.42
33:LF:30:ARG:HG2	33:LF:74:GLU:HG2	2.00	0.42
35:RF:48:ARG:HH21	35:RF:68:TRP:HB3	1.85	0.42
42:LJ:60:ASP:OD1	42:LJ:62:THR:OG1	2.31	0.42
10:LM:90:MET:HE2	10:LM:179:ILE:HG22	2.02	0.42
26:QS:26:ARG:O	28:QT:150:THR:HA	2.20	0.42
30:QU:21:SER:HB2	30:QU:22:PRO:HD3	2.01	0.42
5:A:1117:G:OP1	19:RB:4:SER:HB2	2.20	0.41
29:LE:36:C:H4'	40:LI:155:THR:HG23	2.01	0.41
5:A:723:U:O2'	19:RB:29:TYR:OH	2.31	0.41
5:A:1616:U:H2'	5:A:1617:G:C8	2.55	0.41
24:QQ:133:LYS:HG3	24:QQ:134:HIS:CD2	2.55	0.41
2:LK:136:TYR:CZ	2:LK:231:ASN:HB2	2.55	0.41
5:A:2424:A:OP1	17:JV:90:ASN:ND2	2.54	0.41
5:A:2947:G:N3	36:LG:250:ALA:HB1	2.36	0.41
28:QT:27:LEU:HD11	40:LI:34:LYS:HA	2.03	0.41
29:LE:121:U:OP2	40:LI:265:TYR:OH	2.29	0.41
5:A:1638:A:N1	5:A:1736:G:O2'	2.50	0.41
5:A:2689:A:H2'	5:A:2689:A:N3	2.34	0.41
5:A:2697:A:H2'	5:A:2698:G:C8	2.55	0.41
15:RA:47:LYS:HE2	15:RA:48:TYR:CZ	2.56	0.41
22:QP:76:ALA:HB1	22:QP:138:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:507:U:H2'	5:A:508:U:C6	2.55	0.41
5:A:1571:A:H2'	5:A:1572:U:O4'	2.21	0.41
20:QO:126:ARG:NH1	20:QO:140:GLU:OE2	2.50	0.41
37:RG:3:GLN:NE2	37:RG:30:LEU:H	2.18	0.41
37:RG:46:ASP:HB2	37:RG:84:CYS:SG	2.61	0.41
5:A:1347:U:H2'	5:A:1355:A:H61	1.86	0.41
5:A:2536:A:H2'	5:A:2537:U:C5	2.56	0.41
5:A:3218:A:H5''	5:A:3219:G:C4	2.56	0.41
10:LM:7:GLU:OE2	10:LM:54:LYS:HB3	2.20	0.41
11:QZ:27:LYS:NZ	11:QZ:96:VAL:O	2.37	0.41
32:QV:67:PRO:HA	32:QV:70:ARG:HD3	2.03	0.41
34:QW:57:LYS:HB3	34:QW:57:LYS:HE3	1.73	0.41
5:A:662:U:H2'	5:A:663:C:C6	2.55	0.41
5:A:2407:C:H2'	5:A:2408:U:C6	2.56	0.41
5:A:2768:U:H2'	5:A:2769:A:C8	2.56	0.41
5:A:3356:G:H2'	5:A:3357:U:C6	2.56	0.41
18:LO:133:ARG:NH2	18:LO:158:ASP:OD2	2.47	0.41
38:LH:152:VAL:HG21	38:LH:156:LEU:HD22	2.03	0.41
5:A:421:G:O6	5:A:2383:C:O2'	2.36	0.41
5:A:2108:C:H1'	5:A:3344:A:H8	1.85	0.41
5:A:546:C:OP1	5:A:547:G:N2	2.54	0.41
5:A:629:U:H2'	5:A:630:A:C8	2.56	0.41
5:A:1570:U:O2	5:A:1571:A:H1'	2.21	0.41
5:A:1576:G:H2'	5:A:1577:G:O4'	2.20	0.41
5:A:2947:G:C2	36:LG:250:ALA:HB1	2.55	0.41
18:LO:44:THR:HA	18:LO:45:PRO:HD3	1.92	0.41
5:A:553:U:H2'	5:A:554:A:O4'	2.21	0.41
5:A:633:C:O2'	35:RF:21:ARG:O	2.34	0.41
9:JT:106:GLN:HB3	41:RI:18:THR:HB	2.03	0.41
5:A:1047:A:N3	5:A:2633:U:O2'	2.54	0.40
5:A:1624:G:O2'	5:A:1643:A:N1	2.48	0.40
5:A:2708:C:OP1	12:RQ:100:LYS:NZ	2.54	0.40
18:LO:109:HIS:HA	18:LO:112:LEU:HD23	2.02	0.40
19:RB:24:PRO:HD3	28:QT:84:TYR:HB2	2.03	0.40
19:RB:33:LYS:HB3	19:RB:33:LYS:HE3	1.88	0.40
28:QT:69:LYS:HA	40:LI:40:HIS:CD2	2.56	0.40
36:LG:211:GLN:NE2	36:LG:283:TYR:O	2.45	0.40
5:A:1347:U:H5''	38:LH:303:GLY:H	1.86	0.40
5:A:2129:U:H2'	5:A:2130:G:C8	2.56	0.40
5:A:2510:U:H2'	5:A:2511:A:H8	1.87	0.40
6:LL:162:LEU:HA	17:JV:7:LEU:HD21	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:QZ:23:VAL:HG23	11:QZ:45:GLY:HA3	2.03	0.40
16:RT:49:ARG:HB2	16:RT:55:TRP:CZ3	2.56	0.40
36:LG:173:GLN:HG2	36:LG:175:LYS:H	1.85	0.40
36:LG:236:LYS:HE2	36:LG:236:LYS:HB2	1.96	0.40
5:A:59:G:H2'	25:LD:33:A:O2'	2.22	0.40
7:QY:3:LYS:HD2	7:QY:8:VAL:O	2.21	0.40
2:LK:86:VAL:O	2:LK:114:GLY:HA2	2.22	0.40
5:A:126:U:H1'	17:JV:57:GLN:HE22	1.87	0.40
5:A:2108:C:H1'	5:A:3344:A:C8	2.56	0.40
5:A:2180:G:H2'	5:A:2181:C:C6	2.56	0.40
5:A:3094:A:H2'	5:A:3095:U:C6	2.57	0.40
6:LL:154:ALA:HB2	6:LL:186:LEU:HD12	2.03	0.40
9:JT:49:ARG:HD3	39:RH:116:TYR:CE1	2.57	0.40
11:QZ:9:LYS:HE3	11:QZ:83:THR:O	2.21	0.40
14:LN:34:TYR:HD2	14:LN:89:VAL:HB	1.86	0.40
33:LF:211:HIS:CD2	33:LF:219:ILE:HG23	2.57	0.40
5:A:2512:C:H2'	5:A:2513:U:C6	2.56	0.40
11:QZ:76:ASN:OD1	11:QZ:77:TYR:N	2.54	0.40
17:JV:175:ASN:O	17:JV:184:LYS:HG2	2.21	0.40
26:QS:125:LYS:HE2	26:QS:127:ALA:HB2	2.03	0.40
40:LI:178:ASN:OD1	40:LI:178:ASN:N	2.55	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	
1	2	48/51 (94%)	48 (100%)	0	0	100	100
2	LK	218/244 (89%)	215 (99%)	3 (1%)	0	100	100
3	QX	116/142 (82%)	113 (97%)	3 (3%)	0	100	100
4	RM	75/78 (96%)	74 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	LL	214/256 (84%)	209 (98%)	5 (2%)	0	100	100
7	QY	122/127 (96%)	121 (99%)	1 (1%)	0	100	100
8	RO	48/128 (38%)	48 (100%)	0	0	100	100
9	JT	187/199 (94%)	180 (96%)	7 (4%)	0	100	100
10	LM	186/191 (97%)	179 (96%)	7 (4%)	0	100	100
11	QZ	133/136 (98%)	127 (96%)	6 (4%)	0	100	100
12	RQ	100/106 (94%)	93 (93%)	7 (7%)	0	100	100
13	JU	132/138 (96%)	129 (98%)	3 (2%)	0	100	100
14	LN	200/221 (90%)	197 (98%)	3 (2%)	0	100	100
15	RA	146/149 (98%)	132 (90%)	13 (9%)	1 (1%)	18	13
16	RT	89/92 (97%)	86 (97%)	3 (3%)	0	100	100
17	JV	201/204 (98%)	196 (98%)	5 (2%)	0	100	100
18	LO	166/174 (95%)	161 (97%)	5 (3%)	0	100	100
19	RB	53/59 (90%)	50 (94%)	3 (6%)	0	100	100
20	QO	164/184 (89%)	162 (99%)	2 (1%)	0	100	100
21	JW	195/199 (98%)	192 (98%)	3 (2%)	0	100	100
22	QP	183/186 (98%)	178 (97%)	5 (3%)	0	100	100
23	RC	93/105 (89%)	92 (99%)	1 (1%)	0	100	100
24	QQ	145/189 (77%)	145 (100%)	0	0	100	100
26	QS	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
27	RD	93/113 (82%)	93 (100%)	0	0	100	100
28	QT	157/160 (98%)	150 (96%)	7 (4%)	0	100	100
30	QU	95/121 (78%)	94 (99%)	1 (1%)	0	100	100
31	RE	124/130 (95%)	124 (100%)	0	0	100	100
32	QV	131/137 (96%)	130 (99%)	1 (1%)	0	100	100
33	LF	242/254 (95%)	230 (95%)	12 (5%)	0	100	100
34	QW	59/155 (38%)	59 (100%)	0	0	100	100
35	RF	104/107 (97%)	100 (96%)	4 (4%)	0	100	100
36	LG	383/387 (99%)	375 (98%)	8 (2%)	0	100	100
37	RG	101/121 (84%)	99 (98%)	2 (2%)	0	100	100
38	LH	358/362 (99%)	345 (96%)	13 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	RH	117/120 (98%)	116 (99%)	1 (1%)	0	100	100
40	LI	284/297 (96%)	277 (98%)	7 (2%)	0	100	100
41	RI	94/100 (94%)	91 (97%)	3 (3%)	0	100	100
42	LJ	152/176 (86%)	147 (97%)	5 (3%)	0	100	100
43	RJ	82/88 (93%)	81 (99%)	1 (1%)	0	100	100
All	All	5959/6558 (91%)	5803 (97%)	155 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	RA	15	VAL

