



Full wwPDB EM Validation Report ⓘ

Jan 8, 2025 – 01:07 pm GMT

PDB ID : 9FRA
EMDB ID : EMD-50709
Title : Cryo-EM structure of *Saccharolobus solfataricus* 30S initiation complex bound to Ss-MAP leaderless mRNA
Authors : Bourgeois, G.; Coureux, P.D.; Mechulam, Y.; Schmitt, E.
Deposited on : 2024-06-18
Resolution : 2.80 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

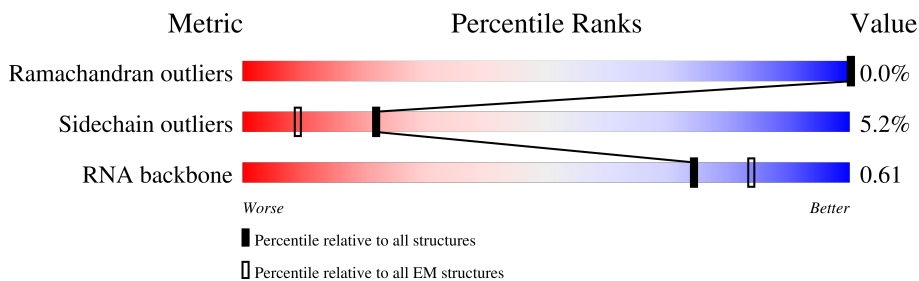
EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)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

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



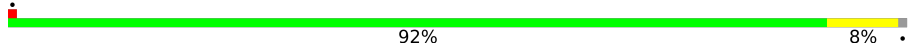
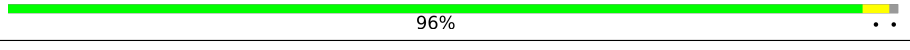
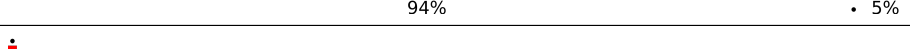
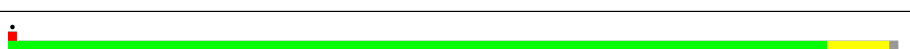
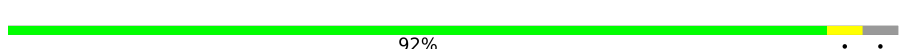
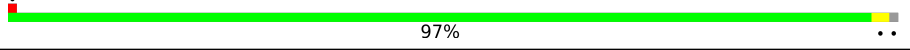

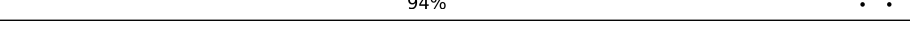



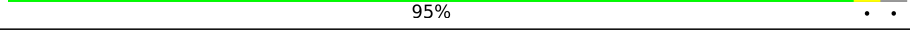

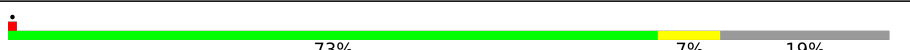


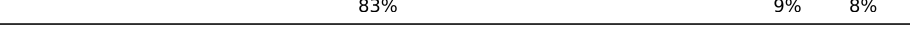







Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	2	1497	
2	A	208	
3	B	231	
4	C	65	
5	D	181	
6	E	239	
7	F	211	
8	G	214	

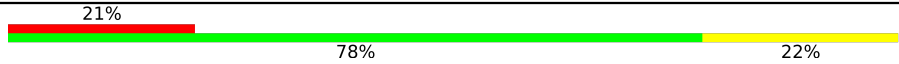

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Mol	Chain	Length	Quality of chain
9	H	193	 92% 8%
10	I	133	 96%
11	J	133	 94% 5%
12	K	137	 91% 6%
13	L	102	 92% 7%
14	M	132	 92%
15	N	147	 97%
16	O	165	 82% 15%
17	P	54	 94%
18	Q	152	 94% 5%
19	R	114	 94% 5%
20	S	79	 77% 6% 16%
21	T	140	 86% 5% 9%
22	U	158	 95%
23	V	120	 84% 5% 11%
24	W	66	 85% 14%
25	X	83	 73% 7% 19%
26	Y	75	 8% 61% 35%
27	Z	229	 83% 14%
28	3	127	 17% 83% 9% 8%
29	a	72	 90% 8%
30	c	110	 25% 95% 5%
31	d	72	 6% 85% 12%
32	e	52	 6% 83% 17%
33	5	15	33% 40% 53% 7%

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Mol	Chain	Length	Quality of chain
34	4	77	 <p>21% 78% 22%</p>
35	s	15	 <p>7% 60% 33%</p>

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 66665 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	1496	32178	14348	5942	10392	1496	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	930	C4J	U	conflict	GB AE006641.1
2	1466	4AC	C	conflict	GB AE006641.1
2	1467	4AC	C	conflict	GB AE006641.1
2	1477	4AC	C	conflict	GB AE006641.1
2	1478	4AC	C	conflict	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
			Total	C	N	O	S		
2	A	186	1515	974	261	278	2	0	0

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

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

- 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
			Total	C	N	O	S		
4	C	58	455	282	84	81	8	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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
			Total	C	N	O	P		
33	5	14	345	146	64	116	19	1	0

- Molecule 34 is a RNA chain called tRNA initiator Met.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
34	4	77	1645	734	296	537	77	1	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	1	A	C	engineered mutation	GB 1334604293
4	72	U	A	engineered mutation	GB 1334604293

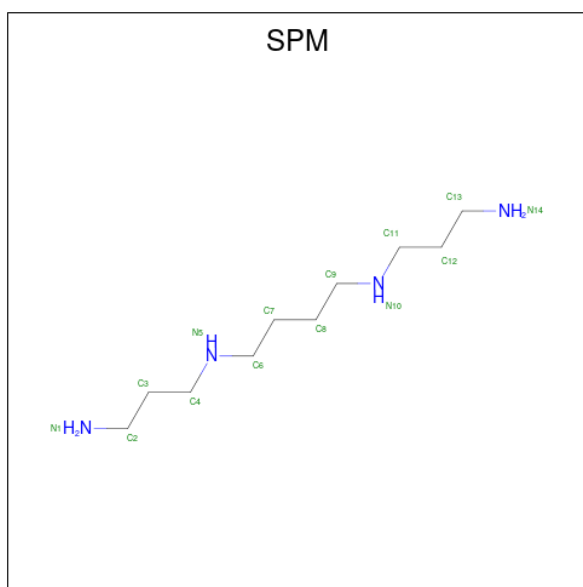
- Molecule 35 is a RNA chain called mRNA_Map.

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

- Molecule 36 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
36	2	53	Total	Mg	0
			53	53	
36	F	2	Total	Mg	0
			2	2	
36	P	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 (three-letter code: 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
			Total	C	N	
37	2	1	Total 14	C 10	N 4	0
37	2	1	Total 14	C 10	N 4	0
37	2	1	Total 14	C 10	N 4	0
37	2	1	Total 14	C 10	N 4	0
37	2	1	Total 14	C 10	N 4	0
37	2	1	Total 14	C 10	N 4	0
37	2	1	Total 14	C 10	N 4	0
37	2	1	Total 14	C 10	N 4	0
37	2	1	Total 14	C 10	N 4	0
37	2	1	Total 14	C 10	N 4	0
37	2	1	Total 14	C 10	N 4	0
37	2	1	Total 14	C 10	N 4	0
37	2	1	Total 14	C 10	N 4	0
37	2	1	Total 14	C 10	N 4	0
37	2	1	Total 14	C 10	N 4	0
37	2	1	Total 14	C 10	N 4	0
37	2	1	Total 14	C 10	N 4	0
37	2	1	Total 14	C 10	N 4	0
37	2	1	Total 14	C 10	N 4	0
37	2	1	Total 14	C 10	N 4	0

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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	

- Molecule 38 is ZINC ION (three-letter code: 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	199	Total	O	0
			199	199	
39	D	1	Total	O	0
			1	1	
39	E	1	Total	O	0
			1	1	
39	H	1	Total	O	0
			1	1	

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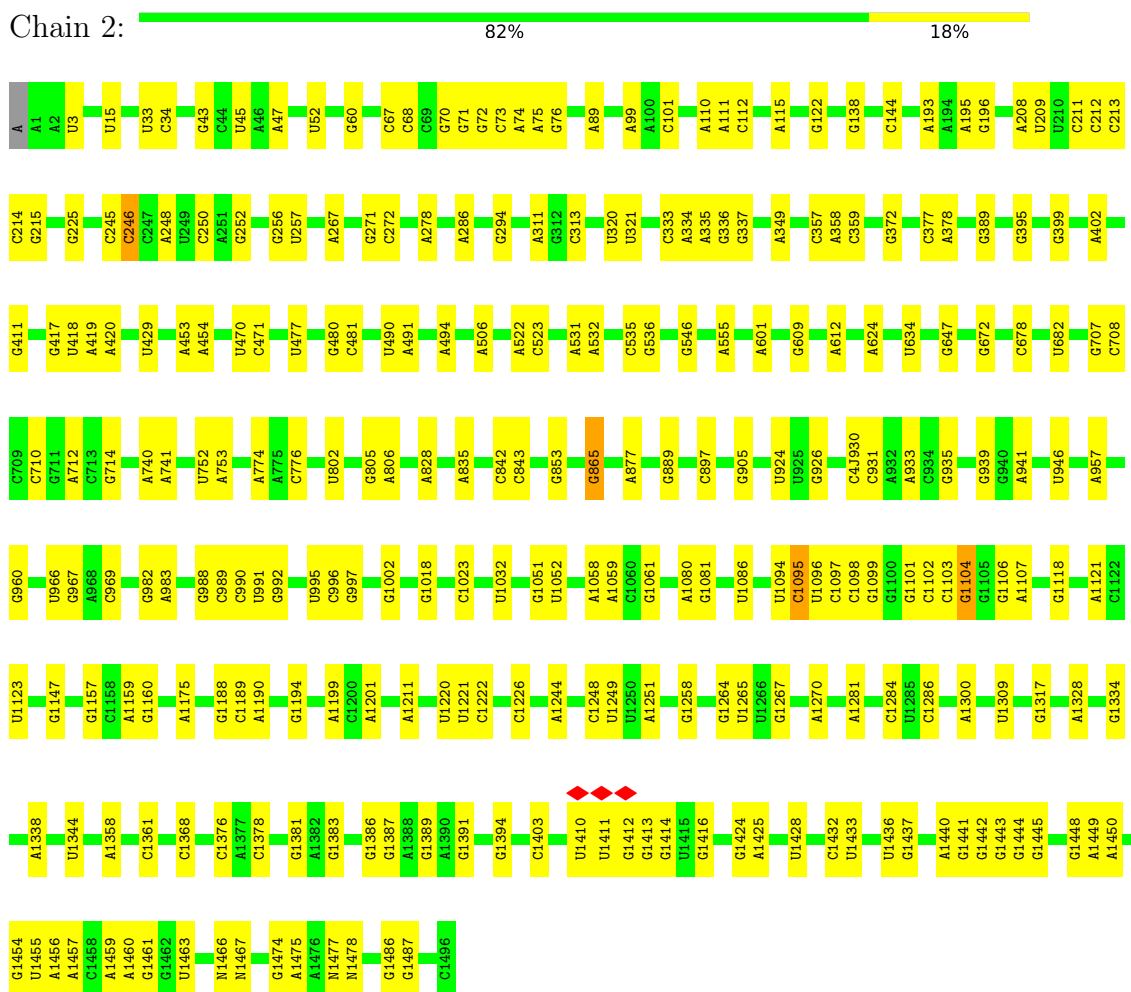
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Mol	Chain	Residues	Atoms		AltConf
39	I	2	Total 2	O 2	0
39	K	2	Total 2	O 2	0
39	P	1	Total 1	O 1	0
39	Q	1	Total 1	O 1	0
39	R	2	Total 2	O 2	0
39	5	8	Total 8	O 8	0
39	4	3	Total 3	O 3	0

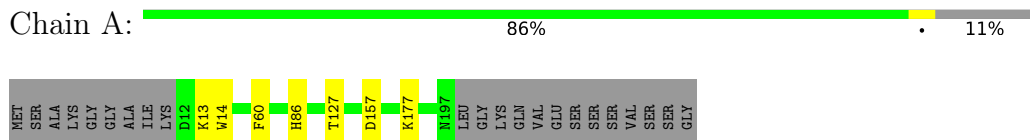
3 Residue-property plots

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



- Molecule 2: Small ribosomal subunit protein eS1




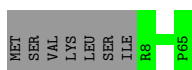
- Molecule 3: Small ribosomal subunit protein uS2

Chain B:  90% 7%




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

Chain C:  89% 11%



- Molecule 5: Small ribosomal subunit protein uS4

Chain D:  87% 8%



- Molecule 6: Small ribosomal subunit protein eS4

Chain E:  99%



- Molecule 7: Small ribosomal subunit protein uS5

Chain F:  96%



- Molecule 8: Small ribosomal subunit protein eS6

Chain G:  94% 5%



- Molecule 9: Small ribosomal subunit protein uS7

Chain H:  92% 8%



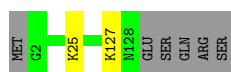
- Molecule 10: Small ribosomal subunit protein uS8

Chain I: 96%



- Molecule 11: Small ribosomal subunit protein eS8

Chain J: 94% • 5%



- Molecule 12: Small ribosomal subunit protein uS9

Chain K: 91% 6% •



- Molecule 13: Small ribosomal subunit protein uS10

Chain L: 92% 7% •



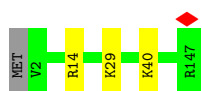
- Molecule 14: Small ribosomal subunit protein uS11

