



Full wwPDB EM Validation Report ⓘ

Jan 8, 2025 – 01:25 pm GMT

PDB ID : 9FS6
EMDB ID : EMD-50724
Title : Cryo-EM structure of *Saccharolobus solfataricus* 30S initiation complex bound to Ss-aIF2beta leaderless mRNA with h44 in up position
Authors : Bourgeois, G.; Coureux, P.D.; Mechulam, Y.; Schmitt, E.
Deposited on : 2024-06-20
Resolution : 2.90 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
buster-report : 1.1.7 (2018)
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

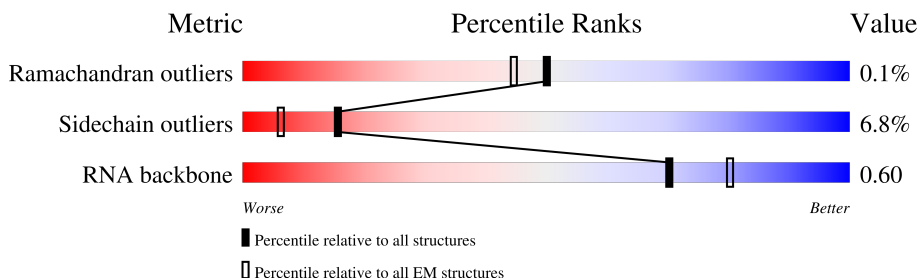
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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	214	
8	G	214	



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Mol	Chain	Length	Quality of chain
9	H	193	
10	I	133	
11	J	133	
12	K	137	
13	L	102	
14	N	147	
15	O	165	
16	Q	152	
17	R	114	
18	S	79	
19	T	140	
20	U	158	
21	V	120	
22	W	66	
23	X	83	
24	Y	75	
25	Z	229	
26	3	127	
27	c	110	
28	d	72	
29	e	52	
30	4	77	
31	a	72	
32	P	54	
33	b	95	

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Mol	Chain	Length	Quality of chain
34	5	14	 14% 7% 79%
35	M	132	 92% . . .

2 Entry composition [i](#)

There are 40 unique types of molecules in this entry. The entry contains 65629 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
1	2	1440	Total	C	N	O	P	0	0
			30982	13818	5732	9992	1440		

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 uS12.

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

- Molecule 15 is a protein called Small ribosomal subunit protein uS13.

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

- Molecule 16 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 17 is a protein called Small ribosomal subunit protein uS17.

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

- Molecule 18 is a protein called Small ribosomal subunit protein eS17.

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

- Molecule 19 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 20 is a protein called Small ribosomal subunit protein eS19.

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

- Molecule 21 is a protein called Small ribosomal subunit protein eS24.

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

- Molecule 22 is a protein called Small ribosomal subunit protein eS27.

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

- Molecule 23 is a protein called Small ribosomal subunit protein eS28.

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

- Molecule 24 is a protein called Small ribosomal subunit protein eS31.

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

- Molecule 25 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 26 is a protein called Large ribosomal subunit protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	3	117	Total	C	N	O	S	0	0
			893	567	149	175	2		

- Molecule 27 is a protein called Small ribosomal subunit protein eS25.

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

- Molecule 28 is a protein called VapB-type antitoxin.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	d	68	Total	C	N	O	S	0	0
			557	362	90	103	2		

- Molecule 29 is a protein called LSU ribosomal protein S30E (Rps30E).

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

- Molecule 30 is a RNA chain called tRNA met initiator.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	4	77	Total	C	N	O	P S	0	0
			1645	734	296	537	77 1		

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 31 is a protein called aS34.

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

- Molecule 32 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 33 is a protein called LSU ribosomal protein S26E (Rps26E).

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	93	Total	C	N	O	S	0	0
			723	449	139	128	7		

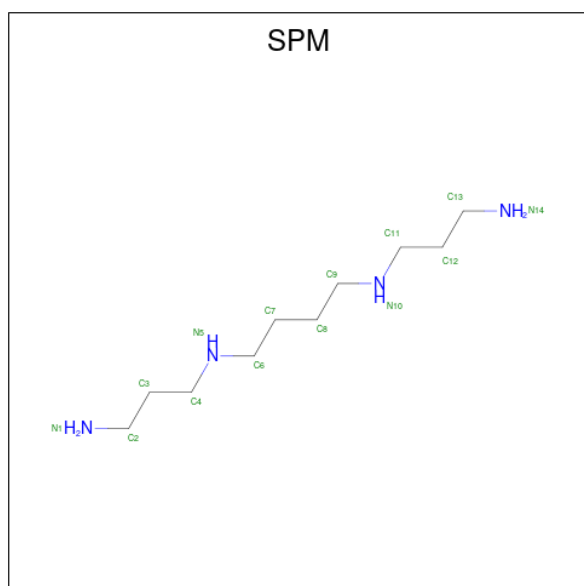
- Molecule 34 is a RNA chain called mRNA Ss-aIF2beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	5	3	Total	C	N	O	P	0	0
			47	19	7	18	3		

- Molecule 35 is a protein called Small ribosomal subunit protein uS11.

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

- Molecule 36 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms			AltConf
36	2	1	Total	C	N	0
			14	10	4	

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Mol	Chain	Residues	Atoms			AltConf
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	

- Molecule 37 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
37	2	54	Total	Mg	0
			54	54	
37	F	1	Total	Mg	0
			1	1	

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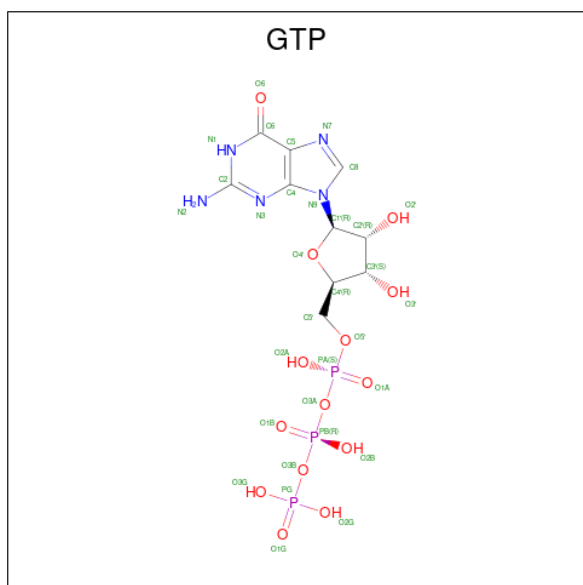
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Mol	Chain	Residues	Atoms		AltConf
37	R	1	Total	Mg	0
			1	1	
37	5	1	Total	Mg	0
			1	1	

- 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	R	1	Total	Zn	0
			1	1	
38	W	1	Total	Zn	0
			1	1	
38	a	2	Total	Zn	0
			2	2	
38	P	1	Total	Zn	0
			1	1	
38	b	1	Total	Zn	0
			1	1	

- Molecule 39 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
39	5	1	Total	C	N	O	P	0
			32	10	5	14	3	

