



Full wwPDB EM Validation Report ⓘ

Dec 18, 2024 – 08:02 pm GMT

PDB ID : 8PFR
EMDB ID : EMD-17653
Title : Mouse RPL39L integrated into the yeast 60S ribosomal subunit
Authors : Rabl, J.; Banerjee, A.; Boehringer, D.; Zavolan, M.
Deposited on : 2023-06-16
Resolution : 2.15 Å(reported)
Based on initial model : 7too

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:

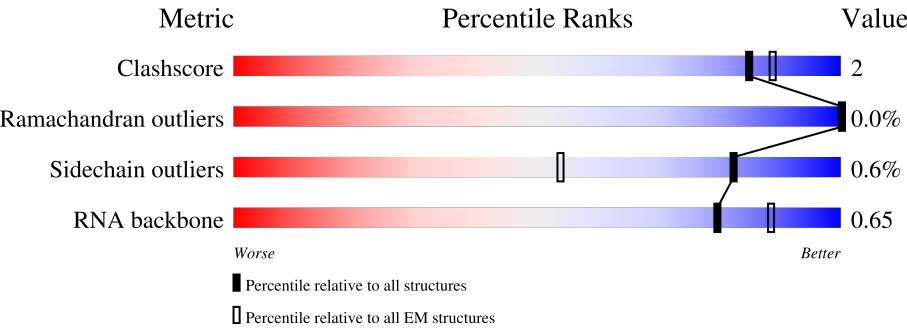
EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

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.



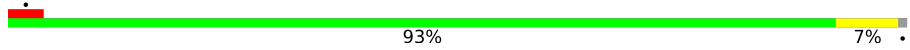

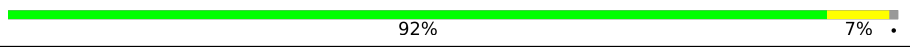



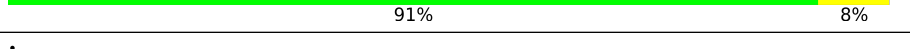
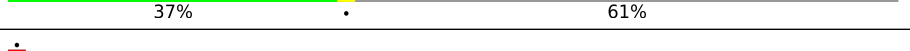
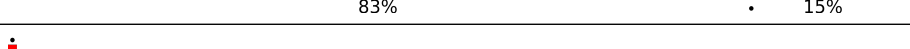
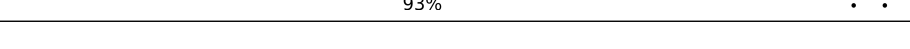
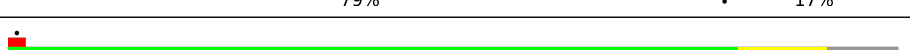

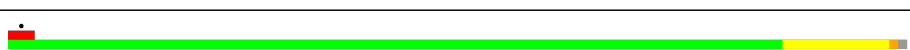
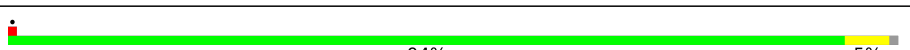
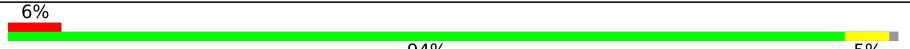

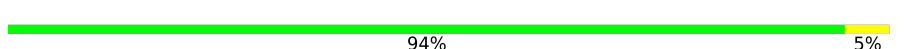
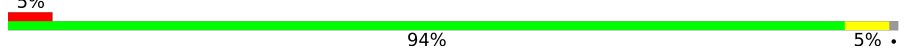


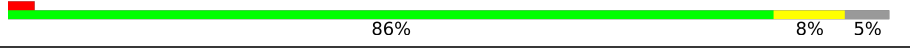
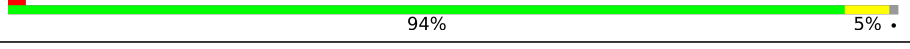
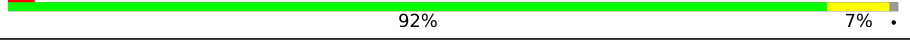


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	A	3396	
2	RE	130	
3	LL	256	
4	QU	121	
5	QY	127	
6	LF	254	
7	RN	51	

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Mol	Chain	Length	Quality of chain
8	QV	137	
9	JT	199	
10	RF	107	
11	LM	191	
12	QW	155	
13	QZ	136	
14	LG	387	
15	RO	128	
16	QX	142	
17	JU	138	
18	RG	121	
19	LN	221	
20	LH	362	
21	RA	149	
22	RH	120	
23	RQ	106	
24	LI	297	
25	JV	204	
26	RI	100	
27	LO	174	
28	LJ	176	
29	RB	59	
30	RJ	88	
31	RT	92	
32	LK	244	

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Mol	Chain	Length	Quality of chain
33	JW	199	 94% 5%
34	RM	78	 92% 6%
35	QO	184	 86% 7% 7%
36	RC	105	 79% 13% 8%
37	QP	186	 92% 8%
38	LD	158	 84% 15%
39	QQ	189	 75% 22%
40	RD	113	 81% 14%
41	QS	172	 92% 8%
42	LE	121	 83% 15%
43	QT	160	 89% 11%

2 Entry composition

There are 49 unique types of molecules in this entry. The entry contains 120018 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3038	Total	C	N	O	P	0	0
			64996	29031	11727	21200	3038		

- Molecule 2 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	RE	127	Total	C	N	O	S	0	0
			1020	647	205	167	1		

- Molecule 3 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	LL	215	Total	C	N	O	S	0	0
			1693	1087	304	299	3		

- Molecule 4 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	QU	100	Total	C	N	O		0	0
			796	516	131	149			

- Molecule 5 is a protein called 60S ribosomal protein L26-A.

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

- Molecule 6 is a protein called 60S ribosomal protein L2-A.

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

- Molecule 7 is a protein called 60S ribosomal protein L39-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	RN	50	Total	C	N	O	S	4	0
			470	300	99	68	3		

- Molecule 8 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	QV	136	Total	C	N	O	S	0	0
			1003	628	189	179	7		

- 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 L33-A.

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

- Molecule 11 is a protein called 60S ribosomal protein L9-A.

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

- Molecule 12 is a protein called 60S ribosomal protein L24-A.

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

- Molecule 13 is a protein called 60S ribosomal protein L27-A.

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

- Molecule 14 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LG	386	Total	C	N	O	S	0	0
			3078	1953	584	533	8		

- Molecule 15 is a protein called Ubiquitin-60S ribosomal protein L40.

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

- Molecule 16 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	QX	120	Total	C	N	O	S	0	0
			959	617	168	172	2		

- Molecule 17 is a protein called 60S ribosomal protein L14-A.

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

- Molecule 18 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	RG	100	Total	C	N	O	S	0	0
			786	486	162	134	4		

- Molecule 19 is a protein called 60S ribosomal protein L10.

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

- Molecule 20 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LH	361	Total	C	N	O	S	0	0
			2748	1729	522	494	3		

- Molecule 21 is a protein called 60S ribosomal protein L28.

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

- Molecule 22 is a protein called 60S ribosomal protein L35-A.

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

- Molecule 23 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	RQ	105	Total	C	N	O	S	0	0
			847	534	170	138	5		

- Molecule 24 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LI	290	Total	C	N	O	S	0	0
			2328	1471	406	449	2		

- Molecule 25 is a protein called 60S ribosomal protein L15-A.

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

- Molecule 26 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	RI	99	Total	C	N	O	S	0	0
			771	481	156	132	2		

- Molecule 27 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LO	160	Total	C	N	O	S	0	0
			1283	800	243	236	4		

- Molecule 28 is a protein called 60S ribosomal protein L6-A.

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

- Molecule 29 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	RB	56	Total	C	N	O		0	0
			444	277	96	71			

- Molecule 30 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	RJ	87	Total	C	N	O	S	0	0
			681	414	148	114	5		

- Molecule 31 is a protein called 60S ribosomal protein L43-A.

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

- Molecule 32 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	LK	222	Total	C	N	O	S	0	0
			1784	1151	324	308	1		

- Molecule 33 is a protein called 60S ribosomal protein L16-A.

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

- Molecule 34 is a protein called 60S ribosomal protein L38.

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

- Molecule 35 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	QO	172	Total	C	N	O	0	0
			1367	848	273	246		

- Molecule 36 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	RC	97	Total	C	N	O	S	0	0
			743	479	124	139	1		

- Molecule 37 is a protein called 60S ribosomal protein L18-A.

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

- Molecule 38 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	LD	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 39 is a protein called 60S ribosomal protein L19-A.

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

- Molecule 40 is a protein called 60S ribosomal protein L31-A.

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

- Molecule 41 is a protein called 60S ribosomal protein L20-A.

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

- Molecule 42 is a RNA chain called 5S rRNA.

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

- Molecule 43 is a protein called 60S ribosomal protein L21-A.

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

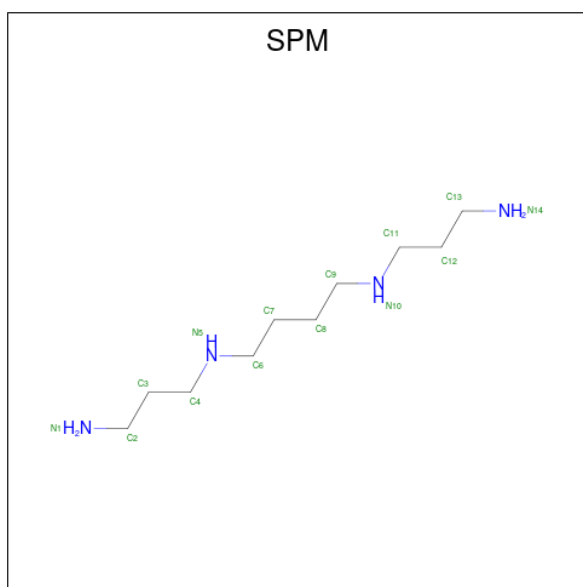
- Molecule 44 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
44	A	164	Total	Mg	0
			164	164	
44	RE	1	Total	Mg	0
			1	1	
44	RA	1	Total	Mg	0
			1	1	
44	RI	1	Total	Mg	0
			1	1	
44	QO	1	Total	Mg	0
			1	1	
44	LD	1	Total	Mg	0
			1	1	
44	LE	1	Total	Mg	0
			1	1	

- Molecule 45 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

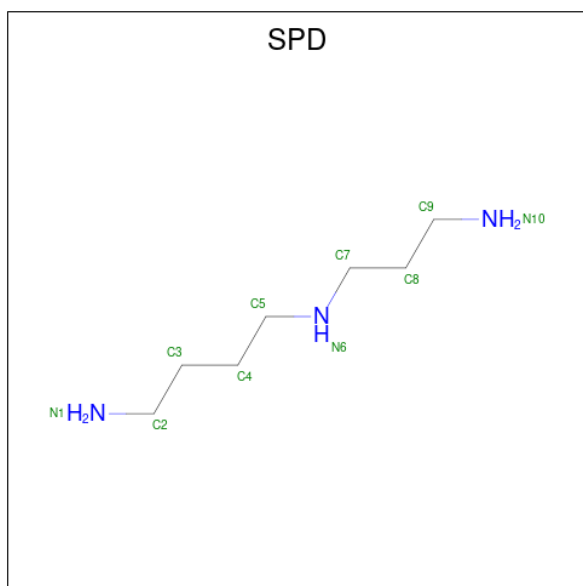
Mol	Chain	Residues	Atoms		AltConf
45	A	21	Total	Cl	0
			21	21	
45	LG	1	Total	Cl	0
			1	1	
45	RQ	1	Total	Cl	0
			1	1	
45	QO	1	Total	Cl	0
			1	1	

- Molecule 46 is SPERMINE (three-letter code: SPM) (formula: C₁₀H₂₆N₄).



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

- Molecule 47 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



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

- Molecule 48 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 49 is water.

Mol	Chain	Residues	Atoms		AltConf
49	A	544	Total 544	O 544	0
49	RE	3	Total 3	O 3	0
49	LF	7	Total 7	O 7	0
49	QX	1	Total 1	O 1	0
49	LH	2	Total 2	O 2	0
49	RA	3	Total 3	O 3	0
49	RQ	1	Total 1	O 1	0
49	LI	1	Total 1	O 1	0
49	JV	2	Total 2	O 2	0
49	RB	1	Total 1	O 1	0
49	RJ	1	Total 1	O 1	0
49	JW	2	Total 2	O 2	0
49	QO	2	Total 2	O 2	0
49	LD	6	Total 6	O 6	0
49	QQ	1	Total 1	O 1	0

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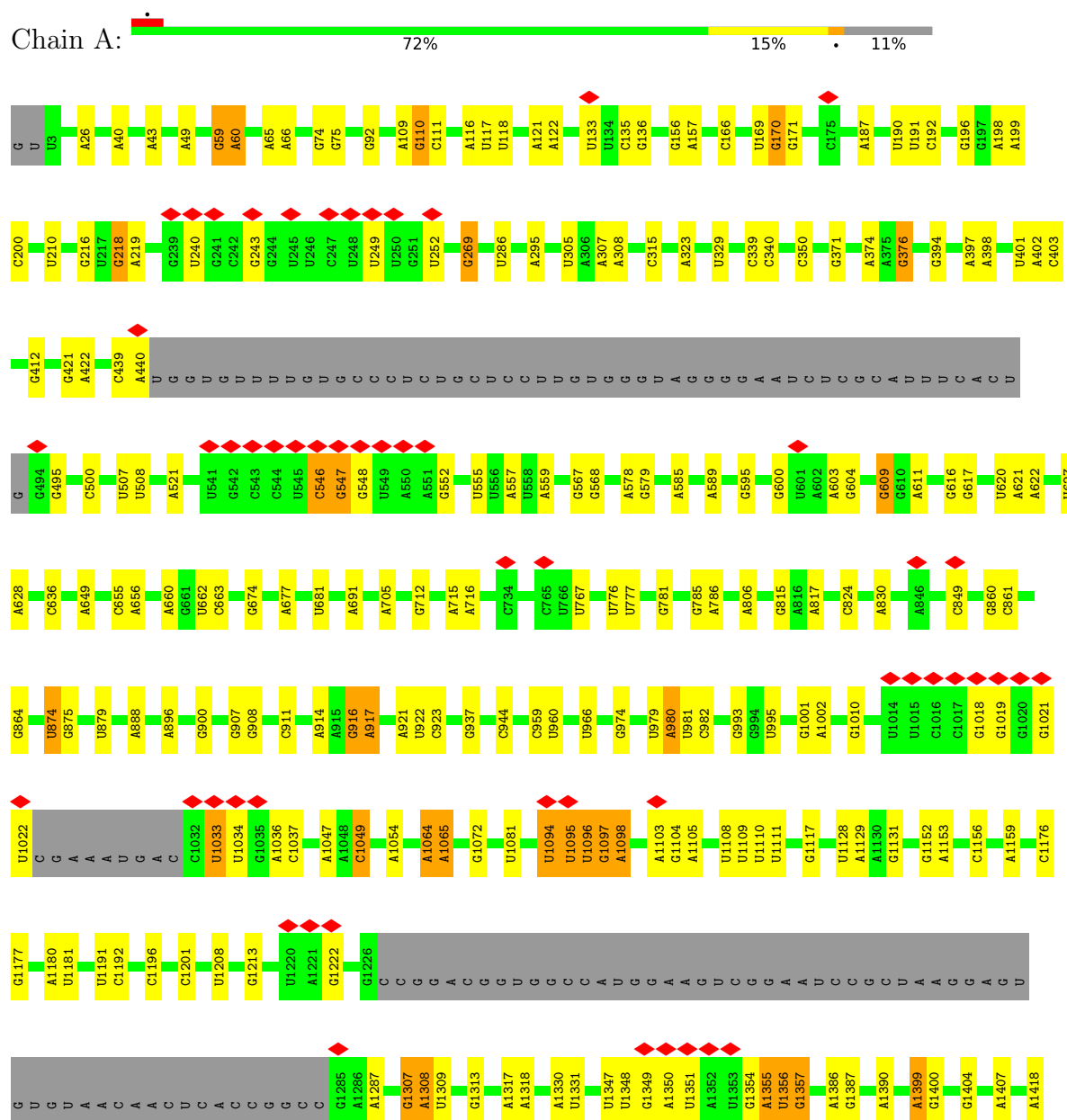
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Mol	Chain	Residues	Atoms		AltConf
49	LE	3	Total	O	0
			3	3	