Chain M: 92% • •




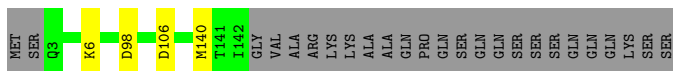
- Molecule 15: Small ribosomal subunit protein uS12

Chain N: 97% • •



- Molecule 16: Small ribosomal subunit protein uS13

Chain O:  82% 15%



- Molecule 17: Small ribosomal subunit protein uS14

Chain P:  94%



- Molecule 18: Small ribosomal subunit protein uS15

Chain Q:  94% 5%




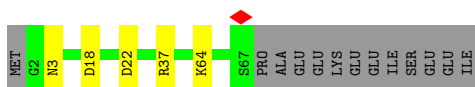
- Molecule 19: Small ribosomal subunit protein uS17

Chain R:  94% 5%




- Molecule 20: Small ribosomal subunit protein eS17

Chain S:  77% 6% 16%



- Molecule 21: Small ribosomal subunit protein uS19

Chain T:  86% 5% 9%




- Molecule 22: Small ribosomal subunit protein eS19

Chain U:  95%




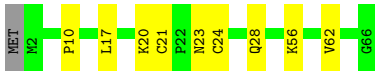
- Molecule 23: Small ribosomal subunit protein eS24

Chain V:  84% 5% 11%




• Molecule 24: Small ribosomal subunit protein eS27

Chain W:  85% 14%



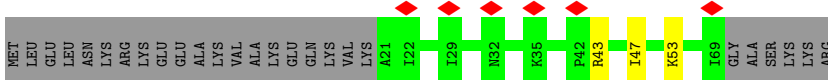
• Molecule 25: Small ribosomal subunit protein eS28

Chain X:  73% 7% 19%




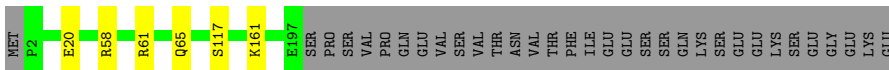
• Molecule 26: Small ribosomal subunit protein eS31

Chain Y:  8% 61% 35%




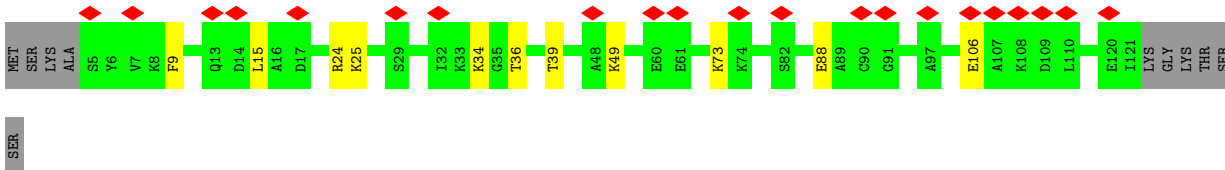
• Molecule 27: Small ribosomal subunit protein uS3

Chain Z:  83% 14%




• Molecule 28: Large ribosomal subunit protein eL8

Chain 3:  17% 83% 9% 8%

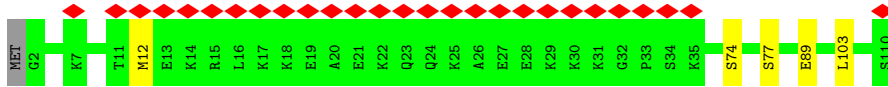


• Molecule 29: aS34

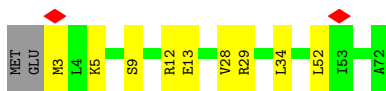
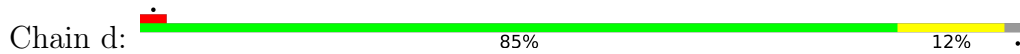
Chain a:  90% 8%



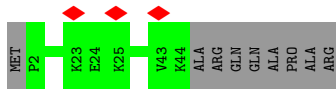
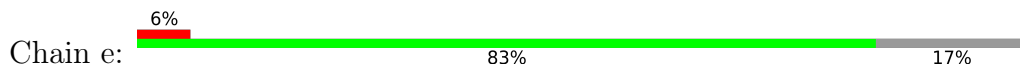
- Molecule 30: Small ribosomal subunit protein eS25



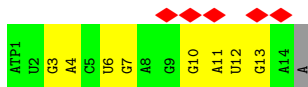
- Molecule 31: VapB-type antitoxin



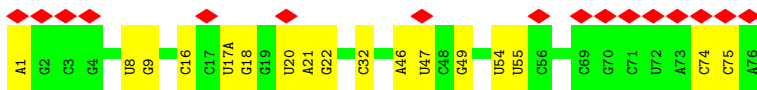
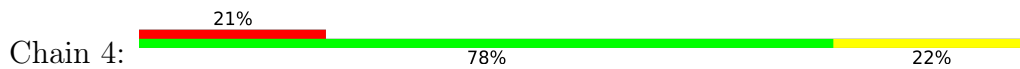
- Molecule 32: LSU ribosomal protein S30E (Rps30E)



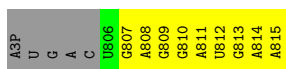
- Molecule 33: mRNA_Map



- Molecule 34: tRNA initiator Met



- Molecule 35: mRNA_Map



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	62000	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	0.050	Depositor
Minimum map value	-0.015	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.006	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 4AC, PSU, 4SU, 6MZ, ZN, ATP, OMU, 5MC, MA6, A2M, SPM, 5MU, C4J, OMC, H2U, OMG, 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	0.47	5/35206 (0.0%)	0.78	7/54930 (0.0%)
2	A	0.31	0/1543	0.55	0/2077
3	B	0.30	0/1731	0.55	0/2349
4	C	0.33	0/466	0.54	0/625
5	D	0.30	0/1380	0.49	0/1859
6	E	0.31	0/1965	0.54	0/2644
7	F	0.31	0/1654	0.52	0/2240
8	G	0.27	0/1684	0.51	0/2265
9	H	0.30	0/1571	0.58	1/2116 (0.0%)
10	I	0.33	0/1070	0.52	0/1444
11	J	0.31	0/994	0.58	0/1337
12	K	0.30	0/1084	0.66	0/1450
13	L	0.33	0/856	0.67	1/1154 (0.1%)
14	M	0.31	0/960	0.66	0/1294
15	N	0.31	0/1155	0.58	0/1540
16	O	0.28	0/1142	0.58	0/1532
17	P	0.35	0/451	0.52	0/600
18	Q	0.31	0/1206	0.53	0/1618
19	R	0.36	0/918	0.57	0/1236
20	S	0.34	0/578	0.64	0/770
21	T	0.29	0/1087	0.52	0/1456
22	U	0.28	0/1270	0.51	0/1710
23	V	0.31	0/843	0.56	0/1124
24	W	0.32	0/511	0.63	0/684
25	X	0.29	0/538	0.67	0/722
26	Y	0.31	0/404	0.66	0/540
27	Z	0.30	0/1584	0.56	0/2124
28	3	0.26	0/902	0.55	0/1216
29	a	0.31	0/574	0.53	0/770
30	c	0.28	0/861	0.56	0/1143
31	d	0.28	0/581	0.67	0/786

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	e	0.29	0/360	0.61	0/477
33	5	0.37	0/317	0.75	0/493
34	4	0.35	1/1725 (0.1%)	0.74	0/2687
35	s	0.25	0/247	0.67	0/384
All	All	0.40	6/69418 (0.0%)	0.70	9/101396 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1095	C	C4'-O4'	14.61	1.64	1.45
1	2	843	C	O3'-P	-14.23	1.44	1.61
34	4	1	A	OP3-P	-10.17	1.49	1.61
1	2	678	C	O3'-P	7.31	1.70	1.61
1	2	842	C	O3'-P	-6.79	1.53	1.61
1	2	843	C	C1'-N1	6.32	1.58	1.48

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1095	C	C1'-O4'-C4'	-12.77	99.68	109.90
1	2	843	C	P-O3'-C3'	-9.03	108.86	119.70
1	2	843	C	O3'-P-O5'	7.49	118.23	104.00
9	H	3	LEU	CA-CB-CG	6.78	130.89	115.30
1	2	1104	G	C5'-C4'-O4'	-6.41	101.40	109.10
1	2	842	C	P-O3'-C3'	6.27	127.23	119.70
1	2	842	C	O3'-P-O5'	-6.01	92.58	104.00
1	2	1095	C	C5'-C4'-O4'	-5.73	102.23	109.10
13	L	79	ASP	CB-CG-OD1	5.20	122.98	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [\(i\)](#)

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	184/208 (88%)	180 (98%)	4 (2%)	0	100	100
3	B	213/231 (92%)	210 (99%)	3 (1%)	0	100	100
4	C	56/65 (86%)	55 (98%)	1 (2%)	0	100	100
5	D	164/181 (91%)	161 (98%)	3 (2%)	0	100	100
6	E	236/239 (99%)	228 (97%)	8 (3%)	0	100	100
7	F	208/211 (99%)	200 (96%)	8 (4%)	0	100	100
8	G	211/214 (99%)	201 (95%)	10 (5%)	0	100	100
9	H	190/193 (98%)	183 (96%)	7 (4%)	0	100	100
10	I	130/133 (98%)	126 (97%)	4 (3%)	0	100	100
11	J	125/133 (94%)	121 (97%)	4 (3%)	0	100	100
12	K	131/137 (96%)	125 (95%)	6 (5%)	0	100	100
13	L	99/102 (97%)	92 (93%)	7 (7%)	0	100	100
14	M	125/132 (95%)	117 (94%)	8 (6%)	0	100	100
15	N	144/147 (98%)	138 (96%)	6 (4%)	0	100	100
16	O	138/165 (84%)	132 (96%)	6 (4%)	0	100	100
17	P	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
18	Q	143/152 (94%)	143 (100%)	0	0	100	100
19	R	111/114 (97%)	110 (99%)	1 (1%)	0	100	100
20	S	64/79 (81%)	63 (98%)	1 (2%)	0	100	100
21	T	126/140 (90%)	126 (100%)	0	0	100	100
22	U	152/158 (96%)	149 (98%)	3 (2%)	0	100	100
23	V	105/120 (88%)	102 (97%)	3 (3%)	0	100	100
24	W	63/66 (96%)	56 (89%)	6 (10%)	1 (2%)	8	27
25	X	65/83 (78%)	58 (89%)	7 (11%)	0	100	100
26	Y	47/75 (63%)	37 (79%)	10 (21%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	Z	194/229 (85%)	190 (98%)	4 (2%)	0	100	100
28	3	115/127 (91%)	102 (89%)	13 (11%)	0	100	100
29	a	69/72 (96%)	69 (100%)	0	0	100	100
30	c	107/110 (97%)	100 (94%)	7 (6%)	0	100	100
31	d	68/72 (94%)	65 (96%)	3 (4%)	0	100	100
32	e	41/52 (79%)	40 (98%)	1 (2%)	0	100	100
All	All	3875/4194 (92%)	3729 (96%)	145 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
24	W	23	ASN

5.3.2 Protein sidechains [i](#)

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%)	161 (96%)	7 (4%)	25	58
3	B	182/198 (92%)	174 (96%)	8 (4%)	24	56
4	C	51/58 (88%)	51 (100%)	0	100	100
5	D	147/158 (93%)	139 (95%)	8 (5%)	18	48
6	E	214/215 (100%)	212 (99%)	2 (1%)	75	92
7	F	180/181 (99%)	172 (96%)	8 (4%)	24	56
8	G	186/187 (100%)	175 (94%)	11 (6%)	16	44
9	H	166/167 (99%)	152 (92%)	14 (8%)	9	28
10	I	113/114 (99%)	109 (96%)	4 (4%)	31	65
11	J	104/110 (94%)	102 (98%)	2 (2%)	52	82
12	K	109/113 (96%)	101 (93%)	8 (7%)	11	34
13	L	93/94 (99%)	87 (94%)	6 (6%)	14	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	M	93/98 (95%)	88 (95%)	5 (5%)	18	48
15	N	122/123 (99%)	119 (98%)	3 (2%)	42	75
16	O	121/142 (85%)	117 (97%)	4 (3%)	33	67
17	P	45/46 (98%)	43 (96%)	2 (4%)	24	56
18	Q	125/129 (97%)	123 (98%)	2 (2%)	58	85
19	R	101/102 (99%)	95 (94%)	6 (6%)	16	44
20	S	63/75 (84%)	58 (92%)	5 (8%)	10	30
21	T	116/126 (92%)	109 (94%)	7 (6%)	16	44
22	U	134/138 (97%)	130 (97%)	4 (3%)	36	70
23	V	92/99 (93%)	86 (94%)	6 (6%)	14	40
24	W	57/58 (98%)	49 (86%)	8 (14%)	3	9
25	X	58/73 (80%)	52 (90%)	6 (10%)	6	19
26	Y	43/65 (66%)	40 (93%)	3 (7%)	12	36
27	Z	163/195 (84%)	157 (96%)	6 (4%)	29	63
28	3	97/105 (92%)	86 (89%)	11 (11%)	4	16
29	a	61/62 (98%)	55 (90%)	6 (10%)	6	21
30	c	95/96 (99%)	90 (95%)	5 (5%)	19	49
31	d	63/65 (97%)	54 (86%)	9 (14%)	2	9
32	e	40/46 (87%)	40 (100%)	0	100	100
All	All	3402/3622 (94%)	3226 (95%)	176 (5%)	22	50

All (176) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	13	LYS
2	A	14	TRP
2	A	60	PHE
2	A	86	HIS
2	A	127	THR
2	A	157	ASP
2	A	177	LYS
3	B	15	GLU
3	B	21	LYS
3	B	26	LYS
3	B	34	GLU

