



wwPDB EM Validation Summary Report ⓘ

Jun 18, 2026 – 02:03 am BST

PDB ID : 9FHL / pdb_00009fhl
EMDB ID : EMD-50445
Title : High-resolution cryo-EM structure of *Saccharolobus solfataricus* 30S ribosomal subunit bound to mRNA and initiator tRNA
Authors : Bourgeois, G.; Coureux, P.D.; Mechulam, Y.; Schmitt, E.
Deposited on : 2024-05-27
Resolution : 2.50 Å(reported)

This is a wwPDB EM Validation Summary 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:

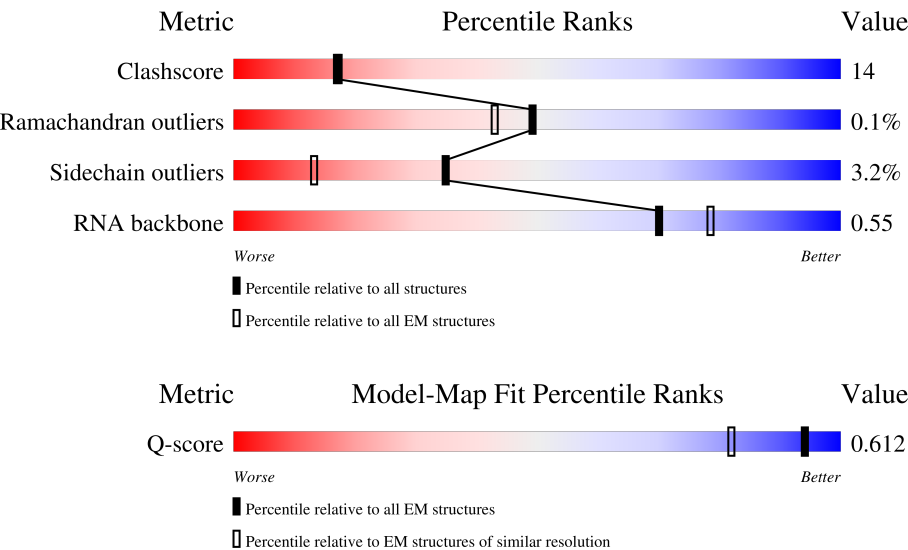
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal 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 i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.50 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	7115 (2.00 - 3.00)

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	1497	53%35%7%.
2	A	208	61%27%.11%
3	B	231	70%23%.7%

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Mol	Chain	Length	Quality of chain
4	C	65	
5	D	181	
6	E	239	
7	F	214	
8	G	214	
9	H	193	
10	I	133	
11	J	133	
12	K	137	
13	L	102	
14	M	132	
15	N	147	
16	O	165	
17	P	54	
18	Q	152	
19	R	114	
20	S	79	
21	T	140	
22	U	158	
23	V	120	
24	W	66	
25	X	83	
26	Y	75	
27	Z	229	
28	3	127	

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Mol	Chain	Length	Quality of chain
29	a	72	
30	c	110	
31	d	72	
32	e	52	
33	5	15	
34	s	15	
35	4	77	

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
37	SPM	2	1570	-	-	X	-
37	SPM	2	1581	-	-	X	-
37	SPM	2	1584	-	-	X	-
37	SPM	2	1589	-	-	X	-
37	SPM	2	1594	-	-	X	-
37	SPM	F	303	-	-	X	-

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 64047 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 rRNA 16S Sso.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1430	Total	C	N	O	P	0	0
			30761	13720	5686	9925	1430		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	843	4AC	C	modified residue	GB AE006641.1
2	930	C4J	U	modified residue	GB AE006641.1
2	1466	4AC	C	modified residue	GB AE006641.1
2	1467	4AC	C	modified residue	GB AE006641.1
2	1477	4AC	C	modified residue	GB AE006641.1
2	1478	4AC	C	modified residue	GB AE006641.1
2	1496	C	A	conflict	GB AE006641.1

- Molecule 2 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	186	Total	C	N	O	S	0	0
			1515	974	261	278	2		

- Molecule 3 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	215	Total	C	N	O	S	0	0
			1698	1092	291	312	3		

- Molecule 4 is a protein called Small zinc finger protein HVO-2753-like zinc-binding pocket domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	58	Total	C	N	O	S	0	0
			455	282	84	81	8		

- Molecule 5 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	166	Total	C	N	O	S	0	0
			1354	864	249	240	1		

- Molecule 6 is a protein called Small ribosomal subunit protein eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	238	Total	C	N	O	S	0	0
			1930	1238	342	344	6		

- Molecule 7 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	210	Total	C	N	O	S	0	0
			1625	1041	275	303	6		

- Molecule 8 is a protein called Small ribosomal subunit protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	213	Total	C	N	O	S	0	0
			1661	1052	292	315	2		

- Molecule 9 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	192	Total	C	N	O	S	0	0
			1543	983	283	274	3		

- Molecule 10 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	132	Total	C	N	O	S	0	0
			1050	675	187	182	6		

- Molecule 11 is a protein called Small ribosomal subunit protein eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	127	Total	C	N	O		0	0
			982	617	186	179			

- Molecule 12 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	133	Total	C	N	O	S	0	0
			1068	675	201	185	7		

- Molecule 13 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	101	Total	C	N	O	S	0	0
			840	536	157	142	5		

- Molecule 14 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	127	Total	C	N	O	S	0	0
			944	587	184	170	3		

- Molecule 15 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	146	Total	C	N	O	S	0	0
			1140	723	220	193	4		

- Molecule 16 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	140	Total	C	N	O	S	0	0
			1124	708	210	202	4		

- Molecule 17 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	53	Total	C	N	O	S	0	0
			440	282	80	74	4		

- Molecule 18 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	145	Total	C	N	O	S	0	0
			1185	753	224	205	3		

- Molecule 19 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	113	Total	C	N	O	S	0	0
			901	570	166	161	4		

- Molecule 20 is a protein called Small ribosomal subunit protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	66	Total	C	N	O	S	0	0
			571	364	101	105	1		

- Molecule 21 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	128	Total	C	N	O	S	0	0
			1064	684	192	184	4		

- Molecule 22 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	154	Total	C	N	O	S	0	0
			1247	805	223	217	2		

- Molecule 23 is a protein called Small ribosomal subunit protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	107	Total	C	N	O	S	0	0
			836	524	154	156	2		

- Molecule 24 is a protein called Small ribosomal subunit protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	65	Total	C	N	O	S	0	0
			503	319	93	84	7		

- Molecule 25 is a protein called Small ribosomal subunit protein eS28.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	X	67	Total	C	N	O	0	0
			535	335	103	97		

- Molecule 26 is a protein called Small ribosomal subunit protein eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	49	Total	C	N	O	S	0	0
			395	252	73	65	5		

- Molecule 27 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	196	Total	C	N	O	S	0	0
			1561	1009	274	272	6		

- Molecule 28 is a protein called Large ribosomal subunit protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	3	117	Total	C	N	O	S	0	0
			893	567	149	175	2		

- Molecule 29 is a protein called aS34.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	a	71	Total	C	N	O	S	0	0
			562	361	98	96	7		

- Molecule 30 is a protein called Small ribosomal subunit protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	c	109	Total	C	N	O	S	0	0
			856	539	152	164	1		

- Molecule 31 is a protein called VapB-type antitoxin.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	d	70	Total	C	N	O	S	0	0
			570	370	92	105	3		

- Molecule 32 is a protein called LSU ribosomal protein S30E (Rps30E).

Mol	Chain	Residues	Atoms				AltConf	Trace
32	e	43	Total	C	N	O	0	0
			354	220	74	60		

- Molecule 33 is a RNA chain called mRNA_Map.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	5	3	Total	C	N	O	P	1	0
			105	39	17	41	8		

- Molecule 34 is a RNA chain called mRNA_Map.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	s	10	Total	C	N	O	P	0	0
			220	98	44	68	10		

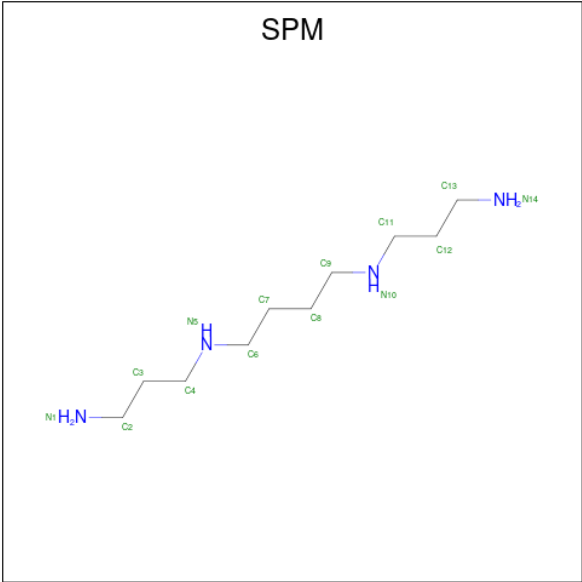
- Molecule 35 is a RNA chain called Initiator tRNA Met.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	4	17	Total	C	N	O	P	0	0
			361	162	64	118	17		

- Molecule 36 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
36	2	56	Total	Mg	0
			56	56	
36	F	1	Total	Mg	0
			1	1	
36	R	1	Total	Mg	0
			1	1	
36	5	1	Total	Mg	0
			1	1	

- Molecule 37 is SPERMINE (CCD ID: SPM) (formula: C₁₀H₂₆N₄).



Mol	Chain	Residues	Atoms			AltConf
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	

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Mol	Chain	Residues	Atoms			AltConf
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	

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Mol	Chain	Residues	Atoms			AltConf
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	F	1	Total	C	N	0
			14	10	4	

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

Mol	Chain	Residues	Atoms		AltConf
38	C	2	Total	Zn	0
			2	2	
38	F	1	Total	Zn	0
			1	1	
38	P	1	Total	Zn	0
			1	1	
38	R	1	Total	Zn	0
			1	1	
38	W	1	Total	Zn	0
			1	1	
38	a	2	Total	Zn	0
			2	2	

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		AltConf
39	2	434	Total	O	0
			434	434	
39	B	1	Total	O	0
			1	1	