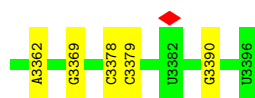
3 Residue-property plots

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

• Molecule 1: 25S rRNA

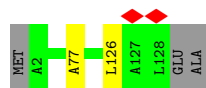






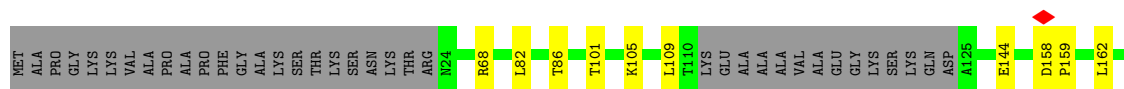
- Molecule 2: 60S ribosomal protein L32

Chain RE: 96%



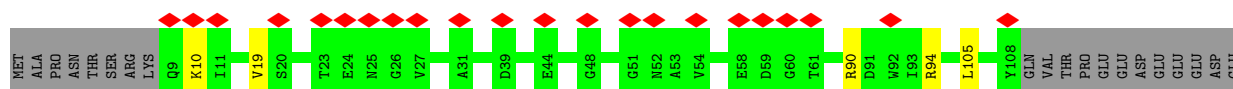
- Molecule 3: 60S ribosomal protein L8-A

Chain LL: 77% 7% 16%



- Molecule 4: 60S ribosomal protein L22-A

Chain QU: 18% 79% 17%



- Molecule 5: 60S ribosomal protein L26-A

Chain QY: 90% 7%



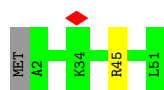
- Molecule 6: 60S ribosomal protein L2-A

Chain LF: 89% 7%



- Molecule 7: 60S ribosomal protein L39-like

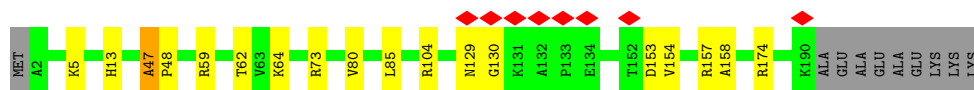
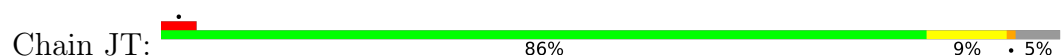
Chain RN: 96%



- Molecule 8: 60S ribosomal protein L23-A



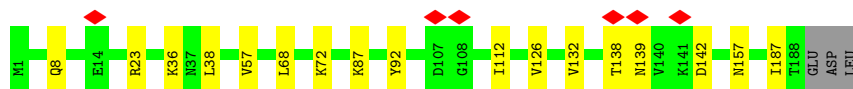
- Molecule 9: 60S ribosomal protein L13-A



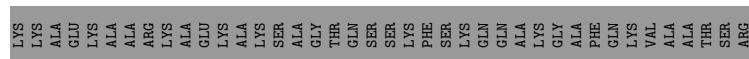
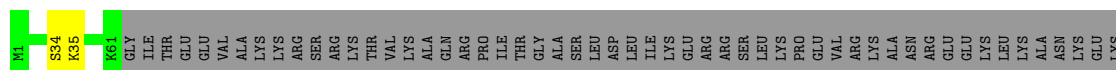
- Molecule 10: 60S ribosomal protein L33-A



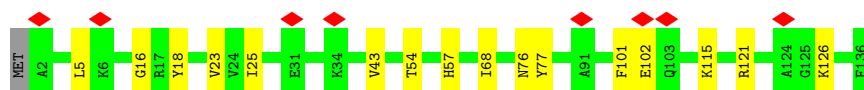
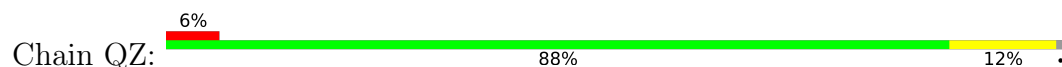
- Molecule 11: 60S ribosomal protein L9-A



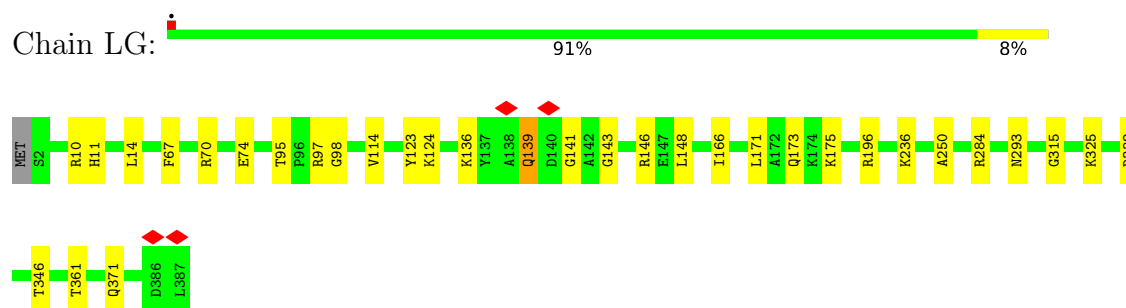
- Molecule 12: 60S ribosomal protein L24-A



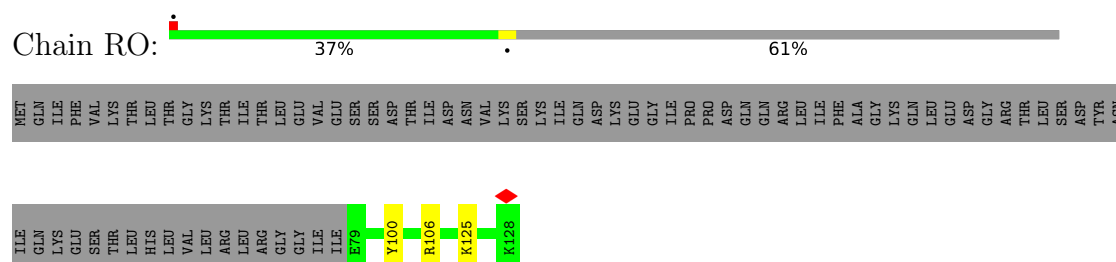
- Molecule 13: 60S ribosomal protein L27-A



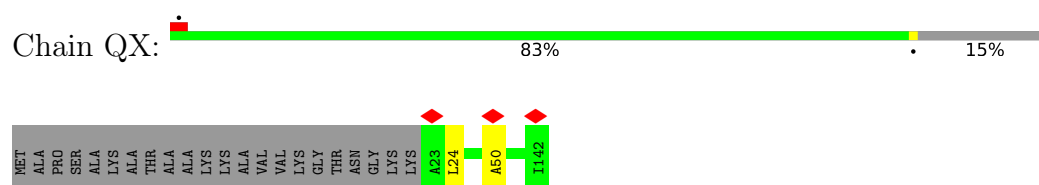
- Molecule 14: 60S ribosomal protein L3



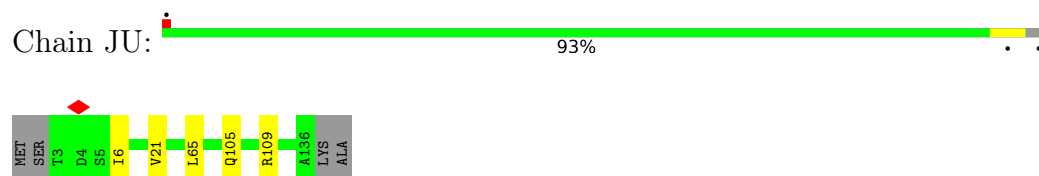
- Molecule 15: Ubiquitin-60S ribosomal protein L40



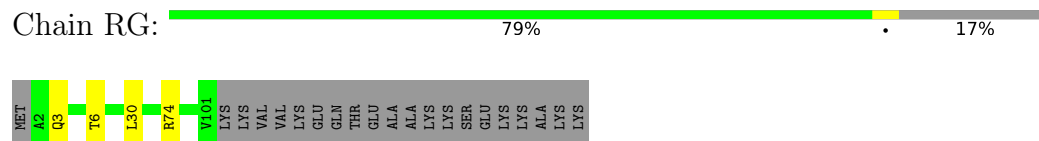
- Molecule 16: 60S ribosomal protein L25



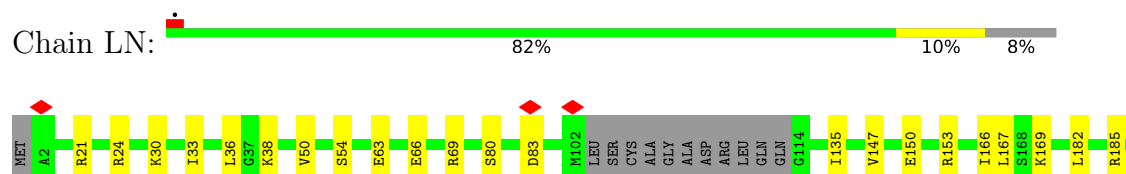
- Molecule 17: 60S ribosomal protein L14-A

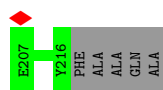


- Molecule 18: 60S ribosomal protein L34-A



- Molecule 19: 60S ribosomal protein L10

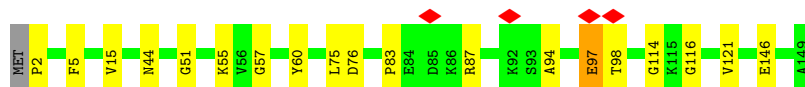




- Molecule 20: 60S ribosomal protein L4-A



- Molecule 21: 60S ribosomal protein L28



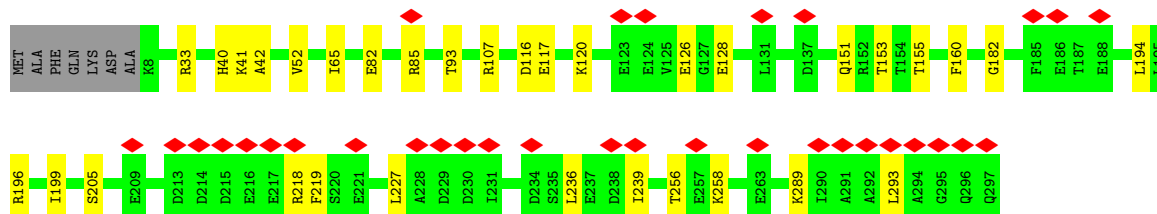
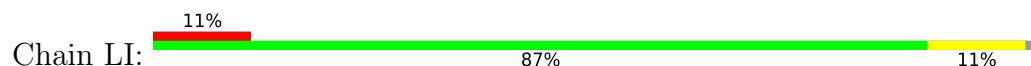
- Molecule 22: 60S ribosomal protein L35-A



- Molecule 23: 60S ribosomal protein L42-A



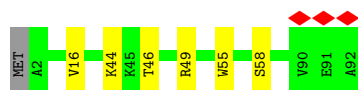
- Molecule 24: 60S ribosomal protein L5



- Molecule 25: 60S ribosomal protein L15-A

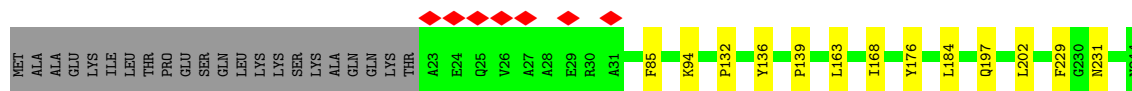






- Molecule 32: 60S ribosomal protein L7-A

Chain LK: 86% 5% 9%



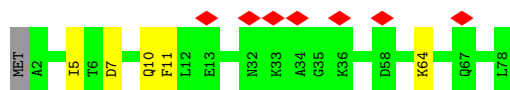
- Molecule 33: 60S ribosomal protein L16-A

Chain JW: 94% 5%



- Molecule 34: 60S ribosomal protein L38

Chain RM: 9% 92% 6%



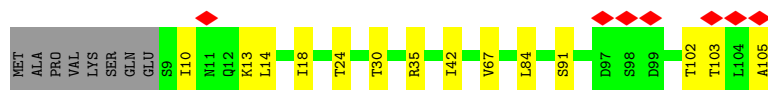
- Molecule 35: 60S ribosomal protein L17-A

Chain QO: 86% 7% 7%



- Molecule 36: 60S ribosomal protein L30

Chain RC: 7% 79% 13% 8%




- Molecule 37: 60S ribosomal protein L18-A

Chain QP: 92% 8%




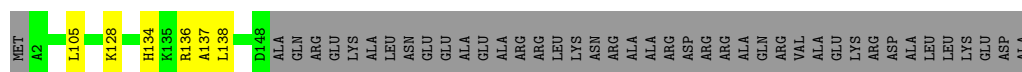
- Molecule 38: 5.8S rRNA

Chain LD:  84% 15%




- Molecule 39: 60S ribosomal protein L19-A

Chain QQ:  75% 22%



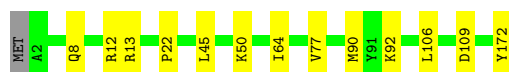
- Molecule 40: 60S ribosomal protein L31-A

Chain RD:  81% 14%




- Molecule 41: 60S ribosomal protein L20-A

Chain QS:  92% 8%




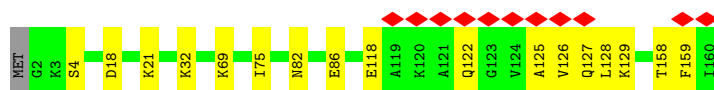
- Molecule 42: 5S rRNA

Chain LE:  83% 15%



- Molecule 43: 60S ribosomal protein L21-A

Chain QT:  7% 89% 11%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	610925	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 ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.085	Depositor
Minimum map value	-2.009	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.092	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: SPM, SPD, CL, 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	A	0.18	0/72753	0.71	3/113421 (0.0%)
2	RE	0.23	0/1041	0.50	0/1394
3	LL	0.24	0/1724	0.45	0/2327
4	QU	0.25	0/812	0.46	0/1099
5	QY	0.23	0/987	0.51	0/1318
6	LF	0.24	0/1889	0.54	0/2539
7	RN	0.22	0/480	0.49	0/635
8	QV	0.25	0/1018	0.51	0/1369
9	JT	0.24	0/1540	0.55	0/2068
10	RF	0.25	0/868	0.52	0/1168
11	LM	0.24	0/1514	0.48	0/2039
12	QW	0.24	0/521	0.50	0/691
13	QZ	0.24	0/1118	0.47	0/1497
14	LG	0.23	0/3149	0.52	0/4233
15	RO	0.24	0/407	0.53	0/540
16	QX	0.23	0/974	0.47	0/1314
17	JU	0.23	0/1054	0.48	0/1420
18	RG	0.23	0/796	0.55	0/1065
19	LN	0.23	0/1699	0.50	0/2277
20	LH	0.23	0/2800	0.49	0/3790
21	RA	0.23	0/1204	0.50	0/1612
22	RH	0.23	0/978	0.47	0/1301
23	RQ	0.24	0/860	0.50	0/1136
24	LI	0.24	0/2377	0.48	0/3207
25	JV	0.23	0/1757	0.56	0/2354
26	RI	0.23	0/778	0.52	0/1034
27	LO	0.23	0/1301	0.53	0/1741
28	LJ	0.24	0/1260	0.47	0/1694
29	RB	0.23	0/455	0.46	0/607
30	RJ	0.24	0/696	0.56	0/923
31	RT	0.23	0/701	0.55	0/934
32	LK	0.24	0/1821	0.47	0/2451

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	JW	0.24	0/1585	0.47	0/2128
34	RM	0.24	0/618	0.51	0/826
35	QO	0.23	0/1389	0.52	0/1865
36	RC	0.24	0/751	0.43	0/1008
37	QP	0.24	0/1465	0.54	0/1965
38	LD	0.17	0/3746	0.69	0/5832
39	QQ	0.22	0/1202	0.51	0/1605
40	RD	0.23	0/804	0.52	0/1077
41	QS	0.24	0/1473	0.50	0/1980
42	LE	0.15	0/2883	0.67	0/4491
43	QT	0.23	0/1300	0.50	0/1743
All	All	0.20	0/128548	0.64	3/189718 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	922	U	C2-N1-C1'	6.33	125.30	117.70
1	A	922	U	N1-C2-O2	5.25	126.48	122.80
1	A	3317	U	P-O3'-C3'	5.07	125.78	119.70