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Mol	Chain	Res	Type
3	B	40	ASP
3	B	211	VAL
3	B	217	ASP
3	B	227	MET
5	D	77	LEU
5	D	85	LYS
5	D	92	ASP
5	D	134	ASN
5	D	151	ASN
5	D	162	LYS
5	D	163	SER
5	D	164	ARG
6	E	8	GLU
6	E	34	GLU
7	F	14	LYS
7	F	16	ARG
7	F	100	ARG
7	F	148	ASP
7	F	190	PHE
7	F	207	LEU
7	F	208	GLN
7	F	210	TRP
8	G	30	LYS
8	G	43	GLN
8	G	49	LYS
8	G	52	GLN
8	G	71	LYS
8	G	95	SER
8	G	142	GLN
8	G	159	SER
8	G	176	LEU
8	G	204	GLU
8	G	214	ARG
9	H	2	SER
9	H	26	SER
9	H	87	ASP
9	H	99	GLN
9	H	116	ARG
9	H	118	MET
9	H	124	TYR
9	H	149	ASP
9	H	151	SER

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Mol	Chain	Res	Type
9	H	173	ASP
9	H	175	LYS
9	H	188	ILE
9	H	191	SER
9	H	192	SER
10	I	28	MET
10	I	43	LYS
10	I	101	GLU
10	I	110	SER
11	J	25	LYS
11	J	127	LYS
12	K	8	VAL
12	K	20	THR
12	K	24	TYR
12	K	27	LYS
12	K	34	ASN
12	K	100	GLU
12	K	101	LYS
12	K	104	ARG
13	L	19	TYR
13	L	28	VAL
13	L	35	MET
13	L	64	LYS
13	L	81	ARG
13	L	85	GLN
14	M	17	SER
14	M	32	GLU
14	M	84	TYR
14	M	123	ARG
14	M	130	ARG
15	N	14	ARG
15	N	29	LYS
15	N	40	LYS
16	O	6	LYS
16	O	98	ASP
16	O	106	ASP
16	O	140	MET
17	P	9	GLU
17	P	14	LYS
18	Q	12	SER
18	Q	25	ARG
19	R	7	THR

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Mol	Chain	Res	Type
19	R	26	GLU
19	R	37	ARG
19	R	65	SER
19	R	75	SER
19	R	88	ARG
20	S	3	ASN
20	S	18	ASP
20	S	22	ASP
20	S	37	ARG
20	S	64	LYS
21	T	9	TRP
21	T	28	ASP
21	T	61	ARG
21	T	68	LYS
21	T	102	THR
21	T	118	LYS
21	T	130	THR
22	U	103	VAL
22	U	106	LEU
22	U	113	LYS
22	U	155	VAL
23	V	4	GLN
23	V	7	VAL
23	V	24	SER
23	V	80	LYS
23	V	101	ARG
23	V	108	LYS
24	W	10	PRO
24	W	17	LEU
24	W	20	LYS
24	W	21	CYS
24	W	24	CYS
24	W	28	GLN
24	W	56	LYS
24	W	62	VAL
25	X	17	PHE
25	X	37	THR
25	X	38	GLN
25	X	51	ARG
25	X	72	THR
25	X	77	ARG
26	Y	43	ARG

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Mol	Chain	Res	Type
26	Y	47	ILE
26	Y	53	LYS
27	Z	20	GLU
27	Z	58	ARG
27	Z	61	ARG
27	Z	65	GLN
27	Z	117	SER
27	Z	161	LYS
28	3	9	PHE
28	3	15	LEU
28	3	24	ARG
28	3	25	LYS
28	3	34	LYS
28	3	36	THR
28	3	39	THR
28	3	49	LYS
28	3	73	LYS
28	3	88	GLU
28	3	106	GLU
29	a	24	CYS
29	a	26	ARG
29	a	40	LYS
29	a	41	CYS
29	a	43	LYS
29	a	51	GLU
30	c	12	MET
30	c	74	SER
30	c	77	SER
30	c	89	GLU
30	c	103	LEU
31	d	3	MET
31	d	5	LYS
31	d	9	SER
31	d	12	ARG
31	d	13	GLU
31	d	28	VAL
31	d	29	ARG
31	d	34	LEU
31	d	52	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
5	D	121	GLN
5	D	134	ASN
7	F	208	GLN
8	G	85	ASN
8	G	142	GLN
13	L	100	GLN
14	M	60	ASN
19	R	86	ASN
20	S	31	ASN
25	X	56	ASN
27	Z	123	ASN
27	Z	157	GLN
29	a	25	ASN
31	d	25	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1488/1497 (99%)	238 (15%)	6 (0%)
33	5	12/15 (80%)	8 (66%)	2 (16%)
34	4	76/77 (98%)	13 (17%)	1 (1%)
35	s	9/15 (60%)	9 (100%)	0
All	All	1585/1604 (98%)	268 (16%)	9 (0%)

All (268) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	3	U
1	2	33	U
1	2	34	C
1	2	43	G
1	2	45	U
1	2	47	A
1	2	60	G
1	2	67	C
1	2	68	C
1	2	70	G
1	2	71	G
1	2	72	G
1	2	73	C
1	2	74	A
1	2	75	A

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Mol	Chain	Res	Type
1	2	76	G
1	2	89	A
1	2	99	A
1	2	101	C
1	2	110	A
1	2	111	A
1	2	112	C
1	2	115	A
1	2	122	G
1	2	138	G
1	2	144	C
1	2	193	A
1	2	195	A
1	2	196	G
1	2	208	A
1	2	209	U
1	2	211	C
1	2	212	C
1	2	213	C
1	2	214	C
1	2	215	G
1	2	225	G
1	2	245	C
1	2	246	OMC
1	2	248	A
1	2	250	C
1	2	252	G
1	2	256	G
1	2	257	U
1	2	267	A
1	2	271	G
1	2	272	C
1	2	278	A
1	2	286	A
1	2	294	G
1	2	311	A
1	2	320	U
1	2	321	U
1	2	333	C
1	2	334	A
1	2	335	A
1	2	336	G

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Mol	Chain	Res	Type
1	2	349	A
1	2	357	C
1	2	358	A
1	2	359	C
1	2	372	G
1	2	377	C
1	2	378	A
1	2	389	G
1	2	395	G
1	2	402	A
1	2	411	G
1	2	417	G
1	2	418	U
1	2	419	A
1	2	420	A
1	2	429	U
1	2	453	A
1	2	454	A
1	2	470	U
1	2	471	C
1	2	477	U
1	2	480	G
1	2	490	U
1	2	491	A
1	2	506	A
1	2	522	A
1	2	523	C
1	2	531	A
1	2	532	A
1	2	535	C
1	2	536	G
1	2	555	A
1	2	601	A
1	2	609	G
1	2	612	A
1	2	624	A
1	2	634	U
1	2	647	G
1	2	682	U
1	2	707	G
1	2	708	C
1	2	712	A

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Mol	Chain	Res	Type
1	2	714	G
1	2	740	A
1	2	741	A
1	2	752	U
1	2	753	A
1	2	774	A
1	2	776	C
1	2	802	U
1	2	805	G
1	2	806	A
1	2	828	A
1	2	835	A
1	2	853	G
1	2	865	OMG
1	2	877	A
1	2	889	G
1	2	897	C
1	2	924	U
1	2	931	C
1	2	933	A
1	2	935	G
1	2	939	G
1	2	941	A
1	2	946	U
1	2	957	A
1	2	960	G
1	2	966	U
1	2	967	G
1	2	969	C
1	2	982	G
1	2	983	A
1	2	988	G
1	2	989	C
1	2	990	C
1	2	991	U
1	2	992	G
1	2	995	U
1	2	996	C
1	2	997	G
1	2	1002	G
1	2	1023	C
1	2	1051	G

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Mol	Chain	Res	Type
1	2	1052	U
1	2	1058	A
1	2	1059	A
1	2	1080	A
1	2	1081	G
1	2	1086	U
1	2	1094	U
1	2	1095	C
1	2	1096	U
1	2	1097	C
1	2	1098	C
1	2	1099	G
1	2	1101	G
1	2	1102	C
1	2	1103	C
1	2	1104	G
1	2	1106	G
1	2	1107	A
1	2	1118	G
1	2	1121	A
1	2	1123	U
1	2	1147	G
1	2	1157	G
1	2	1159	A
1	2	1160	G
1	2	1175	A
1	2	1188	G
1	2	1189	C
1	2	1190	A
1	2	1199	A
1	2	1201	A
1	2	1211	A
1	2	1220	U
1	2	1221	U
1	2	1222	C
1	2	1226	C
1	2	1244	A
1	2	1248	C
1	2	1249	U
1	2	1251	A
1	2	1258	G
1	2	1264	G

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Mol	Chain	Res	Type
1	2	1265	U
1	2	1267	G
1	2	1270	A
1	2	1281	A
1	2	1284	C
1	2	1286	C
1	2	1300	A
1	2	1309	U
1	2	1317	G
1	2	1328	A
1	2	1334	G
1	2	1338	A
1	2	1358	A
1	2	1361	C
1	2	1376	C
1	2	1378	C
1	2	1381	G
1	2	1383	G
1	2	1386	G
1	2	1387	G
1	2	1389	G
1	2	1391	G
1	2	1394	G
1	2	1403	C
1	2	1410	U
1	2	1411	U
1	2	1412	G
1	2	1413	G
1	2	1414	G
1	2	1416	G
1	2	1424	G
1	2	1425	A
1	2	1428	U
1	2	1432	C
1	2	1433	U
1	2	1437	G
1	2	1440	A
1	2	1441	G
1	2	1442	G
1	2	1443	G
1	2	1444	G
1	2	1445	G

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Mol	Chain	Res	Type
1	2	1448	G
1	2	1449	A
1	2	1450	A
1	2	1454	G
1	2	1455	U
1	2	1456	A
1	2	1459	A
1	2	1460	A
1	2	1461	G
1	2	1463	U
1	2	1474	G
1	2	1486	G
1	2	1487	G
33	5	3	G
33	5	4	A
33	5	6	U
33	5	7	G
33	5	10	G
33	5	11	A
33	5	12	U
33	5	13	G
34	4	8	4SU
34	4	9	G
34	4	16	C
34	4	17(A)	U
34	4	18	G
34	4	20	H2U
34	4	21	A
34	4	22	G
34	4	46	A
34	4	47	U
34	4	49	G
34	4	74	C
34	4	75	C
35	s	807	G
35	s	808	A
35	s	809	G
35	s	810	G
35	s	811	A
35	s	812	U
35	s	813	G
35	s	814	A

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Mol	Chain	Res	Type
35	s	815	A

All (9) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	256	G
1	2	1102	C
1	2	1188	G
1	2	1436	U
1	2	1443	G
1	2	1455	U
33	5	3	G
33	5	12	U
34	4	74	C

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

37 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	OMG	2	1061	1	18,26,27	0.95	1 (5%)	19,38,41	1.09	2 (10%)
1	5MC	2	1368	1	18,22,23	0.93	2 (11%)	26,32,35	1.05	3 (11%)
1	OMU	2	52	1	19,22,23	1.25	3 (15%)	26,31,34	1.70	4 (15%)
1	OMC	2	512	1	19,22,23	0.82	0	26,31,34	0.81	0
1	OMU	2	1032	1	19,22,23	1.26	3 (15%)	26,31,34	1.73	4 (15%)
1	4AC	2	1467	1	21,24,25	1.02	2 (9%)	29,34,37	1.34	4 (13%)
1	OMC	2	246	1	19,22,23	0.84	0	26,31,34	0.99	1 (3%)
1	OMC	2	538	1	19,22,23	0.82	0	26,31,34	0.81	0
1	OMC	2	113	1	19,22,23	0.83	0	26,31,34	0.81	0
34	H2U	4	20	34	18,21,22	0.31	0	21,30,33	0.42	0
1	6MZ	2	1457	1,36	18,25,26	0.83	1 (5%)	16,36,39	2.17	3 (18%)
1	MA6	2	1475	1	18,26,27	0.92	1 (5%)	19,38,41	1.23	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMC	2	1060	1	19,22,23	0.82	0	26,31,34	0.75	0
1	OMG	2	1018	1	18,26,27	0.94	1 (5%)	19,38,41	1.08	2 (10%)
1	OMC	2	313	1	19,22,23	0.84	0	26,31,34	0.95	1 (3%)
1	OMG	2	399	1	18,26,27	0.94	1 (5%)	19,38,41	1.08	2 (10%)
1	OMG	2	865	1	18,26,27	0.94	1 (5%)	19,38,41	1.07	2 (10%)
1	OMU	2	15	1	19,22,23	1.26	3 (15%)	26,31,34	1.73	4 (15%)
1	OMG	2	672	1	18,26,27	0.95	1 (5%)	19,38,41	1.07	2 (10%)
1	OMC	2	481	1	19,22,23	0.83	0	26,31,34	0.93	1 (3%)
1	OMG	2	926	1	18,26,27	0.93	1 (5%)	19,38,41	1.14	2 (10%)
1	OMU	2	1344	1	19,22,23	1.23	3 (15%)	26,31,34	1.68	5 (19%)
1	OMG	2	546	1	18,26,27	0.91	1 (5%)	19,38,41	1.15	2 (10%)
1	4AC	2	1477	1	21,24,25	1.02	2 (9%)	29,34,37	1.55	5 (17%)
1	4AC	2	1466	1	21,24,25	1.00	2 (9%)	29,34,37	1.30	4 (13%)
1	OMC	2	1366	1	19,22,23	0.82	0	26,31,34	0.77	0
34	PSU	4	55	34	18,21,22	1.32	2 (11%)	22,30,33	1.88	3 (13%)
1	4AC	2	1478	1	21,24,25	1.02	2 (9%)	29,34,37	1.35	4 (13%)
1	OMG	2	337	1	18,26,27	0.96	1 (5%)	19,38,41	1.13	2 (10%)
34	OMC	4	32	34	19,22,23	0.85	0	26,31,34	1.03	2 (7%)
1	OMC	2	710	1	19,22,23	0.83	0	26,31,34	0.87	1 (3%)
34	4SU	4	8	34	18,21,22	0.27	0	26,30,33	0.34	0
1	OMG	2	1194	1	18,26,27	0.96	1 (5%)	19,38,41	1.14	2 (10%)
1	OMG	2	905	1	18,26,27	0.95	1 (5%)	19,38,41	1.12	2 (10%)
1	C4J	2	930	1	24,29,30	0.65	1 (4%)	29,42,45	0.53	0
34	5MU	4	54	34	19,22,23	1.39	5 (26%)	28,32,35	2.06	7 (25%)
1	A2M	2	494	1	18,25,26	0.95	1 (5%)	18,36,39	1.31	2 (11%)