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	2	47/48 (98%)	47 (100%)	0	100	100
2	LK	185/205 (90%)	184 (100%)	1 (0%)	81	87
3	QX	103/118 (87%)	103 (100%)	0	100	100
4	RM	68/69 (99%)	66 (97%)	2 (3%)	37	39
6	LL	182/208 (88%)	182 (100%)	0	100	100
7	QY	107/110 (97%)	107 (100%)	0	100	100
8	RO	45/116 (39%)	45 (100%)	0	100	100
9	JT	152/159 (96%)	152 (100%)	0	100	100
10	LM	168/171 (98%)	166 (99%)	2 (1%)	63	70
11	QZ	115/116 (99%)	114 (99%)	1 (1%)	70	77
12	RQ	87/91 (96%)	87 (100%)	0	100	100
13	JU	106/109 (97%)	106 (100%)	0	100	100
14	LN	176/187 (94%)	175 (99%)	1 (1%)	78	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	RA	118/119 (99%)	118 (100%)	0	100	100
16	RT	71/72 (99%)	71 (100%)	0	100	100
17	JV	175/176 (99%)	175 (100%)	0	100	100
18	LO	146/150 (97%)	143 (98%)	3 (2%)	47	52
19	RB	44/47 (94%)	44 (100%)	0	100	100
20	QO	135/146 (92%)	134 (99%)	1 (1%)	76	82
21	JW	160/162 (99%)	160 (100%)	0	100	100
22	QP	150/151 (99%)	150 (100%)	0	100	100
23	RC	80/88 (91%)	80 (100%)	0	100	100
24	QQ	122/154 (79%)	121 (99%)	1 (1%)	73	79
26	QS	155/156 (99%)	155 (100%)	0	100	100
27	RD	85/97 (88%)	85 (100%)	0	100	100
28	QT	136/137 (99%)	134 (98%)	2 (2%)	57	64
30	QU	84/107 (78%)	83 (99%)	1 (1%)	63	70
31	RE	108/111 (97%)	108 (100%)	0	100	100
32	QV	102/105 (97%)	102 (100%)	0	100	100
33	LF	187/196 (95%)	187 (100%)	0	100	100
34	QW	54/129 (42%)	54 (100%)	0	100	100
35	RF	90/91 (99%)	90 (100%)	0	100	100
36	LG	321/323 (99%)	320 (100%)	1 (0%)	86	91
37	RG	88/103 (85%)	87 (99%)	1 (1%)	65	72
38	LH	287/289 (99%)	287 (100%)	0	100	100
39	RH	104/105 (99%)	104 (100%)	0	100	100
40	LI	238/245 (97%)	235 (99%)	3 (1%)	61	68
41	RI	78/82 (95%)	78 (100%)	0	100	100
42	LJ	134/153 (88%)	133 (99%)	1 (1%)	76	82
43	RJ	69/71 (97%)	69 (100%)	0	100	100
All	All	5062/5472 (92%)	5041 (100%)	21 (0%)	81	89

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	LK	224	ILE

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Mol	Chain	Res	Type
4	RM	55	VAL
4	RM	78	LEU
10	LM	138	THR
10	LM	157	ASN
11	QZ	23	VAL
14	LN	83	ASP
18	LO	44	THR
18	LO	55	ARG
18	LO	59	ILE
20	QO	182	ILE
24	QQ	51	VAL
28	QT	83	ARG
28	QT	128	LEU
30	QU	56	VAL
36	LG	114	VAL
37	RG	58	ARG
40	LI	93	THR
40	LI	155	THR
40	LI	286	VAL
42	LJ	93	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
2	LK	93	ASN
2	LK	159	GLN
2	LK	186	HIS
2	LK	209	ASN
2	LK	225	GLN
6	LL	28	HIS
6	LL	38	GLN
6	LL	77	GLN
6	LL	240	ASN
9	JT	106	GLN
9	JT	137	GLN
9	JT	160	GLN
10	LM	5	GLN
10	LM	8	GLN
10	LM	51	GLN
10	LM	64	HIS
10	LM	139	ASN
10	LM	183	HIS

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Mol	Chain	Res	Type
11	QZ	123	GLN
12	RQ	38	GLN
12	RQ	90	HIS
13	JU	119	GLN
14	LN	123	HIS
14	LN	209	ASN
15	RA	65	GLN
16	RT	25	GLN
17	JV	11	GLN
17	JV	57	GLN
17	JV	117	ASN
17	JV	138	GLN
18	LO	7	ASN
18	LO	43	GLN
18	LO	152	HIS
19	RB	6	ASN
19	RB	17	HIS
20	QO	45	GLN
20	QO	121	GLN
20	QO	133	HIS
20	QO	137	ASN
22	QP	126	GLN
24	QQ	7	GLN
24	QQ	66	HIS
24	QQ	118	HIS
24	QQ	144	GLN
26	QS	49	HIS
27	RD	56	ASN
27	RD	57	GLN
28	QT	49	GLN
28	QT	98	HIS
28	QT	112	ASN
30	QU	87	ASN
31	RE	20	HIS
31	RE	21	HIS
31	RE	49	ASN
33	LF	97	ASN
35	RF	5	HIS
35	RF	26	ASN
36	LG	139	GLN
36	LG	198	HIS
36	LG	212	ASN

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Mol	Chain	Res	Type
36	LG	224	HIS
36	LG	243	HIS
36	LG	293	ASN
37	RG	3	GLN
38	LH	5	GLN
38	LH	59	GLN
38	LH	115	HIS
38	LH	175	HIS
39	RH	99	GLN
40	LI	40	HIS
40	LI	206	GLN
40	LI	274	GLN
42	LJ	57	HIS
42	LJ	138	GLN
43	RJ	30	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
25	LD	156/158 (98%)	21 (13%)	1 (0%)
29	LE	120/121 (99%)	9 (7%)	0
5	A	3036/3396 (89%)	389 (12%)	23 (0%)
All	All	3312/3675 (90%)	419 (12%)	24 (0%)

All (419) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	A	26	A
5	A	40	A
5	A	43	A
5	A	49	A
5	A	59	G
5	A	60	A
5	A	65	A
5	A	66	A
5	A	92	G
5	A	109	A
5	A	110	G
5	A	111	C
5	A	116	A
5	A	117	U

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Mol	Chain	Res	Type
5	A	118	U
5	A	121	A
5	A	122	A
5	A	133	U
5	A	135	C
5	A	136	G
5	A	154	U
5	A	156	G
5	A	157	A
5	A	166	C
5	A	170	G
5	A	187	A
5	A	190	U
5	A	191	U
5	A	192	C
5	A	200	C
5	A	210	U
5	A	218	G
5	A	219	A
5	A	240	U
5	A	243	G
5	A	245	U
5	A	251	G
5	A	252	U
5	A	269	G
5	A	286	U
5	A	295	A
5	A	305	U
5	A	315	C
5	A	323	A
5	A	329	U
5	A	339	C
5	A	350	C
5	A	376	G
5	A	398	A
5	A	399	A
5	A	401	U
5	A	402	A
5	A	403	C
5	A	421	G
5	A	422	A
5	A	439	C