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	A	64996	0	32660	204	0
2	RE	1020	0	1090	2	0
3	LL	1693	0	1788	10	0
4	QU	796	0	812	4	0
5	QY	976	0	1064	7	0
6	LF	1855	0	1919	14	0
7	RN	470	0	512	1	0
8	QV	1003	0	1048	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	JT	1515	0	1586	13	0
10	RF	850	0	880	5	0
11	LM	1493	0	1566	8	0
12	QW	509	0	537	2	0
13	QZ	1092	0	1155	9	0
14	LG	3078	0	3153	21	0
15	RO	401	0	433	3	0
16	QX	959	0	1023	2	0
17	JU	1039	0	1131	3	0
18	RG	786	0	834	3	0
19	LN	1664	0	1706	15	0
20	LH	2748	0	2859	17	0
21	RA	1173	0	1215	11	0
22	RH	969	0	1078	4	0
23	RQ	847	0	914	3	0
24	LI	2328	0	2281	18	0
25	JV	1720	0	1779	7	0
26	RI	771	0	849	4	0
27	LO	1283	0	1308	16	0
28	LJ	1239	0	1326	7	0
29	RB	444	0	465	3	0
30	RJ	681	0	682	4	0
31	RT	694	0	734	4	0
32	LK	1784	0	1862	7	0
33	JW	1555	0	1659	5	0
34	RM	612	0	682	3	0
35	QO	1367	0	1396	10	0
36	RC	743	0	797	8	0
37	QP	1441	0	1543	9	0
38	LD	3353	0	1695	4	0
39	QQ	1185	0	1269	4	0
40	RD	791	0	852	3	0
41	QS	1437	0	1475	6	0
42	LE	2579	0	1304	7	0
43	QT	1276	0	1323	12	0
44	A	164	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	RA	1	0	0	0	0
44	RE	1	0	0	0	0
44	RI	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	A	21	0	0	4	0
45	LG	1	0	0	1	0
45	QO	1	0	0	0	0
45	RQ	1	0	0	0	0
46	A	14	0	26	0	0
47	A	10	0	19	1	0
48	RG	1	0	0	0	0
48	RJ	1	0	0	0	0
48	RO	1	0	0	0	0
48	RQ	1	0	0	0	0
48	RT	1	0	0	0	0
49	A	544	0	0	1	0
49	JV	2	0	0	0	0
49	JW	2	0	0	0	0
49	LD	6	0	0	0	0
49	LE	3	0	0	0	0
49	LF	7	0	0	0	0
49	LH	2	0	0	0	0
49	LI	1	0	0	0	0
49	QO	2	0	0	0	0
49	QQ	1	0	0	0	0
49	QX	1	0	0	0	0
49	RA	3	0	0	0	0
49	RB	1	0	0	0	0
49	RE	3	0	0	0	0
49	RJ	1	0	0	0	0
49	RQ	1	0	0	0	0
All	All	120018	0	86289	422	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 (422) 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)
9:JT:47:ALA:HB1	9:JT:48:PRO:HD2	1.69	0.75
27:LO:47:GLN:HG3	27:LO:67:VAL:HG22	1.70	0.73
24:LI:40:HIS:HD2	24:LI:42:ALA:H	1.35	0.73
1:A:74:G:H5''	9:JT:104:ARG:HH21	1.54	0.73
1:A:1018:G:H1	1:A:1034:U:H3	1.39	0.70
1:A:1019:G:H1	1:A:1033:U:H3	1.38	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3346:U:H3	1:A:3359:A:H61	1.39	0.70
21:RA:57:GLY:HA3	37:QP:170:ARG:HD2	1.74	0.69
1:A:2969:A:N7	6:LF:215:ASN:ND2	2.41	0.69
1:A:3268:A:OP1	28:LJ:46:ARG:NH2	2.26	0.69
36:RC:13:LYS:NZ	36:RC:103:THR:OG1	2.26	0.67
1:A:3218:A:O2'	1:A:3219:G:OP2	2.11	0.67
16:QX:50:ALA:HB1	22:RH:66:VAL:HG11	1.75	0.67
1:A:2548:C:OP1	6:LF:93:LYS:NZ	2.26	0.66
1:A:674:G:OP1	20:LH:31:ARG:NH1	2.29	0.66
1:A:1757:A:OP1	4:QU:94:ARG:NH2	2.29	0.65
13:QZ:54:THR:H	13:QZ:57:HIS:HD2	1.45	0.65
21:RA:55:LYS:O	37:QP:182:LYS:NZ	2.30	0.64
1:A:2712:U:HO2'	1:A:2743:A:HO2'	1.43	0.64
9:JT:62:THR:HG22	9:JT:64:LYS:H	1.63	0.64
14:LG:361:THR:H	14:LG:371:GLN:HE22	1.44	0.63
1:A:1564:U:H2'	1:A:1565:G:H8	1.64	0.63
19:LN:33:ILE:O	19:LN:69:ARG:NH1	2.32	0.63
22:RH:64:GLU:O	22:RH:68:GLN:NE2	2.32	0.63
24:LI:41:LYS:NZ	43:QT:32:LYS:O	2.27	0.62
1:A:1213:G:H4'	41:QS:90:MET:HG3	1.80	0.62
1:A:2185:G:O2'	1:A:2314:U:OP2	2.17	0.62
27:LO:49:LYS:HB3	27:LO:62:ASN:HA	1.82	0.62
1:A:1152:G:OP2	1:A:1152:G:N2	2.33	0.61
13:QZ:121:ARG:HD3	13:QZ:126:LYS:HE3	1.82	0.61
1:A:2967:A:N6	45:A:3426:CL:CL	2.64	0.61
1:A:3042:U:OP2	1:A:3092:C:N4	2.28	0.61
1:A:1639:C:OP2	18:RG:74:ARG:NH1	2.33	0.60
13:QZ:68:ILE:O	13:QZ:115:LYS:NZ	2.35	0.60
24:LI:205:SER:HB3	24:LI:236:LEU:HD11	1.84	0.60
37:QP:62:VAL:HG13	37:QP:66:ARG:HD2	1.82	0.60
19:LN:30:LYS:HG3	19:LN:63:GLU:HG3	1.84	0.59
1:A:2282:U:OP1	1:A:2973:G:O2'	2.20	0.59
1:A:824:C:H5''	6:LF:21:ARG:HD3	1.83	0.59
1:A:1156:C:OP2	32:LK:94:LYS:NZ	2.35	0.59
14:LG:67:PHE:HA	14:LG:70:ARG:HD3	1.85	0.59
1:A:609:G:OP2	20:LH:315:LYS:NZ	2.30	0.58
9:JT:174:ARG:HG3	26:RI:9:ILE:HD12	1.85	0.57
35:QO:122:ALA:HB3	35:QO:143:PRO:HB2	1.85	0.57
1:A:2631:U:OP2	43:QT:4:SER:OG	2.22	0.57
1:A:1778:G:O2'	1:A:1780:G:OP2	2.19	0.57
1:A:966:U:OP1	21:RA:44:ASN:ND2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:A:3483:CL:CL	6:LF:6:ARG:HB2	2.41	0.57
1:A:2112:U:H4'	1:A:2113:A:O5'	2.05	0.56
1:A:1952:G:O6	1:A:1953:G:N1	2.38	0.56
20:LH:161:LYS:HB2	20:LH:164:GLU:HG2	1.87	0.56
32:LK:163:LEU:HA	32:LK:168:ILE:HD11	1.88	0.56
1:A:2745:G:N2	1:A:2748:A:OP2	2.36	0.56
1:A:2964:G:N2	1:A:2967:A:OP2	2.35	0.56
10:RF:14:LEU:HD11	10:RF:31:LYS:HB2	1.88	0.56
1:A:888:A:N6	45:A:3452:CL:CL	2.69	0.56
20:LH:304:GLN:NE2	20:LH:306:THR:O	2.35	0.56
1:A:3118:C:O2'	15:RO:106:ARG:NH1	2.40	0.55
24:LI:289:LYS:HG3	24:LI:293:LEU:HD13	1.87	0.55
1:A:1387:G:HO2'	28:LJ:2:SER:N	2.05	0.55
11:LM:92:TYR:HB2	11:LM:142:ASP:HB3	1.87	0.55
41:QS:77:VAL:HG11	41:QS:106:LEU:HD22	1.87	0.55
14:LG:284:ARG:NH1	14:LG:293:ASN:O	2.39	0.55
29:RB:20:GLY:HA3	43:QT:82:ASN:HB2	1.87	0.55
14:LG:139:GLN:OE1	14:LG:141:GLY:N	2.39	0.55
41:QS:8:GLN:HB3	41:QS:64:ILE:HD11	1.88	0.55
1:A:864:G:N7	49:A:3621:HOH:O	2.33	0.55
11:LM:132:VAL:HG11	11:LM:157:ASN:HD22	1.72	0.55
1:A:2218:G:OP1	26:RI:68:ARG:NH2	2.40	0.54
27:LO:137:ARG:NH1	42:LE:28:C:OP1	2.40	0.54
24:LI:182:GLY:HA2	24:LI:194:LEU:HD23	1.88	0.54
1:A:3092:C:O2'	1:A:3094:A:OP2	2.17	0.54
20:LH:286:VAL:HG21	37:QP:31:LYS:HE3	1.90	0.54
1:A:3351:U:O2'	1:A:3353:G:N2	2.41	0.54
1:A:3217:C:C5	1:A:3220:G:H1'	2.43	0.54
9:JT:153:ASP:OD1	9:JT:154:VAL:N	2.41	0.54
4:QU:19:VAL:HG12	4:QU:105:LEU:HD23	1.89	0.54
1:A:3218:A:H2'	1:A:3278:C:H5	1.72	0.54
41:QS:12:ARG:HH21	41:QS:22:PRO:HD2	1.72	0.54
42:LE:38:U:N3	42:LE:41:G:OP2	2.36	0.54
1:A:815:G:OP2	30:RJ:31:LYS:NZ	2.39	0.53
19:LN:182:LEU:HD23	19:LN:185:ARG:HD3	1.89	0.53
1:A:3157:U:H4'	1:A:3158:G:H5'	1.90	0.53
3:LL:158:ASP:HB3	3:LL:159:PRO:HD3	1.91	0.53
1:A:585:A:H5''	10:RF:70:LYS:HE2	1.91	0.53
1:A:394:G:N1	1:A:397:A:OP2	2.42	0.53
1:A:2150:G:O2'	1:A:2189:U:OP1	2.24	0.53
6:LF:117:GLU:HG2	6:LF:124:GLY:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:LG:361:THR:H	14:LG:371:GLN:NE2	2.07	0.53
21:RA:2:PRO:HG2	21:RA:5:PHE:HD2	1.73	0.53
1:A:1635:G:N2	1:A:1638:A:OP2	2.37	0.53
25:JV:123:GLN:OE1	25:JV:128:LYS:NZ	2.41	0.53
20:LH:156:LEU:HD12	20:LH:159:ILE:HD12	1.90	0.53
24:LI:33:ARG:NH1	42:LE:7:G:OP1	2.42	0.53
1:A:627:U:H4'	1:A:1399:A:H1'	1.90	0.53
1:A:340:C:OP2	20:LH:195:ARG:NH1	2.34	0.52
1:A:1493:G:OP2	1:A:1493:G:N2	2.39	0.52
1:A:2895:G:O2'	15:RO:100:TYR:O	2.27	0.52
27:LO:54:VAL:HG21	27:LO:57:PHE:HD2	1.74	0.52
1:A:1560:G:N1	1:A:1580:A:N1	2.58	0.52
35:QO:67:ILE:HD11	35:QO:80:LYS:HB3	1.92	0.52
36:RC:24:THR:HB	36:RC:91:SER:HB3	1.90	0.52
6:LF:101:VAL:HG22	6:LF:165:VAL:HG22	1.92	0.52
1:A:198:A:N3	1:A:218:G:O2'	2.43	0.52
1:A:1682:U:O4	4:QU:90:ARG:NH1	2.43	0.52
1:A:2307:G:O2'	1:A:2310:U:OP2	2.24	0.52
1:A:269:G:H5''	25:JV:14:LYS:HE2	1.92	0.52
1:A:1347:U:H5''	20:LH:303:GLY:H	1.75	0.52
1:A:3121:U:H1'	1:A:3122:A:H5''	1.91	0.51
13:QZ:5:LEU:HD11	36:RC:35:ARG:HD2	1.92	0.51
19:LN:66:GLU:OE1	19:LN:69:ARG:NH2	2.42	0.51
1:A:600:G:N2	1:A:603:A:OP2	2.43	0.51
1:A:110:G:OP2	9:JT:73:ARG:NH2	2.34	0.51
32:LK:85:PHE:HB2	32:LK:139:PRO:HG3	1.91	0.51
1:A:2138:A:C4	30:RJ:3:LYS:HB3	2.46	0.51
1:A:374:A:HO2'	1:A:376:G:H8	1.58	0.51
1:A:900:G:H1'	1:A:1589:A:N6	2.26	0.51
1:A:2592:G:H4'	1:A:2594:C:C2	2.45	0.51
1:A:980:A:N6	1:A:1105:A:O4'	2.44	0.51
1:A:2193:U:H5'	1:A:2194:G:H5'	1.93	0.51
2:RE:77:ALA:HB2	28:LJ:3:ALA:HB2	1.93	0.51
9:JT:129:ASN:OD1	9:JT:130:GLY:N	2.45	0.50
22:RH:27:GLU:OE2	22:RH:43:LYS:NZ	2.44	0.50
5:QY:3:LYS:HD2	5:QY:8:VAL:HG23	1.94	0.50
5:QY:74:TYR:OH	38:LD:75:G:OP2	2.24	0.50
13:QZ:25:ILE:HA	13:QZ:43:VAL:HG12	1.93	0.50
1:A:1940:G:H21	1:A:3362:A:H8	1.59	0.50
1:A:3348:G:H1	1:A:3357:U:H3	1.59	0.50
19:LN:150:GLU:OE2	19:LN:153:ARG:NH2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:QQ:134:HIS:HD2	39:QQ:137:ALA:H	1.60	0.50
1:A:916:G:H5'	1:A:917:A:OP1	2.12	0.50
1:A:1021:G:H2'	1:A:1022:U:H4'	1.94	0.50
1:A:1717:U:H2'	1:A:1718:G:C8	2.47	0.50
1:A:3275:U:O2'	10:RF:99:ARG:NH1	2.44	0.50
3:LL:105:LYS:HE2	3:LL:109:LEU:HD11	1.93	0.50
14:LG:74:GLU:OE1	14:LG:325:LYS:NZ	2.39	0.49
19:LN:80:SER:HB3	19:LN:147:VAL:HG11	1.94	0.49
9:JT:157:ARG:NH2	21:RA:146:GLU:OE2	2.45	0.49
1:A:1098:A:OP2	43:QT:129:LYS:HA	2.12	0.49
1:A:1474:A:O2'	40:RD:57:GLN:NE2	2.45	0.49
34:RM:7:ASP:HB3	34:RM:10:GLN:HG2	1.93	0.49
1:A:1913:A:N3	1:A:2120:A:H2'	2.27	0.49
1:A:3199:G:H5''	17:JU:6:ILE:HG21	1.94	0.49
1:A:1927:G:C8	31:RT:16:VAL:HG12	2.48	0.49
16:QX:24:LEU:HD11	38:LD:151:C:C5	2.47	0.49
1:A:2916:U:H5	1:A:2935:U:HO2'	1.60	0.49
33:JW:27:LEU:HD12	33:JW:101:ARG:HB2	1.95	0.49
39:QQ:105:LEU:HD23	39:QQ:138:LEU:HD23	1.93	0.49
1:A:1347:U:H2'	1:A:1355:A:H61	1.78	0.49
1:A:1486:G:H21	18:RG:6:THR:HG22	1.78	0.48
11:LM:138:THR:HG23	11:LM:139:ASN:HD22	1.78	0.48
1:A:2960:C:H2'	1:A:2961:G:C8	2.47	0.48
33:JW:61:ALA:HA	33:JW:70:PRO:HD2	1.95	0.48
40:RD:74:ARG:HH12	40:RD:109:VAL:HG11	1.77	0.48
9:JT:80:VAL:HG13	9:JT:85:LEU:HD12	1.95	0.48
13:QZ:101:PHE:O	13:QZ:102:GLU:HG3	2.14	0.48
19:LN:36:LEU:HD21	19:LN:69:ARG:HH11	1.77	0.48
1:A:371:G:N1	1:A:374:A:OP2	2.40	0.48
1:A:655:C:H2'	1:A:656:A:C8	2.48	0.48
19:LN:169:LYS:HD2	43:QT:159:PHE:HA	1.94	0.48
32:LK:184:LEU:HD21	32:LK:202:LEU:HD21	1.95	0.48
1:A:1597:C:H5'	1:A:1696:A:H1'	1.94	0.48
3:LL:162:LEU:HD23	25:JV:7:LEU:HD11	1.96	0.48
8:QV:10:LYS:NZ	8:QV:56:ASP:OD1	2.42	0.48
19:LN:38:LYS:HD2	19:LN:83:ASP:HB3	1.95	0.48
1:A:1814:A:H4'	1:A:1815:U:H5'	1.96	0.48
37:QP:36:LEU:O	37:QP:40:THR:OG1	2.25	0.48
24:LI:151:GLN:NE2	42:LE:45:A:OP1	2.41	0.48
1:A:412:G:OP1	35:QO:62:ARG:NH1	2.46	0.48
3:LL:144:GLU:OE2	26:RI:36:ARG:NH1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:LH:159:ILE:HG23	20:LH:164:GLU:HG3	1.96	0.48
27:LO:45:PRO:HB3	27:LO:69:VAL:HB	1.95	0.48
1:A:2842:U:OP1	1:A:2844:C:N4	2.47	0.47
24:LI:82:GLU:O	24:LI:85:ARG:HG2	2.14	0.47
40:RD:55:LEU:HB2	40:RD:95:PRO:HD3	1.96	0.47
1:A:1740:U:H1'	1:A:1741:A:H2	1.79	0.47
27:LO:97:SER:OG	27:LO:128:TYR:OH	2.33	0.47
1:A:627:U:H2'	1:A:628:A:C8	2.50	0.47
1:A:1727:G:OP1	31:RT:44:LYS:NZ	2.45	0.47
8:QV:86:ARG:HB2	8:QV:92:PHE:CE2	2.50	0.47
24:LI:219:PHE:HE2	24:LI:227:LEU:HD21	1.79	0.47
42:LE:112:G:H2'	42:LE:113:C:C6	2.49	0.47
1:A:2196:C:O2'	1:A:2270:A:N3	2.41	0.47
33:JW:27:LEU:CD1	33:JW:101:ARG:HB2	2.44	0.47
1:A:974:G:H5'	37:QP:16:ARG:HG3	1.97	0.47
1:A:1554:U:H4'	1:A:1555:U:OP1	2.13	0.47
1:A:1563:C:H2'	1:A:1564:U:O4'	2.15	0.47
1:A:2945:G:O2'	1:A:2948:C:OP2	2.24	0.47
1:A:2201:G:OP1	1:A:2418:G:N1	2.48	0.47
1:A:3332:U:OP1	12:QW:35:LYS:HD3	2.15	0.47
1:A:3350:C:H2'	1:A:3351:U:H2'	1.95	0.47
1:A:1095:U:H4'	1:A:1096:U:H5'	1.97	0.47
1:A:500:C:H4'	28:LJ:80:ASN:HD21	1.78	0.46
33:JW:110:PRO:N	33:JW:111:PRO:HD2	2.30	0.46
1:A:1355:A:H4'	1:A:1356:U:O5'	2.13	0.46
1:A:170:G:H2'	1:A:171:G:H8	1.81	0.46
1:A:2424:A:OP1	25:JV:90:ASN:ND2	2.49	0.46
18:RG:3:GLN:HB2	18:RG:30:LEU:HD12	1.96	0.46
1:A:1580:A:H3'	1:A:2522:G:C8	2.50	0.46
1:A:3379:C:H4'	14:LG:315:GLY:HA2	1.97	0.46
1:A:874:U:OP1	1:A:875:G:H5'	2.16	0.46
1:A:2352:A:H5''	35:QO:83:TRP:O	2.15	0.46
34:RM:5:ILE:HD11	34:RM:11:PHE:HD1	1.80	0.46
35:QO:126:ARG:HA	35:QO:140:GLU:HG2	1.98	0.46
24:LI:196:ARG:O	24:LI:199:ILE:HG12	2.16	0.46
43:QT:125:ALA:O	43:QT:127:GLN:HG2	2.15	0.46
1:A:1108:U:H2'	1:A:1109:U:C6	2.50	0.46
1:A:1390:A:N6	1:A:1418:A:O2'	2.49	0.46
6:LF:2:GLY:HA2	6:LF:207:VAL:HG23	1.97	0.46
8:QV:108:GLU:HA	8:QV:128:ARG:HG3	1.97	0.46
9:JT:158:ALA:HA	21:RA:97:GLU:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:LH:10:SER:OG	20:LH:13:GLY:O	2.20	0.46
36:RC:42:ILE:HD11	36:RC:67:VAL:HG22	1.98	0.46
1:A:1419:A:N6	45:A:3455:CL:CL	2.81	0.45
1:A:1724:U:OP2	39:QQ:128:LYS:NZ	2.38	0.45
11:LM:57:VAL:HG23	11:LM:68:LEU:HD13	1.98	0.45
1:A:616:G:H2'	1:A:617:G:C8	2.51	0.45
13:QZ:54:THR:H	13:QZ:57:HIS:CD2	2.30	0.45
25:JV:153:ASP:OD1	25:JV:154:PRO:HD2	2.17	0.45
35:QO:72:GLN:HE22	35:QO:83:TRP:HE1	1.64	0.45
1:A:1491:A:H5''	30:RJ:14:LYS:HE3	1.97	0.45
6:LF:113:VAL:HG12	6:LF:166:ILE:HD13	1.98	0.45
43:QT:126:VAL:HG13	43:QT:128:LEU:HG	1.99	0.45
1:A:3253:G:H2'	1:A:3254:G:H8	1.81	0.45
14:LG:139:GLN:HE22	14:LG:143:GLY:H	1.64	0.45
1:A:1064:A:H4'	1:A:1065:A:O5'	2.16	0.45
1:A:1621:A:H2'	1:A:1622:U:C6	2.51	0.45
1:A:3317:U:H4'	1:A:3318:G:H5'	1.97	0.45
37:QP:165:ILE:HD11	37:QP:172:PHE:HB3	1.99	0.45
42:LE:12:U:OP2	42:LE:68:C:O2'	2.34	0.45
1:A:911:C:H5''	6:LF:15:ILE:HD13	1.97	0.45
1:A:1191:U:H4'	1:A:1192:C:H5''	1.99	0.45
1:A:2681:U:H5'	27:LO:65:ILE:HD11	1.97	0.45
27:LO:49:LYS:HA	27:LO:64:LYS:HA	1.99	0.45
1:A:1482:A:N1	1:A:1866:C:O2'	2.46	0.45