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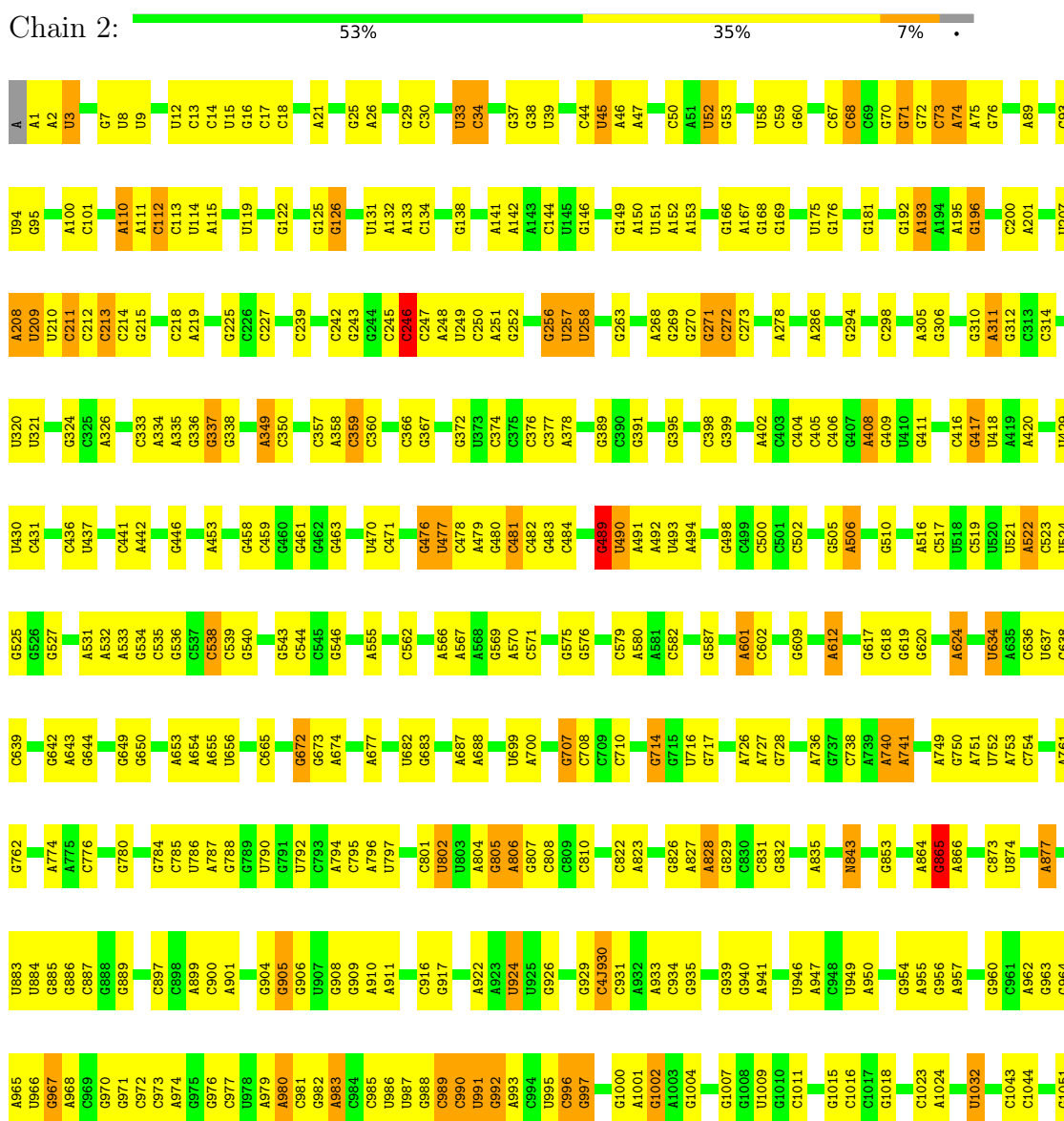
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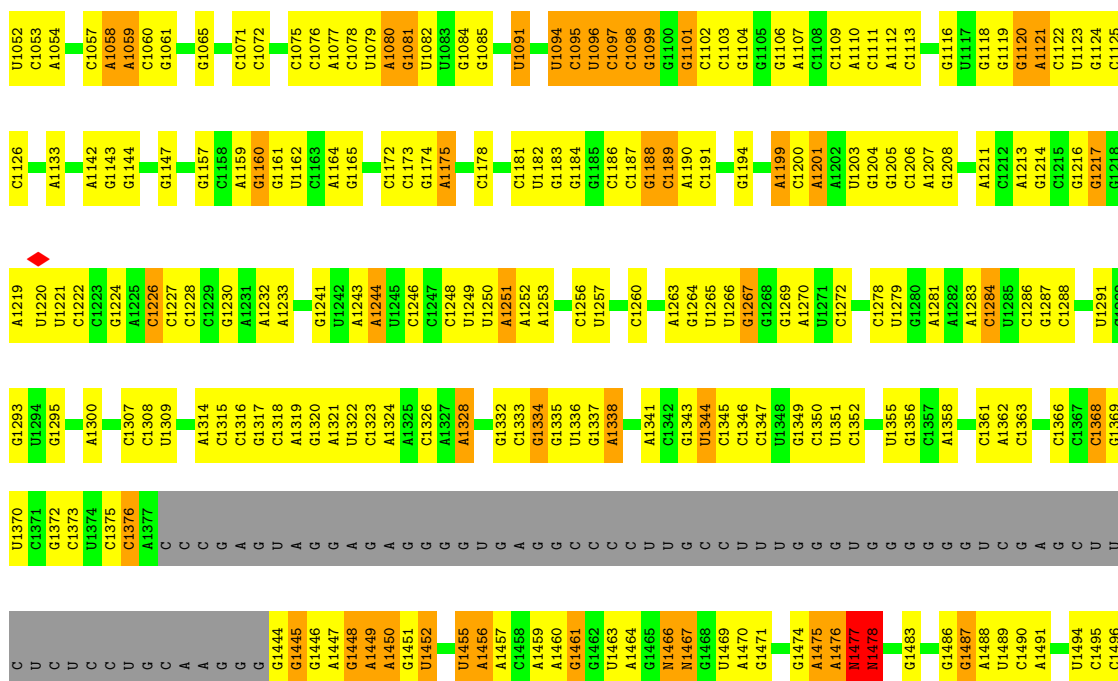
Mol	Chain	Residues	Atoms		AltConf
39	C	4	Total 4	O 4	0
39	D	8	Total 8	O 8	0
39	E	7	Total 7	O 7	0
39	F	15	Total 15	O 15	0
39	H	2	Total 2	O 2	0
39	I	5	Total 5	O 5	0
39	J	2	Total 2	O 2	0
39	K	3	Total 3	O 3	0
39	L	2	Total 2	O 2	0
39	Q	7	Total 7	O 7	0
39	R	4	Total 4	O 4	0
39	U	1	Total 1	O 1	0
39	V	1	Total 1	O 1	0
39	W	3	Total 3	O 3	0
39	5	12	Total 12	O 12	0
39	4	4	Total 4	O 4	0

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.

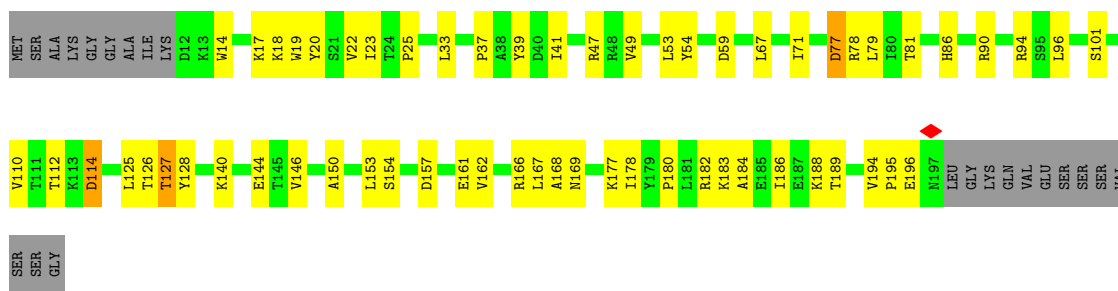
• Molecule 1: rRNA 16S Sso





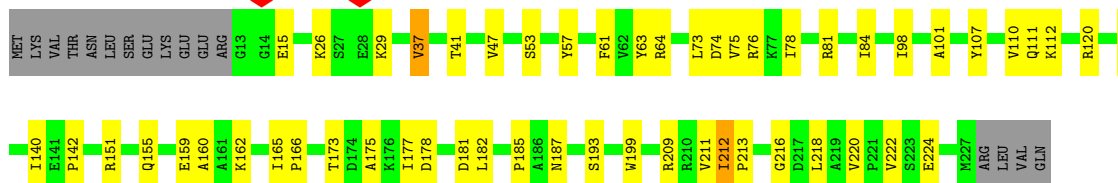
• Molecule 2: Small ribosomal subunit protein eS1

Chain A: 61% 27% 11%



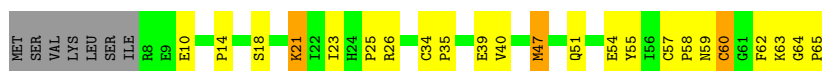
• Molecule 3: Small ribosomal subunit protein uS2

Chain B: 70% 23% 7%



• Molecule 4: Small zinc finger protein HVO-2753-like zinc-binding pocket domain-containing protein

Chain C: 54% 31% 5% 11%



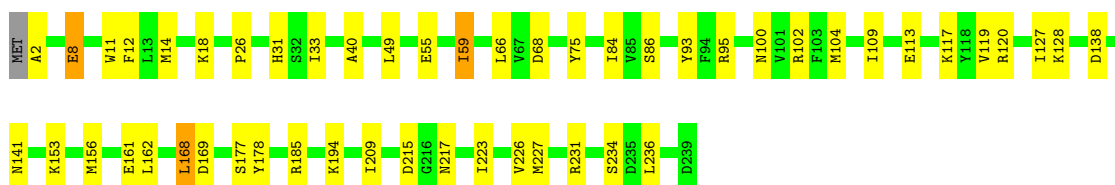
- Molecule 5: Small ribosomal subunit protein uS4

Chain D: 75% 15% 8%



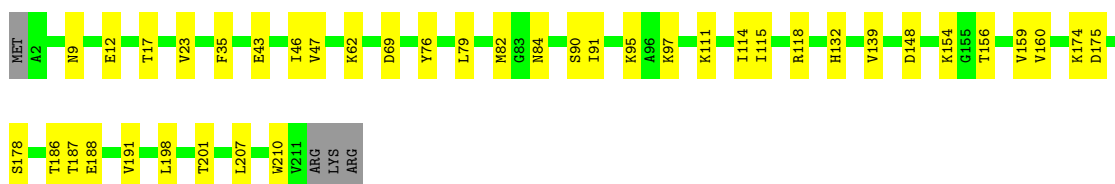
- Molecule 6: Small ribosomal subunit protein eS4

Chain E: 78% 20%



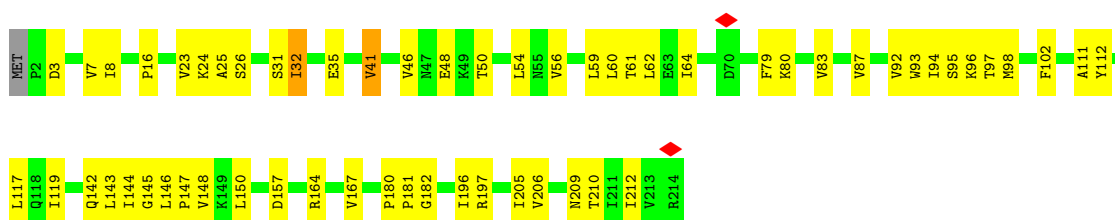
- Molecule 7: Small ribosomal subunit protein uS5

Chain F: 79% 19%



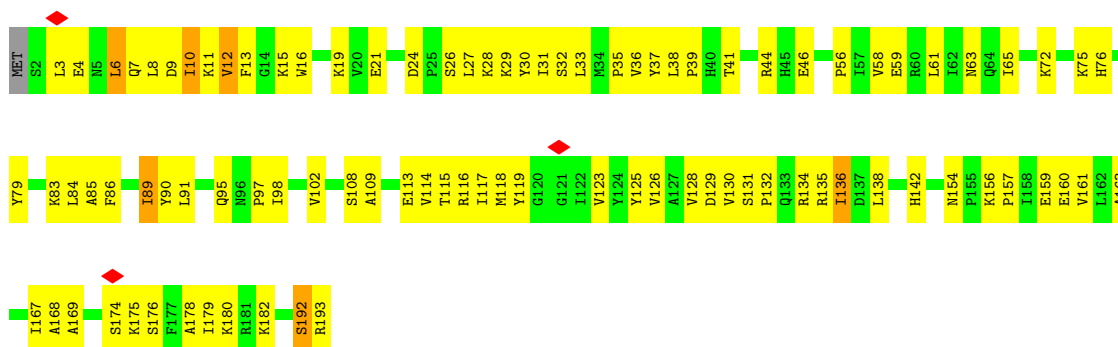
- Molecule 8: Small ribosomal subunit protein eS6

Chain G: 72% 27%



- Molecule 9: Small ribosomal subunit protein uS7

Chain H: 51% 45%



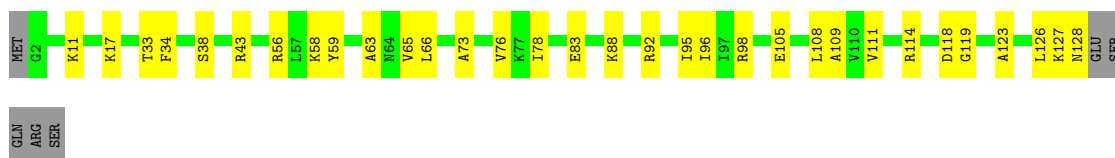
- Molecule 10: Small ribosomal subunit protein uS8

Chain I: 83% 16% .



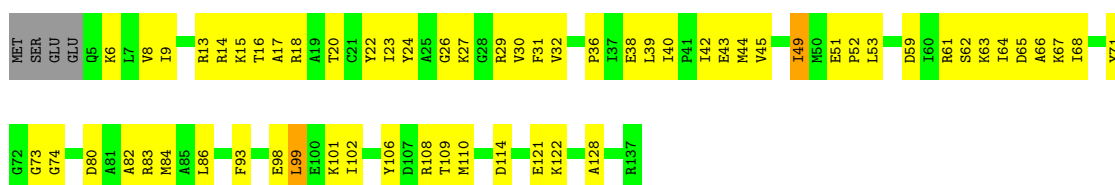
- Molecule 11: Small ribosomal subunit protein eS8

Chain J: 71% 24% 5%



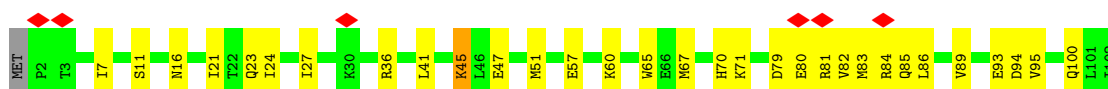
- Molecule 12: Small ribosomal subunit protein uS9

Chain K: 53% 43% . .



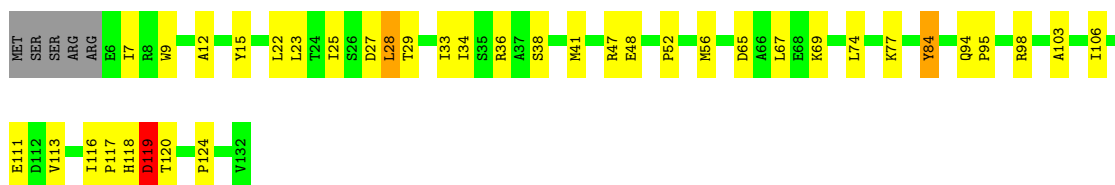
- Molecule 13: Small ribosomal subunit protein uS10

Chain L: 6% 69% 29% . .



- Molecule 14: Small ribosomal subunit protein uS11

Chain M: 67% 27% . . .