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Mol	Chain	Res	Type
5	A	440	A
5	A	521	A
5	A	535	G
5	A	546	C
5	A	547	G
5	A	548	G
5	A	552	G
5	A	555	U
5	A	557	A
5	A	559	A
5	A	578	A
5	A	579	G
5	A	589	A
5	A	604	G
5	A	609	G
5	A	611	A
5	A	612	U
5	A	620	U
5	A	621	A
5	A	622	A
5	A	636	C
5	A	649	A
5	A	660	A
5	A	677	A
5	A	681	U
5	A	691	A
5	A	705	A
5	A	712	G
5	A	715	A
5	A	716	A
5	A	766	U
5	A	767	U
5	A	776	U
5	A	777	U
5	A	781	G
5	A	785	G
5	A	786	A
5	A	806	A
5	A	817	A
5	A	830	A
5	A	849	C
5	A	861	C

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Mol	Chain	Res	Type
5	A	874	U
5	A	879	U
5	A	896	A
5	A	907	G
5	A	908	G
5	A	914	A
5	A	916	G
5	A	917	A
5	A	921	A
5	A	923	C
5	A	925	A
5	A	937	G
5	A	944	C
5	A	959	C
5	A	960	U
5	A	979	U
5	A	980	A
5	A	981	U
5	A	994	G
5	A	995	U
5	A	1001	G
5	A	1002	A
5	A	1010	G
5	A	1022	U
5	A	1033	U
5	A	1037	C
5	A	1047	A
5	A	1049	C
5	A	1064	A
5	A	1065	A
5	A	1072	G
5	A	1081	U
5	A	1082	U
5	A	1094	U
5	A	1095	U
5	A	1096	U
5	A	1097	G
5	A	1098	A
5	A	1103	A
5	A	1104	G
5	A	1117	G
5	A	1131	G

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Mol	Chain	Res	Type
5	A	1153	A
5	A	1159	A
5	A	1180	A
5	A	1181	U
5	A	1196	C
5	A	1201	C
5	A	1209	G
5	A	1221	A
5	A	1222	G
5	A	1287	A
5	A	1307	G
5	A	1308	A
5	A	1309	U
5	A	1313	G
5	A	1330	A
5	A	1331	U
5	A	1348	U
5	A	1349	G
5	A	1351	U
5	A	1352	A
5	A	1356	U
5	A	1357	G
5	A	1386	A
5	A	1392	G
5	A	1399	A
5	A	1400	G
5	A	1419	A
5	A	1434	G
5	A	1437	C
5	A	1446	A
5	A	1481	A
5	A	1484	U
5	A	1508	C
5	A	1536	G
5	A	1555	U
5	A	1556	C
5	A	1557	A
5	A	1562	C
5	A	1563	C
5	A	1564	U
5	A	1569	U
5	A	1572	U

Continued on next page...

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Mol	Chain	Res	Type
5	A	1576	G
5	A	1581	C
5	A	1582	C
5	A	1583	A
5	A	1587	A
5	A	1589	A
5	A	1593	A
5	A	1605	A
5	A	1607	U
5	A	1620	U
5	A	1629	U
5	A	1639	C
5	A	1642	A
5	A	1643	A
5	A	1645	U
5	A	1717	U
5	A	1724	U
5	A	1725	C
5	A	1741	A
5	A	1742	U
5	A	1750	A
5	A	1751	G
5	A	1760	A
5	A	1765	U
5	A	1766	G
5	A	1770	G
5	A	1780	G
5	A	1797	A
5	A	1814	A
5	A	1816	A
5	A	1820	U
5	A	1821	U
5	A	1841	A
5	A	1842	A
5	A	1849	C
5	A	1850	A
5	A	1880	U
5	A	1886	A
5	A	1893	A
5	A	1906	G
5	A	2101	C
5	A	2102	U

Continued on next page...

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Mol	Chain	Res	Type
5	A	2112	U
5	A	2113	A
5	A	2121	G
5	A	2122	G
5	A	2131	A
5	A	2140	U
5	A	2144	A
5	A	2158	A
5	A	2169	G
5	A	2170	U
5	A	2205	U
5	A	2209	U
5	A	2210	G
5	A	2244	A
5	A	2273	G
5	A	2279	A
5	A	2282	U
5	A	2288	G
5	A	2307	G
5	A	2308	C
5	A	2310	U
5	A	2313	A
5	A	2314	U
5	A	2315	G
5	A	2334	U
5	A	2336	U
5	A	2373	A
5	A	2374	C
5	A	2375	G
5	A	2385	G
5	A	2388	U
5	A	2393	G
5	A	2394	G
5	A	2397	A
5	A	2402	A
5	A	2403	G
5	A	2404	A
5	A	2411	U
5	A	2418	G
5	A	2435	G
5	A	2513	U
5	A	2514	U

Continued on next page...

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Mol	Chain	Res	Type
5	A	2522	G
5	A	2523	A
5	A	2531	C
5	A	2537	U
5	A	2538	U
5	A	2539	C
5	A	2540	A
5	A	2541	U
5	A	2542	U
5	A	2549	G
5	A	2552	C
5	A	2555	G
5	A	2561	A
5	A	2569	A
5	A	2570	U
5	A	2571	U
5	A	2572	C
5	A	2573	G
5	A	2585	G
5	A	2593	A
5	A	2606	G
5	A	2607	G
5	A	2614	G
5	A	2652	U
5	A	2656	A
5	A	2674	A
5	A	2677	G
5	A	2689	A
5	A	2691	A
5	A	2696	A
5	A	2704	A
5	A	2705	A
5	A	2714	G
5	A	2728	G
5	A	2729	U
5	A	2752	U
5	A	2753	G
5	A	2755	C
5	A	2762	A
5	A	2777	G
5	A	2778	G
5	A	2796	G

Continued on next page...

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Mol	Chain	Res	Type
5	A	2799	A
5	A	2800	G
5	A	2801	A
5	A	2803	A
5	A	2810	C
5	A	2814	G
5	A	2817	A
5	A	2821	C
5	A	2842	U
5	A	2845	A
5	A	2867	C
5	A	2871	G
5	A	2872	A
5	A	2875	U
5	A	2876	C
5	A	2887	A
5	A	2923	U
5	A	2935	U
5	A	2936	A
5	A	2947	G
5	A	2951	G
5	A	2983	C
5	A	2990	G
5	A	2997	G
5	A	3012	A
5	A	3056	U
5	A	3059	G
5	A	3078	U
5	A	3086	A
5	A	3092	C
5	A	3119	U
5	A	3122	A
5	A	3130	A
5	A	3131	U
5	A	3142	A
5	A	3143	C
5	A	3154	C
5	A	3155	U
5	A	3156	U
5	A	3157	U
5	A	3165	A
5	A	3173	G

Continued on next page...

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Mol	Chain	Res	Type
5	A	3174	A
5	A	3176	G
5	A	3179	U
5	A	3181	C
5	A	3187	A
5	A	3207	U
5	A	3217	C
5	A	3218	A
5	A	3219	G
5	A	3229	G
5	A	3243	A
5	A	3245	A
5	A	3247	G
5	A	3259	U
5	A	3260	G
5	A	3263	G
5	A	3270	U
5	A	3273	A
5	A	3276	G
5	A	3279	A
5	A	3281	U
5	A	3287	U
5	A	3289	G
5	A	3294	A
5	A	3304	U
5	A	3316	A
5	A	3318	G
5	A	3319	U
5	A	3341	U
5	A	3345	G
5	A	3350	C
5	A	3352	U
5	A	3353	G
5	A	3355	U
5	A	3369	G
5	A	3378	C
5	A	3386	G
5	A	3389	U
5	A	3390	G
25	LD	23	U
25	LD	34	U
25	LD	35	C

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Mol	Chain	Res	Type
25	LD	59	A
25	LD	62	C
25	LD	63	G
25	LD	80	A
25	LD	81	U
25	LD	82	U
25	LD	84	C
25	LD	86	U
25	LD	87	G
25	LD	90	U
25	LD	95	G
25	LD	104	A
25	LD	106	C
25	LD	111	A
25	LD	113	U
25	LD	125	U
25	LD	126	A
25	LD	152	G
29	LE	42	A
29	LE	51	A
29	LE	54	U
29	LE	55	A
29	LE	65	G
29	LE	76	A
29	LE	102	A
29	LE	112	G
29	LE	121	U

All (24) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	A	169	U
5	A	916	G
5	A	979	U
5	A	1064	A
5	A	1097	G
5	A	1103	A
5	A	1307	G
5	A	1355	A
5	A	1554	U
5	A	1562	C
5	A	1815	U

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Mol	Chain	Res	Type
5	A	2101	C
5	A	2112	U
5	A	2209	U
5	A	2512	C
5	A	2537	U
5	A	2541	U
5	A	3121	U
5	A	3218	A
5	A	3228	C
5	A	3269	U
5	A	3317	U
5	A	3351	U
25	LD	85	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 179 ligands modelled in this entry, 177 are monoatomic - leaving 2 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	$\# Z > 2$
46	SPD	A	3426	-	9,9,9	0.26	0	8,8,8	0.27	0
47	SPM	A	3547	-	13,13,13	0.36	0	12,12,12	0.80	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	SPD	A	3426	-	-	0/7/7/7	-
47	SPM	A	3547	-	-	0/11/11/11	-

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	A	3426	SPD	1	0

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.