1:A:3217:C:N3	35:QO:182:ILE:HD12	2.31	0.45
3:LL:201:THR:OG1	3:LL:202:GLU:OE1	2.24	0.45
14:LG:95:THR:HG22	14:LG:97:ARG:H	1.81	0.45
14:LG:136:LYS:O	14:LG:139:GLN:NE2	2.49	0.45
1:A:1947:G:OP1	39:QQ:136:ARG:NH1	2.50	0.45
1:A:59:G:H4'	1:A:60:A:H4'	1.99	0.45
11:LM:8:GLN:HB3	11:LM:72:LYS:HD2	1.98	0.45
1:A:1786:G:H2'	1:A:1787:A:C8	2.52	0.44
1:A:2514:U:O2	1:A:2593:A:N6	2.47	0.44
14:LG:173:GLN:HG2	14:LG:175:LYS:H	1.81	0.44
11:LM:87:LYS:HG3	11:LM:187:ILE:HG12	1.99	0.44
13:QZ:16:GLY:C	13:QZ:18:TYR:H	2.20	0.44
19:LN:21:ARG:O	19:LN:24:ARG:NH1	2.49	0.44
36:RC:10:ILE:HD13	36:RC:105:ALA:HB1	1.98	0.44
1:A:196:G:N1	1:A:199:A:OP2	2.50	0.44
1:A:1877:U:H5''	1:A:1878:G:O4'	2.17	0.44
1:A:2514:U:H5'	3:LL:68:ARG:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3228:C:H4'	1:A:3229:G:O5'	2.17	0.44
3:LL:82:LEU:HD13	3:LL:222:PHE:HE2	1.81	0.44
5:QY:53:ASP:O	5:QY:110:HIS:HB2	2.18	0.44
8:QV:104:ASN:OD1	8:QV:108:GLU:N	2.50	0.44
21:RA:94:ALA:HB2	21:RA:121:VAL:HG22	1.98	0.44
1:A:216:G:OP1	5:QY:16:ARG:NH1	2.44	0.44
1:A:662:U:H2'	1:A:663:C:C6	2.52	0.44
1:A:860:G:C6	6:LF:181:LYS:HB2	2.52	0.44
1:A:2177:G:H2'	6:LF:128:ARG:HD3	2.00	0.44
20:LH:3:ARG:NH1	20:LH:22:LEU:O	2.50	0.44
1:A:1094:U:H4'	1:A:1096:U:H5''	1.99	0.44
1:A:2897:A:H5''	15:RO:125:LYS:HD2	1.99	0.44
14:LG:95:THR:HB	14:LG:98:GLY:O	2.17	0.44
1:A:993:G:N3	1:A:2637:A:H2'	2.33	0.44
10:RF:49:ILE:HD11	10:RF:71:VAL:HG22	2.00	0.44
33:JW:79:ILE:HG21	33:JW:138:LEU:HD11	2.00	0.44
1:A:1571:A:H2'	1:A:1572:U:O4'	2.17	0.44
1:A:1624:G:O2'	1:A:1643:A:N1	2.43	0.44
1:A:3231:U:H2'	1:A:3232:G:H8	1.82	0.44
24:LI:40:HIS:CD2	43:QT:69:LYS:HA	2.52	0.44
1:A:546:C:OP1	1:A:547:G:N2	2.50	0.44
1:A:1896:A:H61	1:A:2339:C:H42	1.64	0.44
25:JV:183:THR:HG22	25:JV:187:ARG:HB2	1.98	0.44
41:QS:92:LYS:HE2	41:QS:109:ASP:OD2	2.18	0.44
1:A:595:G:H1	1:A:609:G:H5''	1.82	0.44
1:A:1176:C:H2'	1:A:1177:G:N2	2.32	0.43
19:LN:54:SER:HB2	19:LN:135:ILE:HD11	1.99	0.43
20:LH:12:THR:HA	20:LH:171:ALA:HB1	2.00	0.43
24:LI:126:GLU:HG3	24:LI:128:GLU:HG2	1.99	0.43
1:A:3084:C:H2'	1:A:3085:G:O4'	2.18	0.43
27:LO:161:SER:O	27:LO:165:GLN:HG2	2.18	0.43
1:A:1054:A:H5''	1:A:2637:A:H61	1.82	0.43
1:A:1579:C:N4	1:A:1580:A:H62	2.15	0.43
19:LN:50:VAL:HG22	19:LN:167:LEU:HD13	2.00	0.43
23:RQ:46:LYS:HE3	23:RQ:54:THR:HB	2.00	0.43
25:JV:28:TRP:O	25:JV:32:GLN:HG2	2.18	0.43
35:QO:178:ALA:O	35:QO:182:ILE:HG12	2.19	0.43
1:A:3085:G:OP1	12:QW:34:SER:OG	2.34	0.43
1:A:3356:G:H2'	1:A:3357:U:C6	2.54	0.43
1:A:1779:C:N4	1:A:2102:U:OP2	2.50	0.43
1:A:1863:G:N1	1:A:1866:C:OP2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2585:G:H2'	1:A:2585:G:N3	2.34	0.43
1:A:3218:A:H5''	1:A:3219:G:C4	2.54	0.43
20:LH:179:LEU:HD11	20:LH:183:LYS:HE3	2.00	0.43
24:LI:52:VAL:HG21	24:LI:65:ILE:HD12	2.00	0.43
1:A:1307:G:O2'	1:A:1308:A:OP2	2.34	0.43
1:A:2244:A:H5''	6:LF:243:THR:HB	2.01	0.43
10:RF:37:THR:HG22	10:RF:39:GLN:H	1.84	0.43
24:LI:153:THR:HG23	24:LI:160:PHE:HZ	1.83	0.43
31:RT:46:THR:HB	31:RT:58:SER:HB3	2.00	0.43
1:A:3218:A:H2'	1:A:3278:C:C5	2.53	0.43
1:A:3283:U:H2'	1:A:3284:G:C8	2.53	0.43
3:LL:82:LEU:HG	3:LL:86:THR:HG23	2.01	0.43
6:LF:39:GLY:HA2	6:LF:93:LYS:HD2	2.01	0.43
14:LG:139:GLN:H	14:LG:139:GLN:HG3	1.62	0.43
27:LO:30:LEU:HD11	27:LO:67:VAL:HG23	2.01	0.43
13:QZ:76:ASN:OD1	13:QZ:77:TYR:N	2.51	0.43
27:LO:17:LEU:HD13	27:LO:129:VAL:HG22	2.00	0.43
14:LG:166:ILE:HD11	14:LG:171:LEU:HD12	1.99	0.43
24:LI:256:THR:O	24:LI:258:LYS:NZ	2.48	0.43
32:LK:136:TYR:CZ	32:LK:231:ASN:HB2	2.53	0.43
1:A:307:A:H2'	1:A:308:A:C8	2.54	0.42
1:A:1049:C:OP2	19:LN:21:ARG:NH2	2.51	0.42
1:A:2375:G:O2'	1:A:2377:G:OP2	2.34	0.42
1:A:3162:C:H2'	1:A:3163:A:C8	2.54	0.42
30:RJ:75:LYS:NZ	38:LD:94:C:OP1	2.45	0.42
43:QT:18:ASP:HB2	43:QT:21:LYS:HD2	2.01	0.42
1:A:1110:U:H2'	1:A:1111:U:C6	2.54	0.42
1:A:2565:U:H2'	1:A:2566:C:C6	2.54	0.42
1:A:3283:U:H2'	1:A:3284:G:H8	1.84	0.42
5:QY:69:LYS:HE3	5:QY:69:LYS:HB3	1.86	0.42
9:JT:47:ALA:HB1	9:JT:48:PRO:CD	2.44	0.42
24:LI:117:GLU:HA	24:LI:120:LYS:HE3	2.01	0.42
37:QP:148:GLU:O	37:QP:151:ARG:HG2	2.19	0.42
1:A:1097:G:H4'	1:A:1098:A:O5'	2.18	0.42
31:RT:49:ARG:HB2	31:RT:55:TRP:CZ3	2.54	0.42
1:A:2880:U:H1'	14:LG:250:ALA:HB3	2.01	0.42
8:QV:18:PRO:HA	8:QV:51:ALA:HA	2.00	0.42
24:LI:107:ARG:NH2	24:LI:116:ASP:OD1	2.52	0.42
1:A:1715:A:N7	36:RC:84:LEU:HD12	2.34	0.42
1:A:3152:U:O2'	1:A:3153:U:H5'	2.19	0.42
11:LM:36:LYS:HD3	11:LM:38:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:RC:30:THR:HG23	36:RC:91:SER:HB2	2.02	0.42
1:A:1724:U:H1'	1:A:1725:C:C6	2.55	0.42
23:RQ:25:VAL:HG22	23:RQ:72:LEU:HD22	2.02	0.42
41:QS:13:ARG:NH1	41:QS:50:LYS:O	2.52	0.42
35:QO:60:PHE:HB3	35:QO:64:ASN:HB3	2.01	0.42
1:A:374:A:O2'	1:A:376:G:H5'	2.20	0.42
1:A:616:G:H2'	1:A:617:G:H8	1.84	0.42
1:A:981:U:H2'	1:A:982:C:C6	2.55	0.42
1:A:1792:C:HO2'	1:A:1794:G:H8	1.65	0.42
1:A:2513:U:HO2'	1:A:2514:U:P	2.42	0.42
1:A:2573:G:H2'	1:A:2574:G:H8	1.85	0.42
4:QU:10:LYS:HD2	4:QU:10:LYS:HA	1.74	0.42
5:QY:51:ARG:HG2	5:QY:52:ARG:H	1.83	0.42
14:LG:123:TYR:CZ	14:LG:124:LYS:HG3	2.54	0.42
1:A:3217:C:C2	35:QO:182:ILE:HD12	2.55	0.42
29:RB:35:VAL:O	29:RB:40:ARG:NH2	2.51	0.42
32:LK:132:PRO:HA	32:LK:229:PHE:CG	2.55	0.42
17:JU:105:GLN:HE22	17:JU:109:ARG:NE	2.16	0.42
1:A:2407:C:H2'	1:A:2408:U:C6	2.55	0.41
1:A:2611:U:H2'	1:A:2612:U:C6	2.55	0.41
1:A:3165:A:H2'	1:A:3166:C:C6	2.55	0.41
34:RM:64:LYS:HB3	34:RM:64:LYS:HE3	1.85	0.41
1:A:3107:U:H2'	1:A:3108:G:C8	2.55	0.41
14:LG:148:LEU:HD11	14:LG:196:ARG:HD3	2.02	0.41
14:LG:346:THR:O	14:LG:346:THR:OG1	2.36	0.41
1:A:1111:U:H5''	9:JT:5:LYS:HE2	2.02	0.41
1:A:3259:U:H5''	1:A:3261:C:H5	1.85	0.41
6:LF:68:LYS:HD2	6:LF:70:ARG:CD	2.50	0.41
1:A:3253:G:H2'	1:A:3254:G:C8	2.56	0.41
21:RA:75:LEU:HG	21:RA:114:GLY:HA2	2.01	0.41
27:LO:133:ARG:HB2	27:LO:152:HIS:CE1	2.54	0.41
28:LJ:143:LYS:HE3	28:LJ:143:LYS:HB3	1.91	0.41
38:LD:81:U:H4'	38:LD:82:U:H5'	2.01	0.41
1:A:1616:U:H2'	1:A:1617:G:C8	2.55	0.41
1:A:2689:A:H2'	1:A:2689:A:N3	2.34	0.41
1:A:2716:U:H5'	23:RQ:8:ARG:HH22	1.86	0.41
1:A:3271:G:C5	28:LJ:108:LYS:HE3	2.55	0.41
1:A:507:U:H2'	1:A:508:U:C6	2.55	0.41
1:A:1622:U:H2'	1:A:1623:G:C8	2.55	0.41
1:A:2373:A:N3	1:A:2824:G:O2'	2.45	0.41
1:A:3231:U:H2'	1:A:3232:G:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:LL:251:LYS:HE3	3:LL:251:LYS:HB3	1.77	0.41
5:QY:5:SER:HB3	5:QY:8:VAL:HG22	2.02	0.41
20:LH:180:LYS:HB3	20:LH:180:LYS:HE2	1.88	0.41
20:LH:205:PRO:HD2	20:LH:225:VAL:HG22	2.03	0.41
27:LO:34:SER:HB3	27:LO:67:VAL:HG21	2.02	0.41
1:A:75:G:H5'	9:JT:59:ARG:O	2.21	0.41
1:A:1317:A:O2'	1:A:1318:A:H3'	2.19	0.41
19:LN:33:ILE:HB	19:LN:69:ARG:HH12	1.86	0.41
43:QT:75:ILE:HG23	43:QT:86:GLU:HG3	2.02	0.41
1:A:567:G:H2'	1:A:568:G:C8	2.56	0.41
1:A:2103:U:H2'	1:A:2104:A:C8	2.55	0.41
1:A:2573:G:H2'	1:A:2574:G:C8	2.56	0.41
14:LG:10:ARG:HG2	14:LG:11:HIS:N	2.36	0.41
32:LK:176:TYR:CZ	32:LK:197:GLN:HG2	2.56	0.41
1:A:1615:C:H2'	1:A:1616:U:C6	2.56	0.41
1:A:1895:A:O2'	1:A:3053:G:H4'	2.20	0.41
1:A:2213:A:H2'	1:A:2214:A:C8	2.56	0.41
1:A:2763:U:O2	47:A:3519:SPD:N1	2.54	0.41
2:RE:126:LEU:HD23	2:RE:126:LEU:HA	1.89	0.41
3:LL:189:LEU:HD12	3:LL:190:VAL:HG13	2.03	0.41
17:JU:21:VAL:HG12	17:JU:65:LEU:HD23	2.03	0.41
20:LH:58:HIS:HA	20:LH:90:PHE:HE1	1.86	0.41
28:LJ:8:LYS:HE2	28:LJ:8:LYS:HB2	1.95	0.41
21:RA:76:ASP:HB3	21:RA:116:GLY:HA3	2.02	0.41
1:A:1354:G:H2'	1:A:1357:G:H4'	2.03	0.40
14:LG:14:LEU:N	45:LG:401:CL:CL	2.78	0.40
19:LN:166:ILE:HG21	43:QT:158:THR:HG21	2.04	0.40
20:LH:271:LYS:HB2	20:LH:274:TYR:HB3	2.02	0.40
22:RH:74:LYS:HE3	22:RH:74:LYS:HB2	1.90	0.40
26:RI:5:THR:HG23	26:RI:12:ASN:HB2	2.03	0.40
1:A:1841:A:H1'	7:RN:45:ARG:HH22	1.86	0.40
1:A:2679:A:O2'	27:LO:52:TYR:OH	2.36	0.40
27:LO:96:PHE:HB2	27:LO:156:LYS:HE3	2.03	0.40
1:A:1128:U:H2'	1:A:1129:A:O4'	2.21	0.40
11:LM:112:ILE:HG22	11:LM:126:VAL:O	2.21	0.40
21:RA:51:GLY:HA2	37:QP:175:ALA:O	2.21	0.40
24:LI:236:LEU:HA	24:LI:239:ILE:HG12	2.04	0.40
27:LO:125:MET:HE1	27:LO:127:PHE:HE1	1.86	0.40
42:LE:3:U:H2'	42:LE:4:U:C6	2.56	0.40
43:QT:118:GLU:O	43:QT:122:GLN:NE2	2.54	0.40
1:A:900:G:H1'	1:A:1589:A:H61	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:RB:5:LYS:NZ	29:RB:8:THR:HB	2.36	0.40
1:A:1404:G:N2	1:A:1407:A:OP2	2.45	0.40
1:A:3291:G:H2'	1:A:3292:A:C8	2.56	0.40
14:LG:236:LYS:HE2	14:LG:236:LYS:HB2	1.96	0.40
21:RA:83:PRO:O	21:RA:87:ARG:HG3	2.21	0.40
36:RC:14:LEU:O	36:RC:18:ILE:HG12	2.21	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	
2	RE	125/130 (96%)	125 (100%)	0	0	100	100
3	LL	211/256 (82%)	204 (97%)	7 (3%)	0	100	100
4	QU	98/121 (81%)	94 (96%)	4 (4%)	0	100	100
5	QY	122/127 (96%)	121 (99%)	1 (1%)	0	100	100
6	LF	242/254 (95%)	231 (96%)	11 (4%)	0	100	100
7	RN	52/51 (102%)	51 (98%)	1 (2%)	0	100	100
8	QV	134/137 (98%)	132 (98%)	2 (2%)	0	100	100
9	JT	187/199 (94%)	180 (96%)	6 (3%)	1 (0%)	25	20
10	RF	104/107 (97%)	100 (96%)	4 (4%)	0	100	100
11	LM	186/191 (97%)	178 (96%)	8 (4%)	0	100	100
12	QW	59/155 (38%)	58 (98%)	1 (2%)	0	100	100
13	QZ	133/136 (98%)	122 (92%)	11 (8%)	0	100	100
14	LG	384/387 (99%)	375 (98%)	9 (2%)	0	100	100
15	RO	48/128 (38%)	48 (100%)	0	0	100	100
16	QX	118/142 (83%)	117 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	JU	132/138 (96%)	127 (96%)	5 (4%)	0	100	100
18	RG	98/121 (81%)	96 (98%)	2 (2%)	0	100	100
19	LN	200/221 (90%)	196 (98%)	4 (2%)	0	100	100
20	LH	359/362 (99%)	343 (96%)	16 (4%)	0	100	100
21	RA	146/149 (98%)	133 (91%)	12 (8%)	1 (1%)	19	13
22	RH	117/120 (98%)	116 (99%)	1 (1%)	0	100	100
23	RQ	103/106 (97%)	96 (93%)	7 (7%)	0	100	100
24	LI	288/297 (97%)	281 (98%)	7 (2%)	0	100	100
25	JV	201/204 (98%)	195 (97%)	6 (3%)	0	100	100
26	RI	97/100 (97%)	95 (98%)	2 (2%)	0	100	100
27	LO	156/174 (90%)	149 (96%)	7 (4%)	0	100	100
28	LJ	152/176 (86%)	146 (96%)	6 (4%)	0	100	100
29	RB	54/59 (92%)	51 (94%)	3 (6%)	0	100	100
30	RJ	85/88 (97%)	84 (99%)	1 (1%)	0	100	100
31	RT	89/92 (97%)	84 (94%)	5 (6%)	0	100	100
32	LK	220/244 (90%)	214 (97%)	6 (3%)	0	100	100
33	JW	195/199 (98%)	192 (98%)	3 (2%)	0	100	100
34	RM	75/78 (96%)	71 (95%)	4 (5%)	0	100	100
35	QO	168/184 (91%)	166 (99%)	2 (1%)	0	100	100
36	RC	95/105 (90%)	95 (100%)	0	0	100	100
37	QP	183/186 (98%)	178 (97%)	5 (3%)	0	100	100
39	QQ	145/189 (77%)	144 (99%)	1 (1%)	0	100	100
40	RD	93/113 (82%)	93 (100%)	0	0	100	100
41	QS	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
43	QT	157/160 (98%)	152 (97%)	5 (3%)	0	100	100
All	All	5980/6558 (91%)	5798 (97%)	180 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	JT	47	ALA
21	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	
2	RE	109/111 (98%)	109 (100%)	0	100	100
3	LL	179/208 (86%)	177 (99%)	2 (1%)	70	75
4	QU	87/107 (81%)	87 (100%)	0	100	100
5	QY	107/110 (97%)	106 (99%)	1 (1%)	75	81
6	LF	187/196 (95%)	186 (100%)	1 (0%)	86	91
7	RN	50/47 (106%)	50 (100%)	0	100	100
8	QV	104/105 (99%)	104 (100%)	0	100	100
9	JT	152/159 (96%)	151 (99%)	1 (1%)	81	86
10	RF	90/91 (99%)	90 (100%)	0	100	100
11	LM	168/171 (98%)	167 (99%)	1 (1%)	84	89
12	QW	54/129 (42%)	54 (100%)	0	100	100
13	QZ	115/116 (99%)	114 (99%)	1 (1%)	75	81
14	LG	322/323 (100%)	318 (99%)	4 (1%)	67	73
15	RO	45/116 (39%)	45 (100%)	0	100	100
16	QX	104/118 (88%)	104 (100%)	0	100	100
17	JU	106/109 (97%)	106 (100%)	0	100	100
18	RG	85/103 (82%)	85 (100%)	0	100	100
19	LN	176/187 (94%)	176 (100%)	0	100	100
20	LH	288/289 (100%)	287 (100%)	1 (0%)	91	94
21	RA	118/119 (99%)	115 (98%)	3 (2%)	42	45
22	RH	104/105 (99%)	104 (100%)	0	100	100
23	RQ	90/91 (99%)	90 (100%)	0	100	100
24	LI	240/245 (98%)	237 (99%)	3 (1%)	65	71
25	JV	175/176 (99%)	175 (100%)	0	100	100
26	RI	81/82 (99%)	81 (100%)	0	100	100
27	LO	139/150 (93%)	136 (98%)	3 (2%)	47	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	LJ	134/153 (88%)	131 (98%)	3 (2%)	47	51
29	RB	44/47 (94%)	44 (100%)	0	100	100
30	RJ	70/71 (99%)	70 (100%)	0	100	100
31	RT	71/72 (99%)	71 (100%)	0	100	100
32	LK	186/205 (91%)	186 (100%)	0	100	100
33	JW	160/162 (99%)	159 (99%)	1 (1%)	84	89
34	RM	68/69 (99%)	68 (100%)	0	100	100
35	QO	139/146 (95%)	139 (100%)	0	100	100
36	RC	81/88 (92%)	80 (99%)	1 (1%)	67	73
37	QP	150/151 (99%)	149 (99%)	1 (1%)	81	86
39	QQ	122/154 (79%)	122 (100%)	0	100	100
40	RD	85/97 (88%)	85 (100%)	0	100	100
41	QS	155/156 (99%)	153 (99%)	2 (1%)	65	71
43	QT	136/137 (99%)	136 (100%)	0	100	100
All	All	5076/5471 (93%)	5047 (99%)	29 (1%)	82	89