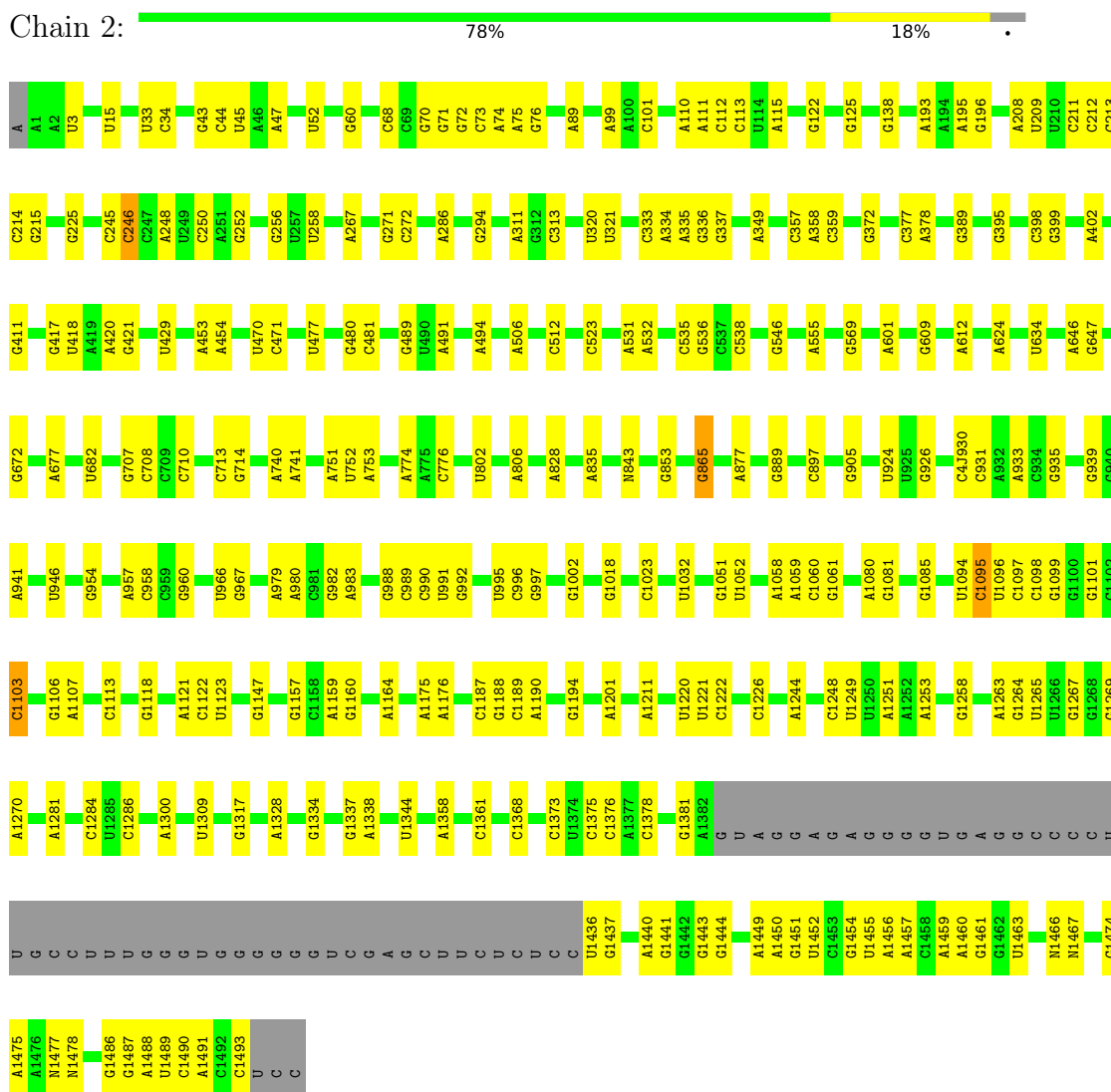
- Molecule 40 is water.

Mol	Chain	Residues	Atoms		AltConf
40	2	181	Total	O	0
			181	181	
40	D	1	Total	O	0
			1	1	
40	E	1	Total	O	0
			1	1	
40	H	1	Total	O	0
			1	1	
40	I	2	Total	O	0
			2	2	
40	J	2	Total	O	0
			2	2	
40	Q	1	Total	O	0
			1	1	
40	R	3	Total	O	0
			3	3	
40	U	1	Total	O	0
			1	1	
40	4	1	Total	O	0
			1	1	
40	b	2	Total	O	0
			2	2	
40	5	3	Total	O	0
			3	3	

3 Residue-property plots

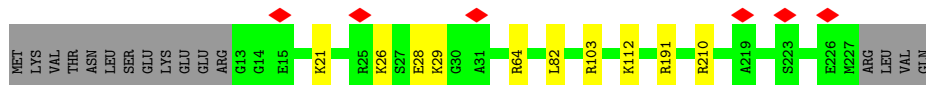
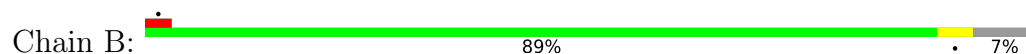
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: rRNA 16S

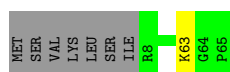
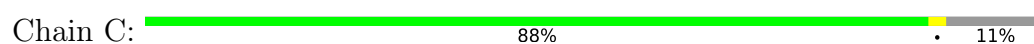




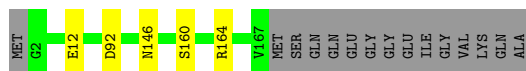
- Molecule 3: Small ribosomal subunit protein uS2



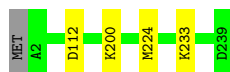
- Molecule 4: Small zinc finger protein HVO-2753-like zinc-binding pocket domain-containing protein



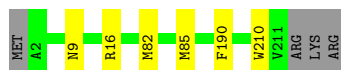
- Molecule 5: Small ribosomal subunit protein uS4



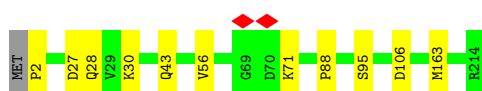
- Molecule 6: Small ribosomal subunit protein eS4



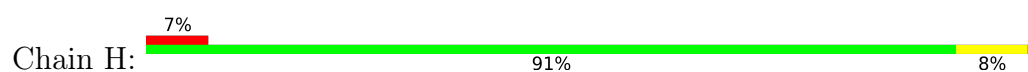
- Molecule 7: Small ribosomal subunit protein uS5



- Molecule 8: Small ribosomal subunit protein eS6



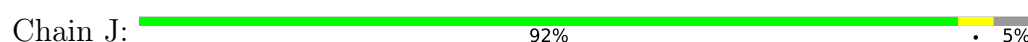
- Molecule 9: Small ribosomal subunit protein uS7



- Molecule 10: Small ribosomal subunit protein uS8



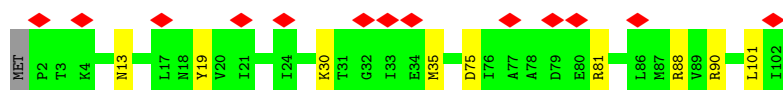
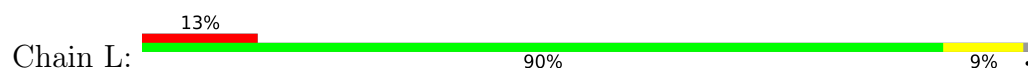
- Molecule 11: Small ribosomal subunit protein eS8



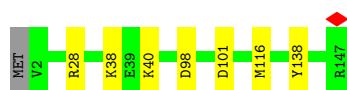
- Molecule 12: Small ribosomal subunit protein uS9



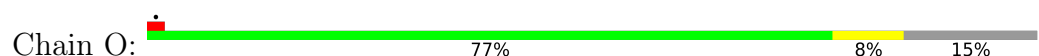
- Molecule 13: Small ribosomal subunit protein uS10



- Molecule 14: Small ribosomal subunit protein uS12

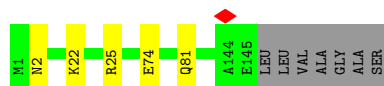


- Molecule 15: Small ribosomal subunit protein uS13



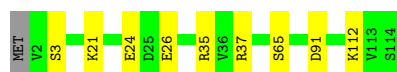
- Molecule 16: Small ribosomal subunit protein uS15

Chain Q:  92% 5%




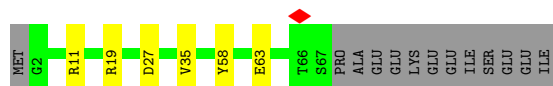
- Molecule 17: Small ribosomal subunit protein uS17

Chain R:  91% 8%




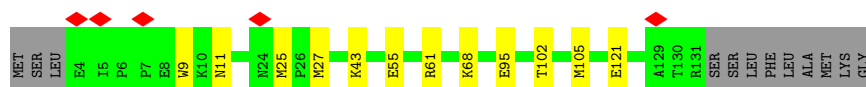
- Molecule 18: Small ribosomal subunit protein eS17