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	OMG	2	1061	1	-	0/5/27/28	0/3/3/3
1	5MC	2	1368	1	-	0/7/25/26	0/2/2/2
1	OMU	2	52	1	-	0/9/27/28	0/2/2/2
1	OMC	2	512	1	-	0/9/27/28	0/2/2/2
1	OMU	2	1032	1	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4AC	2	1467	1	-	0/11/29/30	0/2/2/2
1	OMC	2	246	1	-	4/9/27/28	0/2/2/2
1	OMC	2	538	1	-	0/9/27/28	0/2/2/2
1	OMC	2	113	1	-	0/9/27/28	0/2/2/2
34	H2U	4	20	34	-	3/7/38/39	0/2/2/2
1	6MZ	2	1457	1,36	-	0/5/27/28	0/3/3/3
1	MA6	2	1475	1	-	0/7/29/30	0/3/3/3
1	OMC	2	1060	1	-	0/9/27/28	0/2/2/2
1	OMG	2	1018	1	-	0/5/27/28	0/3/3/3
1	OMC	2	313	1	-	1/9/27/28	0/2/2/2
1	OMG	2	399	1	-	0/5/27/28	0/3/3/3
1	OMG	2	865	1	-	2/5/27/28	0/3/3/3
1	OMU	2	15	1	-	0/9/27/28	0/2/2/2
1	OMG	2	672	1	-	0/5/27/28	0/3/3/3
1	OMC	2	481	1	-	0/9/27/28	0/2/2/2
1	OMG	2	926	1	-	0/5/27/28	0/3/3/3
1	OMU	2	1344	1	-	0/9/27/28	0/2/2/2
1	OMG	2	546	1	-	0/5/27/28	0/3/3/3
1	4AC	2	1477	1	-	2/11/29/30	0/2/2/2
1	4AC	2	1466	1	-	0/11/29/30	0/2/2/2
1	OMC	2	1366	1	-	0/9/27/28	0/2/2/2
34	PSU	4	55	34	-	1/7/25/26	0/2/2/2
1	4AC	2	1478	1	-	0/11/29/30	0/2/2/2
1	OMG	2	337	1	-	1/5/27/28	0/3/3/3
34	OMC	4	32	34	-	3/9/27/28	0/2/2/2
1	OMC	2	710	1	-	0/9/27/28	0/2/2/2
34	4SU	4	8	34	-	0/7/25/26	0/2/2/2
1	OMG	2	1194	1	-	0/5/27/28	0/3/3/3
1	OMG	2	905	1	-	0/5/27/28	0/3/3/3
1	C4J	2	930	1	-	2/16/34/35	0/2/2/2
34	5MU	4	54	34	-	0/7/25/26	0/2/2/2
1	A2M	2	494	1	-	0/5/27/28	0/3/3/3

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	4	55	PSU	C6-C5	3.19	1.39	1.35
1	2	1478	4AC	C5-C4	2.83	1.46	1.40
1	2	15	OMU	C4-N3	-2.80	1.33	1.38
1	2	1467	4AC	C5-C4	2.76	1.46	1.40
1	2	337	OMG	C6-N1	-2.76	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1194	OMG	C6-N1	-2.75	1.33	1.37
1	2	1032	OMU	C4-N3	-2.75	1.33	1.38
1	2	672	OMG	C6-N1	-2.75	1.33	1.37
1	2	1466	4AC	C5-C4	2.73	1.46	1.40
1	2	52	OMU	C4-N3	-2.72	1.33	1.38
1	2	1018	OMG	C6-N1	-2.72	1.33	1.37
1	2	905	OMG	C6-N1	-2.71	1.33	1.37
1	2	1477	4AC	C5-C4	2.69	1.46	1.40
1	2	865	OMG	C6-N1	-2.68	1.33	1.37
1	2	399	OMG	C6-N1	-2.67	1.33	1.37
1	2	930	C4J	O4'-C1'	-2.67	1.40	1.43
34	4	55	PSU	C4-N3	-2.65	1.33	1.38
1	2	1061	OMG	C6-N1	-2.65	1.33	1.37
1	2	926	OMG	C6-N1	-2.64	1.33	1.37
1	2	1344	OMU	C4-N3	-2.64	1.33	1.38
34	4	54	5MU	C6-C5	2.60	1.38	1.34
1	2	1368	5MC	C6-C5	2.52	1.38	1.34
34	4	54	5MU	C4-N3	-2.51	1.34	1.38
1	2	15	OMU	C2-N3	-2.46	1.33	1.38
1	2	546	OMG	C6-N1	-2.44	1.34	1.37
1	2	1475	MA6	C5-C4	2.43	1.47	1.40
1	2	1457	6MZ	C5-C4	2.41	1.47	1.40
1	2	1032	OMU	C2-N3	-2.40	1.33	1.38
1	2	1368	5MC	C6-N1	-2.39	1.34	1.38
34	4	54	5MU	C4-C5	2.38	1.48	1.44
1	2	1467	4AC	C4-N3	-2.33	1.28	1.32
1	2	52	OMU	C2-N3	-2.31	1.33	1.38
1	2	494	A2M	C5-C4	2.29	1.47	1.40
1	2	1344	OMU	C2-N3	-2.28	1.33	1.38
34	4	54	5MU	C6-N1	-2.24	1.34	1.38
1	2	15	OMU	C5-C4	-2.24	1.38	1.43
1	2	1466	4AC	C4-N3	-2.23	1.28	1.32
1	2	1344	OMU	C5-C4	-2.23	1.38	1.43
34	4	54	5MU	C2-N1	2.22	1.42	1.38
1	2	1478	4AC	C4-N3	-2.18	1.29	1.32
1	2	52	OMU	C5-C4	-2.14	1.38	1.43
1	2	1032	OMU	C5-C4	-2.12	1.39	1.43
1	2	1477	4AC	C4-N3	-2.09	1.29	1.32

All (80) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1457	6MZ	C2-N1-C6	7.05	122.63	116.59
34	4	55	PSU	N1-C2-N3	5.84	121.75	115.13
34	4	54	5MU	C4-N3-C2	-5.01	120.87	127.35
34	4	54	5MU	N3-C2-N1	4.71	121.14	114.89
1	2	15	OMU	C4-N3-C2	-4.61	120.50	126.58
1	2	1477	4AC	O7-C7-N4	4.58	129.22	121.82
1	2	1032	OMU	C4-N3-C2	-4.53	120.61	126.58
1	2	1467	4AC	O7-C7-N4	4.45	129.03	121.82
1	2	52	OMU	C4-N3-C2	-4.45	120.71	126.58
1	2	1478	4AC	O7-C7-N4	4.44	129.01	121.82
1	2	1466	4AC	O7-C7-N4	4.37	128.90	121.82
1	2	1344	OMU	C4-N3-C2	-4.32	120.89	126.58
34	4	54	5MU	C5-C4-N3	4.31	118.99	115.31
1	2	1032	OMU	N3-C2-N1	4.07	120.30	114.89
1	2	52	OMU	N3-C2-N1	4.05	120.27	114.89
1	2	1344	OMU	N3-C2-N1	4.03	120.23	114.89
34	4	55	PSU	C4-N3-C2	-3.99	120.59	126.34
1	2	15	OMU	C5-C4-N3	3.96	120.76	114.84
34	4	54	5MU	O4-C4-C5	-3.86	120.43	124.90
1	2	15	OMU	N3-C2-N1	3.84	119.99	114.89
1	2	1032	OMU	C5-C4-N3	3.69	120.36	114.84
1	2	52	OMU	C5-C4-N3	3.68	120.34	114.84
1	2	1477	4AC	N4-C4-N3	3.58	119.86	113.85
1	2	1344	OMU	C5-C4-N3	3.56	120.16	114.84
34	4	54	5MU	C5-C6-N1	-3.51	119.72	123.34
1	2	1457	6MZ	C4-C5-N7	-3.40	105.85	109.40
1	2	1477	4AC	C5-C4-N4	-3.38	117.05	122.92
1	2	1457	6MZ	N3-C2-N1	-3.34	123.45	128.68
1	2	1475	MA6	C4-C5-N7	-3.26	106.00	109.40
1	2	494	A2M	N3-C2-N1	-3.26	123.59	128.68
1	2	1475	MA6	N3-C2-N1	-3.23	123.63	128.68
34	4	55	PSU	O2-C2-N1	-3.19	119.27	122.79
1	2	15	OMU	O4-C4-C5	-3.17	119.58	125.16
1	2	1467	4AC	CM7-C7-N4	-3.12	109.89	115.29
1	2	1344	OMU	O4-C4-C5	-3.05	119.80	125.16
1	2	1478	4AC	N4-C4-N3	3.00	118.88	113.85
1	2	1032	OMU	O4-C4-C5	-2.98	119.92	125.16
1	2	1467	4AC	C5-C4-N4	-2.98	117.75	122.92
1	2	52	OMU	O4-C4-C5	-2.97	119.94	125.16
1	2	1368	5MC	C5-C6-N1	-2.96	120.29	123.34
1	2	1478	4AC	C5-C4-N4	-2.96	117.78	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1466	4AC	N4-C4-N3	2.89	118.71	113.85
1	2	1466	4AC	C5-C4-N4	-2.88	117.91	122.92
1	2	1467	4AC	N4-C4-N3	2.84	118.62	113.85
1	2	1478	4AC	CM7-C7-N4	-2.81	110.43	115.29
1	2	1466	4AC	CM7-C7-N4	-2.74	110.56	115.29
1	2	1368	5MC	C5-C4-N3	-2.70	118.76	121.67
34	4	32	OMC	O2-C2-N3	-2.65	118.02	122.33
1	2	1477	4AC	CM7-C7-N4	-2.61	110.78	115.29
1	2	246	OMC	O2-C2-N3	-2.57	118.15	122.33
1	2	313	OMC	O2-C2-N3	-2.51	118.25	122.33
1	2	494	A2M	C4-C5-N7	-2.49	106.80	109.40
1	2	1194	OMG	C5-C6-N1	2.47	118.32	113.95
1	2	926	OMG	C5-C6-N1	2.47	118.31	113.95
1	2	481	OMC	O2-C2-N3	-2.41	118.42	122.33
1	2	905	OMG	C5-C6-N1	2.40	118.19	113.95
1	2	337	OMG	C5-C6-N1	2.38	118.16	113.95
1	2	672	OMG	C5-C6-N1	2.35	118.11	113.95
1	2	905	OMG	C8-N7-C5	2.35	107.47	102.99
1	2	926	OMG	C8-N7-C5	2.35	107.47	102.99
1	2	1194	OMG	C8-N7-C5	2.35	107.46	102.99
1	2	337	OMG	C8-N7-C5	2.34	107.45	102.99
1	2	546	OMG	C8-N7-C5	2.34	107.44	102.99
1	2	865	OMG	C5-C6-N1	2.33	118.06	113.95
1	2	399	OMG	C8-N7-C5	2.31	107.39	102.99
1	2	399	OMG	C5-C6-N1	2.31	118.03	113.95
1	2	546	OMG	C5-C6-N1	2.31	118.03	113.95
1	2	1061	OMG	C5-C6-N1	2.30	118.02	113.95
1	2	1018	OMG	C5-C6-N1	2.30	118.01	113.95
1	2	672	OMG	C8-N7-C5	2.30	107.36	102.99
1	2	1018	OMG	C8-N7-C5	2.29	107.35	102.99
1	2	1061	OMG	C8-N7-C5	2.29	107.35	102.99
1	2	865	OMG	C8-N7-C5	2.28	107.33	102.99
34	4	54	5MU	O2-C2-N1	-2.26	119.78	122.79
34	4	32	OMC	C1'-N1-C2	2.23	123.41	118.42
1	2	1477	4AC	C1'-N1-C2	2.21	123.35	118.42
1	2	710	OMC	O2-C2-N3	-2.11	118.90	122.33
34	4	54	5MU	C5M-C5-C4	2.11	121.09	118.77
1	2	1344	OMU	O2-C2-N1	-2.05	120.06	122.79
1	2	1368	5MC	O2-C2-N3	-2.04	119.01	122.33