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	LL	101	THR
3	LL	206	GLU
5	QY	74	TYR
6	LF	68	LYS
9	JT	13	HIS
11	LM	23	ARG
13	QZ	23	VAL
14	LG	114	VAL
14	LG	139	GLN
14	LG	146	ARG
14	LG	332	ARG
20	LH	120	TYR
21	RA	60	TYR
21	RA	97	GLU
21	RA	98	THR
24	LI	93	THR
24	LI	155	THR
24	LI	218	ARG

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Mol	Chain	Res	Type
27	LO	40	LEU
27	LO	44	THR
27	LO	155	THR
28	LJ	93	VAL
28	LJ	98	VAL
28	LJ	152	THR
33	JW	117	ARG
36	RC	102	THR
37	QP	135	GLN
41	QS	45	LEU
41	QS	172	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
3	LL	79	GLN
5	QY	81	GLN
6	LF	79	ASN
6	LF	139	HIS
7	RN	25	GLN
8	QV	47	ASN
9	JT	114	GLN
9	JT	137	GLN
10	RF	26	ASN
11	LM	51	GLN
11	LM	64	HIS
11	LM	139	ASN
11	LM	157	ASN
13	QZ	57	HIS
13	QZ	78	ASN
14	LG	371	GLN
16	QX	85	GLN
17	JU	105	GLN
17	JU	119	GLN
18	RG	61	GLN
19	LN	51	HIS
20	LH	92	ASN
20	LH	237	GLN
20	LH	296	GLN
21	RA	39	HIS
22	RH	68	GLN
22	RH	104	GLN

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Mol	Chain	Res	Type
23	RQ	53	GLN
23	RQ	105	GLN
24	LI	40	HIS
24	LI	81	HIS
24	LI	203	HIS
25	JV	11	GLN
26	RI	63	ASN
27	LO	90	GLN
27	LO	152	HIS
30	RJ	13	ASN
32	LK	48	ASN
32	LK	64	GLN
32	LK	159	GLN
32	LK	197	GLN
32	LK	209	ASN
33	JW	26	GLN
33	JW	182	ASN
34	RM	40	GLN
34	RM	67	GLN
35	QO	72	GLN
35	QO	172	GLN
39	QQ	7	GLN
39	QQ	134	HIS
40	RD	57	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	3030/3396 (89%)	368 (12%)	21 (0%)
38	LD	157/158 (99%)	20 (12%)	1 (0%)
42	LE	120/121 (99%)	11 (9%)	0
All	All	3307/3675 (89%)	399 (12%)	22 (0%)

All (399) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	26	A
1	A	40	A
1	A	43	A
1	A	49	A
1	A	59	G

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Mol	Chain	Res	Type
1	A	60	A
1	A	65	A
1	A	66	A
1	A	92	G
1	A	109	A
1	A	110	G
1	A	111	C
1	A	116	A
1	A	117	U
1	A	118	U
1	A	121	A
1	A	122	A
1	A	133	U
1	A	135	C
1	A	136	G
1	A	156	G
1	A	157	A
1	A	166	C
1	A	170	G
1	A	187	A
1	A	190	U
1	A	191	U
1	A	192	C
1	A	200	C
1	A	210	U
1	A	218	G
1	A	219	A
1	A	240	U
1	A	243	G
1	A	249	U
1	A	252	U
1	A	269	G
1	A	286	U
1	A	295	A
1	A	305	U
1	A	315	C
1	A	323	A
1	A	329	U
1	A	339	C
1	A	350	C
1	A	376	G
1	A	398	A

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Mol	Chain	Res	Type
1	A	401	U
1	A	402	A
1	A	403	C
1	A	421	G
1	A	422	A
1	A	439	C
1	A	440	A
1	A	495	G
1	A	521	A
1	A	546	C
1	A	547	G
1	A	548	G
1	A	552	G
1	A	555	U
1	A	557	A
1	A	559	A
1	A	578	A
1	A	579	G
1	A	589	A
1	A	604	G
1	A	609	G
1	A	611	A
1	A	620	U
1	A	621	A
1	A	622	A
1	A	636	C
1	A	649	A
1	A	660	A
1	A	677	A
1	A	681	U
1	A	691	A
1	A	705	A
1	A	712	G
1	A	715	A
1	A	716	A
1	A	767	U
1	A	776	U
1	A	777	U
1	A	781	G
1	A	785	G
1	A	786	A
1	A	806	A

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Mol	Chain	Res	Type
1	A	817	A
1	A	830	A
1	A	849	C
1	A	861	C
1	A	874	U
1	A	879	U
1	A	896	A
1	A	907	G
1	A	908	G
1	A	914	A
1	A	916	G
1	A	917	A
1	A	921	A
1	A	923	C
1	A	937	G
1	A	944	C
1	A	959	C
1	A	960	U
1	A	979	U
1	A	980	A
1	A	995	U
1	A	1001	G
1	A	1002	A
1	A	1010	G
1	A	1033	U
1	A	1036	A
1	A	1037	C
1	A	1047	A
1	A	1049	C
1	A	1064	A
1	A	1065	A
1	A	1072	G
1	A	1081	U
1	A	1094	U
1	A	1095	U
1	A	1096	U
1	A	1097	G
1	A	1098	A
1	A	1103	A
1	A	1104	G
1	A	1117	G
1	A	1131	G

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Mol	Chain	Res	Type
1	A	1153	A
1	A	1159	A
1	A	1180	A
1	A	1181	U
1	A	1196	C
1	A	1201	C
1	A	1208	U
1	A	1222	G
1	A	1287	A
1	A	1307	G
1	A	1308	A
1	A	1309	U
1	A	1313	G
1	A	1330	A
1	A	1331	U
1	A	1348	U
1	A	1349	G
1	A	1350	A
1	A	1351	U
1	A	1356	U
1	A	1357	G
1	A	1386	A
1	A	1399	A
1	A	1400	G
1	A	1419	A
1	A	1434	G
1	A	1437	C
1	A	1446	A
1	A	1481	A
1	A	1484	U
1	A	1508	C
1	A	1536	G
1	A	1555	U
1	A	1556	C
1	A	1557	A
1	A	1562	C
1	A	1563	C
1	A	1566	A
1	A	1569	U
1	A	1580	A
1	A	1581	C
1	A	1582	C

Continued on next page...