Chain S:  76% 8% 16%




- Molecule 19: Small ribosomal subunit protein uS19

Chain T:  83% 9% 9%




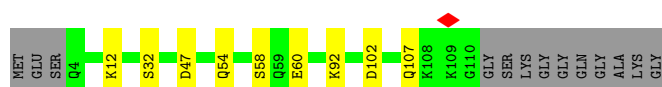
- Molecule 20: Small ribosomal subunit protein eS19

Chain U:  89% 8%



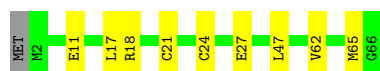
- Molecule 21: Small ribosomal subunit protein eS24

Chain V:  82% 8% 11%

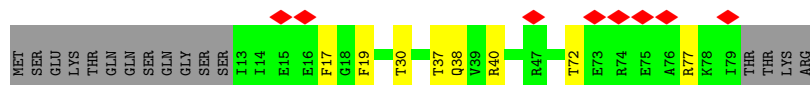


- Molecule 22: Small ribosomal subunit protein eS27

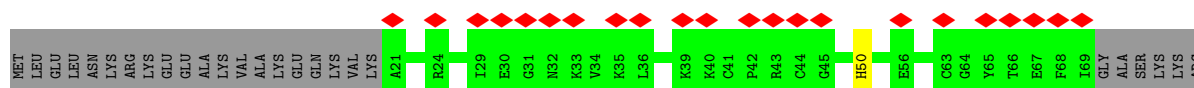
Chain W:  85% 14%



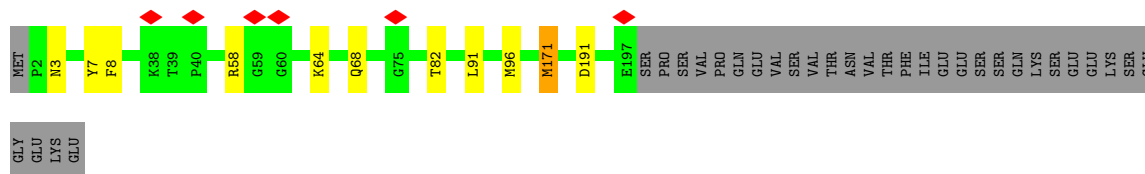
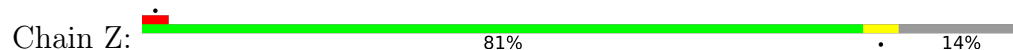
- Molecule 23: Small ribosomal subunit protein eS28



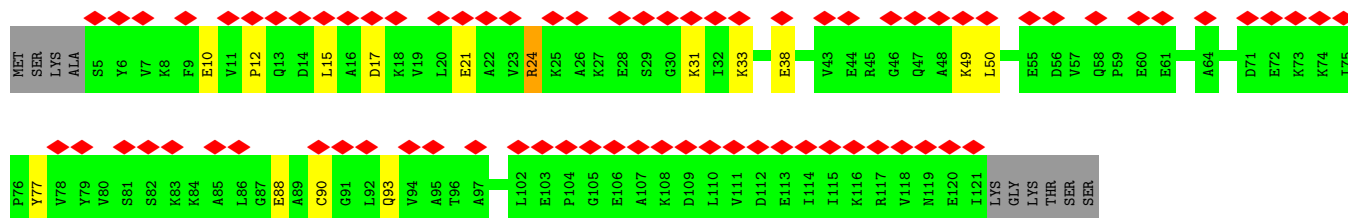
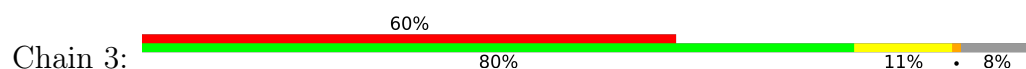
- Molecule 24: Small ribosomal subunit protein eS31



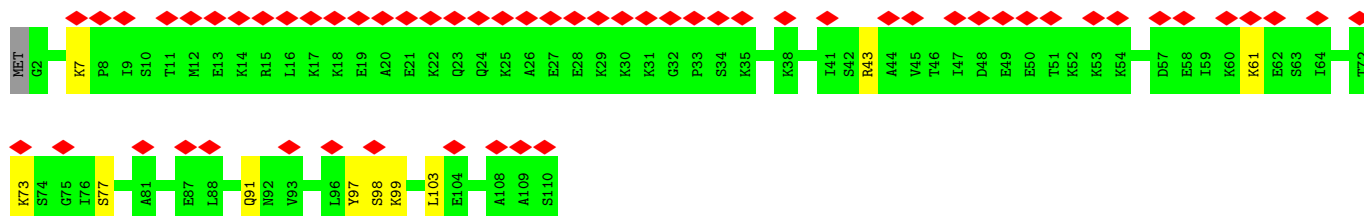
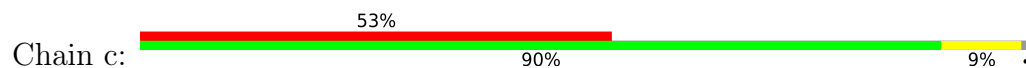
- Molecule 25: Small ribosomal subunit protein uS3



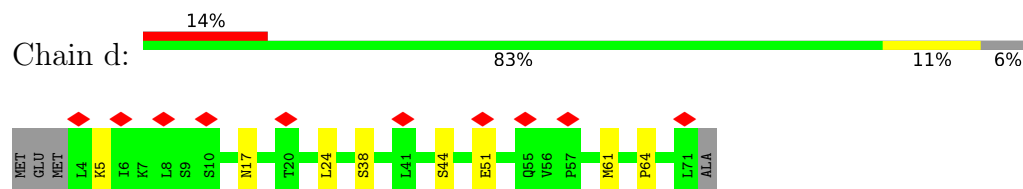
- Molecule 26: Large ribosomal subunit protein eL8



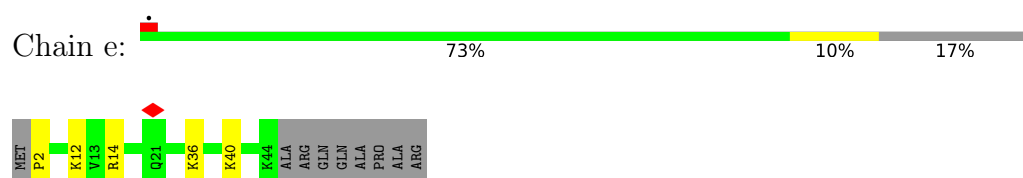
- Molecule 27: Small ribosomal subunit protein eS25



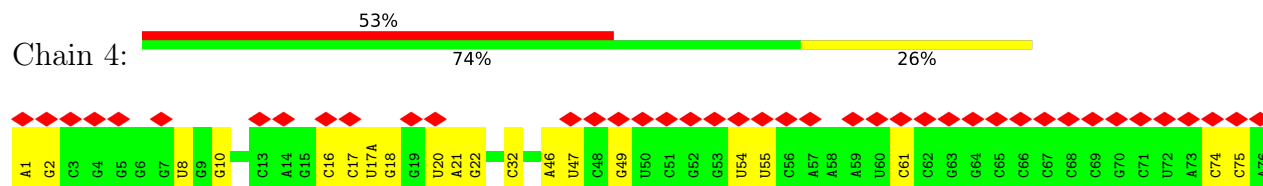
- Molecule 28: VapB-type antitoxin



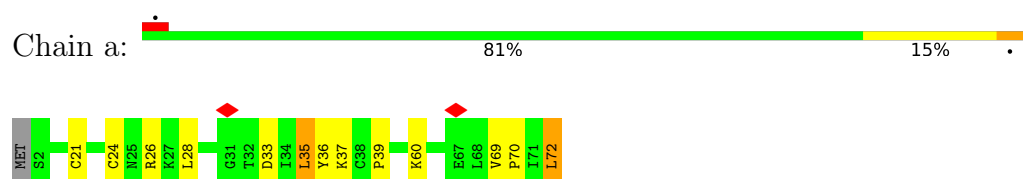
- Molecule 29: LSU ribosomal protein S30E (Rps30E)