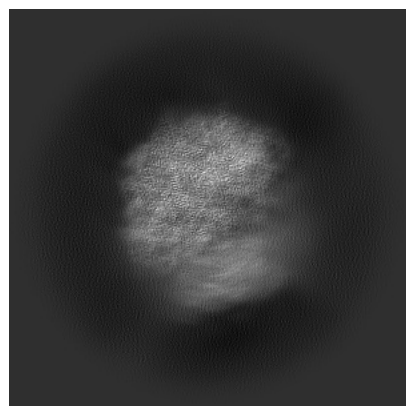
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17550. These allow visual inspection of the internal detail of the map and identification of artifacts.

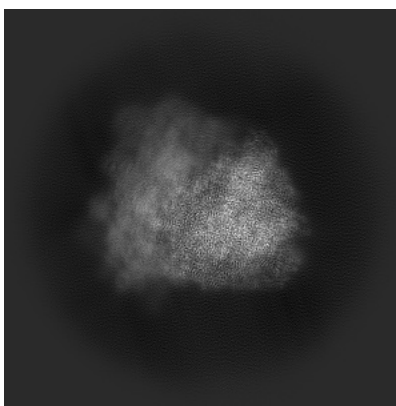
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

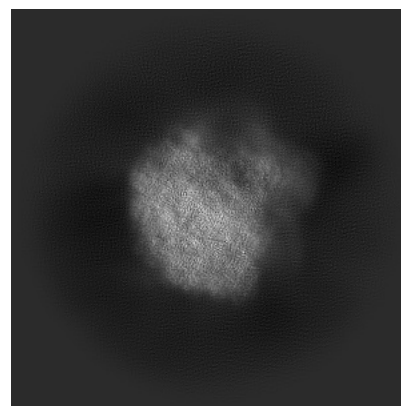
6.1.1 Primary map



X

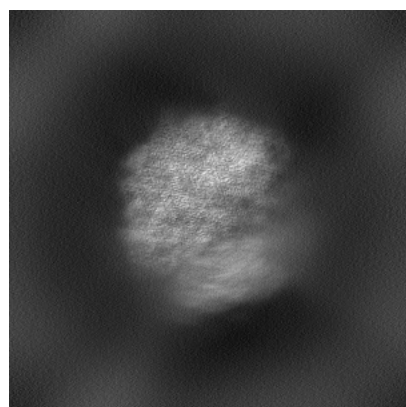


Y

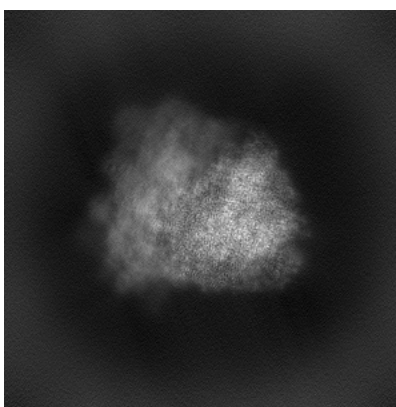


Z

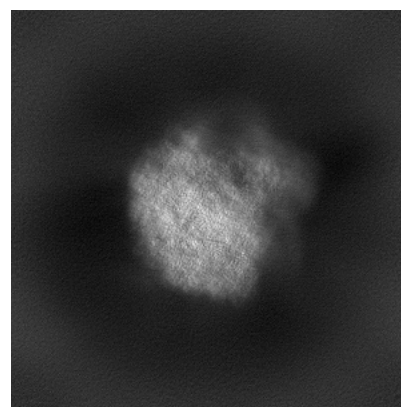
6.1.2 Raw map



X



Y

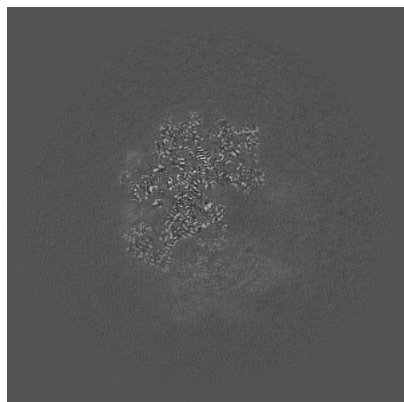


Z

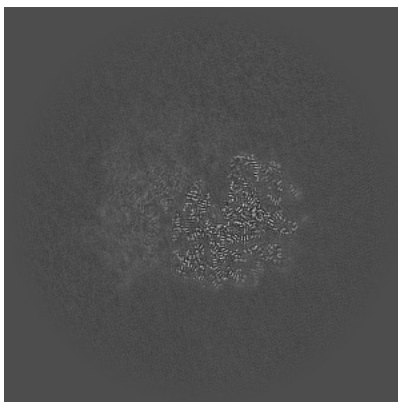
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

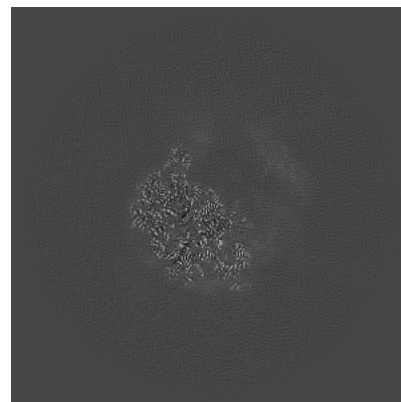
6.2.1 Primary map



X Index: 300

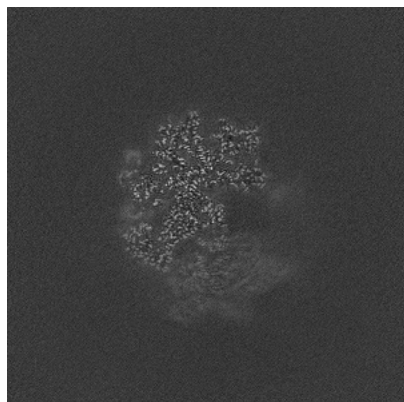


Y Index: 300

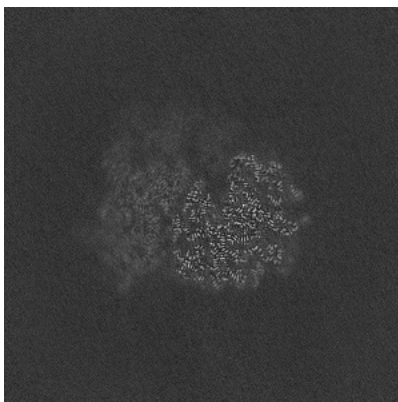


Z Index: 300

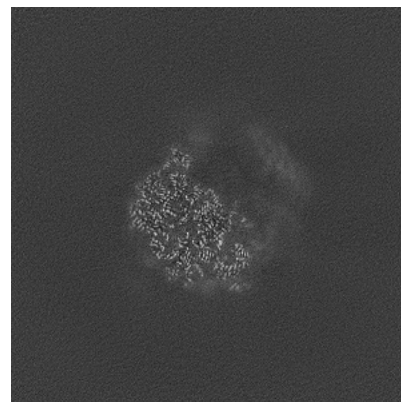
6.2.2 Raw map



X Index: 300



Y Index: 300

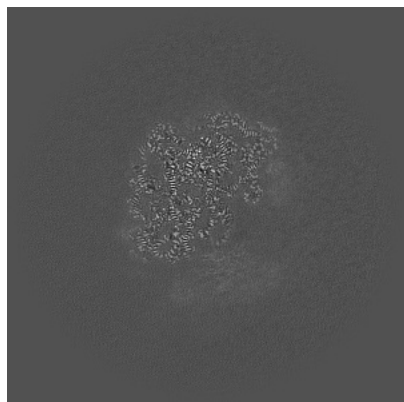


Z Index: 300

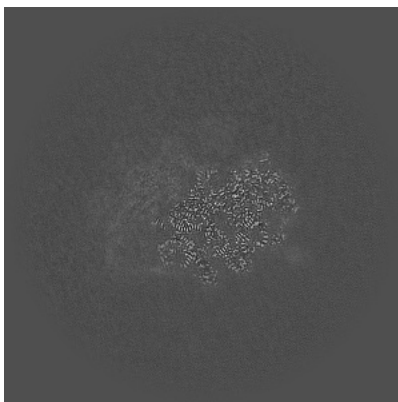
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