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Mol	Chain	Res	Type
1	A	1583	A
1	A	1587	A
1	A	1589	A
1	A	1593	A
1	A	1607	U
1	A	1620	U
1	A	1629	U
1	A	1639	C
1	A	1643	A
1	A	1717	U
1	A	1724	U
1	A	1725	C
1	A	1741	A
1	A	1750	A
1	A	1751	G
1	A	1765	U
1	A	1770	G
1	A	1775	G
1	A	1778	G
1	A	1780	G
1	A	1797	A
1	A	1814	A
1	A	1816	A
1	A	1820	U
1	A	1821	U
1	A	1841	A
1	A	1842	A
1	A	1849	C
1	A	1850	A
1	A	1880	U
1	A	1886	A
1	A	1893	A
1	A	1906	G
1	A	1952	G
1	A	2101	C
1	A	2102	U
1	A	2112	U
1	A	2113	A
1	A	2114	C
1	A	2121	G
1	A	2122	G
1	A	2131	A

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Mol	Chain	Res	Type
1	A	2140	U
1	A	2158	A
1	A	2169	G
1	A	2170	U
1	A	2205	U
1	A	2209	U
1	A	2210	G
1	A	2244	A
1	A	2272	G
1	A	2273	G
1	A	2279	A
1	A	2282	U
1	A	2288	G
1	A	2307	G
1	A	2308	C
1	A	2310	U
1	A	2313	A
1	A	2314	U
1	A	2315	G
1	A	2334	U
1	A	2335	G
1	A	2336	U
1	A	2373	A
1	A	2374	C
1	A	2375	G
1	A	2385	G
1	A	2388	U
1	A	2393	G
1	A	2397	A
1	A	2402	A
1	A	2403	G
1	A	2404	A
1	A	2411	U
1	A	2418	G
1	A	2435	G
1	A	2513	U
1	A	2514	U
1	A	2515	A
1	A	2522	G
1	A	2523	A
1	A	2531	C
1	A	2549	G

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Mol	Chain	Res	Type
1	A	2552	C
1	A	2554	A
1	A	2555	G
1	A	2561	A
1	A	2569	A
1	A	2570	U
1	A	2571	U
1	A	2572	C
1	A	2573	G
1	A	2585	G
1	A	2593	A
1	A	2606	G
1	A	2607	G
1	A	2614	G
1	A	2652	U
1	A	2656	A
1	A	2674	A
1	A	2677	G
1	A	2689	A
1	A	2691	A
1	A	2696	A
1	A	2704	A
1	A	2705	A
1	A	2714	G
1	A	2728	G
1	A	2729	U
1	A	2752	U
1	A	2753	G
1	A	2755	C
1	A	2762	A
1	A	2777	G
1	A	2778	G
1	A	2796	G
1	A	2799	A
1	A	2800	G
1	A	2801	A
1	A	2803	A
1	A	2810	C
1	A	2814	G
1	A	2817	A
1	A	2842	U
1	A	2845	A

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Mol	Chain	Res	Type
1	A	2867	C
1	A	2871	G
1	A	2872	A
1	A	2875	U
1	A	2876	C
1	A	2887	A
1	A	2923	U
1	A	2935	U
1	A	2936	A
1	A	2942	C
1	A	2947	G
1	A	2951	G
1	A	2983	C
1	A	2990	G
1	A	2996	U
1	A	2997	G
1	A	3012	A
1	A	3056	U
1	A	3059	G
1	A	3078	U
1	A	3086	A
1	A	3092	C
1	A	3122	A
1	A	3130	A
1	A	3131	U
1	A	3142	A
1	A	3143	C
1	A	3154	C
1	A	3155	U
1	A	3156	U
1	A	3157	U
1	A	3165	A
1	A	3173	G
1	A	3174	A
1	A	3176	G
1	A	3179	U
1	A	3181	C
1	A	3187	A
1	A	3207	U
1	A	3217	C
1	A	3218	A
1	A	3219	G

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Mol	Chain	Res	Type
1	A	3229	G
1	A	3243	A
1	A	3245	A
1	A	3247	G
1	A	3259	U
1	A	3263	G
1	A	3270	U
1	A	3273	A
1	A	3276	G
1	A	3279	A
1	A	3281	U
1	A	3287	U
1	A	3289	G
1	A	3294	A
1	A	3304	U
1	A	3316	A
1	A	3318	G
1	A	3319	U
1	A	3341	U
1	A	3345	G
1	A	3351	U
1	A	3352	U
1	A	3353	G
1	A	3355	U
1	A	3369	G
1	A	3378	C
1	A	3390	G
38	LD	23	U
38	LD	34	U
38	LD	35	C
38	LD	59	A
38	LD	62	C
38	LD	63	G
38	LD	80	A
38	LD	81	U
38	LD	84	C
38	LD	86	U
38	LD	87	G
38	LD	90	U
38	LD	95	G
38	LD	104	A
38	LD	106	C

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Mol	Chain	Res	Type
38	LD	111	A
38	LD	113	U
38	LD	125	U
38	LD	126	A
38	LD	152	G
42	LE	7	G
42	LE	33	U
42	LE	42	A
42	LE	51	A
42	LE	54	U
42	LE	55	A
42	LE	65	G
42	LE	76	A
42	LE	102	A
42	LE	112	G
42	LE	121	U

All (22) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	65	A
1	A	169	U
1	A	547	G
1	A	916	G
1	A	1064	A
1	A	1097	G
1	A	1307	G
1	A	1355	A
1	A	1554	U
1	A	1562	C
1	A	1815	U
1	A	2101	C
1	A	2112	U
1	A	2209	U
1	A	2512	C
1	A	3121	U
1	A	3218	A
1	A	3228	C
1	A	3269	U
1	A	3317	U
1	A	3351	U
38	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 201 ligands modelled in this entry, 199 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	$\# Z > 2$
47	SPD	A	3519	-	9,9,9	0.27	0	8,8,8	0.32	0
46	SPM	A	3470	-	13,13,13	0.36	0	12,12,12	0.81	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
47	SPD	A	3519	-	-	0/7/7/7	-
46	SPM	A	3470	-	-	1/11/11/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	3470	SPM	C12-C11-N10-C9

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	A	3519	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.

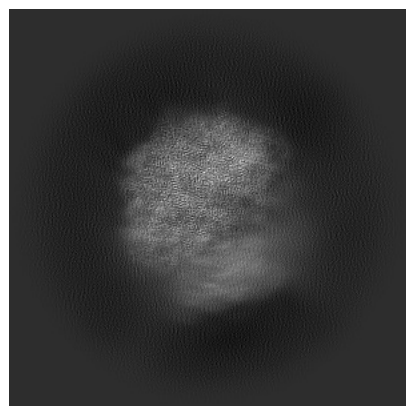
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17653. These allow visual inspection of the internal detail of the map and identification of artifacts.

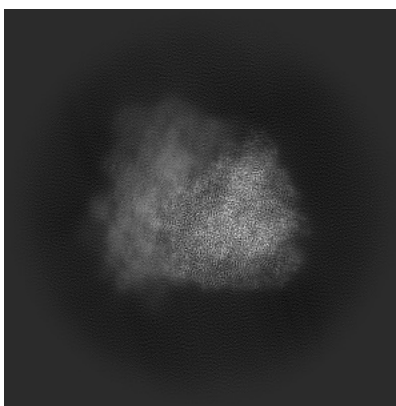
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

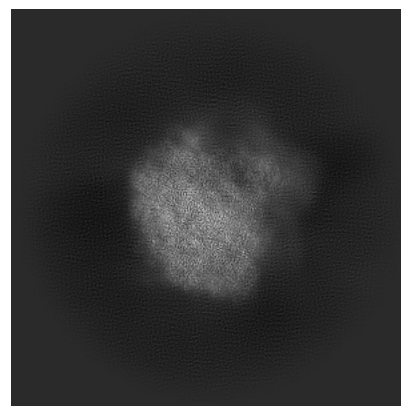
6.1.1 Primary map



X

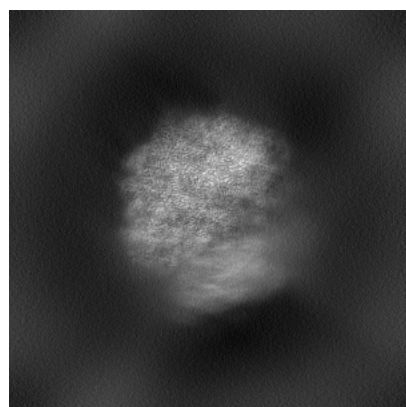


Y

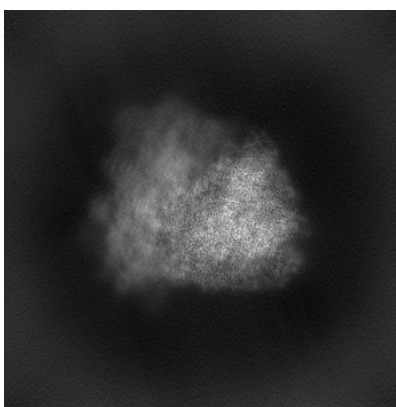


Z

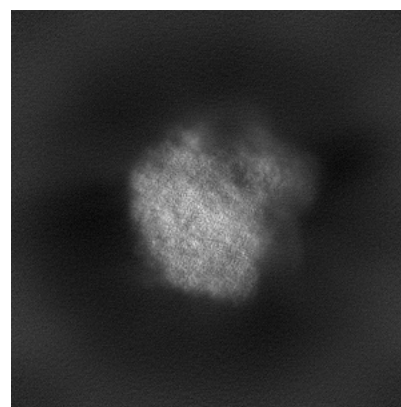
6.1.2 Raw map



X



Y

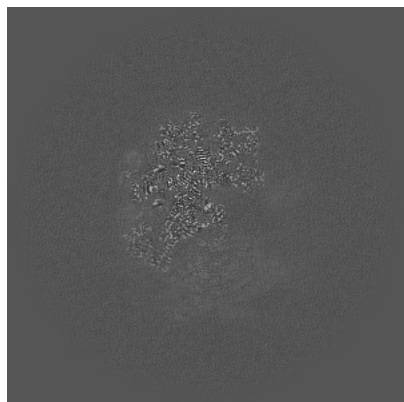


Z

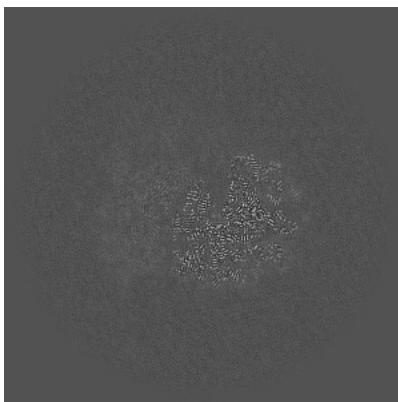
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

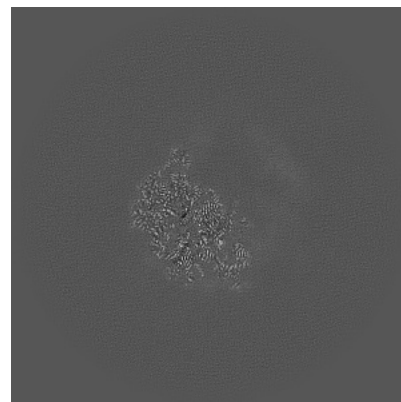
6.2.1 Primary map



X Index: 300

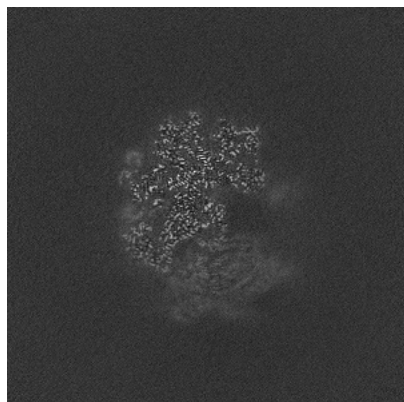


Y Index: 300

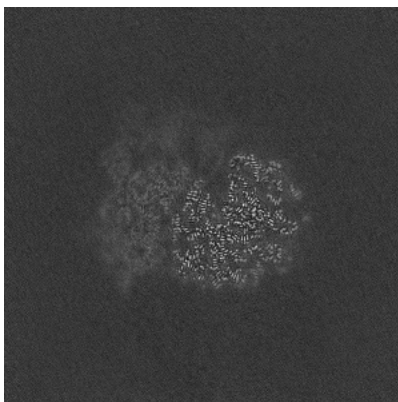


Z Index: 300

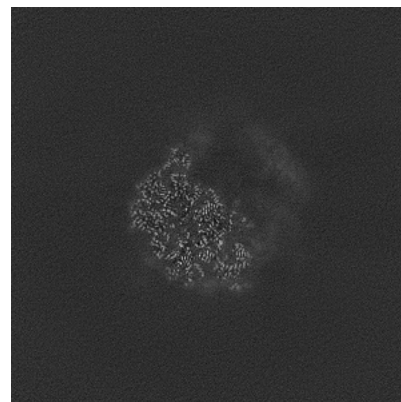
6.2.2 Raw map



X Index: 300



Y Index: 300

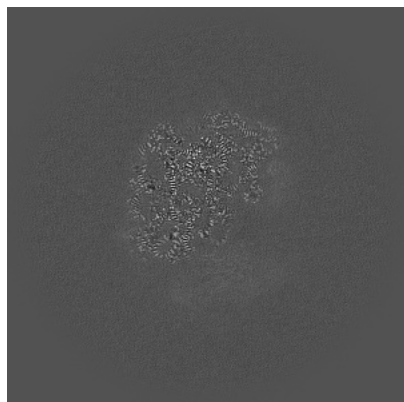


Z Index: 300

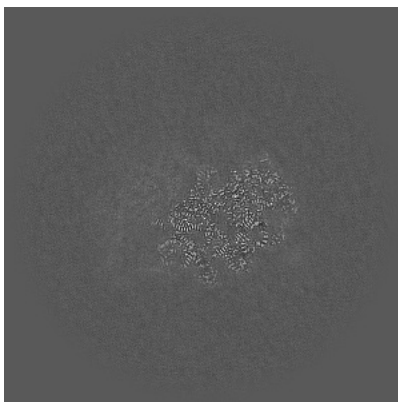
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

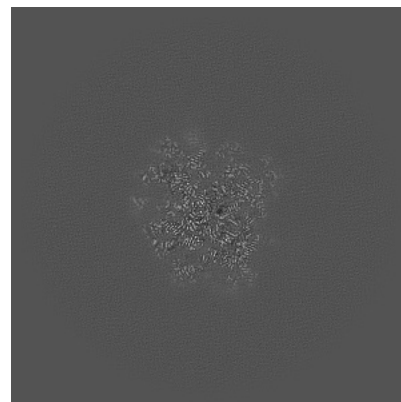
6.3.1 Primary map



X Index: 273

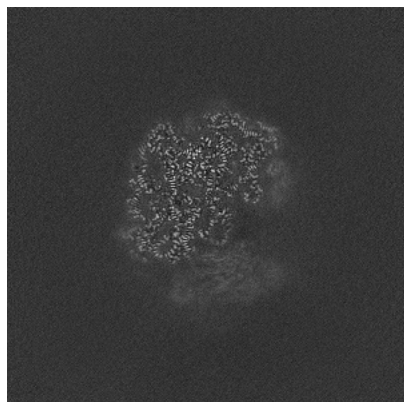


Y Index: 273

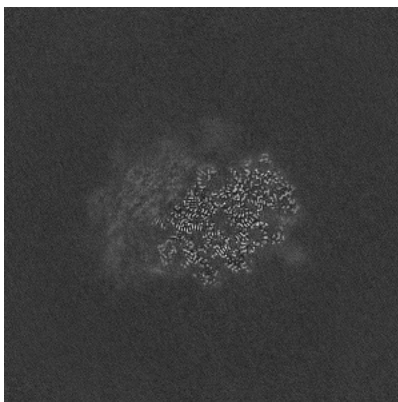


Z Index: 361

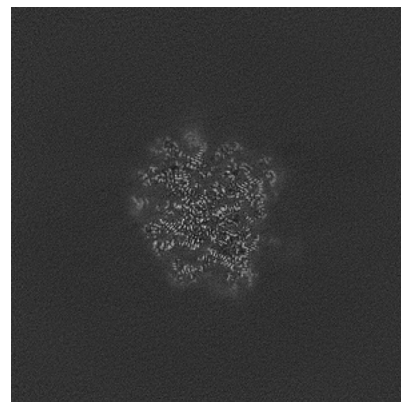
6.3.2 Raw map



X Index: 273



Y Index: 274

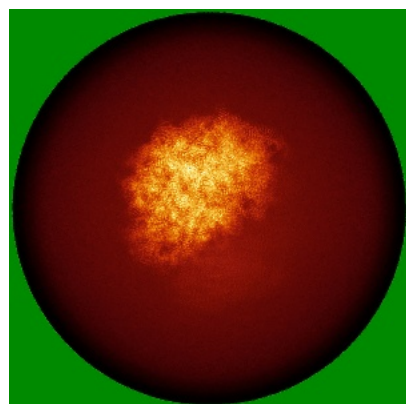


Z Index: 360

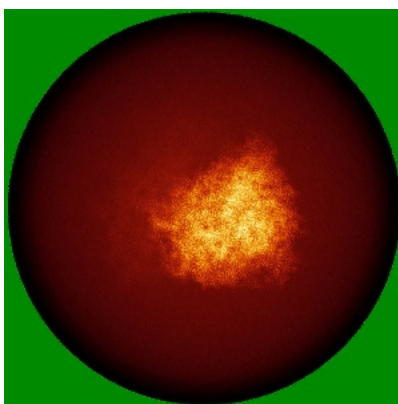
The images above show the largest variance slices of the map in three orthogonal directions.