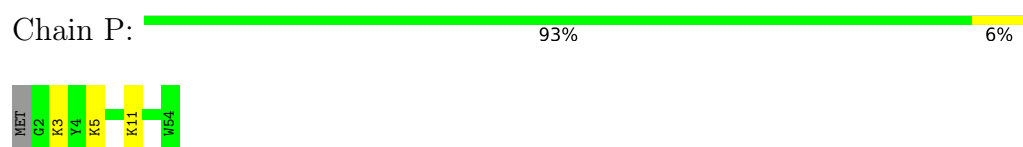
- Molecule 30: tRNA met initiator



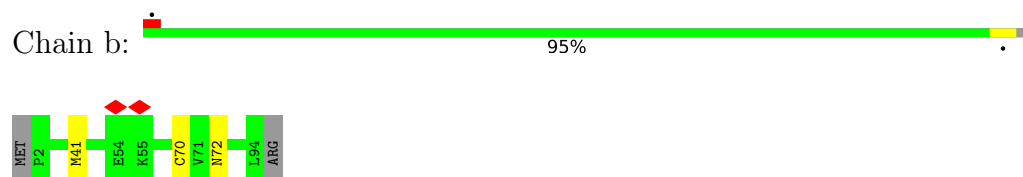
- Molecule 31: aS34



- Molecule 32: Small ribosomal subunit protein uS14



- Molecule 33: LSU ribosomal protein S26E (Rps26E)



- Molecule 34: mRNA Ss-aIF2beta



- Molecule 35: Small ribosomal subunit protein uS11

Chain M:  92% ...

MET	SER	SER	ARG	ARG	E6	Y63	Y64	E111	D119	R130	R131	V132
-----	-----	-----	-----	-----	----	-----	-----	------	------	------	------	------

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	49401	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	0.048	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0045	Depositor
Map size (Å)	361.19998, 361.19998, 361.19998	wwPDB
Map dimensions	516, 516, 516	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.7, 0.7, 0.7	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 6MZ, OMG, MG, OMU, ZN, 4AC, SPM, H2U, A2M, 5MC, MA6, GTP, OMC, 4SU, C4J, PSU, 5MU

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	0.74	0/33843	0.81	11/52798 (0.0%)
2	A	0.38	0/1543	0.61	0/2077
3	B	0.34	0/1731	0.60	0/2349
4	C	0.39	0/466	0.57	0/625
5	D	0.39	0/1380	0.52	0/1859
6	E	0.41	0/1965	0.56	0/2644
7	F	0.40	0/1654	0.56	0/2240
8	G	0.36	1/1684 (0.1%)	0.64	3/2265 (0.1%)
9	H	0.66	3/1571 (0.2%)	0.80	5/2116 (0.2%)
10	I	0.44	0/1070	0.56	0/1444
11	J	0.39	0/994	0.62	0/1337
12	K	0.33	0/1084	0.76	1/1450 (0.1%)
13	L	0.34	0/856	0.70	0/1154
14	N	0.41	0/1155	0.59	0/1540
15	O	0.32	0/1142	0.65	0/1532
16	Q	0.37	0/1206	0.58	0/1618
17	R	0.46	0/918	0.59	0/1236
18	S	0.36	0/578	0.64	0/770
19	T	0.31	0/1087	0.59	0/1456
20	U	0.32	0/1270	0.65	1/1710 (0.1%)
21	V	0.38	0/843	0.60	0/1124
22	W	0.38	0/511	0.64	0/684
23	X	0.32	0/538	0.72	0/722
24	Y	0.34	0/404	0.63	0/540
25	Z	0.37	0/1584	0.64	2/2124 (0.1%)
26	3	0.75	2/902 (0.2%)	1.19	6/1216 (0.5%)
27	c	0.27	0/861	0.57	0/1143
28	d	0.32	0/568	0.74	1/769 (0.1%)
29	e	0.39	0/360	0.89	2/477 (0.4%)
30	4	0.37	1/1725 (0.1%)	0.76	1/2687 (0.0%)
31	a	0.80	3/574 (0.5%)	1.26	8/770 (1.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	P	0.42	0/451	0.66	0/600
33	b	0.35	0/732	0.63	0/976
34	5	0.21	0/51	0.66	0/78
35	M	0.32	0/960	0.67	0/1294
All	All	0.60	10/68261 (0.0%)	0.75	41/99424 (0.0%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	3	12	PRO	CB-CG	17.14	2.35	1.50
9	H	39	PRO	CG-CD	-15.10	1.00	1.50
9	H	39	PRO	CB-CG	14.71	2.23	1.50
30	4	1	A	OP3-P	-10.62	1.48	1.61
26	3	12	PRO	CG-CD	-10.35	1.16	1.50
31	a	70	PRO	CG-CD	-10.08	1.17	1.50
9	H	39	PRO	N-CD	6.89	1.57	1.47
31	a	36	TYR	CE1-CZ	-5.92	1.30	1.38
31	a	36	TYR	CD2-CE2	-5.55	1.31	1.39
8	G	88	PRO	CG-CD	-5.31	1.33	1.50

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	3	12	PRO	CA-N-CD	-23.50	78.60	111.50
26	3	12	PRO	CB-CG-CD	-19.52	30.37	106.50
9	H	39	PRO	N-CD-CG	-16.07	79.09	103.20
26	3	12	PRO	N-CD-CG	12.98	122.67	103.20
29	e	2	PRO	CA-N-CD	-12.70	93.72	111.50
31	a	70	PRO	CA-N-CD	-11.84	94.92	111.50
31	a	35	LEU	CA-CB-CG	10.99	140.57	115.30
8	G	88	PRO	CA-N-CD	-9.48	98.23	111.50
9	H	39	PRO	CB-CG-CD	-8.72	72.50	106.50
31	a	69	VAL	C-N-CD	8.59	146.44	128.40
9	H	39	PRO	CA-CB-CG	-8.41	88.02	104.00
8	G	88	PRO	N-CD-CG	-8.11	91.04	103.20
26	3	12	PRO	N-CA-CB	-7.60	94.18	103.30
1	2	1373	C	C2-N1-C1'	7.39	126.93	118.80
1	2	1095	C	O4'-C1'-N1	7.16	113.93	108.20
9	H	39	PRO	N-CA-CB	-7.07	94.81	103.30
1	2	1122	C	C2-N1-C1'	6.84	126.32	118.80
26	3	50	LEU	CA-CB-CG	6.57	130.41	115.30
29	e	2	PRO	N-CD-CG	-6.42	93.56	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1378	C	N1-C2-O2	6.41	122.75	118.90
31	a	70	PRO	N-CD-CG	-6.39	93.61	103.20
31	a	39	PRO	CA-N-CD	-6.26	102.73	111.50
1	2	1122	C	N1-C2-O2	6.08	122.55	118.90
1	2	1373	C	C6-N1-C1'	-5.84	113.80	120.80
8	G	2	PRO	CA-N-CD	-5.82	103.36	111.50
28	d	51	GLU	CA-CB-CG	5.77	126.09	113.40
1	2	1122	C	N3-C2-O2	-5.68	117.92	121.90
31	a	21	CYS	CA-CB-SG	-5.59	103.94	114.00
9	H	190	LEU	CA-CB-CG	5.55	128.06	115.30
31	a	28	LEU	CA-CB-CG	5.50	127.96	115.30
25	Z	91	LEU	CA-CB-CG	5.38	127.67	115.30
20	U	5	MET	CG-SD-CE	5.35	108.76	100.20
1	2	1122	C	C6-N1-C2	-5.34	118.16	120.30
31	a	72	LEU	CB-CG-CD1	-5.23	102.12	111.00
25	Z	171	MET	CA-CB-CG	5.20	122.14	113.30
1	2	1085	G	N1-C6-O6	-5.13	116.83	119.90
1	2	713	C	C2-N1-C1'	5.12	124.43	118.80
26	3	24	ARG	CA-CB-CG	5.07	124.56	113.40
12	K	90	LEU	CA-CB-CG	5.05	126.91	115.30
1	2	1103	C	C2-N1-C1'	5.04	124.35	118.80
30	4	17	C	C2-N1-C1'	5.02	124.32	118.80