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	246	OMC	C3'-C4'-C5'-O5'
34	4	20	H2U	O4'-C1'-N1-C6
1	2	930	C4J	C4'-C5'-O5'-P
1	2	246	OMC	O4'-C4'-C5'-O5'
34	4	20	H2U	O4'-C1'-N1-C2
1	2	930	C4J	C3'-C4'-C5'-O5'
1	2	865	OMG	C4'-C5'-O5'-P
34	4	20	H2U	C4'-C5'-O5'-P
34	4	32	OMC	C3'-C2'-O2'-CM2
1	2	337	OMG	C4'-C5'-O5'-P
1	2	865	OMG	C3'-C4'-C5'-O5'
34	4	32	OMC	C2'-C1'-N1-C6
34	4	55	PSU	O4'-C1'-C5-C4
1	2	313	OMC	C2'-C1'-N1-C2
1	2	246	OMC	C2'-C1'-N1-C2
34	4	32	OMC	C2'-C1'-N1-C2
1	2	1477	4AC	C2'-C1'-N1-C2
1	2	246	OMC	C3'-C2'-O2'-CM2
1	2	1477	4AC	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 108 ligands modelled in this entry, 66 are monoatomic - leaving 42 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	1565	-	13,13,13	0.10	0	12,12,12	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	SPM	2	1574	-	13,13,13	0.10	0	12,12,12	0.11	0
37	SPM	2	1584	1	13,13,13	0.11	0	12,12,12	0.13	0
37	SPM	2	1564	-	13,13,13	0.09	0	12,12,12	0.08	0
37	SPM	2	1589	-	13,13,13	0.10	0	12,12,12	0.12	0
37	SPM	2	1562	-	13,13,13	0.09	0	12,12,12	0.10	0
37	SPM	2	1572	-	13,13,13	0.11	0	12,12,12	0.09	0
37	SPM	2	1580	-	13,13,13	0.11	0	12,12,12	0.09	0
37	SPM	2	1573	-	13,13,13	0.10	0	12,12,12	0.09	0
37	SPM	2	1558	-	13,13,13	0.07	0	12,12,12	0.12	0
37	SPM	2	1577	-	13,13,13	0.11	0	12,12,12	0.10	0
37	SPM	2	1593	-	13,13,13	0.12	0	12,12,12	0.09	0
37	SPM	2	1586	-	13,13,13	0.10	0	12,12,12	0.10	0
37	SPM	2	1554	-	13,13,13	0.07	0	12,12,12	0.11	0
37	SPM	2	1568	-	13,13,13	0.09	0	12,12,12	0.11	0
37	SPM	2	1594	-	13,13,13	0.10	0	12,12,12	0.06	0
37	SPM	2	1560	-	13,13,13	0.08	0	12,12,12	0.12	0
37	SPM	2	1583	-	13,13,13	0.09	0	12,12,12	0.08	0
37	SPM	2	1555	-	13,13,13	0.11	0	12,12,12	0.09	0
37	SPM	2	1559	-	13,13,13	0.08	0	12,12,12	0.07	0
37	SPM	2	1592	-	13,13,13	0.11	0	12,12,12	0.07	0
37	SPM	2	1570	-	13,13,13	0.09	0	12,12,12	0.09	0
37	SPM	2	1563	-	13,13,13	0.08	0	12,12,12	0.10	0
37	SPM	2	1569	-	13,13,13	0.06	0	12,12,12	0.15	0
37	SPM	2	1582	-	13,13,13	0.11	0	12,12,12	0.12	0
37	SPM	2	1567	-	13,13,13	0.10	0	12,12,12	0.07	0
37	SPM	2	1581	-	13,13,13	0.11	0	12,12,12	0.06	0
37	SPM	2	1575	-	13,13,13	0.10	0	12,12,12	0.08	0
37	SPM	2	1587	-	13,13,13	0.10	0	12,12,12	0.09	0
37	SPM	2	1588	-	13,13,13	0.12	0	12,12,12	0.10	0
37	SPM	2	1576	-	13,13,13	0.07	0	12,12,12	0.12	0
37	SPM	2	1578	-	13,13,13	0.11	0	12,12,12	0.07	0
37	SPM	2	1585	-	13,13,13	0.12	0	12,12,12	0.11	0
37	SPM	2	1571	-	13,13,13	0.09	0	12,12,12	0.11	0
37	SPM	2	1566	-	13,13,13	0.11	0	12,12,12	0.10	0
37	SPM	2	1595	-	13,13,13	0.10	0	12,12,12	0.13	0
37	SPM	2	1590	-	13,13,13	0.11	0	12,12,12	0.08	0
37	SPM	2	1556	-	13,13,13	0.09	0	12,12,12	0.13	0
37	SPM	2	1591	-	13,13,13	0.11	0	12,12,12	0.08	0
37	SPM	2	1579	-	13,13,13	0.08	0	12,12,12	0.11	0
37	SPM	2	1557	-	13,13,13	0.10	0	12,12,12	0.08	0
37	SPM	2	1561	-	13,13,13	0.09	0	12,12,12	0.10	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	SPM	2	1565	-	-	4/11/11/11	-
37	SPM	2	1574	-	-	2/11/11/11	-
37	SPM	2	1584	1	-	4/11/11/11	-
37	SPM	2	1564	-	-	3/11/11/11	-
37	SPM	2	1589	-	-	1/11/11/11	-
37	SPM	2	1562	-	-	2/11/11/11	-
37	SPM	2	1572	-	-	4/11/11/11	-
37	SPM	2	1580	-	-	1/11/11/11	-
37	SPM	2	1573	-	-	4/11/11/11	-
37	SPM	2	1558	-	-	2/11/11/11	-
37	SPM	2	1577	-	-	4/11/11/11	-
37	SPM	2	1593	-	-	1/11/11/11	-
37	SPM	2	1586	-	-	1/11/11/11	-
37	SPM	2	1554	-	-	2/11/11/11	-
37	SPM	2	1568	-	-	0/11/11/11	-
37	SPM	2	1594	-	-	4/11/11/11	-
37	SPM	2	1560	-	-	1/11/11/11	-
37	SPM	2	1583	-	-	2/11/11/11	-
37	SPM	2	1555	-	-	3/11/11/11	-
37	SPM	2	1559	-	-	4/11/11/11	-
37	SPM	2	1592	-	-	1/11/11/11	-
37	SPM	2	1570	-	-	5/11/11/11	-
37	SPM	2	1563	-	-	2/11/11/11	-
37	SPM	2	1569	-	-	1/11/11/11	-
37	SPM	2	1582	-	-	2/11/11/11	-
37	SPM	2	1567	-	-	3/11/11/11	-
37	SPM	2	1581	-	-	2/11/11/11	-
37	SPM	2	1575	-	-	3/11/11/11	-
37	SPM	2	1587	-	-	3/11/11/11	-
37	SPM	2	1588	-	-	4/11/11/11	-
37	SPM	2	1576	-	-	3/11/11/11	-
37	SPM	2	1578	-	-	3/11/11/11	-
37	SPM	2	1585	-	-	4/11/11/11	-
37	SPM	2	1571	-	-	3/11/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	SPM	2	1566	-	-	1/11/11/11	-
37	SPM	2	1595	-	-	5/11/11/11	-
37	SPM	2	1590	-	-	2/11/11/11	-
37	SPM	2	1556	-	-	3/11/11/11	-
37	SPM	2	1591	-	-	1/11/11/11	-
37	SPM	2	1579	-	-	3/11/11/11	-
37	SPM	2	1557	-	-	3/11/11/11	-
37	SPM	2	1561	-	-	3/11/11/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (109) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
37	2	1562	SPM	C12-C11-N10-C9
37	2	1571	SPM	C7-C6-N5-C4
37	2	1577	SPM	C3-C4-N5-C6
37	2	1577	SPM	C12-C11-N10-C9
37	2	1554	SPM	C8-C9-N10-C11
37	2	1555	SPM	C12-C11-N10-C9
37	2	1571	SPM	C3-C4-N5-C6
37	2	1572	SPM	C7-C6-N5-C4
37	2	1572	SPM	C12-C11-N10-C9
37	2	1574	SPM	C7-C6-N5-C4
37	2	1575	SPM	C7-C6-N5-C4
37	2	1585	SPM	C7-C6-N5-C4
37	2	1587	SPM	C3-C4-N5-C6
37	2	1588	SPM	C3-C4-N5-C6
37	2	1594	SPM	C3-C4-N5-C6
37	2	1595	SPM	C12-C11-N10-C9
37	2	1557	SPM	C3-C4-N5-C6
37	2	1560	SPM	C12-C11-N10-C9
37	2	1562	SPM	C8-C9-N10-C11
37	2	1563	SPM	C3-C4-N5-C6
37	2	1576	SPM	C7-C6-N5-C4
37	2	1578	SPM	C3-C4-N5-C6
37	2	1578	SPM	C8-C9-N10-C11
37	2	1579	SPM	C12-C11-N10-C9

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Mol	Chain	Res	Type	Atoms
37	2	1582	SPM	C3-C4-N5-C6
37	2	1583	SPM	C3-C4-N5-C6
37	2	1588	SPM	C12-C11-N10-C9
37	2	1590	SPM	C7-C6-N5-C4
37	2	1592	SPM	C3-C4-N5-C6
37	2	1595	SPM	N5-C6-C7-C8
37	2	1556	SPM	C12-C11-N10-C9
37	2	1557	SPM	C8-C9-N10-C11
37	2	1577	SPM	C7-C6-N5-C4
37	2	1581	SPM	C3-C4-N5-C6
37	2	1586	SPM	C7-C6-N5-C4
37	2	1555	SPM	C3-C4-N5-C6
37	2	1559	SPM	C12-C11-N10-C9
37	2	1565	SPM	C7-C6-N5-C4
37	2	1574	SPM	C3-C4-N5-C6
37	2	1575	SPM	C8-C9-N10-C11
37	2	1580	SPM	C7-C6-N5-C4
37	2	1583	SPM	C12-C11-N10-C9
37	2	1588	SPM	C7-C6-N5-C4
37	2	1594	SPM	C7-C6-N5-C4
37	2	1559	SPM	C3-C4-N5-C6
37	2	1559	SPM	C7-C6-N5-C4
37	2	1590	SPM	C12-C11-N10-C9
37	2	1573	SPM	C6-C7-C8-C9
37	2	1567	SPM	C8-C9-N10-C11
37	2	1556	SPM	C8-C9-N10-C11
37	2	1563	SPM	C7-C6-N5-C4
37	2	1564	SPM	C7-C6-N5-C4
37	2	1565	SPM	C3-C4-N5-C6
37	2	1570	SPM	C3-C4-N5-C6
37	2	1573	SPM	C12-C11-N10-C9
37	2	1577	SPM	C8-C9-N10-C11
37	2	1582	SPM	C7-C6-N5-C4
37	2	1595	SPM	C3-C4-N5-C6
37	2	1561	SPM	C7-C6-N5-C4
37	2	1573	SPM	C7-C8-C9-N10
37	2	1576	SPM	C6-C7-C8-C9
37	2	1556	SPM	C3-C4-N5-C6
37	2	1564	SPM	C3-C4-N5-C6
37	2	1570	SPM	C7-C6-N5-C4
37	2	1573	SPM	C3-C4-N5-C6
37	2	1576	SPM	C8-C9-N10-C11

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Mol	Chain	Res	Type	Atoms
37	2	1570	SPM	N10-C11-C12-C13
37	2	1557	SPM	C7-C6-N5-C4
37	2	1565	SPM	C12-C11-N10-C9
37	2	1587	SPM	C7-C6-N5-C4
37	2	1565	SPM	C8-C9-N10-C11
37	2	1585	SPM	C3-C4-N5-C6
37	2	1585	SPM	C8-C9-N10-C11
37	2	1587	SPM	C8-C9-N10-C11
37	2	1595	SPM	C8-C9-N10-C11
37	2	1566	SPM	C8-C9-N10-C11
37	2	1567	SPM	C7-C6-N5-C4
37	2	1579	SPM	C3-C4-N5-C6
37	2	1584	SPM	C7-C6-N5-C4
37	2	1591	SPM	C3-C4-N5-C6
37	2	1594	SPM	C12-C11-N10-C9
37	2	1589	SPM	C6-C7-C8-C9
37	2	1558	SPM	C8-C9-N10-C11
37	2	1561	SPM	C3-C4-N5-C6
37	2	1569	SPM	C3-C4-N5-C6
37	2	1570	SPM	C8-C9-N10-C11
37	2	1579	SPM	C7-C6-N5-C4
37	2	1585	SPM	C6-C7-C8-C9
37	2	1554	SPM	C12-C11-N10-C9
37	2	1567	SPM	C12-C11-N10-C9
37	2	1595	SPM	C6-C7-C8-C9
37	2	1561	SPM	C12-C11-N10-C9
37	2	1578	SPM	C12-C11-N10-C9
37	2	1593	SPM	C7-C6-N5-C4
37	2	1559	SPM	C6-C7-C8-C9
37	2	1555	SPM	C8-C9-N10-C11
37	2	1564	SPM	C8-C9-N10-C11
37	2	1572	SPM	C3-C4-N5-C6
37	2	1584	SPM	C6-C7-C8-C9
37	2	1558	SPM	C7-C6-N5-C4
37	2	1570	SPM	C12-C11-N10-C9
37	2	1575	SPM	C12-C11-N10-C9
37	2	1584	SPM	C3-C4-N5-C6
37	2	1584	SPM	C8-C9-N10-C11
37	2	1588	SPM	C8-C9-N10-C11
37	2	1594	SPM	C6-C7-C8-C9
37	2	1581	SPM	C8-C9-N10-C11
37	2	1571	SPM	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
37	2	1572	SPM	C6-C7-C8-C9

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

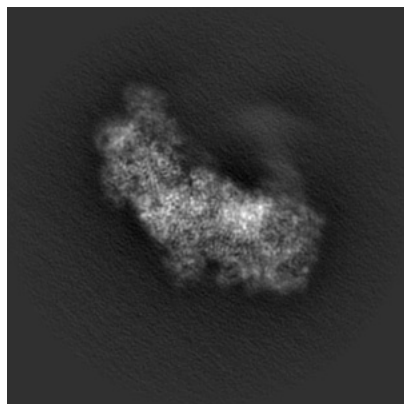
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50709. These allow visual inspection of the internal detail of the map and identification of artifacts.