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

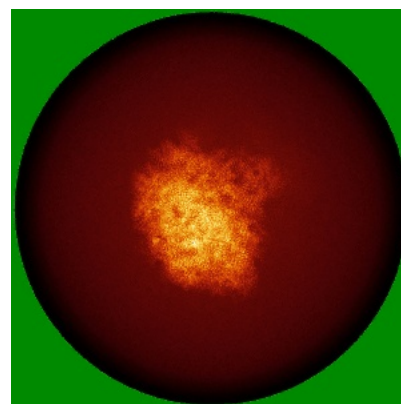
6.4.1 Primary map



X

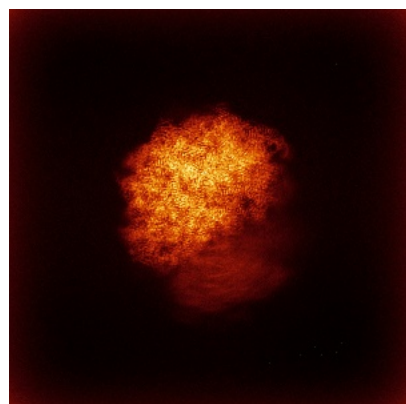


Y

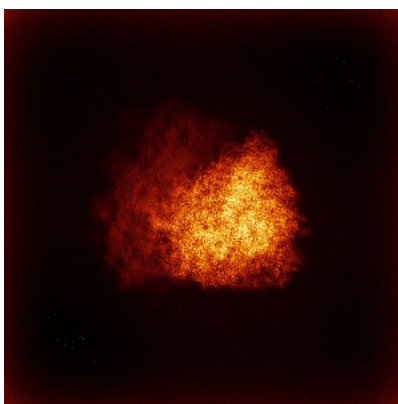


Z

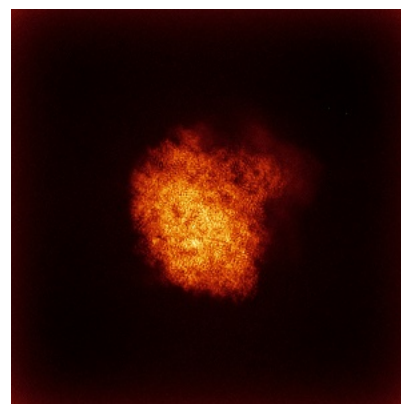
6.4.2 Raw map



X



Y

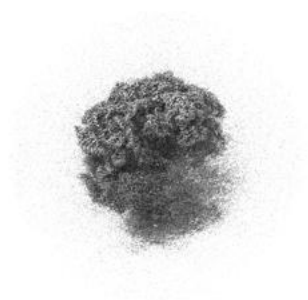


Z

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](#)

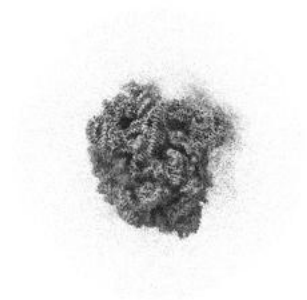
6.5.1 Primary map



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.

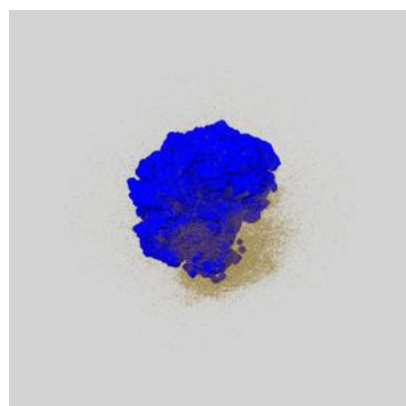
6.6 Mask visualisation [i](#)

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

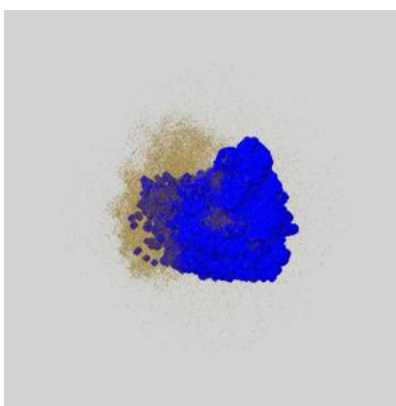
A mask typically either:

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

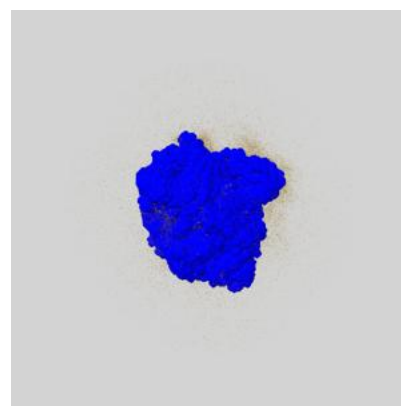
6.6.1 emd_17653_msk_1.map [i](#)



X



Y

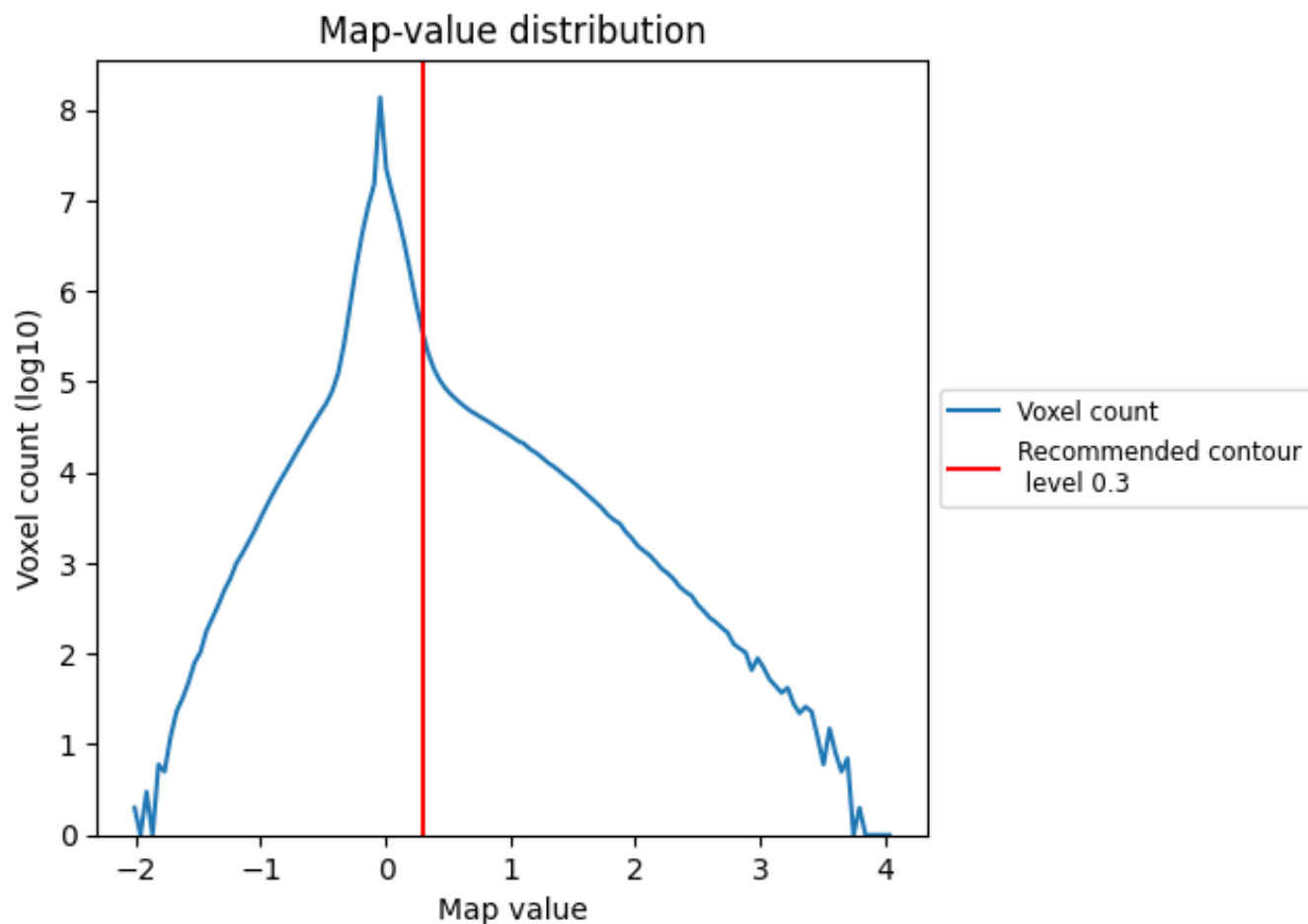


Z

7 Map analysis [i](#)

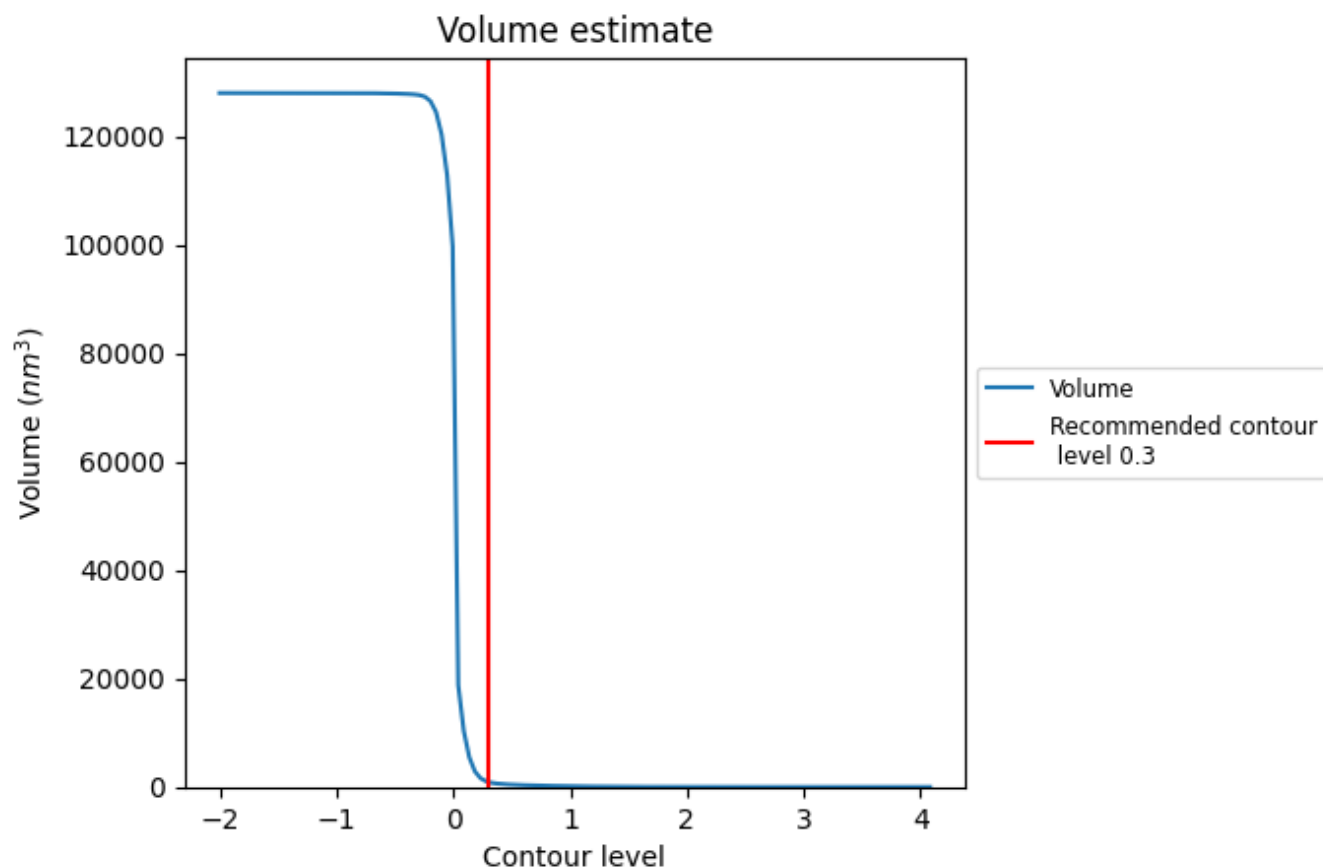
This section contains the results of statistical analysis of the map.

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.