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 [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%)	179 (97%)	5 (3%)	0	100	100
3	B	213/231 (92%)	205 (96%)	8 (4%)	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%)	230 (98%)	6 (2%)	0	100	100
7	F	208/214 (97%)	202 (97%)	6 (3%)	0	100	100
8	G	211/214 (99%)	200 (95%)	11 (5%)	0	100	100
9	H	190/193 (98%)	182 (96%)	8 (4%)	0	100	100
10	I	130/133 (98%)	126 (97%)	4 (3%)	0	100	100
11	J	125/133 (94%)	123 (98%)	2 (2%)	0	100	100
12	K	131/137 (96%)	123 (94%)	8 (6%)	0	100	100
13	L	99/102 (97%)	92 (93%)	7 (7%)	0	100	100
14	N	144/147 (98%)	138 (96%)	6 (4%)	0	100	100
15	O	138/165 (84%)	130 (94%)	8 (6%)	0	100	100
16	Q	143/152 (94%)	142 (99%)	1 (1%)	0	100	100
17	R	111/114 (97%)	108 (97%)	3 (3%)	0	100	100
18	S	64/79 (81%)	63 (98%)	1 (2%)	0	100	100
19	T	126/140 (90%)	123 (98%)	3 (2%)	0	100	100
20	U	152/158 (96%)	146 (96%)	6 (4%)	0	100	100
21	V	105/120 (88%)	102 (97%)	3 (3%)	0	100	100
22	W	63/66 (96%)	58 (92%)	5 (8%)	0	100	100
23	X	65/83 (78%)	57 (88%)	8 (12%)	0	100	100
24	Y	47/75 (63%)	36 (77%)	11 (23%)	0	100	100
25	Z	194/229 (85%)	191 (98%)	3 (2%)	0	100	100
26	3	115/127 (91%)	103 (90%)	12 (10%)	0	100	100
27	c	107/110 (97%)	99 (92%)	8 (8%)	0	100	100
28	d	66/72 (92%)	60 (91%)	5 (8%)	1 (2%)	8	29
29	e	41/52 (79%)	41 (100%)	0	0	100	100
31	a	69/72 (96%)	64 (93%)	5 (7%)	0	100	100
32	P	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
33	b	91/95 (96%)	90 (99%)	1 (1%)	0	100	100
35	M	125/132 (95%)	118 (94%)	6 (5%)	1 (1%)	16	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3964/4292 (92%)	3794 (96%)	168 (4%)	2 (0%)	50 77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
35	M	119	ASP
28	d	17	ASN

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%)	155 (92%)	13 (8%)	10 31
3	B	182/198 (92%)	172 (94%)	10 (6%)	18 48
4	C	51/58 (88%)	50 (98%)	1 (2%)	50 79
5	D	147/158 (93%)	142 (97%)	5 (3%)	32 67
6	E	214/215 (100%)	210 (98%)	4 (2%)	52 81
7	F	180/184 (98%)	174 (97%)	6 (3%)	33 68
8	G	186/187 (100%)	177 (95%)	9 (5%)	21 54
9	H	166/167 (99%)	152 (92%)	14 (8%)	9 28
10	I	113/114 (99%)	111 (98%)	2 (2%)	54 82
11	J	104/110 (94%)	99 (95%)	5 (5%)	21 54
12	K	109/113 (96%)	103 (94%)	6 (6%)	18 48
13	L	93/94 (99%)	84 (90%)	9 (10%)	6 22
14	N	122/123 (99%)	115 (94%)	7 (6%)	17 47
15	O	121/142 (85%)	108 (89%)	13 (11%)	5 17
16	Q	125/129 (97%)	120 (96%)	5 (4%)	27 61
17	R	101/102 (99%)	92 (91%)	9 (9%)	8 26
18	S	63/75 (84%)	57 (90%)	6 (10%)	7 22
19	T	116/126 (92%)	104 (90%)	12 (10%)	6 19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	U	134/138 (97%)	122 (91%)	12 (9%)	8	25
21	V	92/99 (93%)	83 (90%)	9 (10%)	6	21
22	W	57/58 (98%)	48 (84%)	9 (16%)	2	6
23	X	58/73 (80%)	50 (86%)	8 (14%)	3	9
24	Y	43/65 (66%)	42 (98%)	1 (2%)	45	77
25	Z	163/195 (84%)	153 (94%)	10 (6%)	15	43
26	3	97/105 (92%)	84 (87%)	13 (13%)	3	9
27	c	95/96 (99%)	85 (90%)	10 (10%)	5	18
28	d	62/65 (95%)	56 (90%)	6 (10%)	6	22
29	e	40/46 (87%)	36 (90%)	4 (10%)	6	20
31	a	61/62 (98%)	54 (88%)	7 (12%)	4	15
32	P	45/46 (98%)	42 (93%)	3 (7%)	13	39
33	b	77/79 (98%)	74 (96%)	3 (4%)	27	62
35	M	93/98 (95%)	88 (95%)	5 (5%)	18	49
All	All	3478/3704 (94%)	3242 (93%)	236 (7%)	16	38

All (236) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	12	ASP
2	A	14	TRP
2	A	16	MET
2	A	19	TRP
2	A	26	LYS
2	A	43	GLN
2	A	49	VAL
2	A	54	TYR
2	A	87	GLU
2	A	109	ASP
2	A	169	ASN
2	A	173	GLU
2	A	183	LYS
3	B	21	LYS
3	B	26	LYS
3	B	28	GLU
3	B	29	LYS
3	B	64	ARG

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Mol	Chain	Res	Type
3	B	82	LEU
3	B	103	ARG
3	B	112	LYS
3	B	191	ARG
3	B	210	ARG
4	C	63	LYS
5	D	12	GLU
5	D	92	ASP
5	D	146	ASN
5	D	160	SER
5	D	164	ARG
6	E	112	ASP
6	E	200	LYS
6	E	224	MET
6	E	233	LYS
7	F	9	ASN
7	F	16	ARG
7	F	82	MET
7	F	85	MET
7	F	190	PHE
7	F	210	TRP
8	G	27	ASP
8	G	28	GLN
8	G	30	LYS
8	G	43	GLN
8	G	56	VAL
8	G	71	LYS
8	G	95	SER
8	G	106	ASP
8	G	163	MET
9	H	11	LYS
9	H	17	ASP
9	H	34	MET
9	H	71	ASN
9	H	113	GLU
9	H	118	MET
9	H	119	TYR
9	H	124	TYR
9	H	149	ASP
9	H	154	ASN
9	H	173	ASP
9	H	181	ARG

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Mol	Chain	Res	Type
9	H	187	ARG
9	H	192	SER
10	I	28	MET
10	I	110	SER
11	J	25	LYS
11	J	67	ASP
11	J	83	GLU
11	J	98	ARG
11	J	101	LYS
12	K	15	LYS
12	K	24	TYR
12	K	39	LEU
12	K	43	GLU
12	K	107	ASP
12	K	110	MET
13	L	13	ASN
13	L	19	TYR
13	L	30	LYS
13	L	35	MET
13	L	75	ASP
13	L	81	ARG
13	L	88	ARG
13	L	90	ARG
13	L	101	LEU
14	N	28	ARG
14	N	38	LYS
14	N	40	LYS
14	N	98	ASP
14	N	101	ASP
14	N	116	MET
14	N	138	TYR
15	O	4	GLN
15	O	5	PHE
15	O	10	ARG
15	O	15	ASP
15	O	19	THR
15	O	42	ARG
15	O	54	GLU
15	O	68	SER
15	O	86	TYR
15	O	87	GLU
15	O	90	LEU