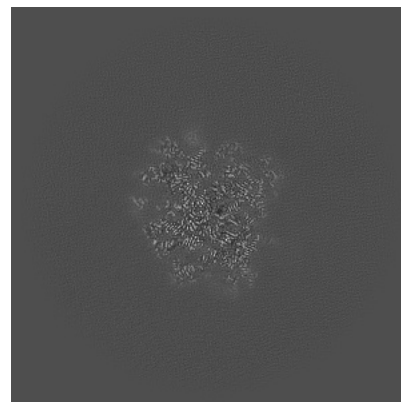
6.3.1 Primary map



X Index: 273

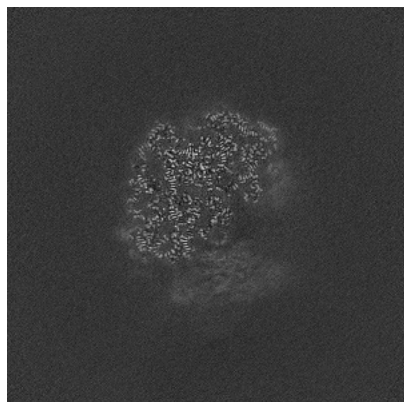


Y Index: 273

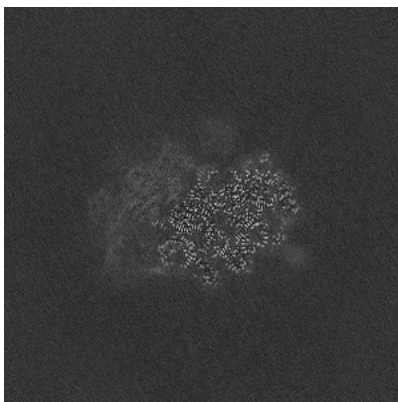


Z Index: 361

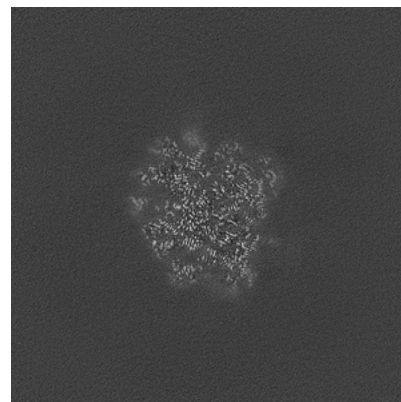
6.3.2 Raw map



X Index: 273



Y Index: 273

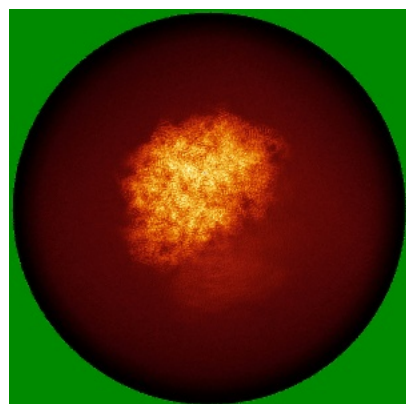


Z Index: 361

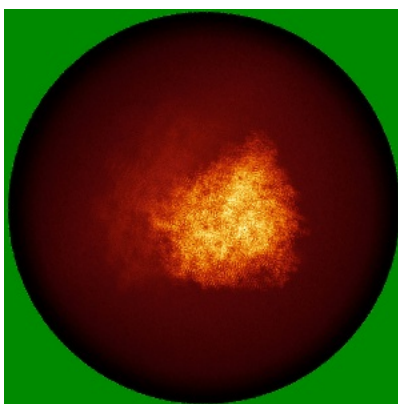
The images above show the largest variance slices of the map in three orthogonal directions.

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

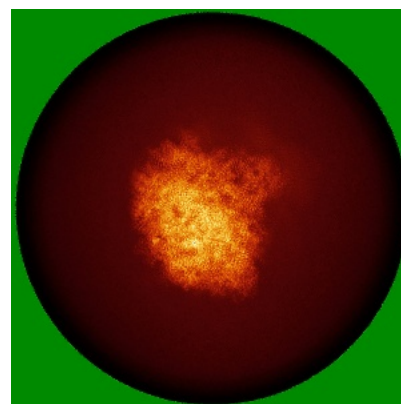
6.4.1 Primary map



X

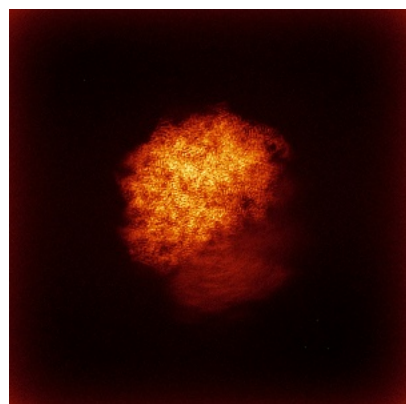


Y

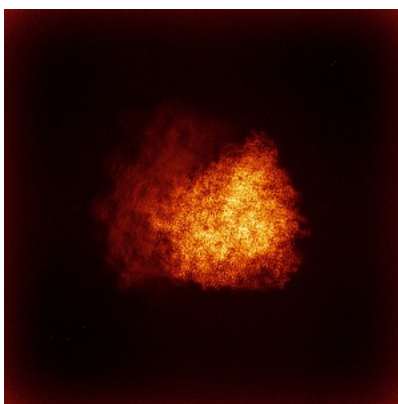


Z

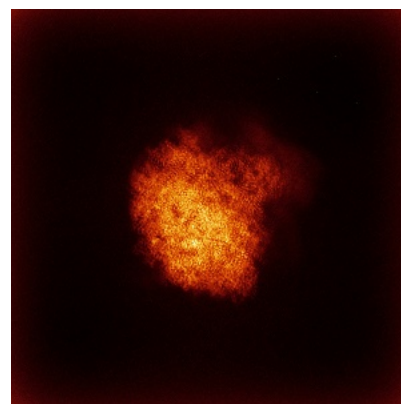
6.4.2 Raw map



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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3. 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



X



Y



Z

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.

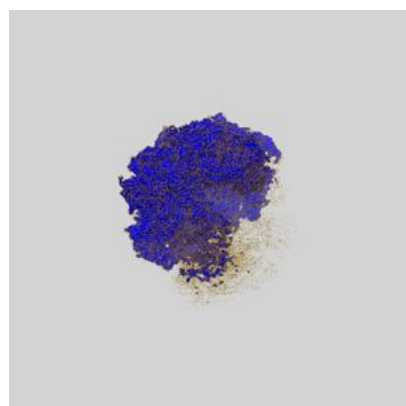
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

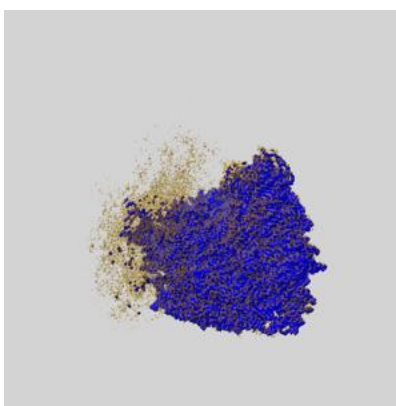
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

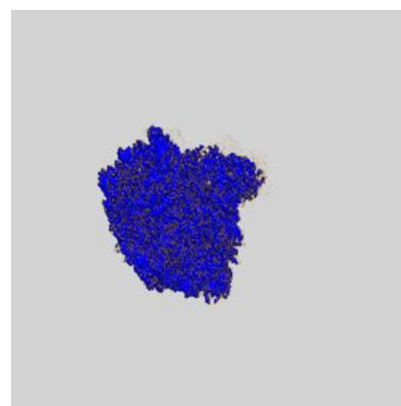
6.6.1 emd_17550_msk_1.map [i](#)