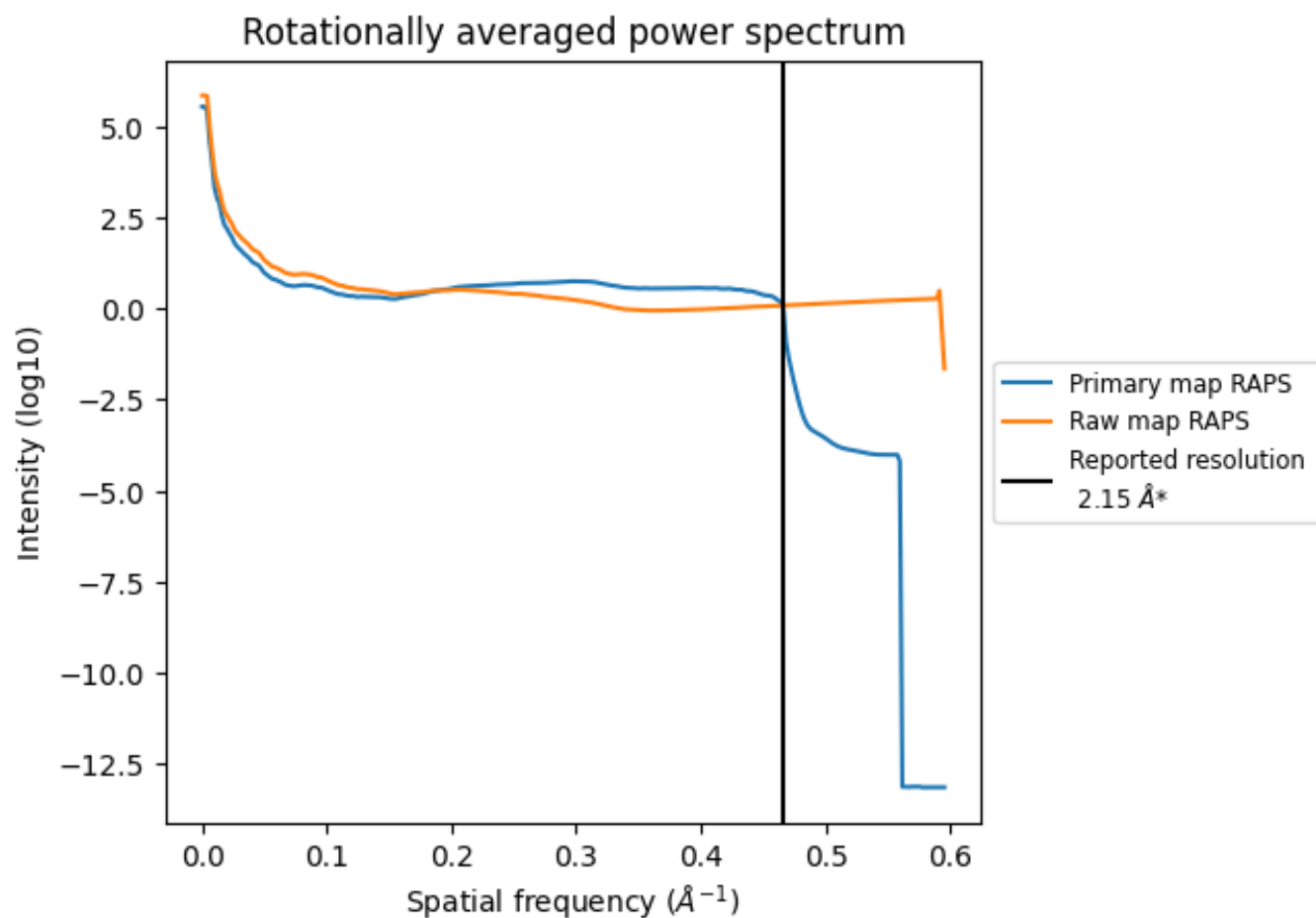
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 911 nm^3 ; this corresponds to an approximate mass of 823 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 ⓘ

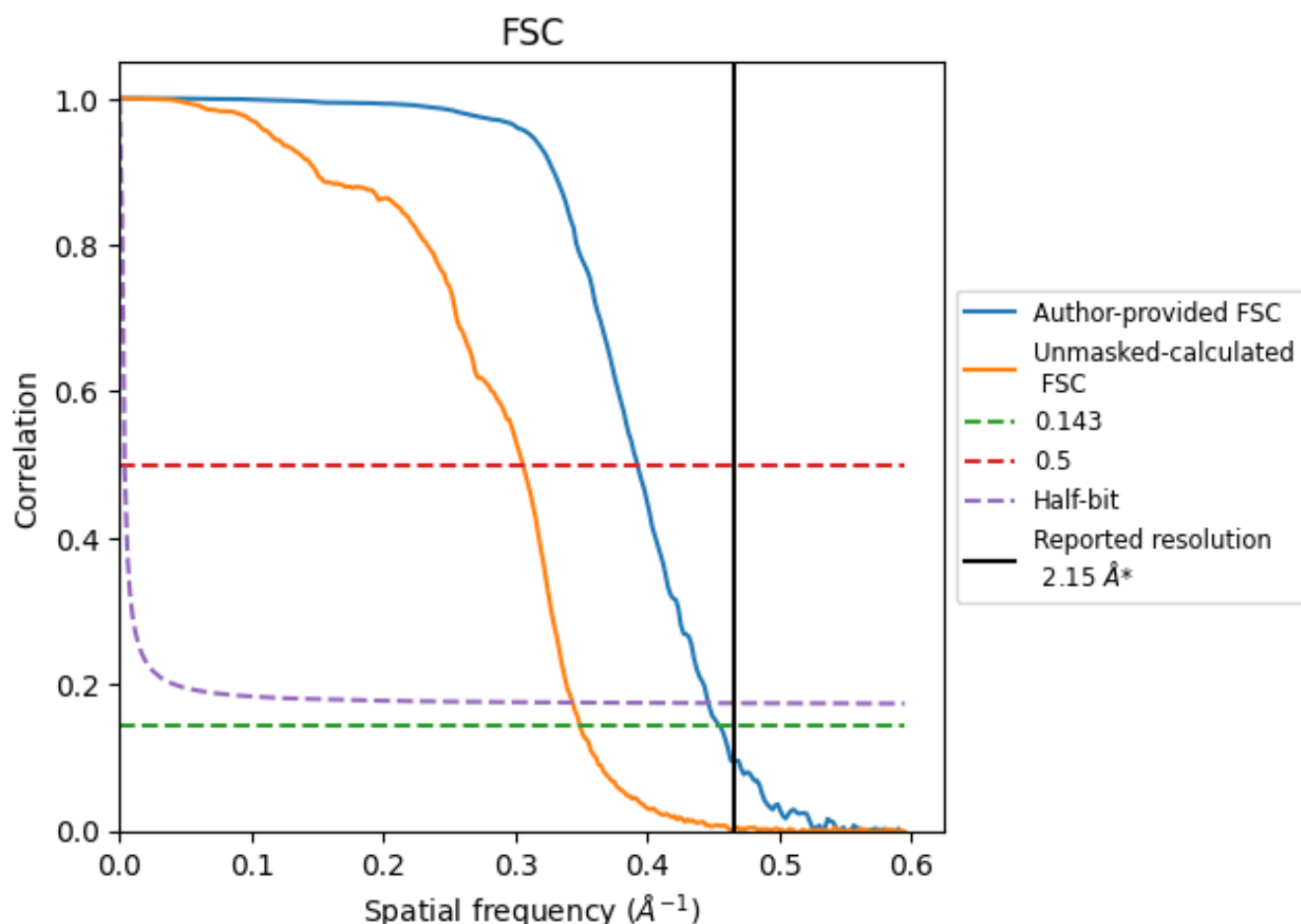


*Reported resolution corresponds to spatial frequency of 0.465 Å⁻¹

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 0.465 \AA^{-1}

8.2 Resolution estimates [i](#)

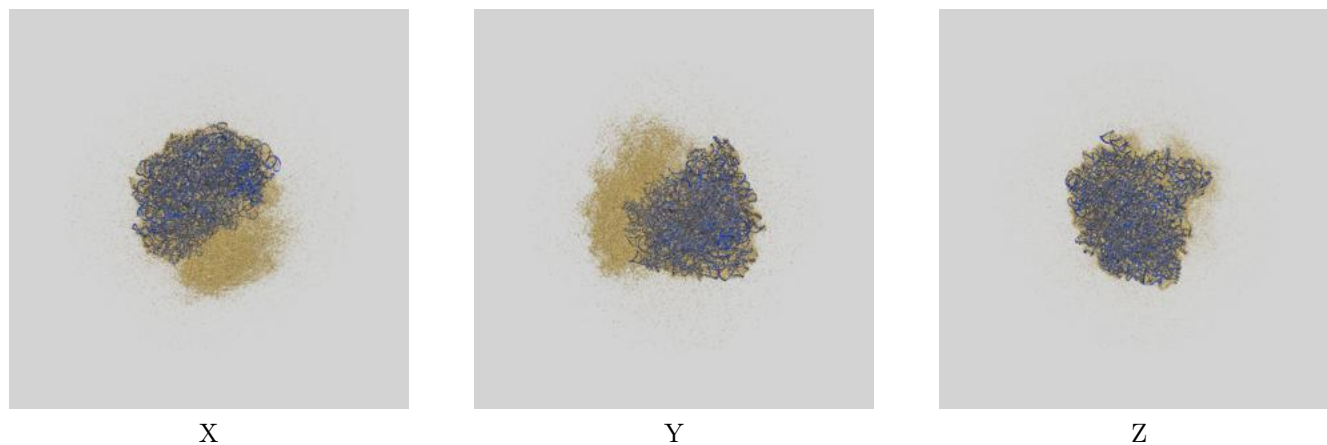
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.15	-	-
Author-provided FSC curve	2.20	2.55	2.24
Unmasked-calculated*	2.86	3.27	2.91

*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 2.86 differs from the reported value 2.15 by more than 10 %

9 Map-model fit [i](#)

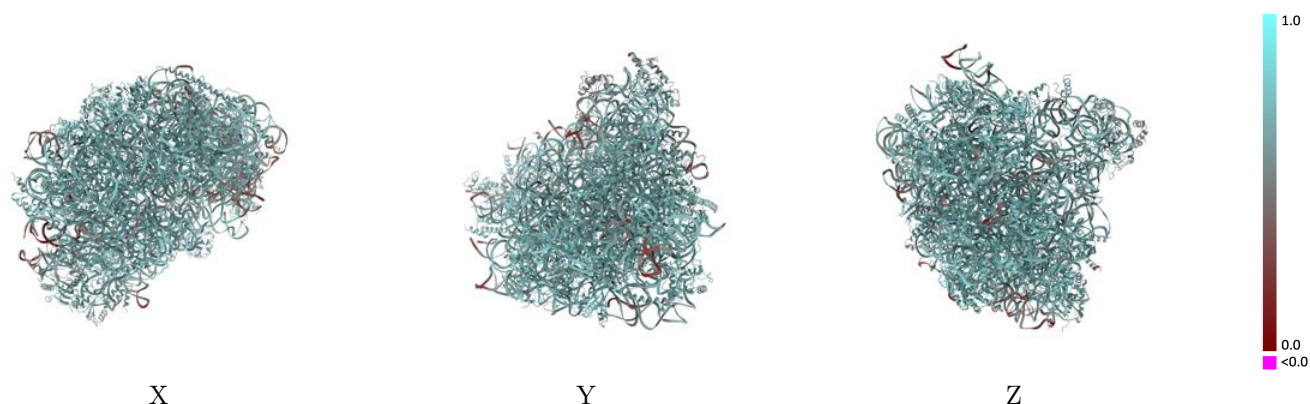
This section contains information regarding the fit between EMDB map EMD-17653 and PDB model 8PFR. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



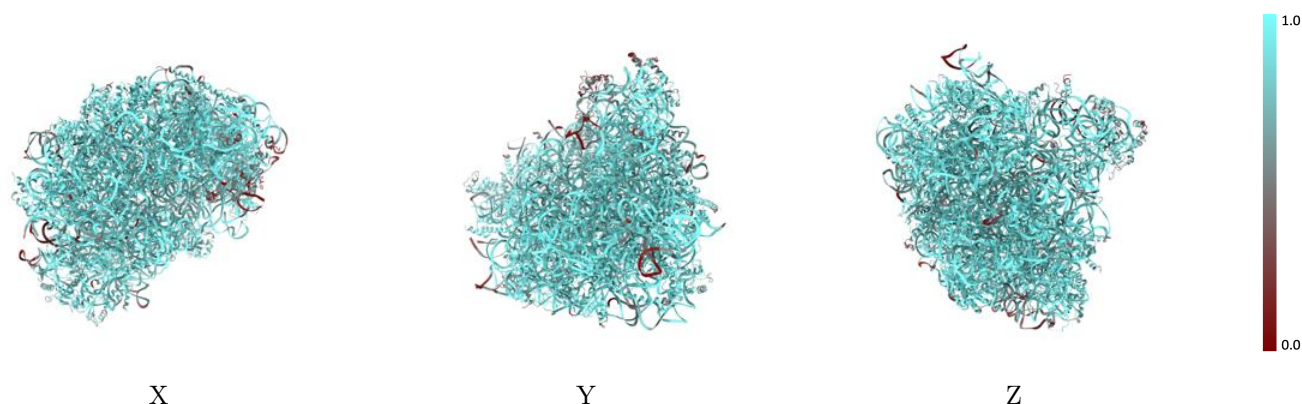
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



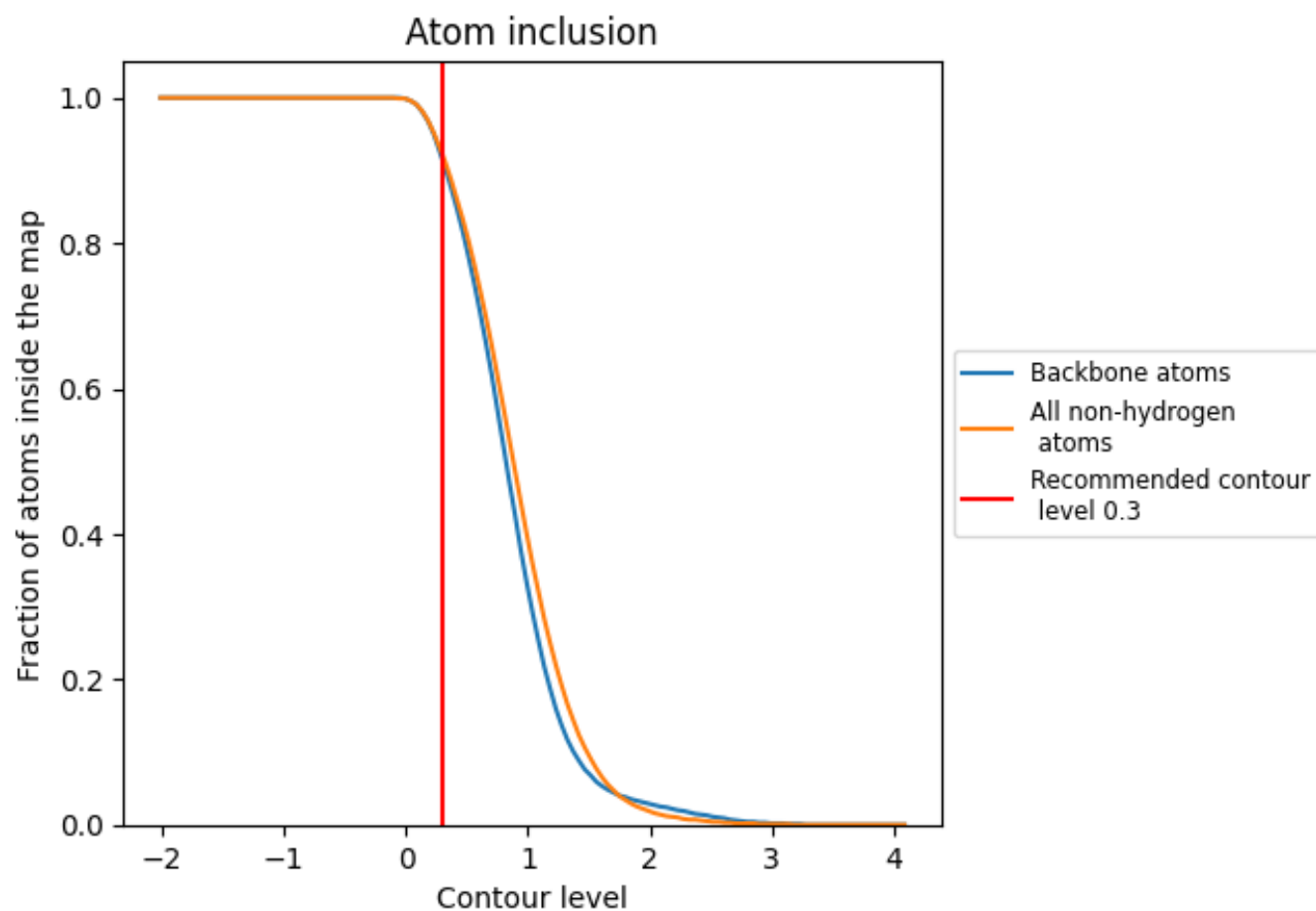
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 92% 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	 0.9220	 0.6750
A	 0.9310	 0.6700
JT	 0.9130	 0.6870
JU	 0.9240	 0.6810
JV	 0.9860	 0.7290
JW	 0.9520	 0.7100
LD	 0.9560	 0.6860
LE	 0.9600	 0.6690
LF	 0.9730	 0.7180
LG	 0.9510	 0.7070
LH	 0.9420	 0.7020
LI	 0.7870	 0.6060
LJ	 0.8620	 0.6520
LK	 0.9390	 0.7030
LL	 0.8930	 0.6620
LM	 0.8870	 0.6540
LN	 0.9040	 0.6830
LO	 0.5590	 0.5090
QO	 0.9550	 0.7180
QP	 0.9680	 0.7180
QQ	 0.9550	 0.7090
QS	 0.9480	 0.7020
QT	 0.8920	 0.6770
QU	 0.6380	 0.5750
QV	 0.9220	 0.6960
QW	 0.9150	 0.6950
QX	 0.9330	 0.6910
QY	 0.9380	 0.7030
QZ	 0.8300	 0.6310
RA	 0.9410	 0.7040
RB	 0.8940	 0.6480
RC	 0.8260	 0.6260
RD	 0.9490	 0.7070
RE	 0.9610	 0.7230
RF	 0.9710	 0.7200



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Chain	Atom inclusion	Q-score
RG	 0.9750	 0.7160
RH	 0.9160	 0.6910
RI	 0.8780	 0.6460
RJ	 0.9650	 0.7290
RM	 0.7480	 0.6030
RN	 0.9140	 0.6900
RO	 0.9360	 0.6920
RQ	 0.8770	 0.6620
RT	 0.9220	 0.6900