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Mol	Chain	Res	Type
15	O	112	LYS
15	O	140	MET
16	Q	2	ASN
16	Q	22	LYS
16	Q	25	ARG
16	Q	74	GLU
16	Q	81	GLN
17	R	3	SER
17	R	21	LYS
17	R	24	GLU
17	R	26	GLU
17	R	35	ARG
17	R	37	ARG
17	R	65	SER
17	R	91	ASP
17	R	112	LYS
18	S	11	ARG
18	S	19	ARG
18	S	27	ASP
18	S	35	VAL
18	S	58	TYR
18	S	63	GLU
19	T	9	TRP
19	T	11	ASN
19	T	25	MET
19	T	27	MET
19	T	43	LYS
19	T	55	GLU
19	T	61	ARG
19	T	68	LYS
19	T	95	GLU
19	T	102	THR
19	T	105	MET
19	T	121	GLU
20	U	11	VAL
20	U	14	ASP
20	U	19	ARG
20	U	23	TYR
20	U	26	GLU
20	U	30	THR
20	U	103	VAL
20	U	121	LYS

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Mol	Chain	Res	Type
20	U	130	LYS
20	U	136	ASP
20	U	143	PHE
20	U	156	TYR
21	V	12	LYS
21	V	32	SER
21	V	47	ASP
21	V	54	GLN
21	V	58	SER
21	V	60	GLU
21	V	92	LYS
21	V	102	ASP
21	V	107	GLN
22	W	11	GLU
22	W	17	LEU
22	W	18	ARG
22	W	21	CYS
22	W	24	CYS
22	W	27	GLU
22	W	47	LEU
22	W	62	VAL
22	W	65	MET
23	X	17	PHE
23	X	19	PHE
23	X	30	THR
23	X	37	THR
23	X	38	GLN
23	X	40	ARG
23	X	72	THR
23	X	77	ARG
24	Y	50	HIS
25	Z	3	ASN
25	Z	7	TYR
25	Z	8	PHE
25	Z	58	ARG
25	Z	64	LYS
25	Z	68	GLN
25	Z	82	THR
25	Z	96	MET
25	Z	171	MET
25	Z	191	ASP
26	3	10	GLU

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Mol	Chain	Res	Type
26	3	15	LEU
26	3	17	ASP
26	3	21	GLU
26	3	24	ARG
26	3	31	LYS
26	3	33	LYS
26	3	38	GLU
26	3	49	LYS
26	3	77	TYR
26	3	88	GLU
26	3	90	CYS
26	3	93	GLN
27	c	7	LYS
27	c	43	ARG
27	c	61	LYS
27	c	73	LYS
27	c	77	SER
27	c	91	GLN
27	c	97	TYR
27	c	98	SER
27	c	99	LYS
27	c	103	LEU
28	d	5	LYS
28	d	24	LEU
28	d	38	SER
28	d	44	SER
28	d	61	MET
28	d	64	PRO
29	e	12	LYS
29	e	14	ARG
29	e	36	LYS
29	e	40	LYS
31	a	24	CYS
31	a	26	ARG
31	a	33	ASP
31	a	35	LEU
31	a	37	LYS
31	a	60	LYS
31	a	72	LEU
32	P	3	LYS
32	P	5	LYS
32	P	11	LYS

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Mol	Chain	Res	Type
33	b	41	MET
33	b	70	CYS
33	b	72	ASN
35	M	53	TYR
35	M	84	TYR
35	M	111	GLU
35	M	119	ASP
35	M	130	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	86	HIS
2	A	105	ASN
6	E	19	GLN
6	E	58	HIS
6	E	220	GLN
8	G	209	ASN
9	H	5	ASN
9	H	40	HIS
9	H	71	ASN
9	H	95	GLN
9	H	172	ASN
13	L	100	GLN
15	O	14	GLN
15	O	121	HIS
18	S	31	ASN
19	T	52	HIS
20	U	150	ASN
21	V	22	GLN
24	Y	50	HIS
25	Z	3	ASN
27	c	91	GLN
27	c	100	ASN
29	e	16	GLN
31	a	5	ASN
31	a	25	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1431/1497 (95%)	232 (16%)	4 (0%)
30	4	76/77 (98%)	15 (19%)	1 (1%)
34	5	1/14 (7%)	1 (100%)	0
All	All	1508/1588 (94%)	248 (16%)	5 (0%)

All (248) 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	44	C
1	2	45	U
1	2	47	A
1	2	60	G
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
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	125	G
1	2	138	G
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

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Mol	Chain	Res	Type
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	258	U
1	2	267	A
1	2	271	G
1	2	272	C
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
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	398	C
1	2	402	A
1	2	411	G
1	2	417	G
1	2	418	U
1	2	420	A
1	2	421	G
1	2	429	U
1	2	453	A
1	2	454	A
1	2	470	U
1	2	471	C

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Mol	Chain	Res	Type
1	2	477	U
1	2	480	G
1	2	489	G
1	2	491	A
1	2	506	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	569	G
1	2	601	A
1	2	609	G
1	2	612	A
1	2	624	A
1	2	634	U
1	2	646	A
1	2	647	G
1	2	677	A
1	2	682	U
1	2	707	G
1	2	708	C
1	2	714	G
1	2	740	A
1	2	741	A
1	2	751	A
1	2	752	U
1	2	753	A
1	2	774	A
1	2	776	C
1	2	802	U
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

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Mol	Chain	Res	Type
1	2	933	A
1	2	935	G
1	2	939	G
1	2	941	A
1	2	946	U
1	2	954	G
1	2	957	A
1	2	958	C
1	2	960	G
1	2	966	U
1	2	967	G
1	2	979	A
1	2	980	A
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
1	2	1052	U
1	2	1058	A
1	2	1059	A
1	2	1080	A
1	2	1081	G
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	1103	C
1	2	1106	G
1	2	1107	A
1	2	1113	C

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Mol	Chain	Res	Type
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	1164	A
1	2	1175	A
1	2	1176	A
1	2	1187	C
1	2	1188	G
1	2	1189	C
1	2	1190	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	1253	A
1	2	1258	G
1	2	1263	A
1	2	1264	G
1	2	1265	U
1	2	1267	G
1	2	1269	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	1337	G
1	2	1338	A

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Mol	Chain	Res	Type
1	2	1358	A
1	2	1361	C
1	2	1375	C
1	2	1376	C
1	2	1381	G
1	2	1437	G
1	2	1440	A
1	2	1441	G
1	2	1443	G
1	2	1444	G
1	2	1449	A
1	2	1450	A
1	2	1451	G
1	2	1452	U
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
1	2	1488	A
1	2	1489	U
1	2	1490	C
1	2	1491	A
1	2	1493	C
30	4	2	G
30	4	8	4SU
30	4	10	G
30	4	16	C
30	4	17(A)	U
30	4	18	G
30	4	20	H2U
30	4	21	A
30	4	22	G
30	4	46	A
30	4	47	U
30	4	49	G
30	4	61	C

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Mol	Chain	Res	Type
30	4	74	C
30	4	75	C
34	5	3	G

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	44	C
1	2	979	A
1	2	1188	G
1	2	1436	U
30	4	74	C