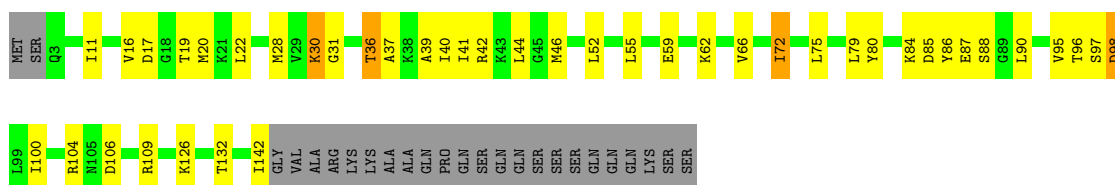
- Molecule 15: Small ribosomal subunit protein uS12

Chain N: 79% 20% ..



- Molecule 16: Small ribosomal subunit protein uS13

Chain O: 59% 24% 15%



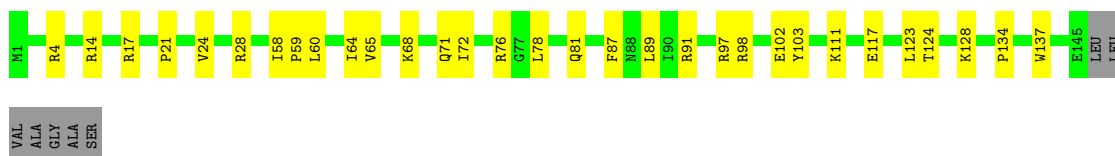
- Molecule 17: Small ribosomal subunit protein uS14

Chain P: 59% 37% ..



- Molecule 18: Small ribosomal subunit protein uS15

Chain Q: 75% 20% 5%

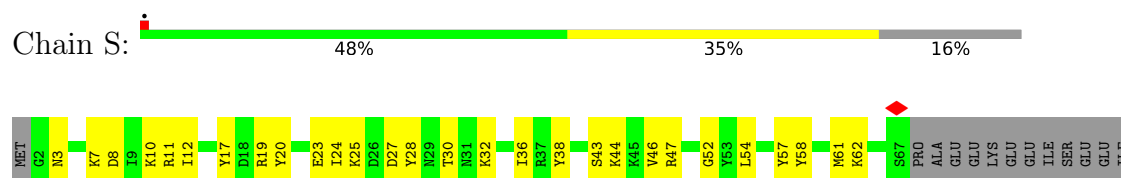


- Molecule 19: Small ribosomal subunit protein uS17

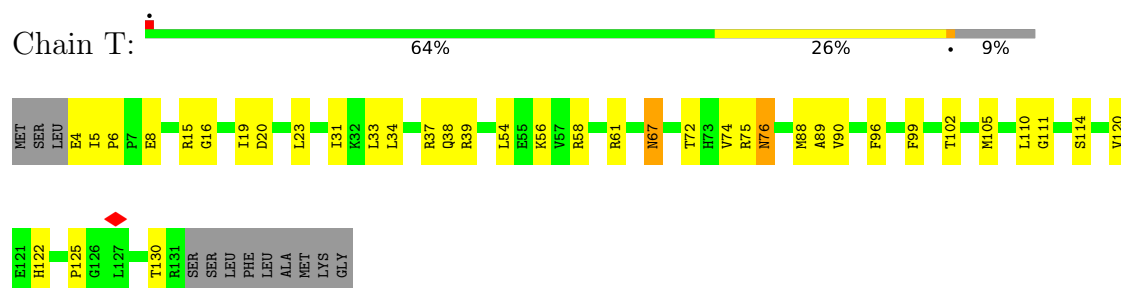
Chain R: 83% 16%



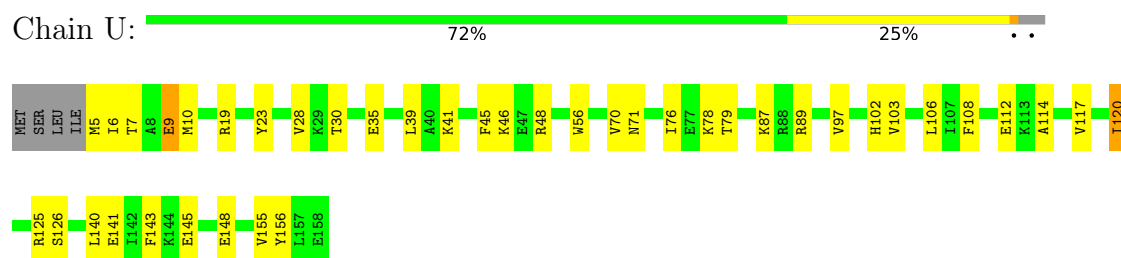
- Molecule 20: Small ribosomal subunit protein eS17



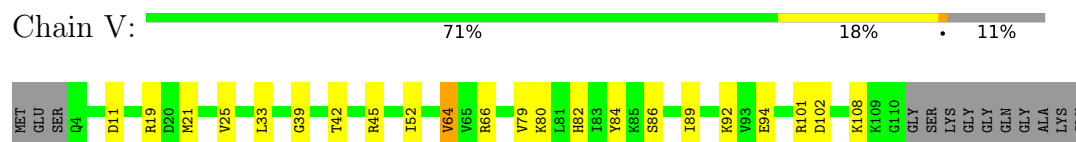
- Molecule 21: Small ribosomal subunit protein uS19



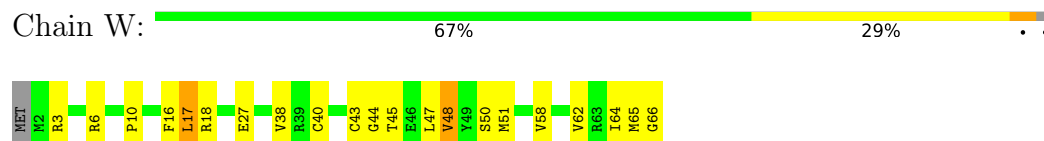
- Molecule 22: Small ribosomal subunit protein eS19



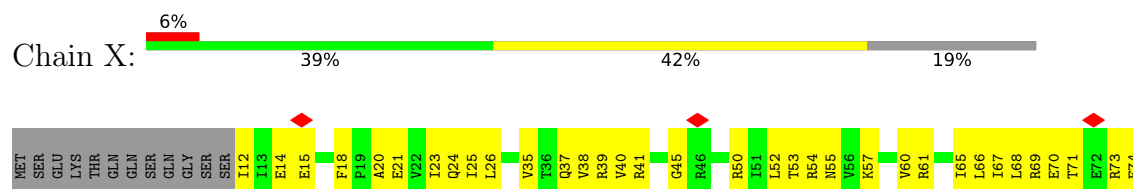
- Molecule 23: Small ribosomal subunit protein eS24

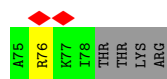


- Molecule 24: Small ribosomal subunit protein eS27

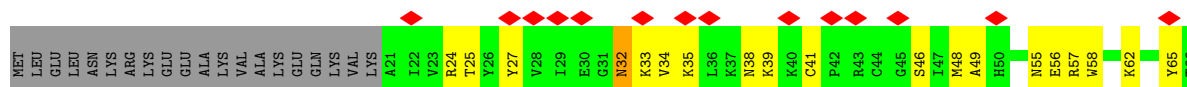


- Molecule 25: Small ribosomal subunit protein eS28

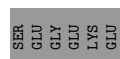
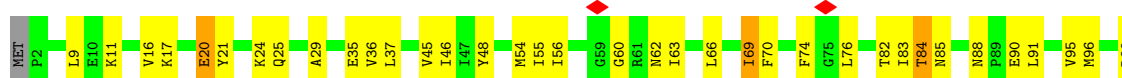




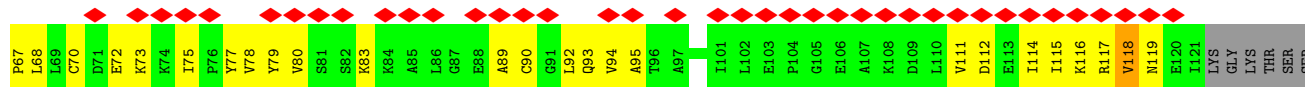
- Molecule 26: Small ribosomal subunit protein eS31



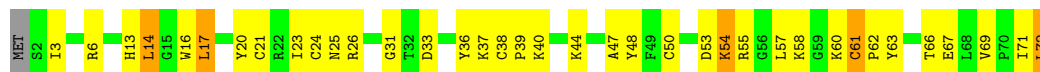
- Molecule 27: Small ribosomal subunit protein uS3



- Molecule 28: Large ribosomal subunit protein eL8



- Molecule 29: aS34



- Molecule 30: Small ribosomal subunit protein eS25



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	766000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.177	Depositor
Minimum map value	-0.086	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.007	Depositor
Map size (Å)	365.292, 365.292, 365.292	wwPDB
Map dimensions	438, 438, 438	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.834, 0.834, 0.834	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, 4AC, OMU, 5MC, OMC, MA6, OMG, SPM, ZN, 6MZ, C4J, A2M, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	2	0.36	2/33594 (0.0%)	0.38	4/52408 (0.0%)
2	A	0.25	0/1543	0.42	0/2077
3	B	0.22	0/1731	0.47	1/2349 (0.0%)
4	C	0.27	0/466	0.63	2/625 (0.3%)
5	D	0.28	0/1380	0.39	0/1859
6	E	0.31	0/1965	0.48	0/2644
7	F	0.36	0/1654	0.55	3/2240 (0.1%)
8	G	0.20	0/1684	0.42	0/2265
9	H	0.21	0/1571	0.50	2/2116 (0.1%)
10	I	0.32	0/1070	0.41	0/1444
11	J	0.29	0/994	0.45	0/1337
12	K	0.24	0/1084	0.47	0/1450
13	L	0.22	0/856	0.43	1/1154 (0.1%)
14	M	0.29	0/960	0.67	2/1294 (0.2%)
15	N	0.32	0/1155	0.50	1/1540 (0.1%)
16	O	0.21	0/1142	0.42	0/1532
17	P	0.26	0/451	0.59	2/600 (0.3%)
18	Q	0.29	0/1206	0.38	0/1618
19	R	0.32	0/918	0.44	0/1236
20	S	0.22	0/578	0.40	0/770
21	T	0.20	0/1087	0.37	0/1456
22	U	0.22	0/1270	0.40	0/1710
23	V	0.23	0/843	0.44	0/1124
24	W	0.27	0/511	0.42	0/684
25	X	0.20	0/538	0.52	0/722
26	Y	0.24	0/404	0.67	0/540
27	Z	0.24	0/1584	0.42	0/2124
28	3	0.24	0/902	0.57	0/1216
29	a	0.79	0/574	0.97	2/770 (0.3%)
30	c	0.36	1/861 (0.1%)	0.64	3/1143 (0.3%)
31	d	0.24	0/581	0.59	0/786
32	e	0.28	0/360	0.62	1/477 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	5	0.34	0/47	0.51	0/71
34	s	0.38	0/247	0.84	2/384 (0.5%)
35	4	0.24	0/379	0.30	0/588
All	All	0.33	3/66190 (0.0%)	0.44	26/96353 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	c	9	ILE	CA-C	-6.91	1.44	1.52
1	2	1450	A	O3'-P	-6.47	1.51	1.61
1	2	1373	C	O3'-P	5.16	1.68	1.61

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1450	A	O3'-P-O5'	9.53	118.29	104.00
29	a	24	CYS	N-CA-C	7.89	119.96	111.36
1	2	489	G	C2'-C3'-O3'	7.50	120.75	109.50
30	c	9	ILE	N-CA-C	7.02	117.16	110.42
14	M	118	HIS	CA-C-N	6.62	134.18	121.54

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	30761	0	15566	542	0
2	A	1515	0	1565	54	0
3	B	1698	0	1753	37	0
4	C	455	0	438	19	0
5	D	1354	0	1419	24	0
6	E	1930	0	2013	37	0
7	F	1625	0	1689	33	0
8	G	1661	0	1737	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	H	1543	0	1611	156	0
10	I	1050	0	1100	15	0
11	J	982	0	1046	21	0
12	K	1068	0	1125	65	0
13	L	840	0	893	32	0
14	M	944	0	978	31	0
15	N	1140	0	1244	26	0
16	O	1124	0	1162	42	0
17	P	440	0	436	29	0
18	Q	1185	0	1260	22	0
19	R	901	0	935	15	0
20	S	571	0	598	26	0
21	T	1064	0	1107	34	0
22	U	1247	0	1329	47	0
23	V	836	0	894	18	0
24	W	503	0	531	16	0
25	X	535	0	572	33	0
26	Y	395	0	405	37	0
27	Z	1561	0	1667	53	0
28	3	893	0	940	66	0
29	a	562	0	574	49	0
30	c	856	0	941	69	0
31	d	570	0	590	86	0
32	e	354	0	386	11	0
33	5	105	0	44	0	0
34	s	220	0	109	8	0
35	4	361	0	187	3	0
36	2	56	0	0	1	0
36	5	1	0	0	0	0
36	F	1	0	0	0	0
36	R	1	0	0	0	0
37	2	602	0	1117	152	0
37	F	14	0	26	11	0
38	C	2	0	0	0	0
38	F	1	0	0	0	0
38	P	1	0	0	0	0
38	R	1	0	0	0	0
38	W	1	0	0	0	0
38	a	2	0	0	0	0
39	2	434	0	0	21	0
39	4	4	0	0	0	0
39	5	12	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	B	1	0	0	0	0
39	C	4	0	0	1	0
39	D	8	0	0	1	0
39	E	7	0	0	1	0
39	F	15	0	0	0	0
39	H	2	0	0	0	0
39	I	5	0	0	0	0
39	J	2	0	0	0	0
39	K	3	0	0	0	0
39	L	2	0	0	1	0
39	Q	7	0	0	0	0
39	R	4	0	0	0	0
39	U	1	0	0	0	0
39	V	1	0	0	0	0
39	W	3	0	0	1	0
All	All	64047	0	49987	1553	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 14.