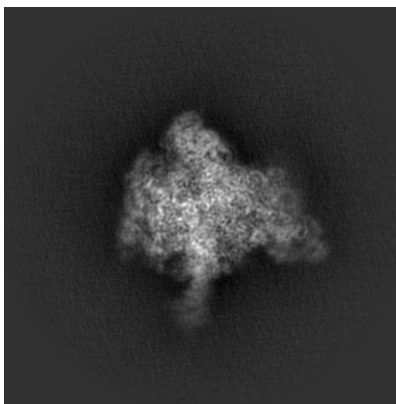
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

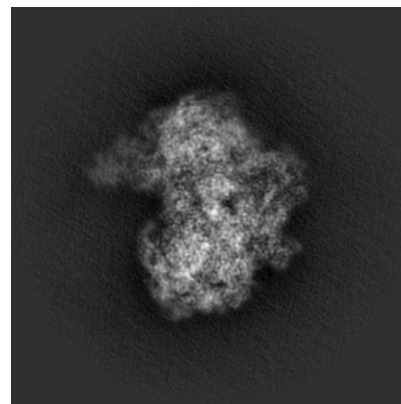
6.1.1 Primary map



X

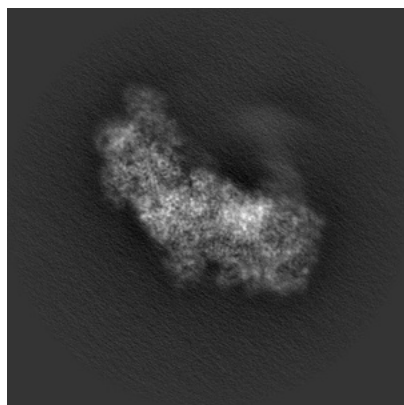


Y

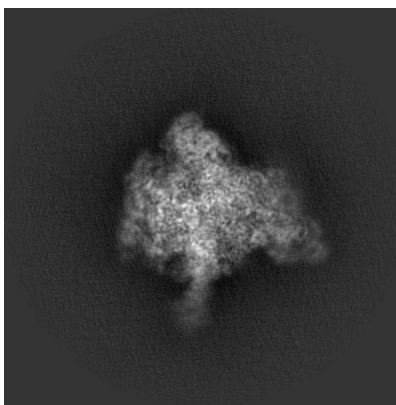


Z

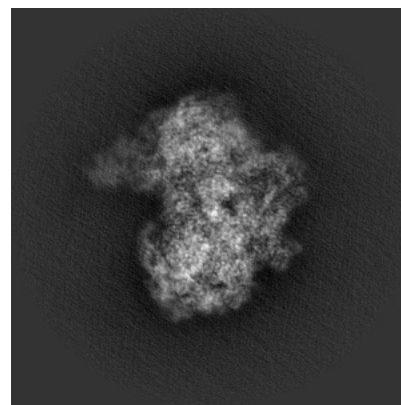
6.1.2 Raw map



X



Y

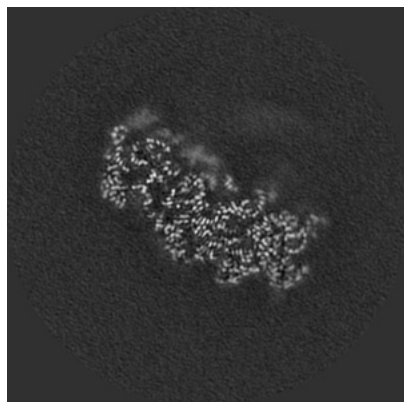


Z

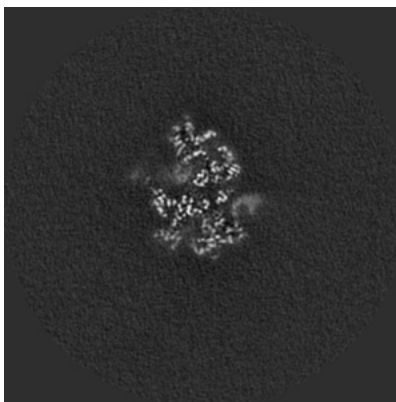
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

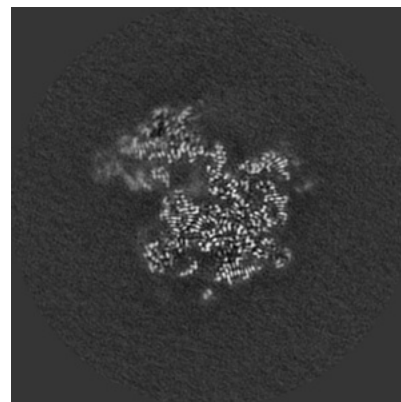
6.2.1 Primary map



X Index: 219

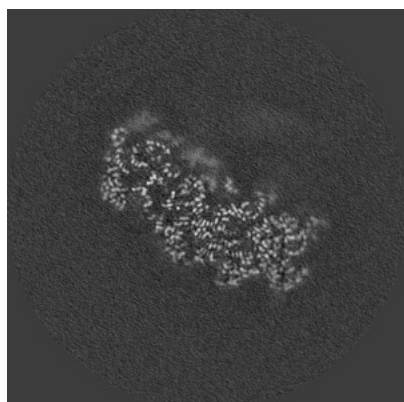


Y Index: 219

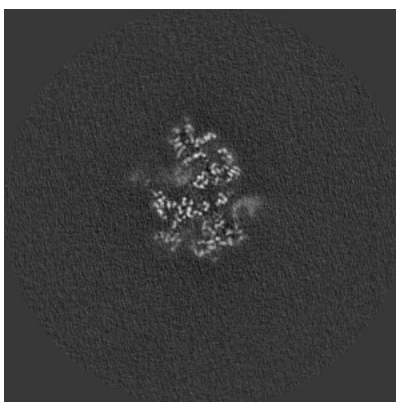


Z Index: 219

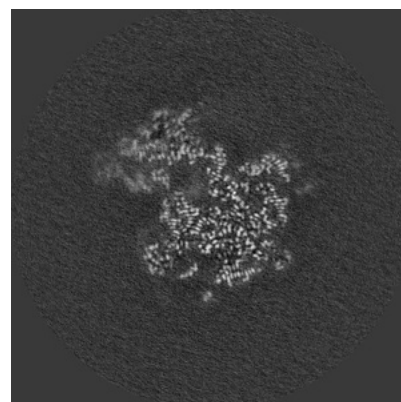
6.2.2 Raw map



X Index: 219



Y Index: 219

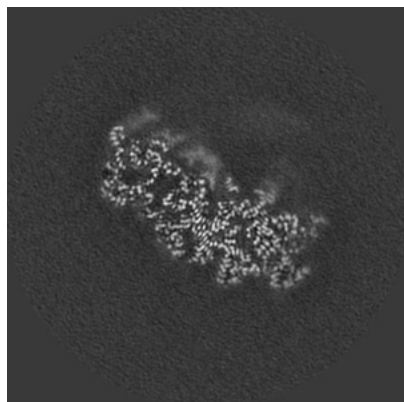


Z Index: 219

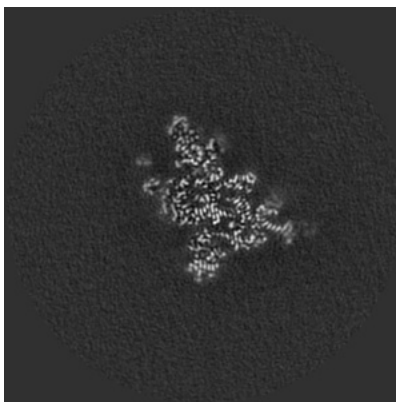
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

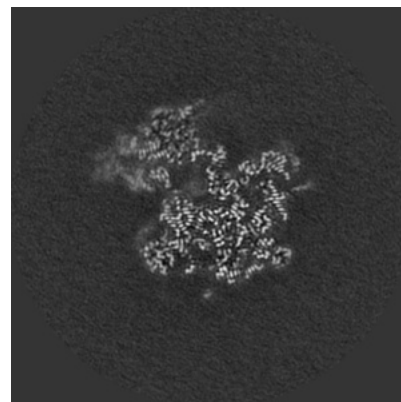
6.3.1 Primary map



X Index: 221

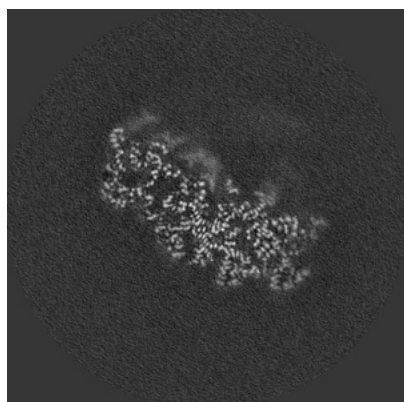


Y Index: 176

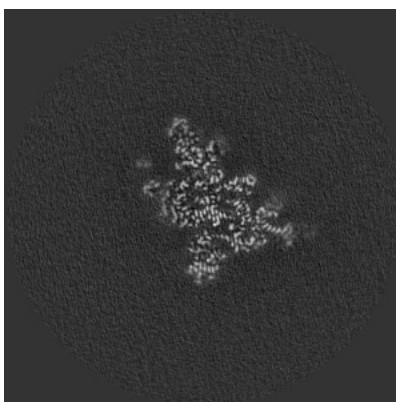


Z Index: 217

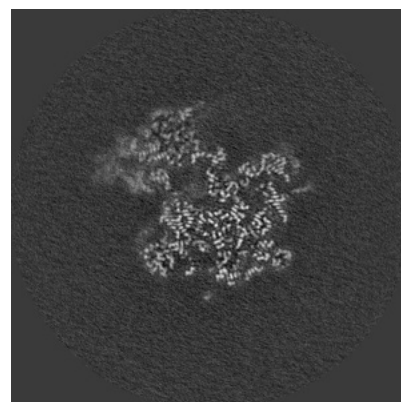
6.3.2 Raw map



X Index: 221



Y Index: 176



Z Index: 217

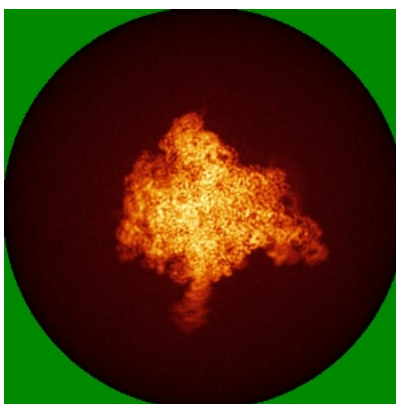
The images above show the largest variance slices of the map in three orthogonal directions.

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

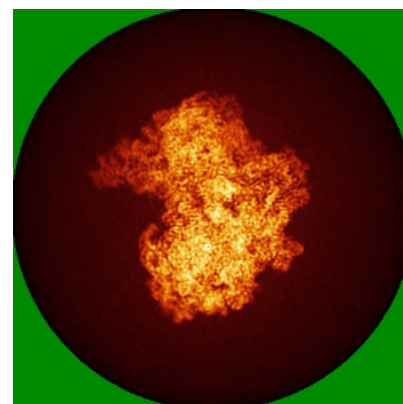
6.4.1 Primary map



X

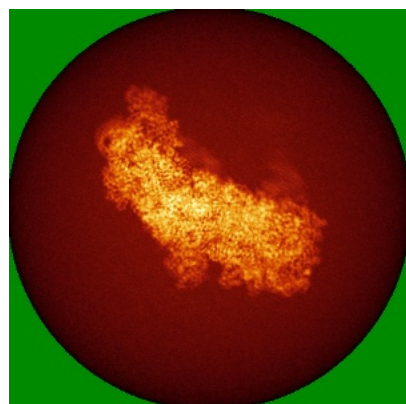


Y

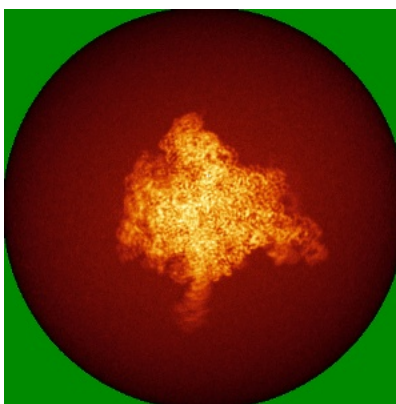


Z

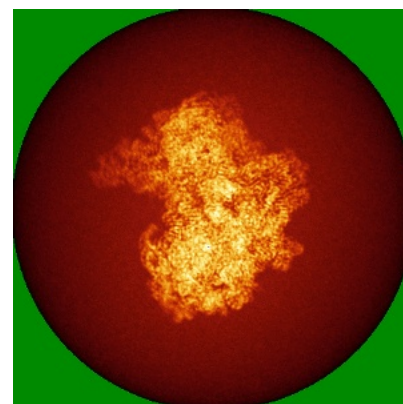
6.4.2 Raw map



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



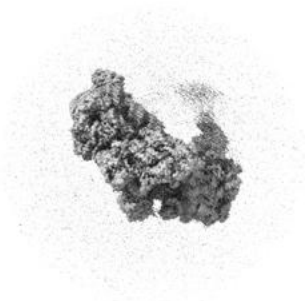
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.006. 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.