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

38 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	546	1	18,26,27	0.98	1 (5%)	19,38,41	1.14	2 (10%)
1	OMU	2	52	1	19,22,23	1.28	3 (15%)	26,31,34	1.75	5 (19%)
1	OMC	2	538	1	19,22,23	0.88	2 (10%)	26,31,34	0.87	1 (3%)
30	OMC	4	32	30	19,22,23	0.84	0	26,31,34	1.04	2 (7%)
1	OMC	2	1060	1	19,22,23	0.85	1 (5%)	26,31,34	0.73	0
30	5MU	4	54	30	19,22,23	1.39	5 (26%)	28,32,35	2.10	8 (28%)
30	PSU	4	55	30	18,21,22	1.31	2 (11%)	22,30,33	1.89	3 (13%)
1	5MC	2	1368	1	18,22,23	0.92	2 (11%)	26,32,35	1.05	2 (7%)
1	OMG	2	905	1	18,26,27	0.97	1 (5%)	19,38,41	1.10	2 (10%)
1	OMU	2	15	1	19,22,23	1.35	4 (21%)	26,31,34	1.82	5 (19%)
1	OMC	2	512	1	19,22,23	0.86	2 (10%)	26,31,34	0.86	0
1	OMG	2	926	1	18,26,27	0.96	1 (5%)	19,38,41	1.12	2 (10%)
1	OMU	2	1344	1	19,22,23	1.22	3 (15%)	26,31,34	1.67	6 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMC	2	1366	1	19,22,23	0.81	0	26,31,34	0.74	0
1	6MZ	2	1457	37,1	18,25,26	0.82	1 (5%)	16,36,39	2.10	3 (18%)
1	C4J	2	930	1	24,29,30	0.65	1 (4%)	29,42,45	0.55	0
1	OMU	2	1032	1	19,22,23	1.29	3 (15%)	26,31,34	1.74	4 (15%)
1	OMC	2	313	1	19,22,23	0.89	2 (10%)	26,31,34	0.95	1 (3%)
1	OMG	2	1018	1	18,26,27	0.98	1 (5%)	19,38,41	1.08	2 (10%)
1	MA6	2	1475	1	18,26,27	0.94	1 (5%)	19,38,41	1.26	3 (15%)
1	4AC	2	1477	1	21,24,25	1.03	2 (9%)	29,34,37	1.60	7 (24%)
1	OMG	2	672	1	18,26,27	0.98	1 (5%)	19,38,41	1.07	2 (10%)
1	4AC	2	1466	1	21,24,25	1.03	2 (9%)	29,34,37	1.30	4 (13%)
1	OMC	2	113	1	19,22,23	0.86	1 (5%)	26,31,34	0.86	0
1	4AC	2	843	1	21,24,25	1.11	3 (14%)	29,34,37	1.39	4 (13%)
1	OMG	2	865	1	18,26,27	0.96	1 (5%)	19,38,41	1.10	2 (10%)
1	OMG	2	1194	1	18,26,27	0.94	1 (5%)	19,38,41	1.11	2 (10%)
1	4AC	2	1467	1	21,24,25	1.04	2 (9%)	29,34,37	1.27	4 (13%)
1	OMG	2	337	1	18,26,27	0.97	1 (5%)	19,38,41	1.17	2 (10%)
1	4AC	2	1478	1	21,24,25	1.03	2 (9%)	29,34,37	1.35	4 (13%)
1	A2M	2	494	1	18,25,26	0.93	1 (5%)	18,36,39	1.32	2 (11%)
30	H2U	4	20	30	18,21,22	0.30	0	21,30,33	0.44	0
1	OMG	2	399	1	18,26,27	1.00	1 (5%)	19,38,41	1.15	3 (15%)
1	OMC	2	710	1	19,22,23	0.88	2 (10%)	26,31,34	0.79	0
30	4SU	4	8	30	18,21,22	0.28	0	26,30,33	0.35	0
1	OMG	2	1061	1	18,26,27	0.98	1 (5%)	19,38,41	1.13	2 (10%)
1	OMC	2	246	1	19,22,23	0.88	1 (5%)	26,31,34	1.03	1 (3%)
1	OMC	2	481	1	19,22,23	0.94	1 (5%)	26,31,34	1.05	3 (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	546	1	-	0/5/27/28	0/3/3/3
1	OMU	2	52	1	-	0/9/27/28	0/2/2/2
1	OMC	2	538	1	-	0/9/27/28	0/2/2/2
30	OMC	4	32	30	-	4/9/27/28	0/2/2/2
1	OMC	2	1060	1	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	5MU	4	54	30	-	0/7/25/26	0/2/2/2
30	PSU	4	55	30	-	1/7/25/26	0/2/2/2
1	5MC	2	1368	1	-	0/7/25/26	0/2/2/2
1	OMG	2	905	1	-	0/5/27/28	0/3/3/3
1	OMU	2	15	1	-	0/9/27/28	0/2/2/2
1	OMC	2	512	1	-	0/9/27/28	0/2/2/2
1	OMG	2	926	1	-	1/5/27/28	0/3/3/3
1	OMU	2	1344	1	-	0/9/27/28	0/2/2/2
1	OMC	2	1366	1	-	0/9/27/28	0/2/2/2
1	6MZ	2	1457	37,1	-	0/5/27/28	0/3/3/3
1	C4J	2	930	1	-	3/16/34/35	0/2/2/2
1	OMU	2	1032	1	-	0/9/27/28	0/2/2/2
1	OMC	2	313	1	-	1/9/27/28	0/2/2/2
1	OMG	2	1018	1	-	0/5/27/28	0/3/3/3
1	MA6	2	1475	1	-	0/7/29/30	0/3/3/3
1	4AC	2	1477	1	-	2/11/29/30	0/2/2/2
1	OMG	2	672	1	-	0/5/27/28	0/3/3/3
1	4AC	2	1466	1	-	0/11/29/30	0/2/2/2
1	OMC	2	113	1	-	0/9/27/28	0/2/2/2
1	4AC	2	843	1	-	0/11/29/30	0/2/2/2
1	OMG	2	865	1	-	3/5/27/28	0/3/3/3
1	OMG	2	1194	1	-	0/5/27/28	0/3/3/3
1	4AC	2	1467	1	-	0/11/29/30	0/2/2/2
1	OMG	2	337	1	-	1/5/27/28	0/3/3/3
1	4AC	2	1478	1	-	0/11/29/30	0/2/2/2
1	A2M	2	494	1	-	0/5/27/28	0/3/3/3
30	H2U	4	20	30	-	3/7/38/39	0/2/2/2
1	OMG	2	399	1	-	0/5/27/28	0/3/3/3
1	OMC	2	710	1	-	0/9/27/28	0/2/2/2
30	4SU	4	8	30	-	0/7/25/26	0/2/2/2
1	OMG	2	1061	1	-	0/5/27/28	0/3/3/3
1	OMC	2	246	1	-	3/9/27/28	0/2/2/2
1	OMC	2	481	1	-	0/9/27/28	0/2/2/2