The worst 5 of 1553 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:H:19:LYS:NZ	31:d:71:LEU:CD1	1.87	1.34
1:2:7:G:OP1	37:2:1586:SPM:H131	1.40	1.20
31:d:56:VAL:HG22	31:d:57:PRO:CD	1.69	1.20
9:H:10:ILE:HG23	9:H:37:TYR:CD1	1.79	1.18
1:2:904:G:OP2	37:2:1583:SPM:N1	1.79	1.15

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	A	184/208 (88%)	181 (98%)	3 (2%)	0	100	100
3	B	213/231 (92%)	209 (98%)	4 (2%)	0	100	100
4	C	56/65 (86%)	55 (98%)	1 (2%)	0	100	100
5	D	164/181 (91%)	162 (99%)	2 (1%)	0	100	100
6	E	236/239 (99%)	229 (97%)	7 (3%)	0	100	100
7	F	208/214 (97%)	201 (97%)	7 (3%)	0	100	100
8	G	211/214 (99%)	201 (95%)	10 (5%)	0	100	100
9	H	190/193 (98%)	181 (95%)	9 (5%)	0	100	100
10	I	130/133 (98%)	128 (98%)	2 (2%)	0	100	100
11	J	125/133 (94%)	116 (93%)	9 (7%)	0	100	100
12	K	131/137 (96%)	125 (95%)	6 (5%)	0	100	100
13	L	99/102 (97%)	95 (96%)	4 (4%)	0	100	100
14	M	125/132 (95%)	118 (94%)	6 (5%)	1 (1%)	16	31
15	N	144/147 (98%)	138 (96%)	5 (4%)	1 (1%)	18	34
16	O	138/165 (84%)	130 (94%)	8 (6%)	0	100	100
17	P	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
18	Q	143/152 (94%)	142 (99%)	1 (1%)	0	100	100
19	R	111/114 (97%)	108 (97%)	3 (3%)	0	100	100
20	S	64/79 (81%)	62 (97%)	2 (3%)	0	100	100
21	T	126/140 (90%)	119 (94%)	7 (6%)	0	100	100
22	U	152/158 (96%)	147 (97%)	5 (3%)	0	100	100
23	V	105/120 (88%)	102 (97%)	3 (3%)	0	100	100
24	W	63/66 (96%)	57 (90%)	6 (10%)	0	100	100
25	X	65/83 (78%)	57 (88%)	8 (12%)	0	100	100
26	Y	47/75 (63%)	40 (85%)	7 (15%)	0	100	100
27	Z	194/229 (85%)	189 (97%)	5 (3%)	0	100	100
28	3	115/127 (91%)	103 (90%)	12 (10%)	0	100	100
29	a	69/72 (96%)	69 (100%)	0	0	100	100
30	c	107/110 (97%)	99 (92%)	8 (8%)	0	100	100
31	d	68/72 (94%)	64 (94%)	4 (6%)	0	100	100
32	e	41/52 (79%)	40 (98%)	1 (2%)	0	100	100
All	All	3875/4197 (92%)	3717 (96%)	156 (4%)	2 (0%)	49	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	N	64	GLN
14	M	119	ASP

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	A	168/184 (91%)	162 (96%)	6 (4%)	31	58
3	B	182/198 (92%)	179 (98%)	3 (2%)	55	79
4	C	51/58 (88%)	47 (92%)	4 (8%)	11	24
5	D	147/158 (93%)	145 (99%)	2 (1%)	59	81
6	E	214/215 (100%)	211 (99%)	3 (1%)	59	81
7	F	180/184 (98%)	179 (99%)	1 (1%)	78	91
8	G	186/187 (100%)	181 (97%)	5 (3%)	39	67
9	H	166/167 (99%)	159 (96%)	7 (4%)	26	52
10	I	113/114 (99%)	112 (99%)	1 (1%)	70	87
11	J	104/110 (94%)	103 (99%)	1 (1%)	68	86
12	K	109/113 (96%)	106 (97%)	3 (3%)	38	66
13	L	93/94 (99%)	92 (99%)	1 (1%)	65	84
14	M	93/98 (95%)	89 (96%)	4 (4%)	26	51
15	N	122/123 (99%)	119 (98%)	3 (2%)	42	69
16	O	121/142 (85%)	116 (96%)	5 (4%)	27	53
17	P	45/46 (98%)	45 (100%)	0	100	100
18	Q	125/129 (97%)	125 (100%)	0	100	100
19	R	101/102 (99%)	100 (99%)	1 (1%)	68	86
20	S	63/75 (84%)	62 (98%)	1 (2%)	55	79
21	T	116/126 (92%)	111 (96%)	5 (4%)	26	51
22	U	134/138 (97%)	131 (98%)	3 (2%)	45	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	V	92/99 (93%)	90 (98%)	2 (2%)	45	73
24	W	57/58 (98%)	54 (95%)	3 (5%)	20	42
25	X	58/73 (80%)	57 (98%)	1 (2%)	53	78
26	Y	43/65 (66%)	42 (98%)	1 (2%)	44	72
27	Z	163/195 (84%)	159 (98%)	4 (2%)	42	69
28	3	97/105 (92%)	96 (99%)	1 (1%)	68	86
29	a	61/62 (98%)	51 (84%)	10 (16%)	2	4
30	c	95/96 (99%)	89 (94%)	6 (6%)	16	34
31	d	63/65 (97%)	44 (70%)	19 (30%)	0	0
32	e	40/46 (87%)	38 (95%)	2 (5%)	22	44
All	All	3402/3625 (94%)	3294 (97%)	108 (3%)	35	62

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	U	106	LEU
29	a	14	LEU
31	d	33	THR
23	V	64	VAL
26	Y	32	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
14	M	60	ASN
15	N	100	HIS
15	N	27	GLN
16	O	3	GLN
9	H	71	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1428/1497 (95%)	227 (15%)	7 (0%)
33	5	1/15 (6%)	0	0
34	s	9/15 (60%)	8 (88%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
35	4	16/77 (20%)	0	0
All	All	1454/1604 (90%)	235 (16%)	7 (0%)

5 of 235 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	3	U
1	2	14	C
1	2	33	U
1	2	34	C
1	2	45	U

5 of 7 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	804	A
1	2	1188	G
1	2	1477	4AC
1	2	1455	U
1	2	522	A

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

34 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	OMU	2	1344	1	19,22,23	1.24	3 (15%)	26,31,34	1.75	5 (19%)
1	OMU	2	15	1	19,22,23	1.41	3 (15%)	26,31,34	1.78	4 (15%)
1	OMG	2	1194	1	23,26,27	1.22	3 (13%)	33,38,41	2.04	7 (21%)
1	OMC	2	481	1	19,22,23	1.10	2 (10%)	26,31,34	1.84	6 (23%)
1	A2M	2	494	1	22,25,26	1.46	4 (18%)	31,36,39	2.11	9 (29%)
1	OMU	2	52	1	19,22,23	1.25	3 (15%)	26,31,34	1.72	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMG	2	546	1	23,26,27	1.23	4 (17%)	33,38,41	1.91	6 (18%)
1	4AC	2	1477	1	21,24,25	1.08	2 (9%)	29,34,37	1.48	4 (13%)
1	OMG	2	1018	1	23,26,27	1.20	3 (13%)	33,38,41	2.01	7 (21%)
1	OMG	2	672	1	23,26,27	1.21	3 (13%)	33,38,41	1.94	5 (15%)
1	MA6	2	1475	1	23,26,27	1.44	4 (17%)	34,38,41	2.25	11 (32%)
1	5MC	2	1368	1	18,22,23	0.91	2 (11%)	26,32,35	1.10	2 (7%)
1	OMG	2	905	1	23,26,27	1.19	3 (13%)	33,38,41	1.99	8 (24%)
1	OMG	2	1061	1	23,26,27	1.19	4 (17%)	33,38,41	1.89	6 (18%)
1	OMC	2	113	1	19,22,23	0.79	0	26,31,34	0.91	0
1	OMC	2	1366	1	19,22,23	0.80	0	26,31,34	0.83	1 (3%)
1	4AC	2	1478	1	21,24,25	1.05	2 (9%)	29,34,37	1.28	4 (13%)
1	OMG	2	337	1	23,26,27	1.24	4 (17%)	33,38,41	1.98	7 (21%)
1	OMG	2	399	1	23,26,27	1.21	3 (13%)	33,38,41	1.95	6 (18%)
1	OMG	2	865	1	23,26,27	1.25	3 (13%)	33,38,41	1.95	6 (18%)
1	OMC	2	710	1	19,22,23	0.82	0	26,31,34	0.78	1 (3%)
1	C4J	2	930	1	24,29,30	0.23	0	29,42,45	0.54	0
1	4AC	2	1466	1	21,24,25	1.01	2 (9%)	29,34,37	1.16	3 (10%)
1	6MZ	2	1457	36,1	22,25,26	1.42	4 (18%)	30,36,39	2.23	10 (33%)
1	OMC	2	1060	1	19,22,23	0.81	0	26,31,34	0.75	0
1	OMG	2	926	1	23,26,27	1.23	3 (13%)	33,38,41	1.96	6 (18%)
1	OMC	2	313	1	19,22,23	0.83	0	26,31,34	0.79	0
1	OMU	2	1032	1	19,22,23	1.33	3 (15%)	26,31,34	1.71	4 (15%)
1	OMC	2	246	1	19,22,23	0.87	1 (5%)	26,31,34	1.00	1 (3%)
1	4AC	2	843	1	21,24,25	1.09	2 (9%)	29,34,37	1.40	4 (13%)
1	OMC	2	538	1	19,22,23	0.81	0	26,31,34	0.83	1 (3%)
1	4AC	2	1467	1	21,24,25	1.10	3 (14%)	29,34,37	1.22	4 (13%)
35	OMC	4	32	35	19,22,23	0.88	1 (5%)	26,31,34	1.12	2 (7%)
1	OMC	2	512	1	19,22,23	0.81	0	26,31,34	0.86	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
1	OMU	2	1344	1	-	0/9/27/28	0/2/2/2
1	OMU	2	15	1	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	2	1194	1	-	0/9/27/28	0/3/3/3
1	OMC	2	481	1	-	0/9/27/28	0/2/2/2
1	A2M	2	494	1	-	1/9/27/28	0/3/3/3
1	OMU	2	52	1	-	0/9/27/28	0/2/2/2
1	OMG	2	546	1	-	0/9/27/28	0/3/3/3
1	4AC	2	1477	1	-	0/11/29/30	0/2/2/2
1	OMG	2	1018	1	-	0/9/27/28	0/3/3/3
1	OMG	2	672	1	-	0/9/27/28	0/3/3/3
1	MA6	2	1475	1	-	0/11/29/30	0/3/3/3
1	5MC	2	1368	1	-	0/7/25/26	0/2/2/2
1	OMG	2	905	1	-	0/9/27/28	0/3/3/3
1	OMG	2	1061	1	-	0/9/27/28	0/3/3/3
1	OMC	2	113	1	-	0/9/27/28	0/2/2/2
1	OMC	2	1366	1	-	0/9/27/28	0/2/2/2
1	4AC	2	1478	1	-	0/11/29/30	0/2/2/2
1	OMG	2	337	1	-	1/9/27/28	0/3/3/3
1	OMG	2	399	1	-	0/9/27/28	0/3/3/3
1	OMG	2	865	1	-	2/9/27/28	0/3/3/3
1	OMC	2	710	1	-	0/9/27/28	0/2/2/2
1	C4J	2	930	1	-	3/16/34/35	0/2/2/2
1	4AC	2	1466	1	-	0/11/29/30	0/2/2/2
1	6MZ	2	1457	36,1	-	0/9/27/28	0/3/3/3
1	OMC	2	1060	1	-	0/9/27/28	0/2/2/2
1	OMG	2	926	1	-	0/9/27/28	0/3/3/3
1	OMC	2	313	1	-	0/9/27/28	0/2/2/2
1	OMU	2	1032	1	-	0/9/27/28	0/2/2/2
1	OMC	2	246	1	-	3/9/27/28	0/2/2/2
1	4AC	2	843	1	-	0/11/29/30	0/2/2/2
1	OMC	2	538	1	-	0/9/27/28	0/2/2/2
1	4AC	2	1467	1	-	0/11/29/30	0/2/2/2
35	OMC	4	32	35	-	3/9/27/28	0/2/2/2
1	OMC	2	512	1	-	0/9/27/28	0/2/2/2

The worst 5 of 74 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	494	A2M	C5-C4	4.44	1.47	1.39
1	2	1475	MA6	C5-C4	4.38	1.47	1.39
1	2	1457	6MZ	C5-C4	4.08	1.46	1.39
1	2	15	OMU	C4-N3	-3.47	1.32	1.38
1	2	15	OMU	C2-N3	-3.22	1.32	1.38

The worst 5 of 144 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1475	MA6	C5-C4-N3	-6.28	118.56	126.75
1	2	926	OMG	C5-C4-N3	-6.18	118.43	128.46
1	2	494	A2M	C5-C4-N3	-6.16	118.71	126.75
1	2	1018	OMG	C5-C4-N3	-6.13	118.51	128.46
1	2	865	OMG	C5-C4-N3	-6.11	118.55	128.46

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	246	OMC	C3'-C4'-C5'-O5'
1	2	246	OMC	O4'-C4'-C5'-O5'
1	2	930	C4J	C4'-C5'-O5'-P
1	2	930	C4J	C3'-C4'-C5'-O5'
1	2	930	C4J	O4'-C4'-C5'-O5'

There are no ring outliers.