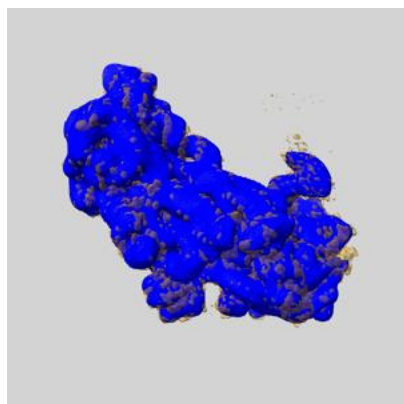
6.6 Mask visualisation [i](#)

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

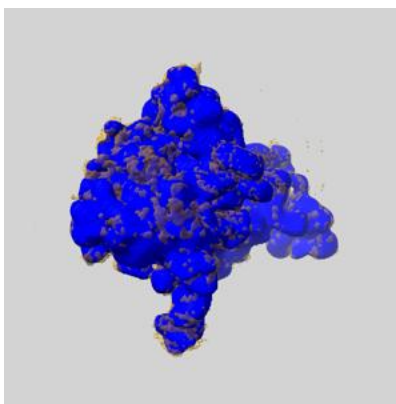
A mask typically either:

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

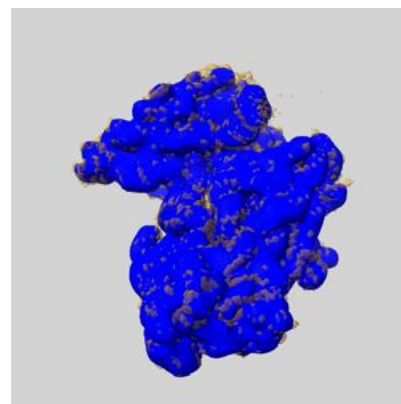
6.6.1 emd_50709_msk_1.map [i](#)



X



Y

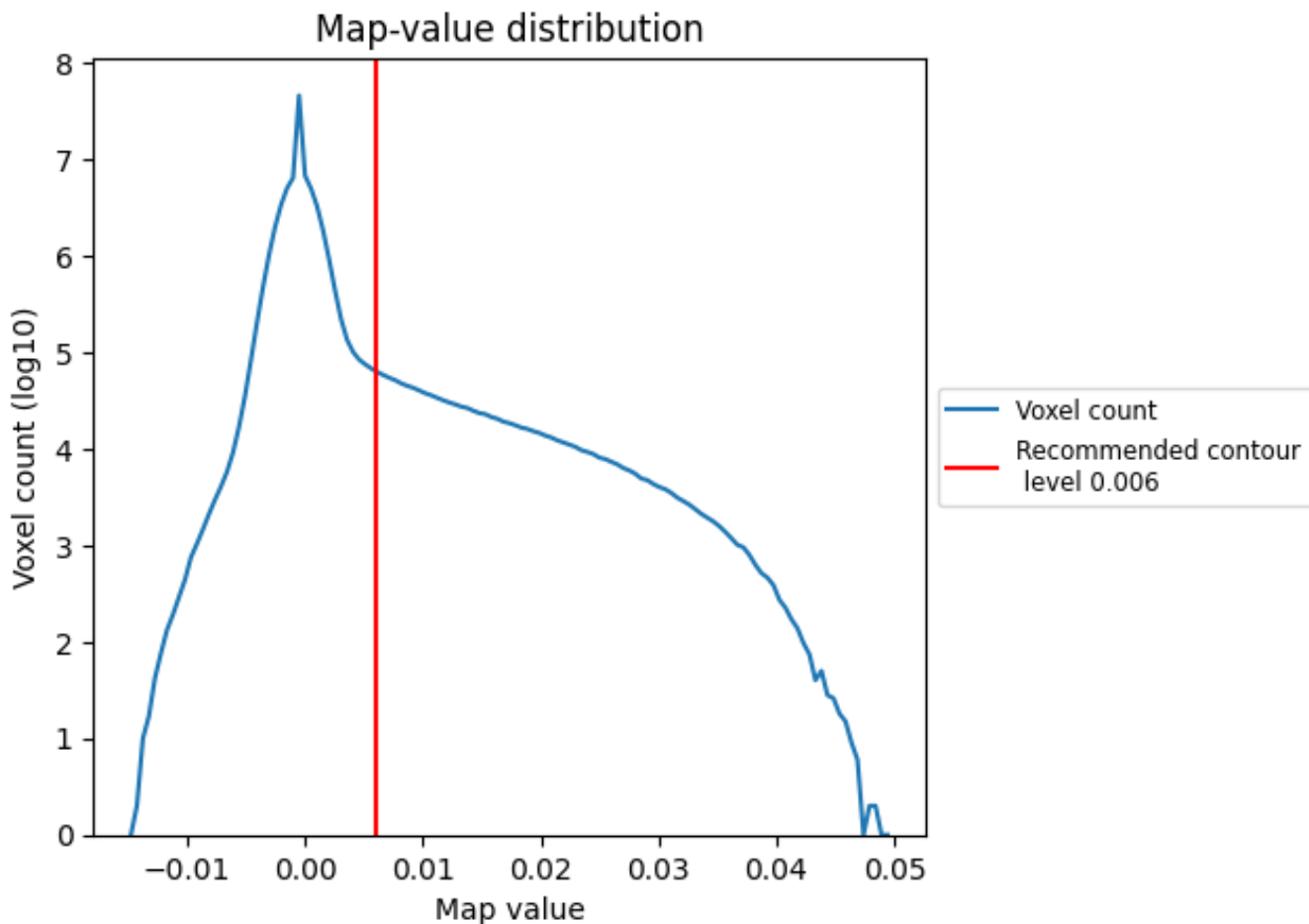


Z

7 Map analysis [i](#)

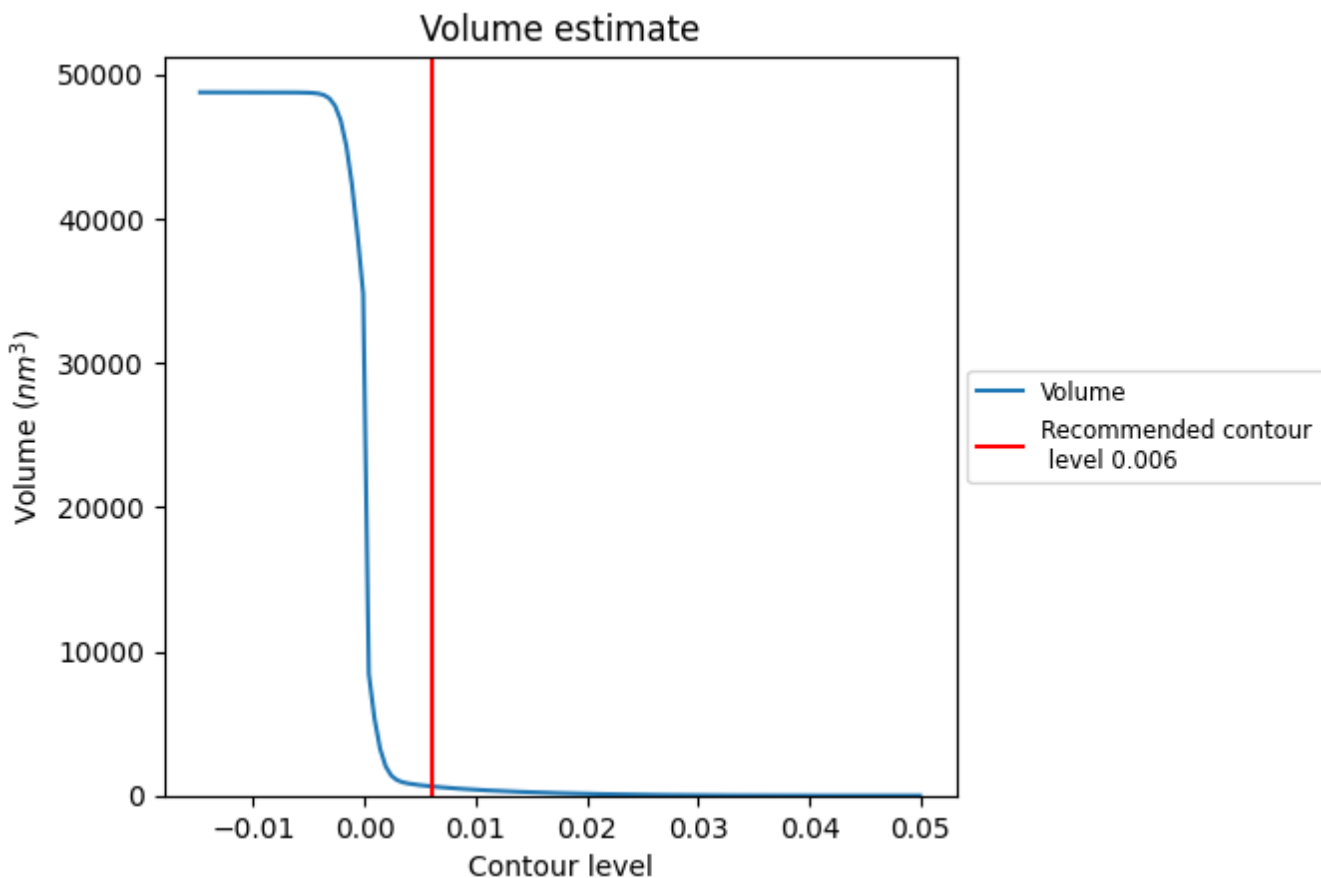
This section contains the results of statistical analysis of the map.

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.

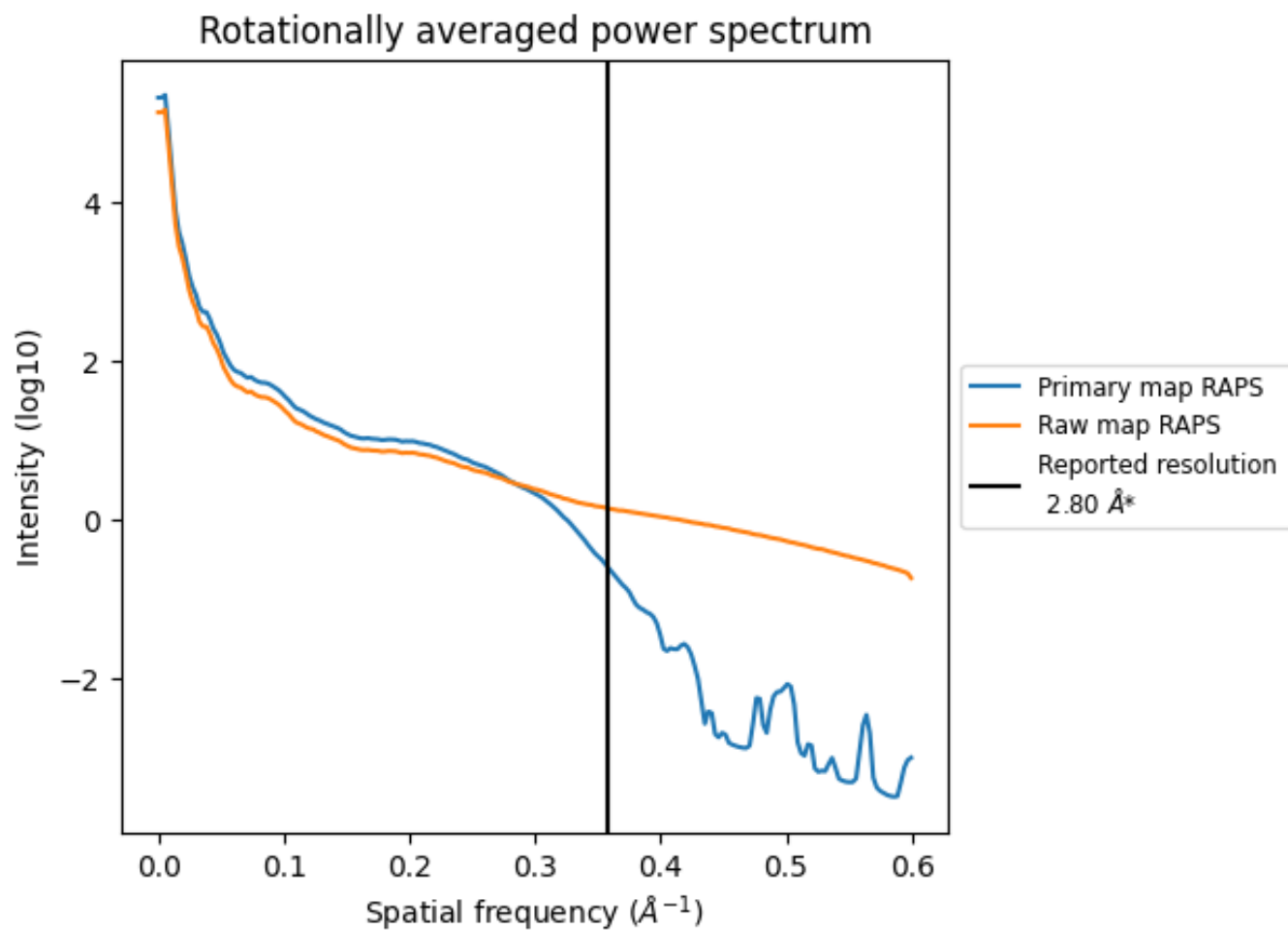
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 638 nm³; this corresponds to an approximate mass of 576 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 i