X



Y

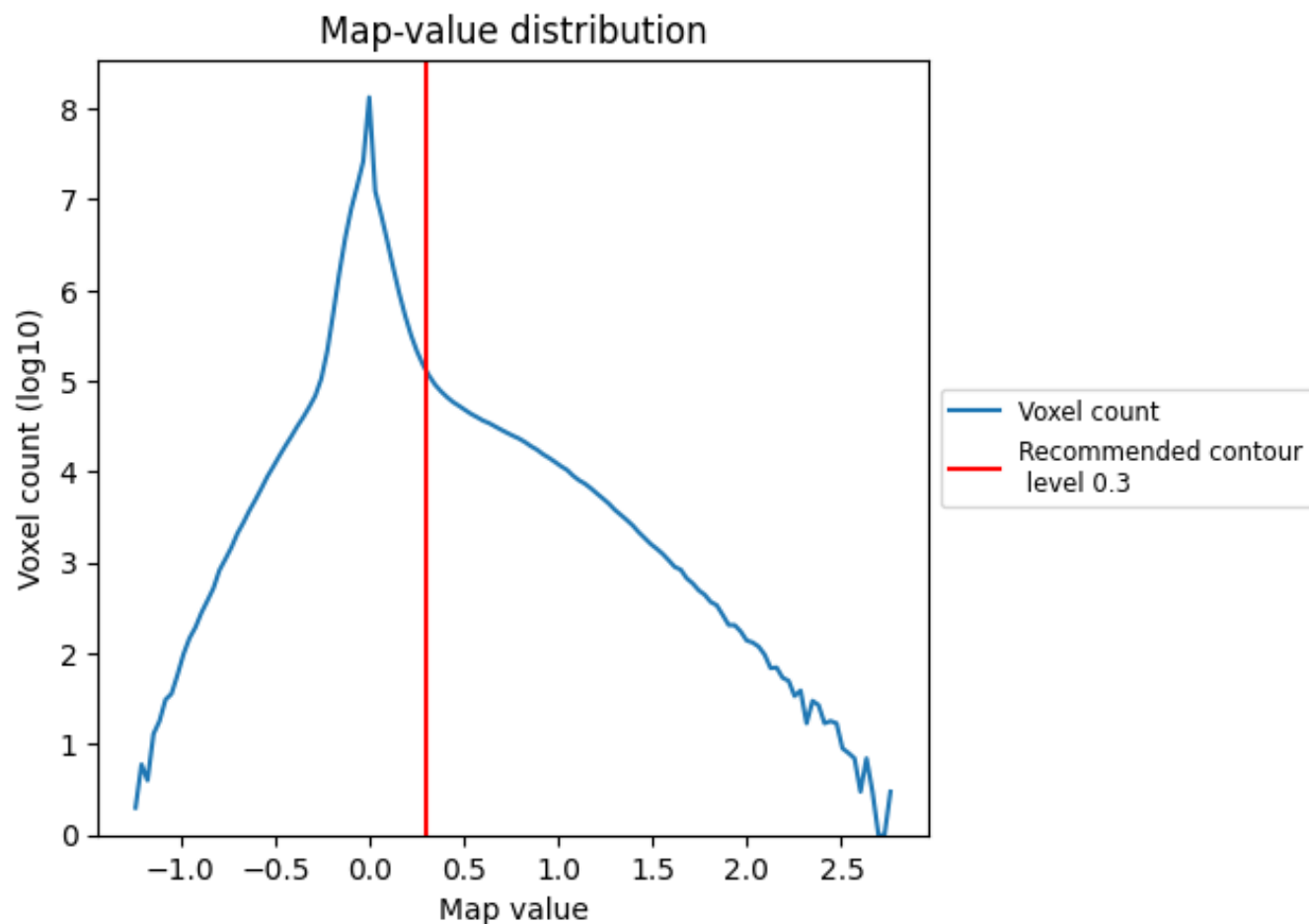


Z

7 Map analysis [i](#)

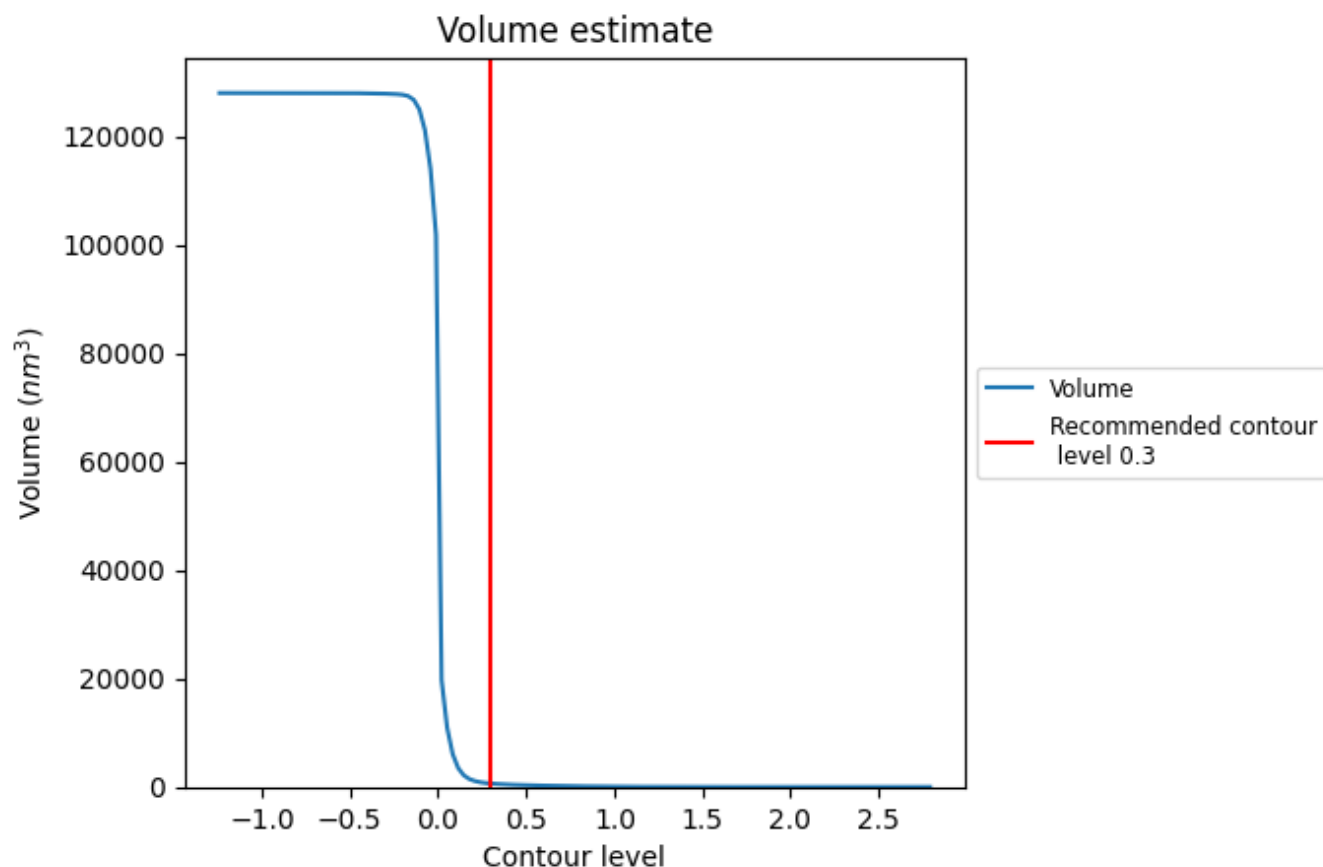
This section contains the results of statistical analysis of the map.

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.