21 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	1344	OMU	3	0
1	2	481	OMC	3	0
1	2	52	OMU	1	0
1	2	1477	4AC	2	0
1	2	672	OMG	1	0
1	2	1475	MA6	1	0
1	2	1368	5MC	1	0
1	2	905	OMG	2	0
1	2	113	OMC	2	0
1	2	1478	4AC	2	0
1	2	337	OMG	3	0
1	2	865	OMG	3	0
1	2	930	C4J	2	0
1	2	1466	4AC	1	0
1	2	1060	OMC	2	0
1	2	1032	OMU	1	0
1	2	246	OMC	2	0
1	2	843	4AC	1	0
1	2	538	OMC	2	0
1	2	1467	4AC	1	0
35	4	32	OMC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 111 ligands modelled in this entry, 67 are monoatomic - leaving 44 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	$\# Z > 2$
37	SPM	2	1589	-	13,13,13	0.11	0	12,12,12	0.08	0
37	SPM	2	1560	-	13,13,13	0.12	0	12,12,12	0.11	0
37	SPM	2	1575	-	13,13,13	0.12	0	12,12,12	0.07	0
37	SPM	2	1576	-	13,13,13	0.11	0	12,12,12	0.07	0
37	SPM	2	1599	-	13,13,13	0.10	0	12,12,12	0.21	0
37	SPM	2	1598	-	13,13,13	0.12	0	12,12,12	0.07	0
37	SPM	F	303	-	13,13,13	0.09	0	12,12,12	0.21	0
37	SPM	2	1580	-	13,13,13	0.11	0	12,12,12	0.13	0
37	SPM	2	1597	-	13,13,13	0.16	0	12,12,12	0.14	0
37	SPM	2	1581	-	13,13,13	0.10	0	12,12,12	0.07	0
37	SPM	2	1591	-	13,13,13	0.06	0	12,12,12	0.13	0
37	SPM	2	1565	-	13,13,13	0.07	0	12,12,12	0.22	0
37	SPM	2	1566	-	13,13,13	0.09	0	12,12,12	0.08	0
37	SPM	2	1571	-	13,13,13	0.09	0	12,12,12	0.13	0
37	SPM	2	1573	-	13,13,13	0.07	0	12,12,12	0.13	0
37	SPM	2	1559	-	13,13,13	0.08	0	12,12,12	0.30	0
37	SPM	2	1578	-	13,13,13	0.10	0	12,12,12	0.09	0
37	SPM	2	1574	-	13,13,13	0.07	0	12,12,12	0.23	0
37	SPM	2	1588	1	13,13,13	0.12	0	12,12,12	0.14	0
37	SPM	2	1568	-	13,13,13	0.11	0	12,12,12	0.08	0
37	SPM	2	1594	-	13,13,13	0.11	0	12,12,12	0.05	0
37	SPM	2	1570	-	13,13,13	0.10	0	12,12,12	0.07	0
37	SPM	2	1561	-	13,13,13	0.07	0	12,12,12	0.11	0
37	SPM	2	1562	-	13,13,13	0.06	0	12,12,12	0.11	0
37	SPM	2	1587	-	13,13,13	0.11	0	12,12,12	0.10	0
37	SPM	2	1584	-	13,13,13	0.16	0	12,12,12	0.30	0
37	SPM	2	1586	-	13,13,13	0.10	0	12,12,12	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	SPM	2	1569	-	13,13,13	0.12	0	12,12,12	0.32	0
37	SPM	2	1557	-	13,13,13	0.11	0	12,12,12	0.14	0
37	SPM	2	1579	-	13,13,13	0.12	0	12,12,12	0.29	0
37	SPM	2	1590	-	13,13,13	0.10	0	12,12,12	0.17	0
37	SPM	2	1582	-	13,13,13	0.10	0	12,12,12	0.08	0
37	SPM	2	1564	-	13,13,13	0.06	0	12,12,12	0.13	0
37	SPM	2	1567	-	13,13,13	0.06	0	12,12,12	0.18	0
37	SPM	2	1558	-	13,13,13	0.13	0	12,12,12	0.06	0
37	SPM	2	1592	-	13,13,13	0.12	0	12,12,12	0.06	0
37	SPM	2	1595	-	13,13,13	0.12	0	12,12,12	0.06	0
37	SPM	2	1572	-	13,13,13	0.10	0	12,12,12	0.28	0
37	SPM	2	1563	-	13,13,13	0.09	0	12,12,12	0.08	0
37	SPM	2	1596	-	13,13,13	0.10	0	12,12,12	0.08	0
37	SPM	2	1577	-	13,13,13	0.09	0	12,12,12	0.11	0
37	SPM	2	1583	-	13,13,13	0.11	0	12,12,12	0.08	0
37	SPM	2	1593	-	13,13,13	0.10	0	12,12,12	0.16	0
37	SPM	2	1585	-	13,13,13	0.09	0	12,12,12	0.12	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
37	SPM	2	1589	-	-	3/11/11/11	-
37	SPM	2	1560	-	-	3/11/11/11	-
37	SPM	2	1575	-	-	3/11/11/11	-
37	SPM	2	1576	-	-	4/11/11/11	-
37	SPM	2	1599	-	-	6/11/11/11	-
37	SPM	2	1598	-	-	3/11/11/11	-
37	SPM	F	303	-	-	3/11/11/11	-
37	SPM	2	1580	-	-	4/11/11/11	-
37	SPM	2	1597	-	-	2/11/11/11	-
37	SPM	2	1581	-	-	3/11/11/11	-
37	SPM	2	1591	-	-	3/11/11/11	-
37	SPM	2	1565	-	-	3/11/11/11	-
37	SPM	2	1566	-	-	2/11/11/11	-
37	SPM	2	1571	-	-	1/11/11/11	-
37	SPM	2	1573	-	-	5/11/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	SPM	2	1559	-	-	4/11/11/11	-
37	SPM	2	1578	-	-	4/11/11/11	-
37	SPM	2	1574	-	-	4/11/11/11	-
37	SPM	2	1588	1	-	4/11/11/11	-
37	SPM	2	1568	-	-	2/11/11/11	-
37	SPM	2	1594	-	-	3/11/11/11	-
37	SPM	2	1570	-	-	4/11/11/11	-
37	SPM	2	1561	-	-	5/11/11/11	-
37	SPM	2	1562	-	-	3/11/11/11	-
37	SPM	2	1587	-	-	2/11/11/11	-
37	SPM	2	1584	-	-	5/11/11/11	-
37	SPM	2	1586	-	-	3/11/11/11	-
37	SPM	2	1569	-	-	2/11/11/11	-
37	SPM	2	1557	-	-	2/11/11/11	-
37	SPM	2	1579	-	-	6/11/11/11	-
37	SPM	2	1590	-	-	4/11/11/11	-
37	SPM	2	1582	-	-	3/11/11/11	-
37	SPM	2	1564	-	-	3/11/11/11	-
37	SPM	2	1567	-	-	3/11/11/11	-
37	SPM	2	1558	-	-	3/11/11/11	-
37	SPM	2	1592	-	-	4/11/11/11	-
37	SPM	2	1595	-	-	0/11/11/11	-
37	SPM	2	1572	-	-	2/11/11/11	-
37	SPM	2	1563	-	-	3/11/11/11	-
37	SPM	2	1596	-	-	2/11/11/11	-
37	SPM	2	1577	-	-	3/11/11/11	-
37	SPM	2	1583	-	-	2/11/11/11	-
37	SPM	2	1593	-	-	4/11/11/11	-
37	SPM	2	1585	-	-	3/11/11/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 140 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
37	2	1562	SPM	C3-C4-N5-C6
37	2	1568	SPM	C8-C9-N10-C11
37	2	1574	SPM	C7-C6-N5-C4
37	2	1575	SPM	C3-C4-N5-C6
37	2	1576	SPM	C8-C9-N10-C11

There are no ring outliers.

37 monomers are involved in 160 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	2	1589	SPM	10	0
37	2	1560	SPM	2	0
37	2	1575	SPM	5	0
37	2	1576	SPM	2	0
37	2	1599	SPM	3	0
37	F	303	SPM	11	0
37	2	1580	SPM	1	0
37	2	1597	SPM	2	0
37	2	1581	SPM	11	0
37	2	1591	SPM	3	0
37	2	1565	SPM	2	0
37	2	1566	SPM	6	0
37	2	1571	SPM	4	0
37	2	1573	SPM	2	0
37	2	1578	SPM	1	0
37	2	1574	SPM	1	0
37	2	1588	SPM	5	0
37	2	1568	SPM	5	0
37	2	1594	SPM	11	0
37	2	1570	SPM	11	0
37	2	1587	SPM	5	0
37	2	1584	SPM	14	0
37	2	1586	SPM	8	0
37	2	1569	SPM	3	0
37	2	1579	SPM	1	0
37	2	1582	SPM	1	0
37	2	1564	SPM	2	0
37	2	1567	SPM	1	0
37	2	1558	SPM	8	0
37	2	1595	SPM	2	0
37	2	1572	SPM	5	0
37	2	1563	SPM	1	0
37	2	1596	SPM	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	2	1577	SPM	3	0
37	2	1583	SPM	8	0
37	2	1593	SPM	2	0
37	2	1585	SPM	4	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.

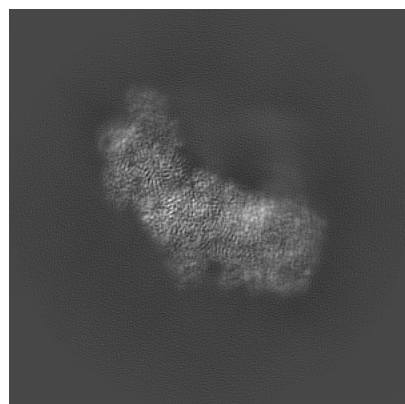
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50445. These allow visual inspection of the internal detail of the map and identification of artifacts.

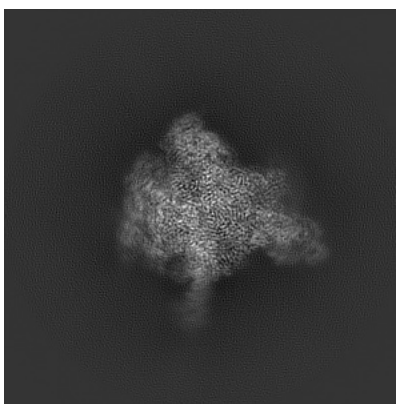
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

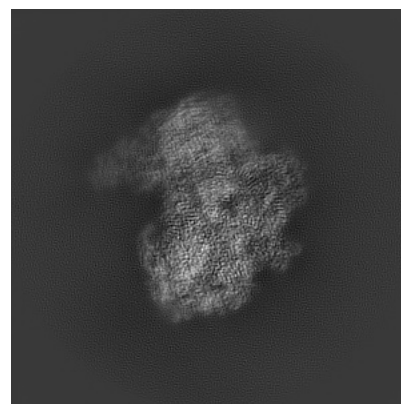
6.1.1 Primary map



X

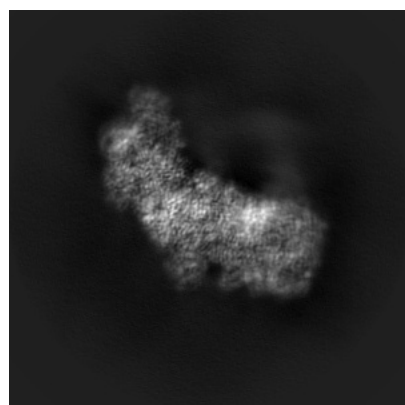


Y

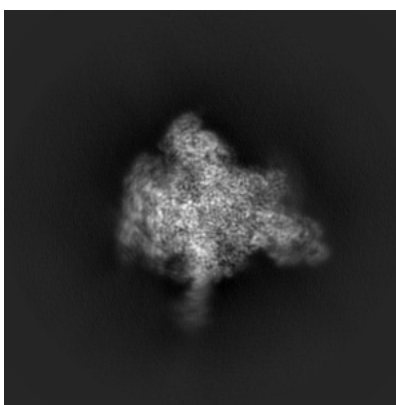


Z

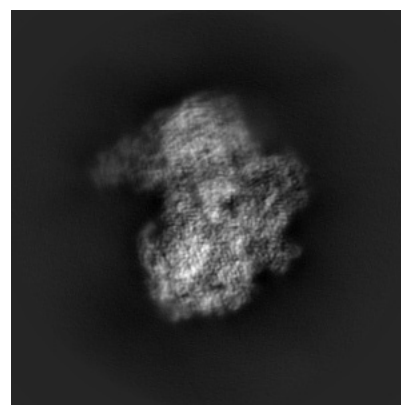
6.1.2 Raw map



X



Y

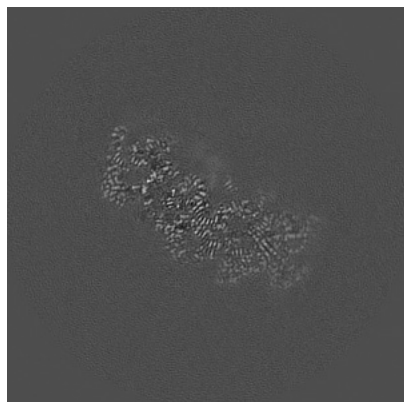


Z

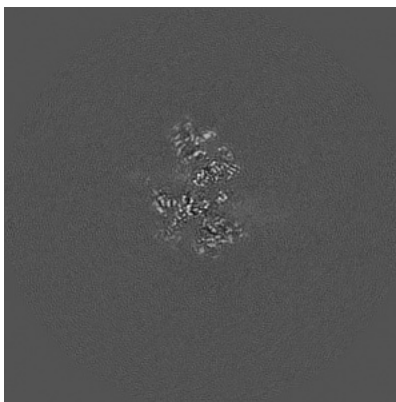
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