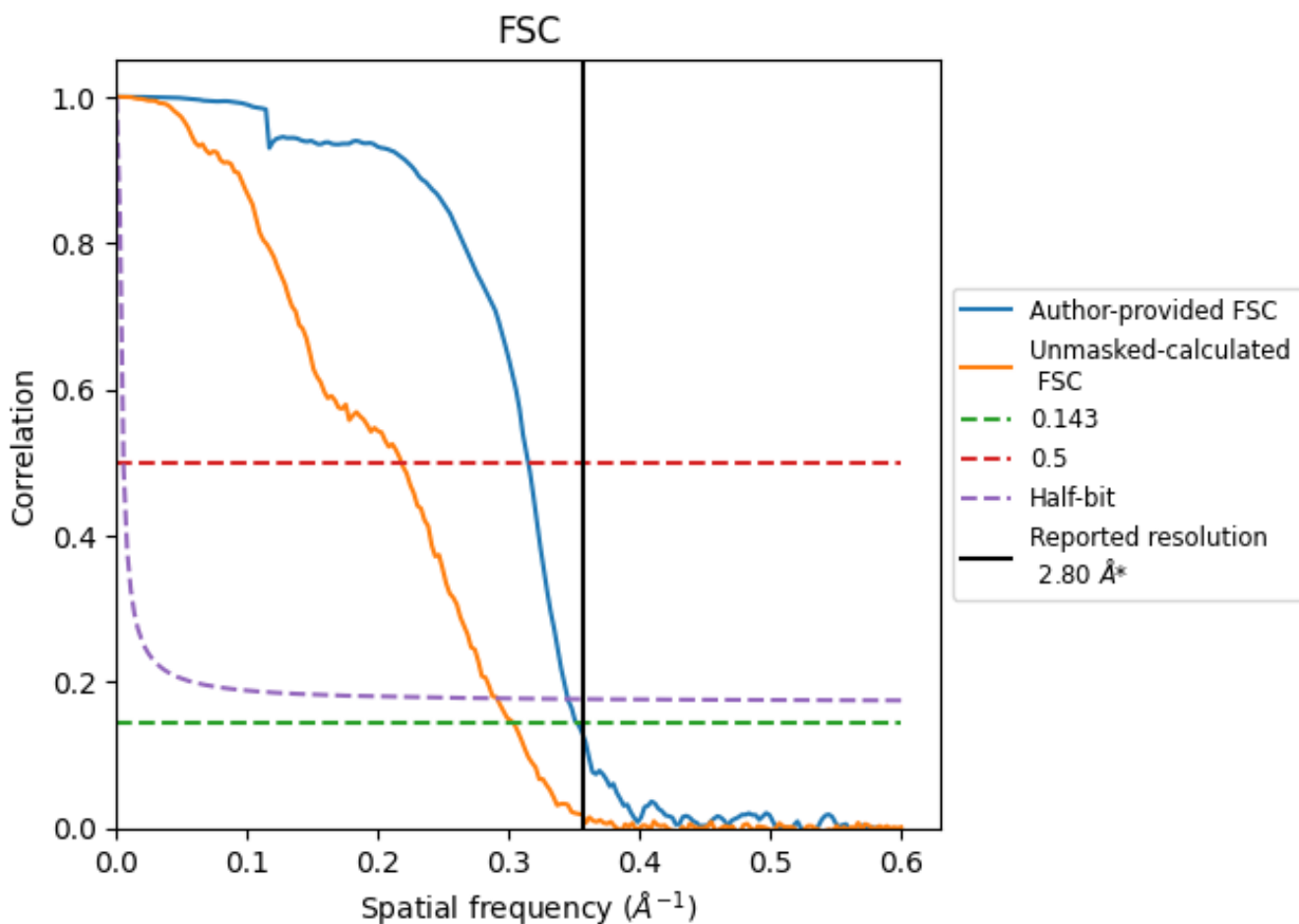


*Reported resolution corresponds to spatial frequency of 0.357 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

8.2 Resolution estimates [i](#)

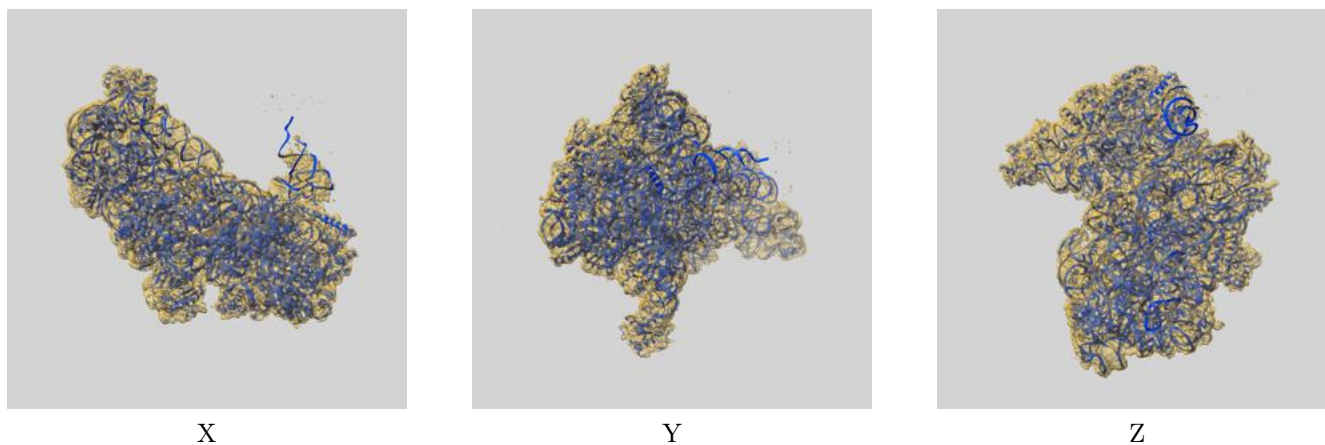
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.84	3.18	2.90
Unmasked-calculated*	3.30	4.59	3.44

*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 3.30 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

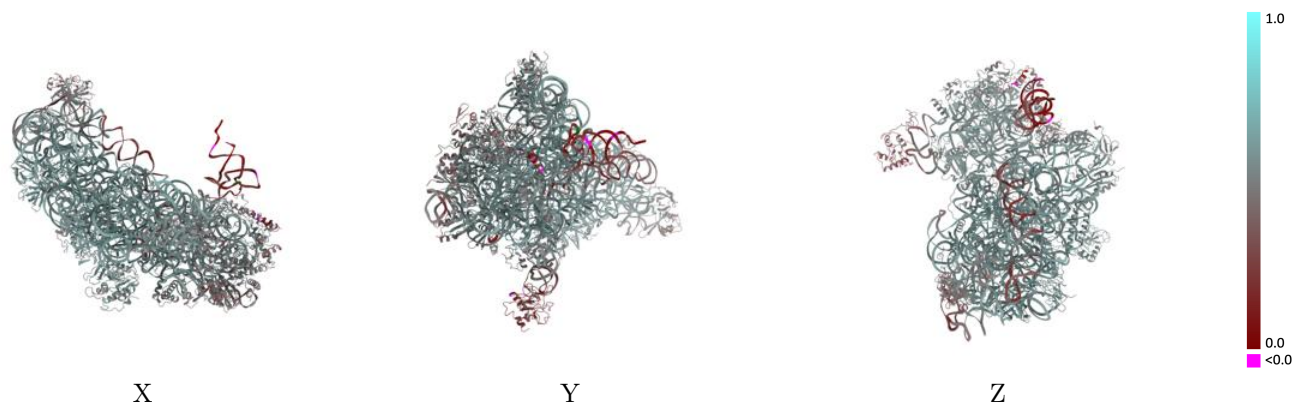
This section contains information regarding the fit between EMDB map EMD-50709 and PDB model 9FRA. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



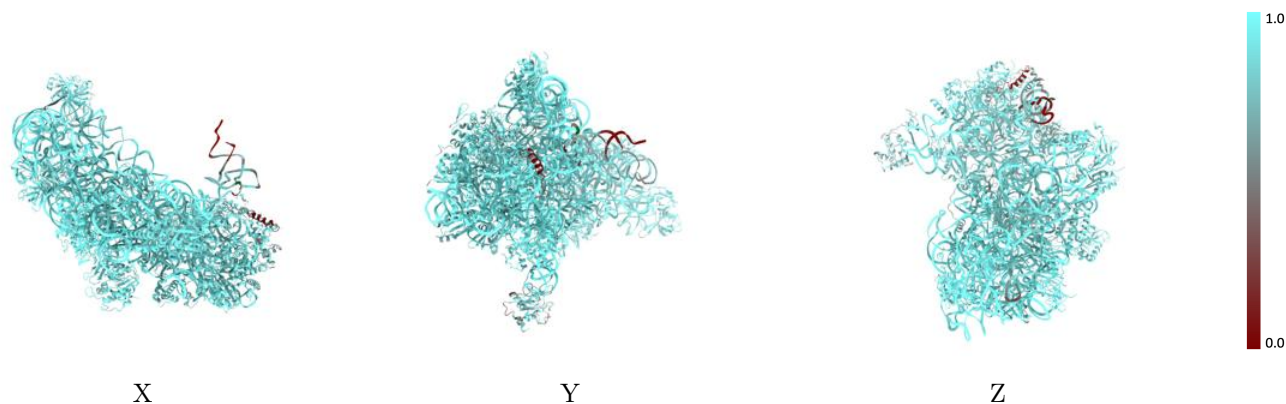
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



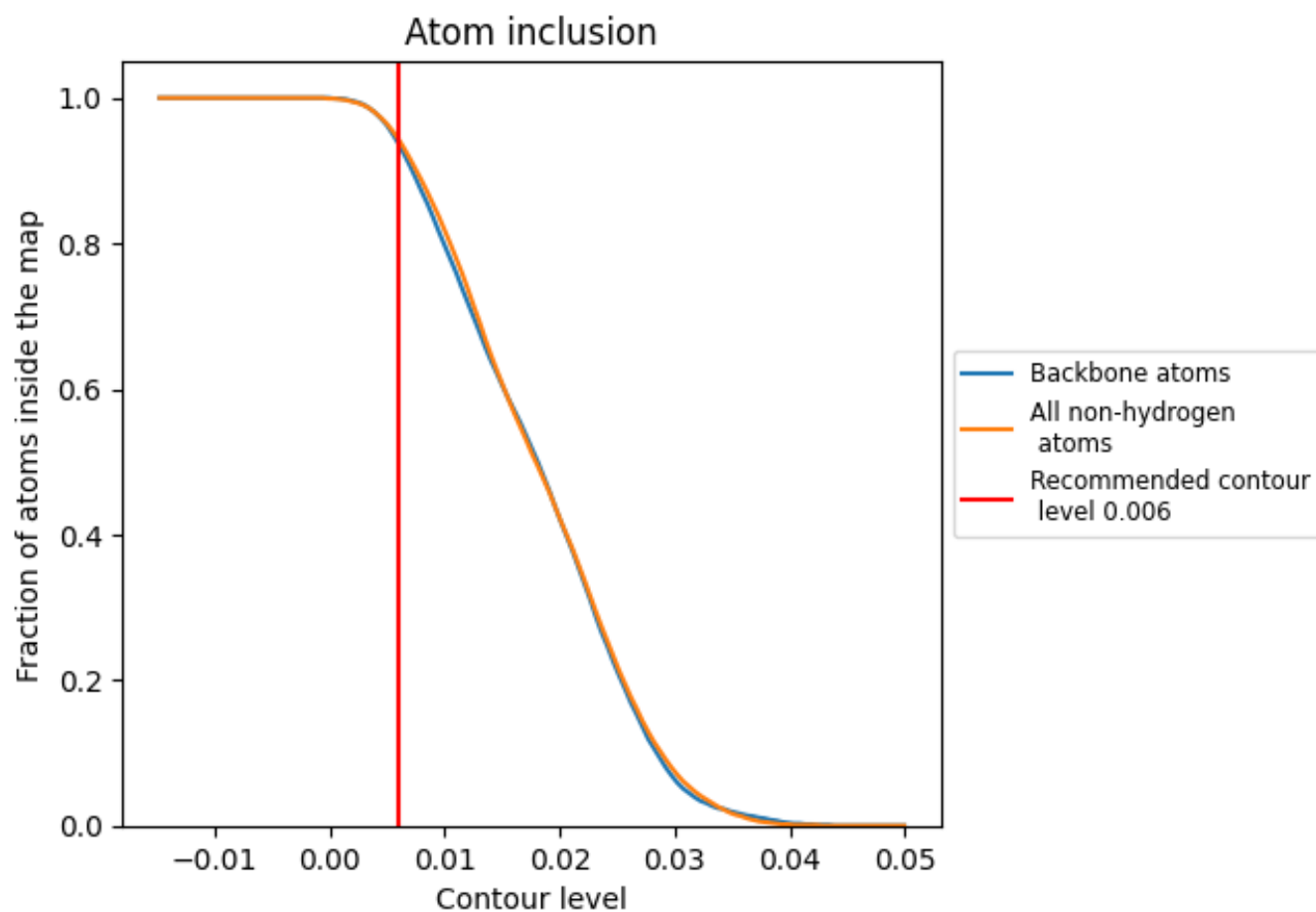
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.006).









































































9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 94% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9430	 0.5330
2	 0.9850	 0.5580
3	 0.6710	 0.2530
4	 0.6830	 0.2520
5	 0.5970	 0.3660
A	 0.9450	 0.5280
B	 0.9240	 0.5430
C	 0.9600	 0.5740
D	 0.9670	 0.5800
E	 0.9700	 0.5840
F	 0.9660	 0.5880
G	 0.9100	 0.4540
H	 0.9020	 0.4940
I	 0.9760	 0.6000
J	 0.9670	 0.5700
K	 0.9510	 0.5230
L	 0.8990	 0.5110
M	 0.9440	 0.5370
N	 0.9630	 0.5820
O	 0.9440	 0.5230
P	 0.9790	 0.5870
Q	 0.9560	 0.5630
R	 0.9730	 0.5950
S	 0.9310	 0.5170
T	 0.9130	 0.5180
U	 0.9430	 0.5230
V	 0.9470	 0.5600
W	 0.9780	 0.5640
X	 0.8970	 0.4650
Y	 0.7120	 0.2570
Z	 0.9380	 0.5450
a	 0.9580	 0.5300
c	 0.5710	 0.3810
d	 0.8480	 0.4180
e	 0.7490	 0.5440
s	 0.7770	 0.2740