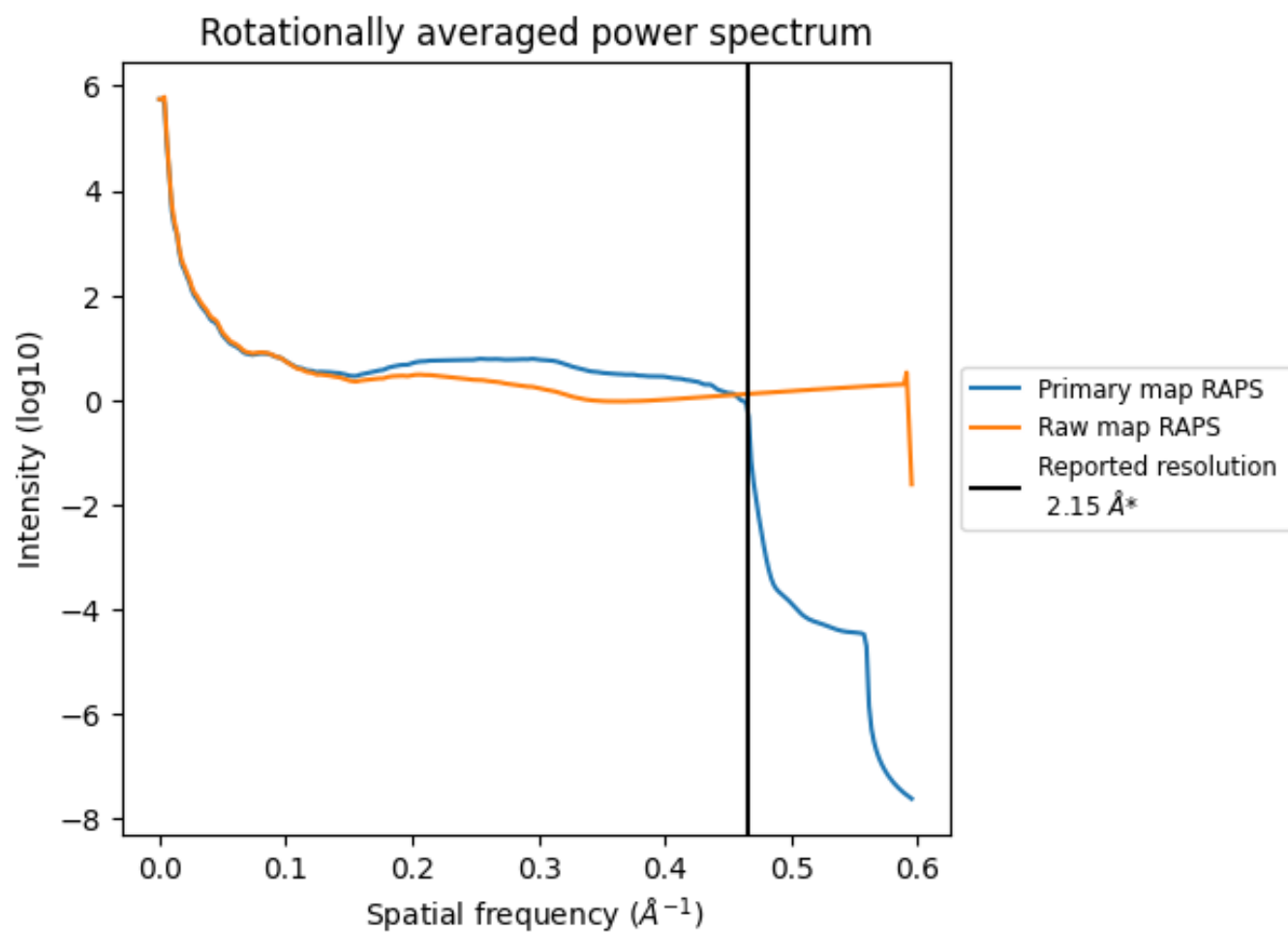
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 634 nm^3 ; this corresponds to an approximate mass of 573 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 ⓘ

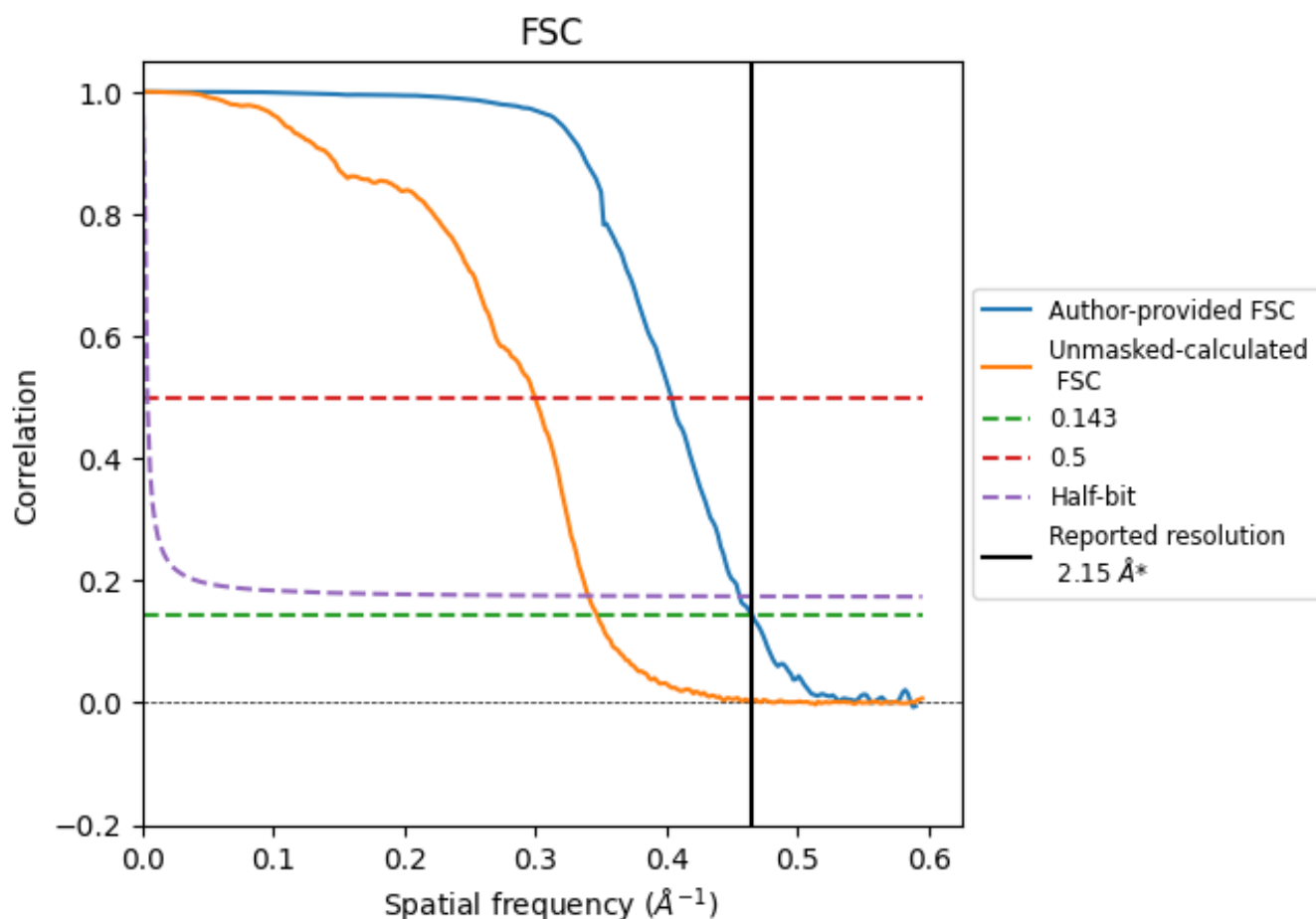


*Reported resolution corresponds to spatial frequency of 0.465 $\text{\AA}^{-1}$

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 0.465 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

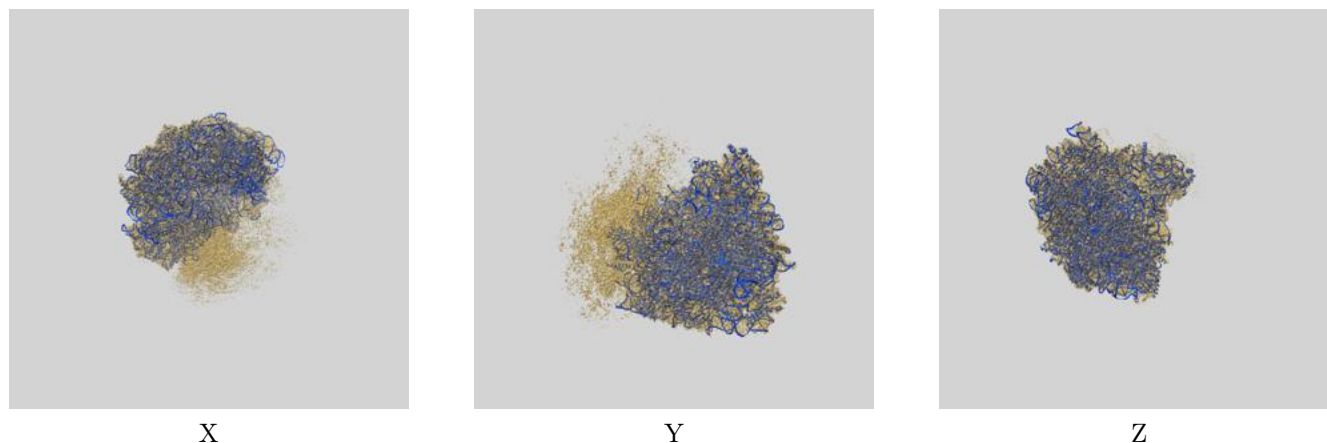
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.15	-	-
Author-provided FSC curve	2.15	2.48	2.19
Unmasked-calculated*	2.88	3.34	2.94

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.88 differs from the reported value 2.15 by more than 10 %