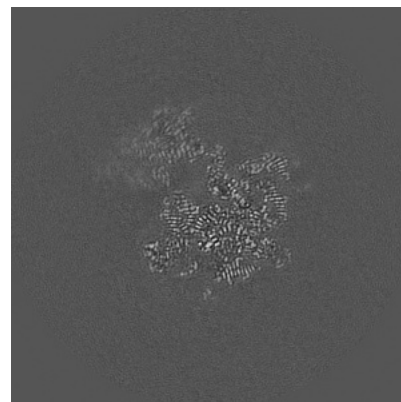
6.2.1 Primary map



X Index: 219

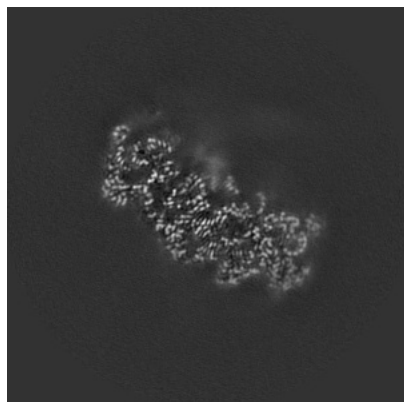


Y Index: 219

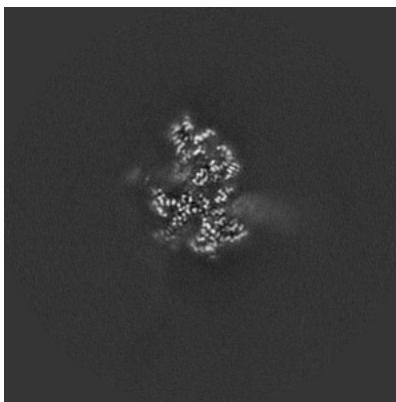


Z Index: 219

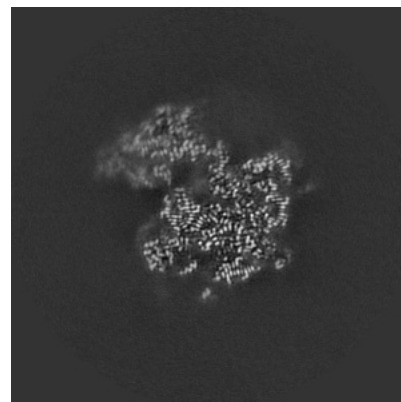
6.2.2 Raw map



X Index: 219



Y Index: 219

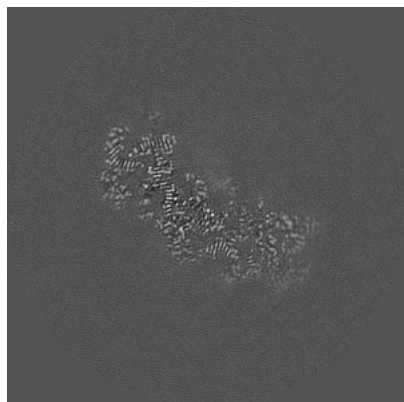


Z Index: 219

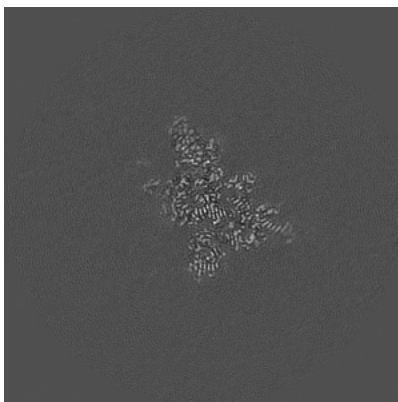
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

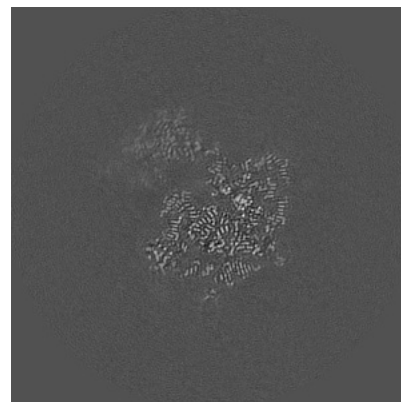
6.3.1 Primary map



X Index: 214

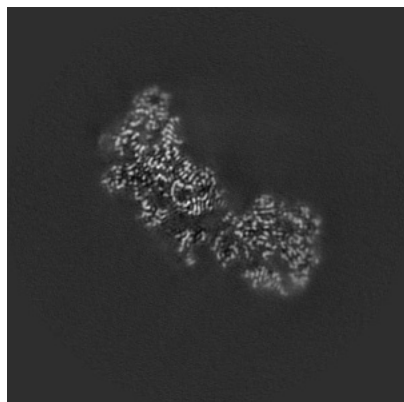


Y Index: 176

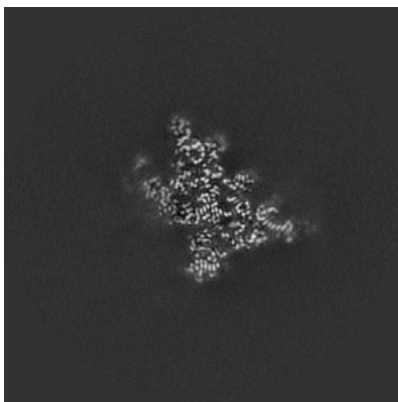


Z Index: 222

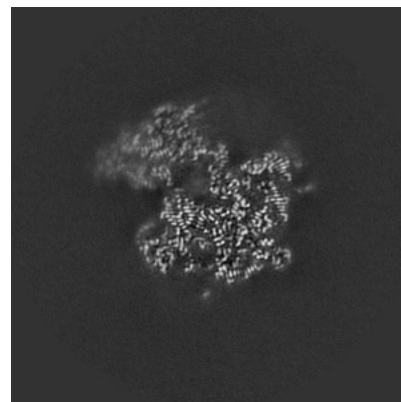
6.3.2 Raw map



X Index: 197



Y Index: 179

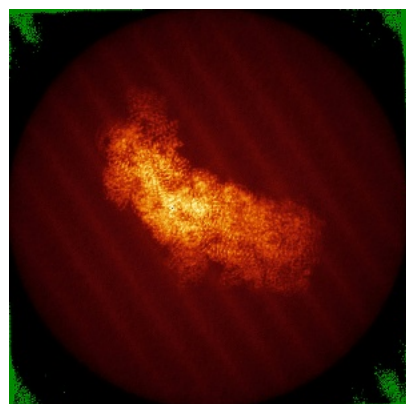


Z Index: 217

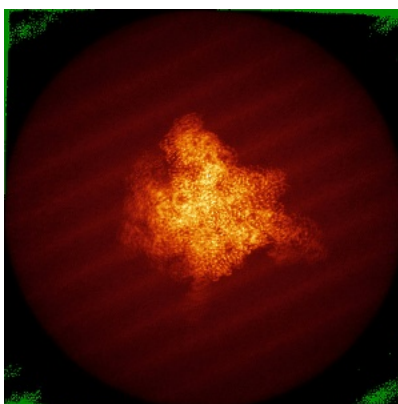
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

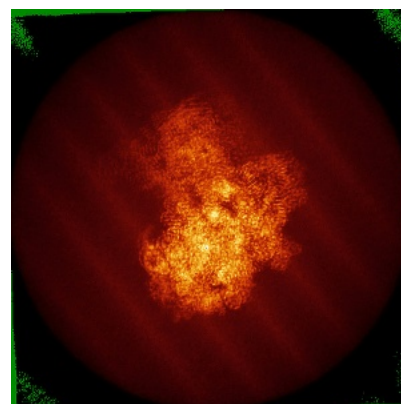
6.4.1 Primary map



X



Y

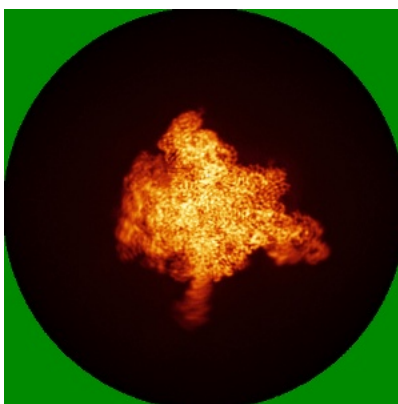


Z

6.4.2 Raw map



X



Y

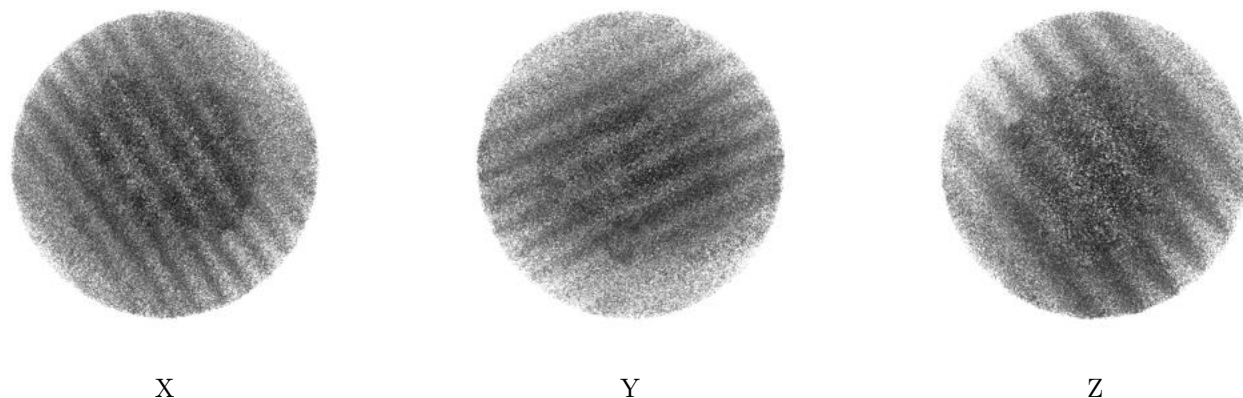


Z

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

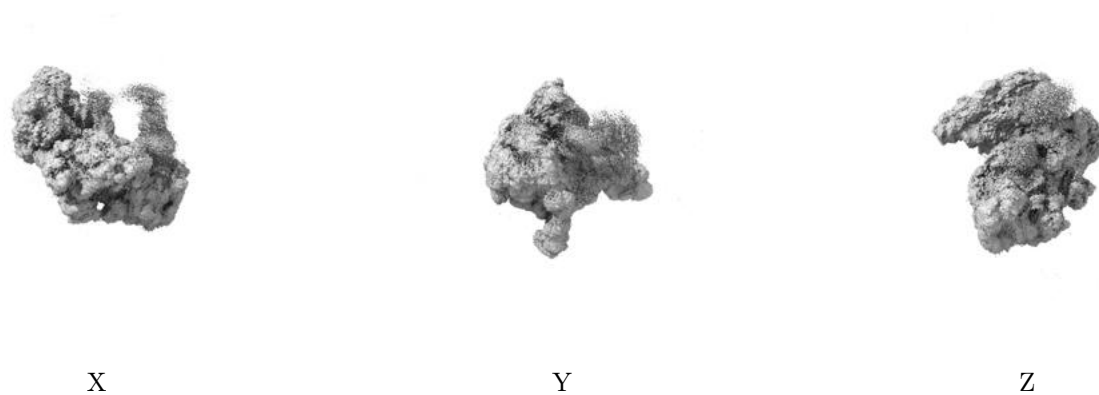
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.007. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

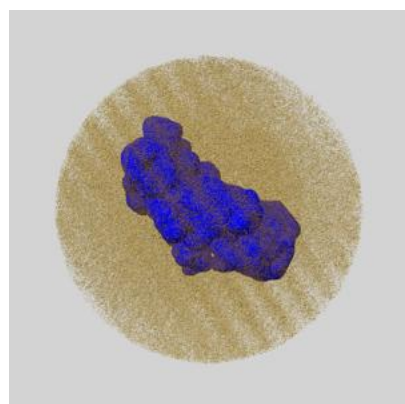
6.6 Mask visualisation [i](#)

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

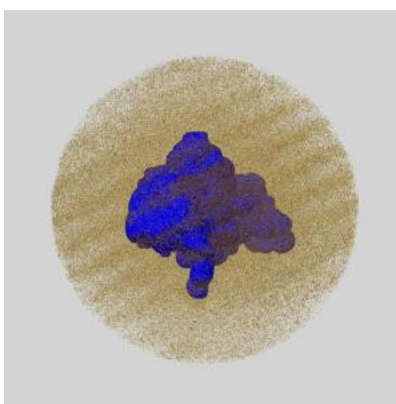
A mask typically either:

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

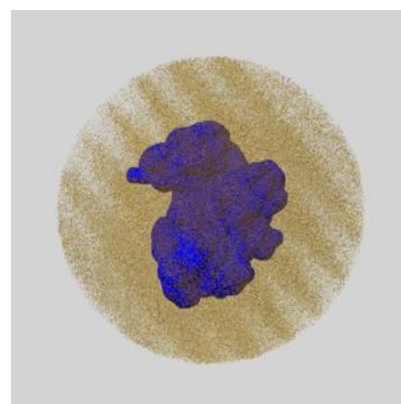
6.6.1 emd_50445_msk_1.map [i](#)



X



Y

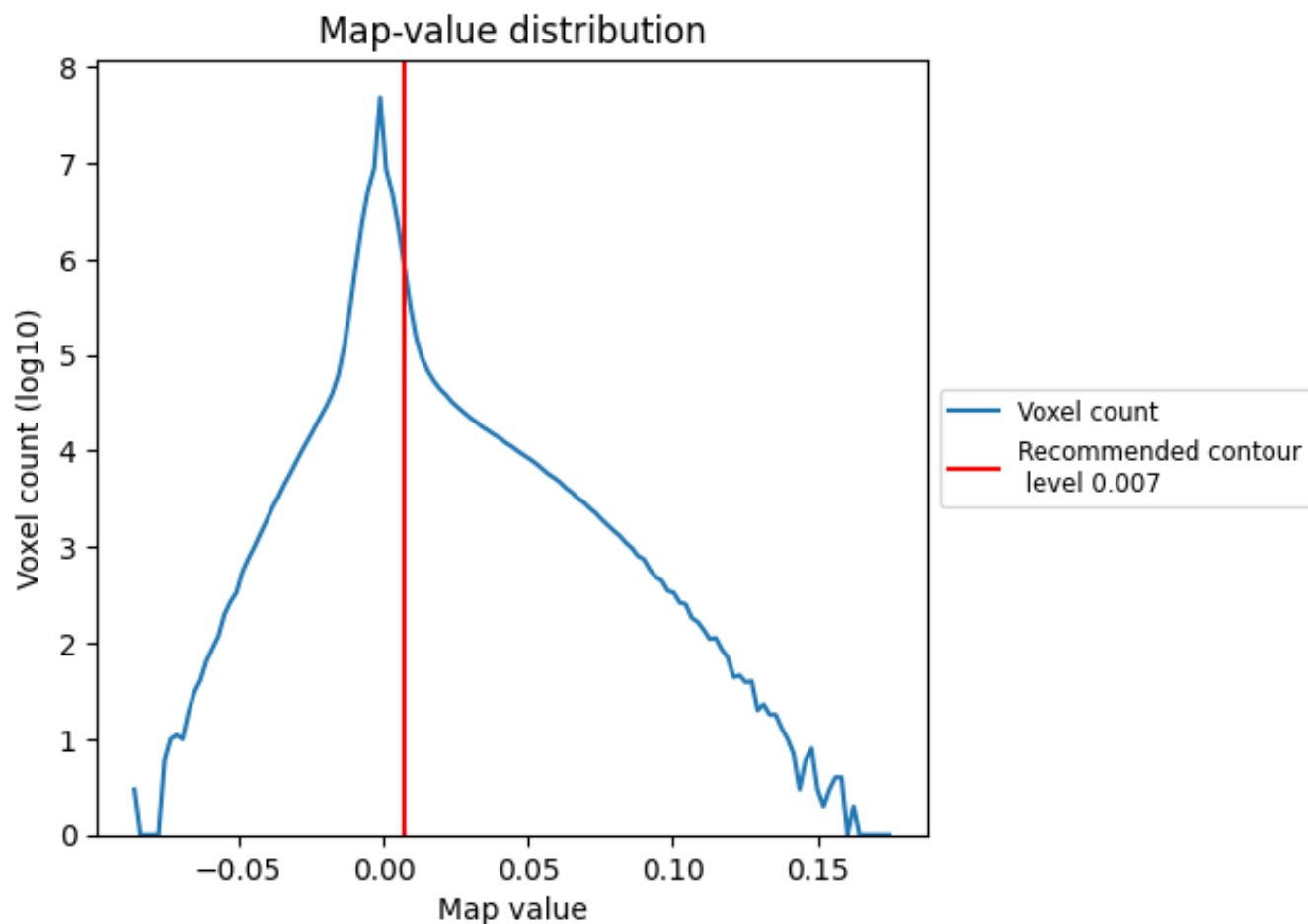


Z

7 Map analysis [i](#)

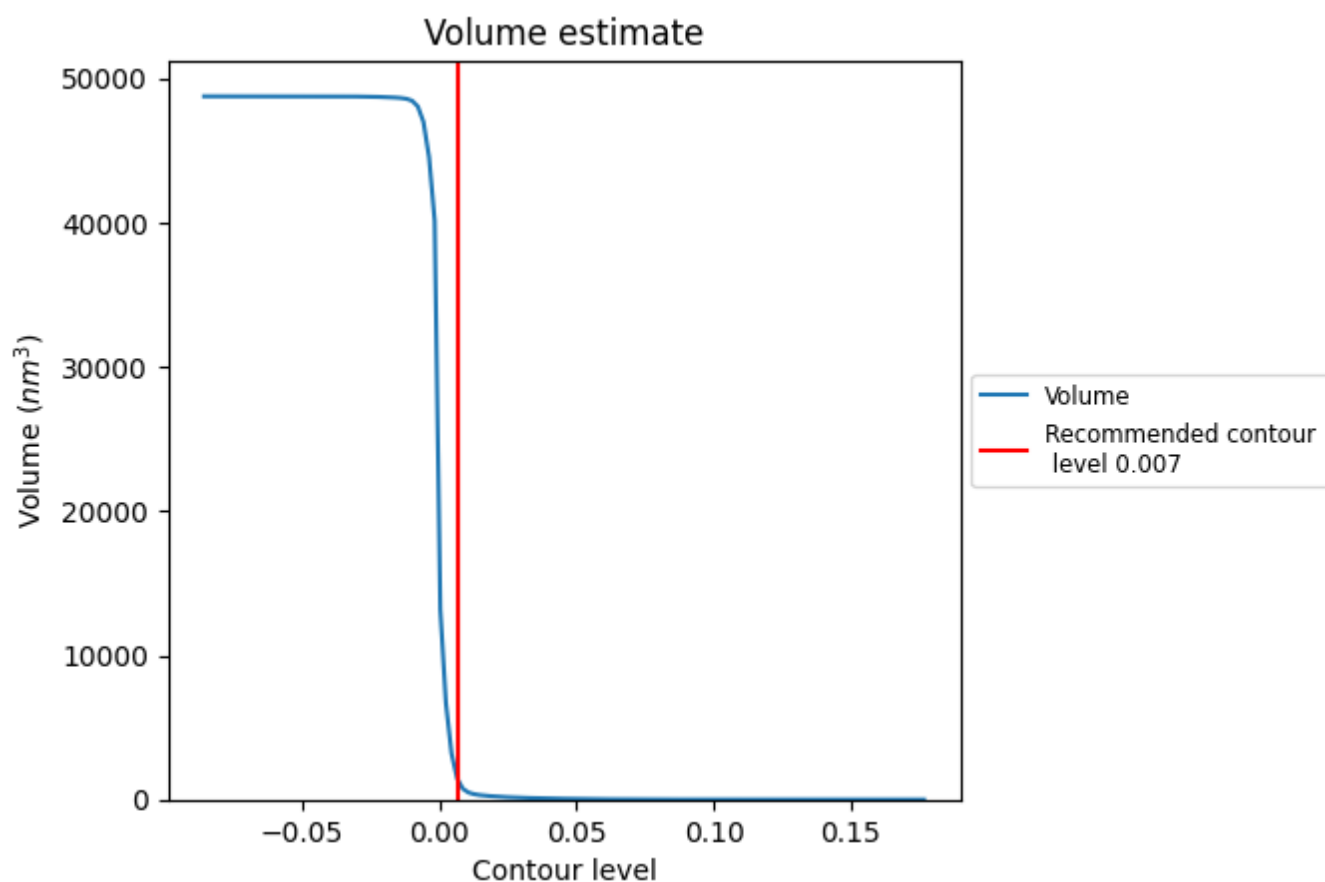
This section contains the results of statistical analysis of the map.

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.

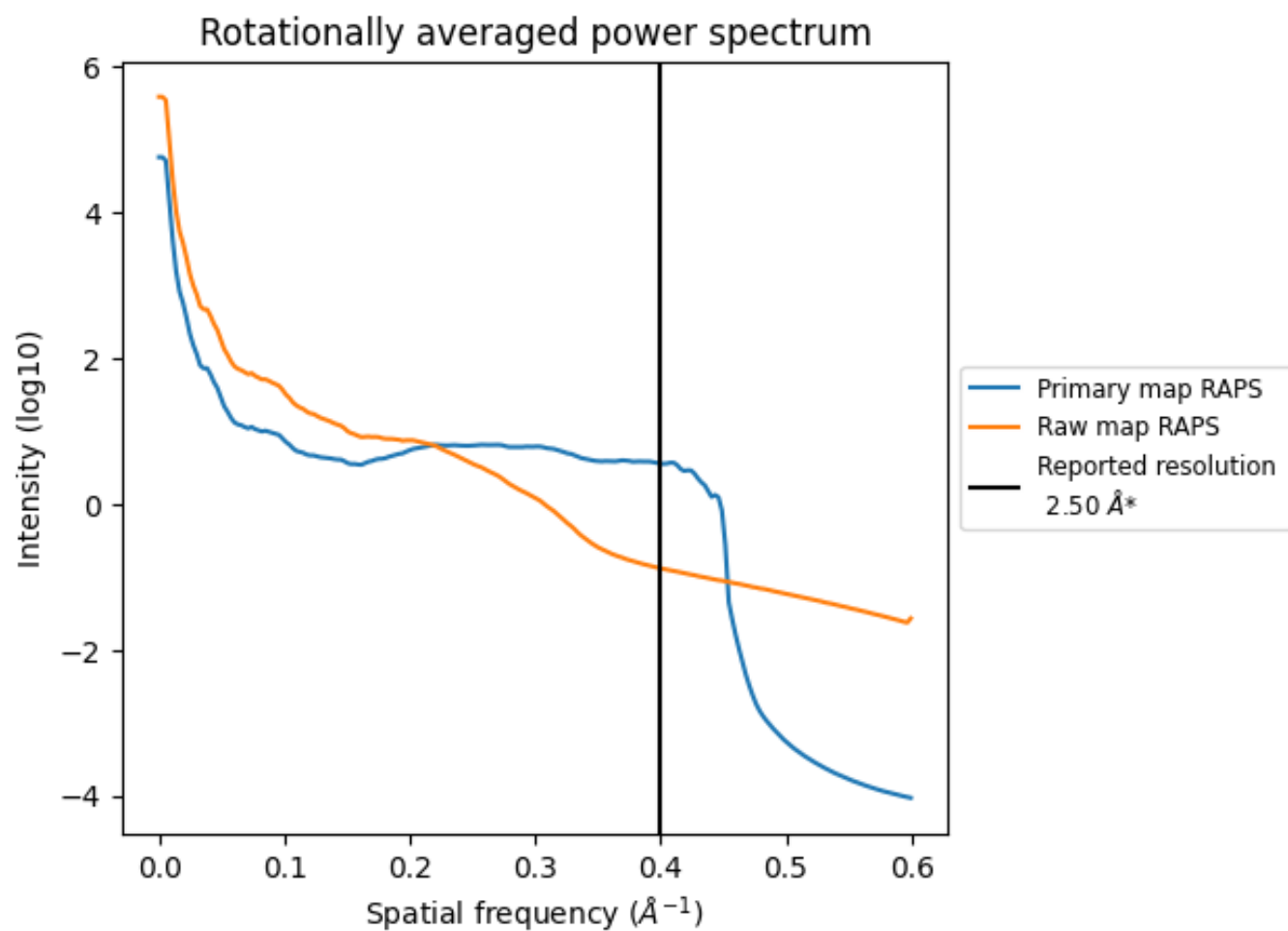
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1269 nm^3 ; this corresponds to an approximate mass of 1146 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 ⓘ