9 Map-model fit [i](#)

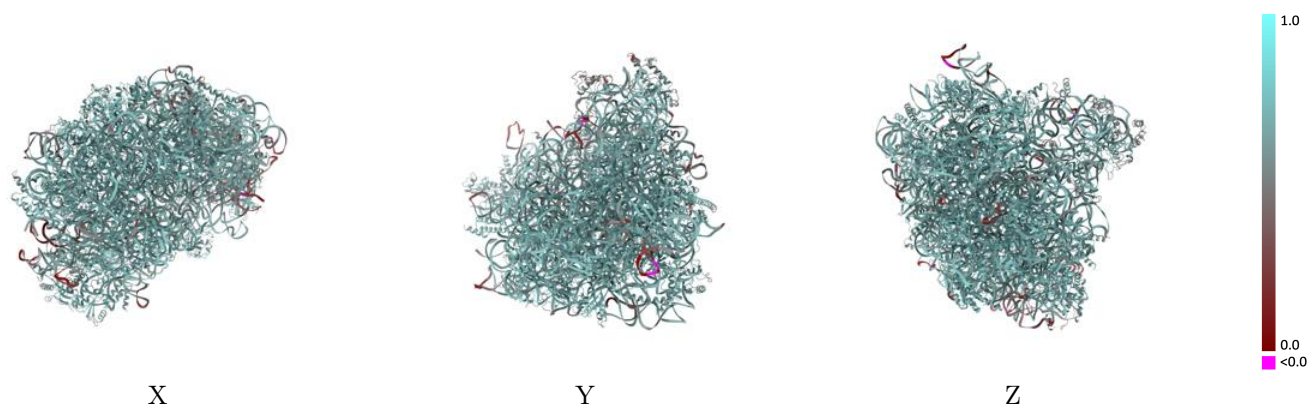
This section contains information regarding the fit between EMDB map EMD-17550 and PDB model 8P8N. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



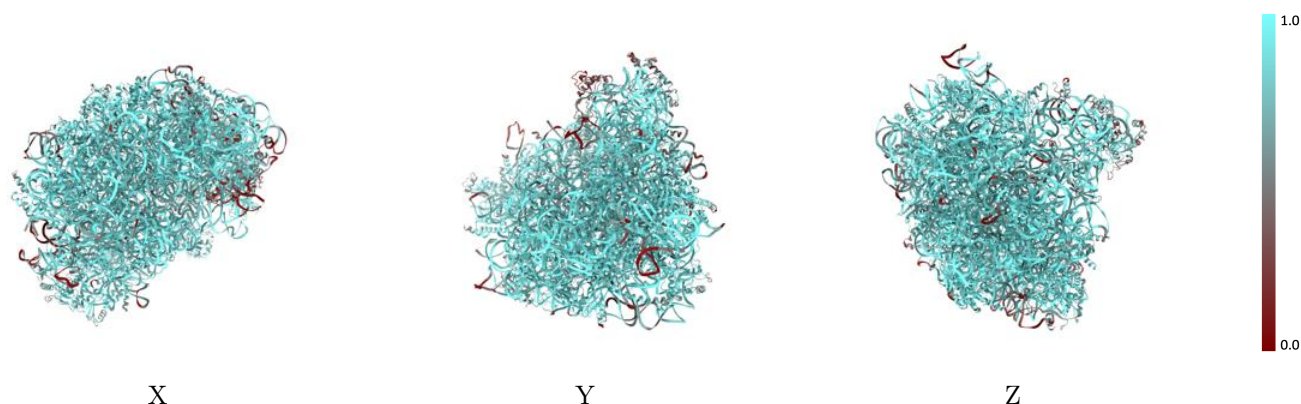
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



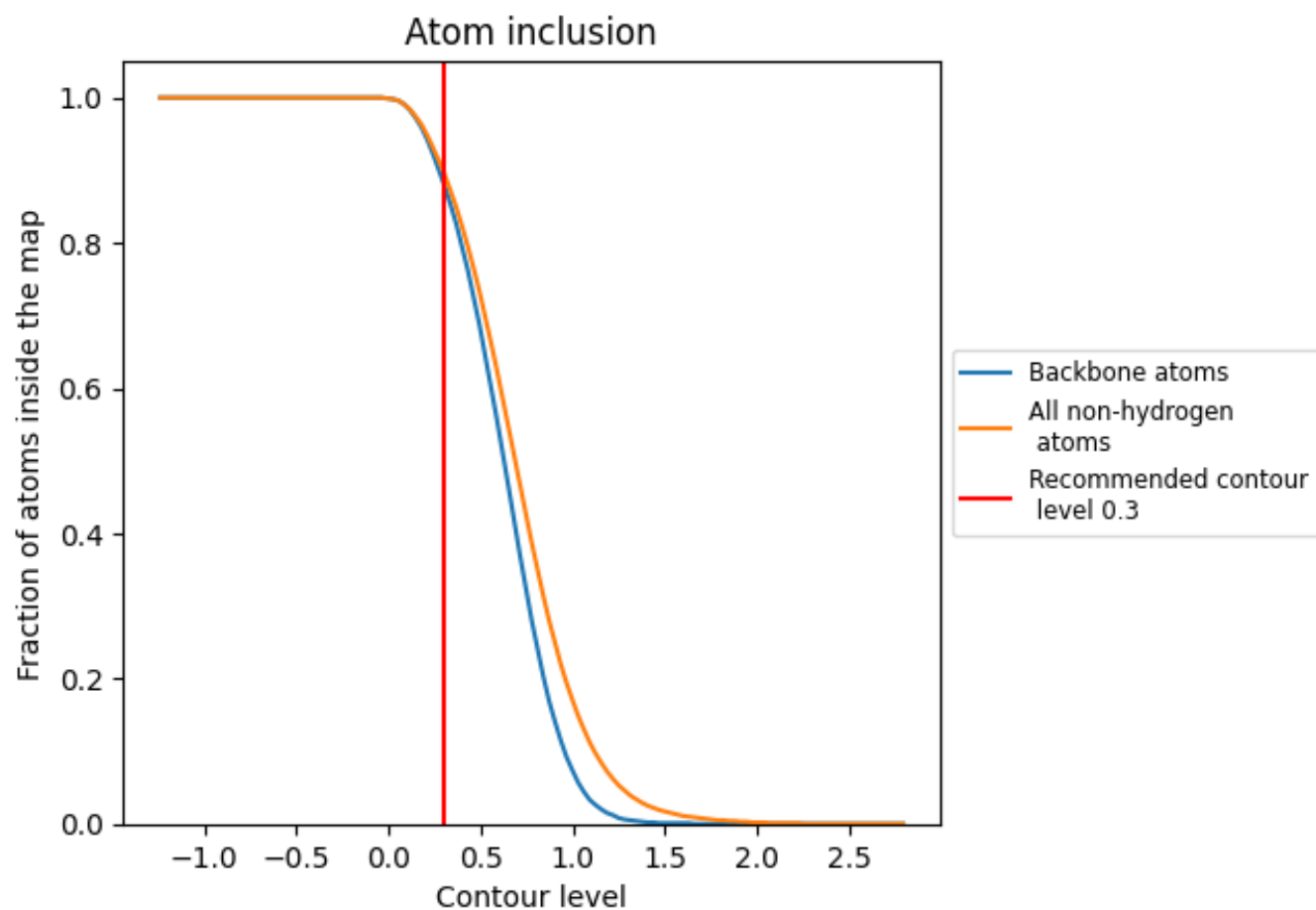
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

9.4 Atom inclusion ⓘ



At the recommended contour level, 88% of all backbone atoms, 90% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8970	 0.6650
2	 0.8840	 0.6780
A	 0.9120	 0.6600
JT	 0.8770	 0.6640
JU	 0.8790	 0.6720
JV	 0.9770	 0.7140
JW	 0.9180	 0.6880
LD	 0.9510	 0.6810
LE	 0.9400	 0.6580
LF	 0.9540	 0.7070
LG	 0.9250	 0.6940
LH	 0.9170	 0.6910
LI	 0.7120	 0.5940
LJ	 0.7950	 0.6380
LK	 0.9240	 0.6900
LL	 0.8350	 0.6480
LM	 0.8430	 0.6490
LN	 0.8620	 0.6680
LO	 0.4720	 0.5210
QO	 0.9410	 0.7100
QP	 0.9480	 0.7040
QQ	 0.9350	 0.7020
QS	 0.9200	 0.6880
QT	 0.8690	 0.6570
QU	 0.5780	 0.5850
QV	 0.8960	 0.6880
QW	 0.8760	 0.6950
QX	 0.9030	 0.6830
QY	 0.9070	 0.6890
QZ	 0.7800	 0.6310
RA	 0.9290	 0.6920
RB	 0.8490	 0.6420
RC	 0.8010	 0.6380
RD	 0.9180	 0.6940
RE	 0.9470	 0.7090



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Chain	Atom inclusion	Q-score
RF	 0.9570	 0.7060
RG	 0.9410	 0.7030
RH	 0.8810	 0.6780
RI	 0.8760	 0.6570
RJ	 0.9700	 0.7250
RM	 0.6460	 0.6040
RO	 0.8920	 0.6720
RQ	 0.8560	 0.6600
RT	 0.8880	 0.6790