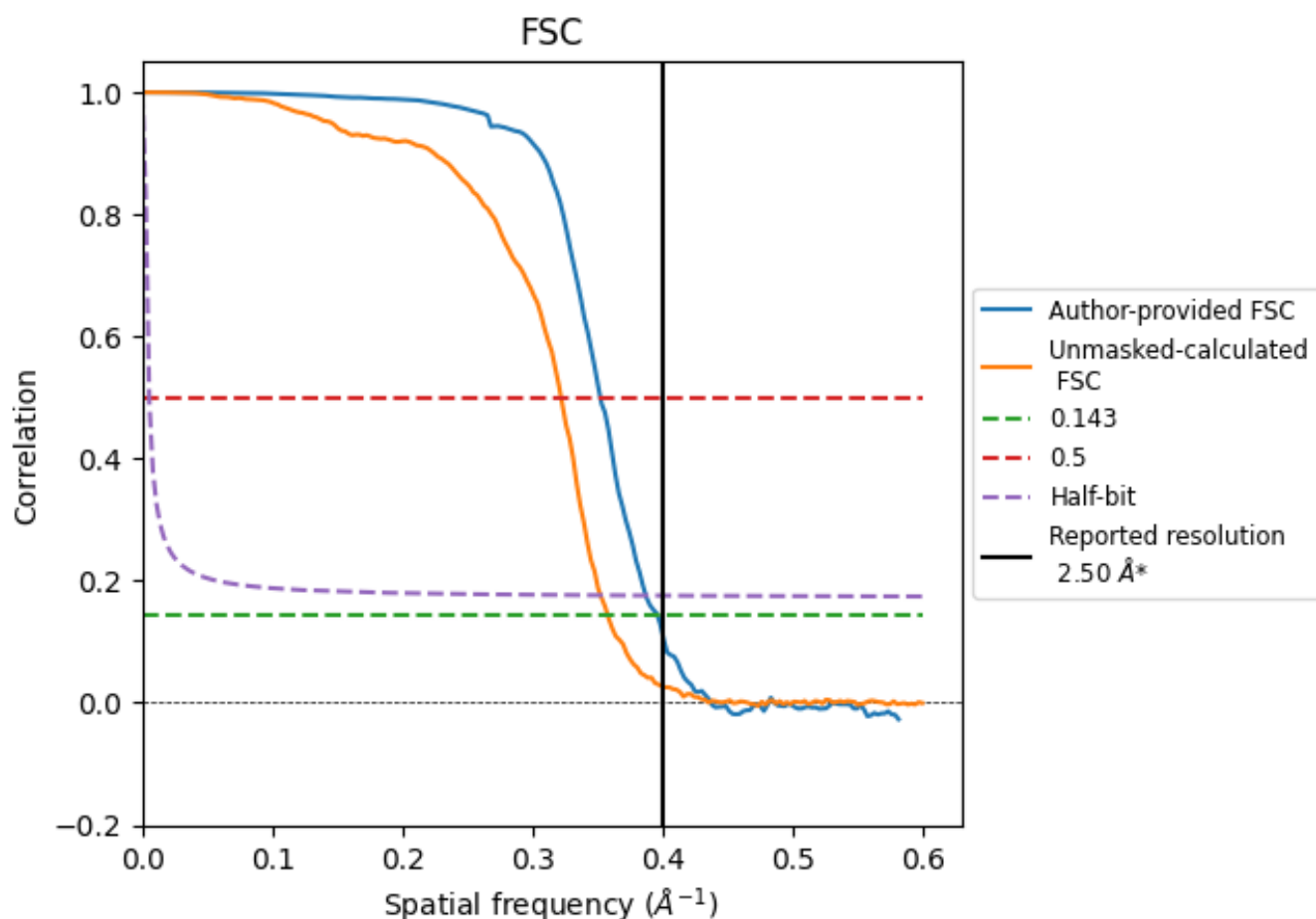


*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

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 $0.400 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.53	2.84	2.58
Unmasked-calculated*	2.79	3.10	2.84

*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 2.79 differs from the reported value 2.5 by more than 10 %

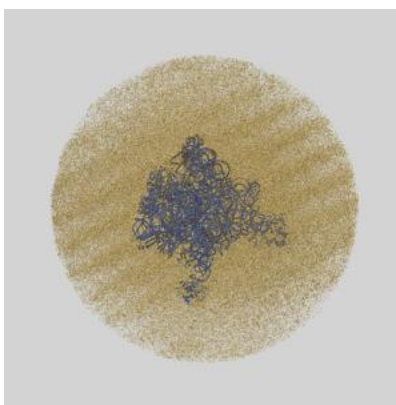
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-50445 and PDB model 9FHL. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

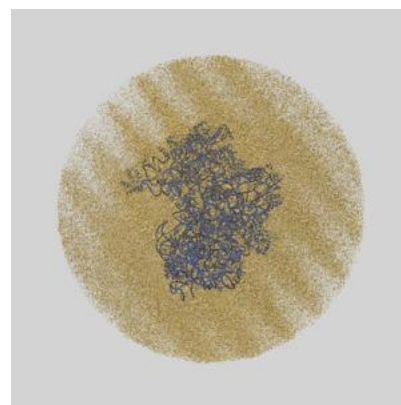
9.1 Map-model overlay [i](#)



X



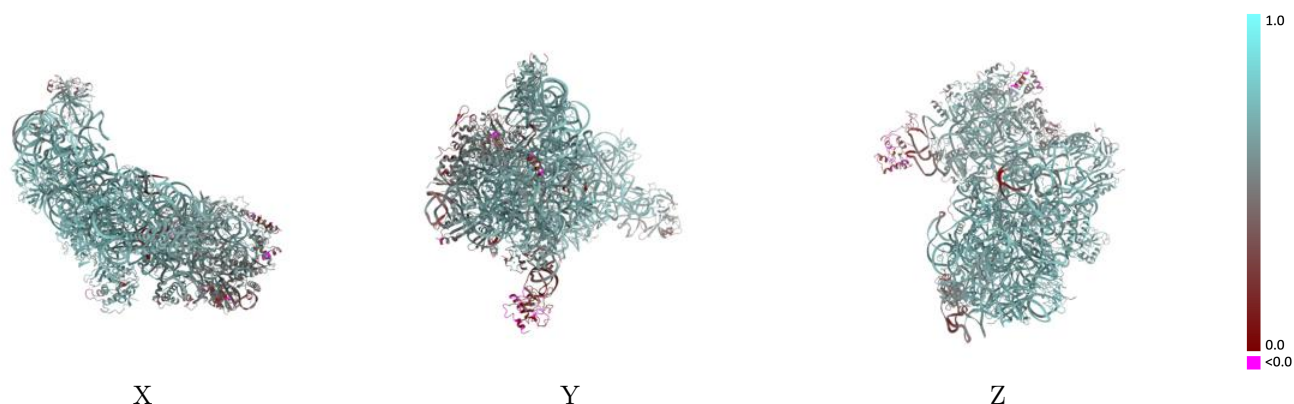
Y



Z

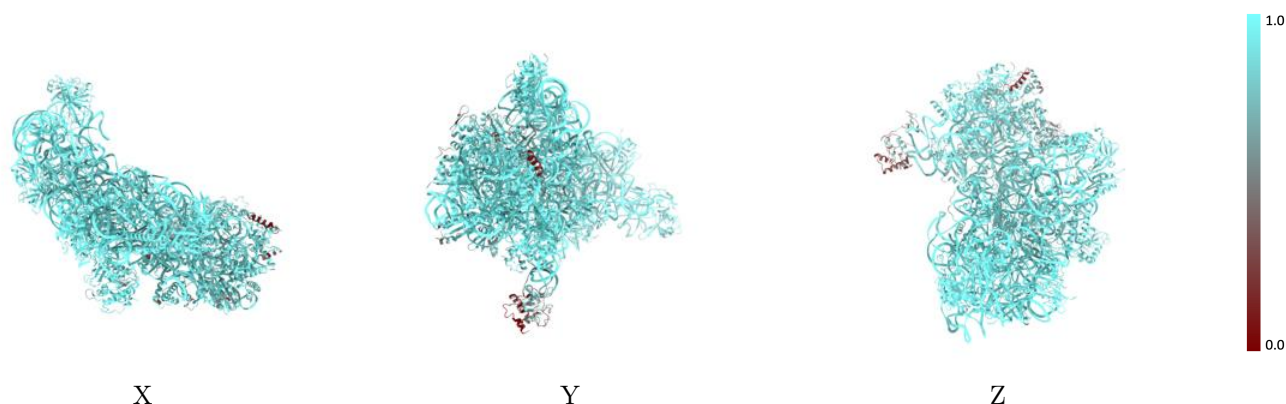
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



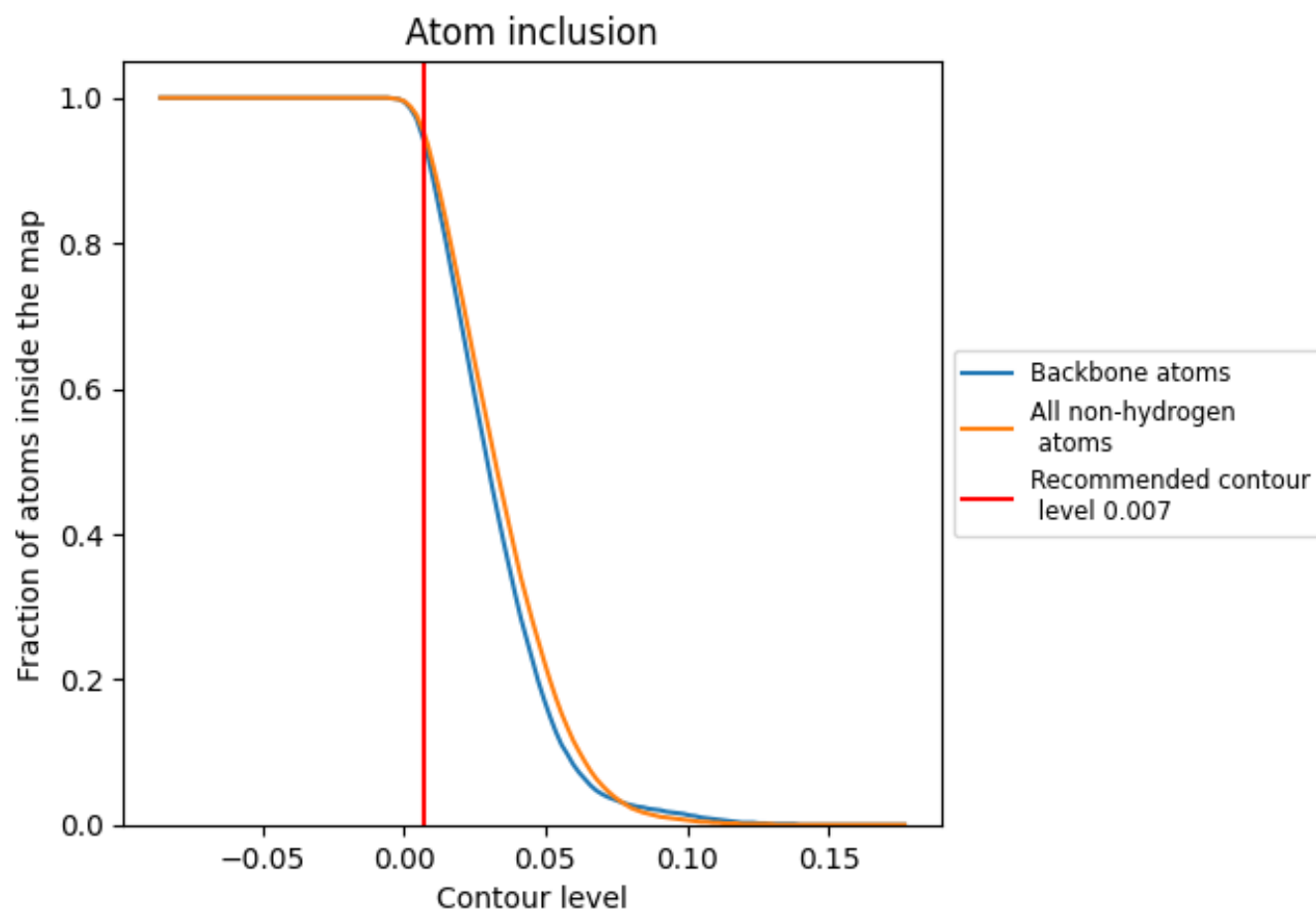
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.007).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 95% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9530	 0.6120
2	 0.9880	 0.6460
3	 0.3310	 0.1370
4	 0.9950	 0.6270
5	 0.9870	 0.6710
A	 0.9710	 0.6080
B	 0.9610	 0.6180
C	 0.9840	 0.6550
D	 0.9890	 0.6810
E	 0.9960	 0.6880
F	 0.9870	 0.6870
G	 0.9310	 0.5190
H	 0.8860	 0.5060
I	 0.9950	 0.6990
J	 0.9840	 0.6660
K	 0.9260	 0.5510
L	 0.8730	 0.5130
M	 0.9730	 0.6110
N	 0.9790	 0.6690
O	 0.9490	 0.5800
P	 0.9760	 0.6480
Q	 0.9820	 0.6590
R	 0.9900	 0.6860
S	 0.9360	 0.5700
T	 0.9290	 0.5520
U	 0.9700	 0.5900
V	 0.9760	 0.6520
W	 0.9940	 0.6540
X	 0.8210	 0.4370
Y	 0.5090	 0.1660
Z	 0.9460	 0.5940
a	 0.9130	 0.5270
c	 0.6350	 0.3770
d	 0.7830	 0.3710
e	 0.8660	 0.5770
s	 0.5910	 0.1810