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	15	OMU	C4-N3	-3.15	1.32	1.38
1	2	399	OMG	C6-N1	-3.13	1.33	1.37
30	4	55	PSU	C6-C5	3.12	1.39	1.35
1	2	1018	OMG	C6-N1	-3.01	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1061	OMG	C6-N1	-3.00	1.33	1.37
1	2	672	OMG	C6-N1	-2.99	1.33	1.37
1	2	1032	OMU	C4-N3	-2.99	1.33	1.38
1	2	337	OMG	C6-N1	-2.97	1.33	1.37
1	2	546	OMG	C6-N1	-2.93	1.33	1.37
1	2	843	4AC	C4-N3	-2.91	1.27	1.32
1	2	865	OMG	C6-N1	-2.89	1.33	1.37
1	2	52	OMU	C4-N3	-2.86	1.33	1.38
1	2	905	OMG	C6-N1	-2.84	1.33	1.37
1	2	15	OMU	C2-N3	-2.82	1.32	1.38
1	2	926	OMG	C6-N1	-2.78	1.33	1.37
1	2	1467	4AC	C4-N3	-2.71	1.28	1.32
1	2	1194	OMG	C6-N1	-2.71	1.33	1.37
30	4	54	5MU	C6-C5	2.63	1.38	1.34
30	4	55	PSU	C4-N3	-2.61	1.34	1.38
1	2	52	OMU	C2-N3	-2.60	1.33	1.38
1	2	1478	4AC	C5-C4	2.58	1.46	1.40
1	2	1344	OMU	C4-N3	-2.58	1.33	1.38
1	2	843	4AC	C5-C4	2.58	1.46	1.40
1	2	930	C4J	O4'-C1'	-2.57	1.40	1.43
1	2	1467	4AC	C5-C4	2.56	1.46	1.40
1	2	1032	OMU	C2-N3	-2.56	1.33	1.38
1	2	1466	4AC	C4-N3	-2.55	1.28	1.32
1	2	1478	4AC	C4-N3	-2.55	1.28	1.32
30	4	54	5MU	C4-N3	-2.54	1.34	1.38
1	2	1466	4AC	C5-C4	2.54	1.46	1.40
1	2	1368	5MC	C6-N1	-2.52	1.33	1.38
1	2	15	OMU	C5-C4	-2.50	1.38	1.43
1	2	1477	4AC	C5-C4	2.44	1.46	1.40
1	2	1477	4AC	C4-N3	-2.38	1.28	1.32
30	4	54	5MU	C4-C5	2.38	1.48	1.44
1	2	1475	MA6	C5-C4	2.36	1.47	1.40
1	2	1457	6MZ	C5-C4	2.32	1.47	1.40
1	2	1344	OMU	C2-N3	-2.31	1.33	1.38
1	2	1032	OMU	C5-C4	-2.31	1.38	1.43
1	2	1368	5MC	C6-C5	2.31	1.38	1.34
30	4	54	5MU	C6-N1	-2.28	1.34	1.38
1	2	52	OMU	C5-C4	-2.27	1.38	1.43
30	4	54	5MU	C2-N1	2.25	1.42	1.38
1	2	1344	OMU	C5-C4	-2.24	1.38	1.43
1	2	843	4AC	C4-N4	-2.11	1.36	1.39
1	2	538	OMC	C6-N1	-2.11	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	313	OMC	C6-N1	-2.10	1.32	1.38
1	2	246	OMC	C5-C4	-2.09	1.38	1.42
1	2	494	A2M	C5-C4	2.09	1.46	1.40
1	2	15	OMU	C6-N1	-2.07	1.33	1.38
1	2	481	OMC	C6-N1	-2.07	1.33	1.38
1	2	313	OMC	C5-C4	-2.07	1.38	1.42
1	2	512	OMC	C5-C4	-2.05	1.38	1.42
1	2	538	OMC	C5-C4	-2.05	1.38	1.42
1	2	113	OMC	C6-N1	-2.03	1.33	1.38
1	2	710	OMC	C5-C4	-2.03	1.38	1.42
1	2	1060	OMC	C6-N1	-2.02	1.33	1.38
1	2	512	OMC	C6-N1	-2.02	1.33	1.38
1	2	710	OMC	C6-N1	-2.02	1.33	1.38

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1457	6MZ	C2-N1-C6	6.67	122.31	116.59
30	4	55	PSU	N1-C2-N3	5.78	121.67	115.13
30	4	54	5MU	C4-N3-C2	-5.17	120.66	127.35
1	2	15	OMU	C4-N3-C2	-4.88	120.14	126.58
30	4	54	5MU	N3-C2-N1	4.85	121.33	114.89
1	2	843	4AC	O7-C7-N4	4.71	129.44	121.82
1	2	1478	4AC	O7-C7-N4	4.64	129.32	121.82
1	2	52	OMU	C4-N3-C2	-4.56	120.56	126.58
1	2	1032	OMU	C4-N3-C2	-4.54	120.59	126.58
1	2	1477	4AC	O7-C7-N4	4.49	129.08	121.82
1	2	1466	4AC	O7-C7-N4	4.40	128.94	121.82
30	4	54	5MU	C5-C4-N3	4.39	119.06	115.31
1	2	1344	OMU	C4-N3-C2	-4.32	120.88	126.58
1	2	1467	4AC	O7-C7-N4	4.30	128.78	121.82
1	2	52	OMU	N3-C2-N1	4.16	120.42	114.89
1	2	15	OMU	N3-C2-N1	4.15	120.40	114.89
1	2	1032	OMU	N3-C2-N1	4.15	120.40	114.89
1	2	15	OMU	C5-C4-N3	4.10	120.98	114.84
30	4	55	PSU	C4-N3-C2	-4.01	120.56	126.34
1	2	1344	OMU	N3-C2-N1	3.84	119.99	114.89
1	2	1032	OMU	C5-C4-N3	3.78	120.50	114.84
30	4	54	5MU	O4-C4-C5	-3.75	120.56	124.90
1	2	52	OMU	C5-C4-N3	3.71	120.40	114.84
1	2	1344	OMU	C5-C4-N3	3.66	120.32	114.84
30	4	54	5MU	C5-C6-N1	-3.60	119.64	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1477	4AC	N4-C4-N3	3.57	119.85	113.85
1	2	1457	6MZ	C4-C5-N7	-3.47	105.78	109.40
1	2	1477	4AC	C5-C4-N4	-3.41	117.00	122.92
1	2	494	A2M	N3-C2-N1	-3.38	123.39	128.68
30	4	55	PSU	O2-C2-N1	-3.33	119.12	122.79
1	2	1475	MA6	N3-C2-N1	-3.27	123.56	128.68
1	2	15	OMU	O4-C4-C5	-3.26	119.43	125.16
1	2	1467	4AC	CM7-C7-N4	-3.25	109.67	115.29
1	2	1475	MA6	C4-C5-N7	-3.25	106.01	109.40
1	2	1368	5MC	C5-C6-N1	-3.08	120.17	123.34
1	2	1344	OMU	O4-C4-C5	-3.07	119.76	125.16
1	2	52	OMU	O4-C4-C5	-3.06	119.78	125.16
1	2	1457	6MZ	N3-C2-N1	-2.97	124.03	128.68
1	2	1466	4AC	C5-C4-N4	-2.88	117.91	122.92
1	2	843	4AC	CM7-C7-N4	-2.88	110.32	115.29
1	2	1478	4AC	C5-C4-N4	-2.87	117.93	122.92
1	2	1466	4AC	N4-C4-N3	2.85	118.63	113.85
1	2	1032	OMU	O4-C4-C5	-2.85	120.16	125.16
1	2	1466	4AC	CM7-C7-N4	-2.84	110.38	115.29
30	4	32	OMC	O2-C2-N3	-2.75	117.86	122.33
1	2	246	OMC	O2-C2-N3	-2.75	117.86	122.33
1	2	1478	4AC	CM7-C7-N4	-2.74	110.55	115.29
1	2	1477	4AC	C1'-N1-C2	2.74	124.53	118.42
1	2	1478	4AC	N4-C4-N3	2.70	118.39	113.85
1	2	843	4AC	C5-C4-N4	-2.66	118.30	122.92
1	2	399	OMG	C5-C6-N1	2.57	118.50	113.95
1	2	1467	4AC	C5-C4-N4	-2.54	118.51	122.92
1	2	337	OMG	C5-C6-N1	2.52	118.41	113.95
1	2	1368	5MC	C5-C4-N3	-2.52	118.96	121.67
1	2	1477	4AC	CM7-C7-N4	-2.51	110.96	115.29
30	4	54	5MU	O2-C2-N1	-2.48	119.48	122.79
1	2	926	OMG	C8-N7-C5	2.47	107.69	102.99
1	2	313	OMC	O2-C2-N3	-2.44	118.36	122.33
1	2	1061	OMG	C5-C6-N1	2.42	118.23	113.95
1	2	546	OMG	C5-C6-N1	2.42	118.23	113.95
1	2	1467	4AC	N4-C4-N3	2.39	117.86	113.85
1	2	865	OMG	C5-C6-N1	2.38	118.16	113.95
1	2	1194	OMG	C8-N7-C5	2.38	107.53	102.99
1	2	481	OMC	C5-C4-N3	-2.37	117.29	121.33
1	2	481	OMC	C6-C5-C4	2.37	121.33	117.50
1	2	905	OMG	C5-C6-N1	2.35	118.10	113.95
1	2	15	OMU	O2-C2-N1	-2.34	119.67	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	865	OMG	C8-N7-C5	2.33	107.43	102.99
30	4	54	5MU	C5M-C5-C4	2.33	121.33	118.77
1	2	1018	OMG	C5-C6-N1	2.33	118.06	113.95
1	2	926	OMG	C5-C6-N1	2.30	118.02	113.95
30	4	32	OMC	C1'-N1-C2	2.30	123.56	118.42
1	2	1194	OMG	C5-C6-N1	2.30	118.01	113.95
1	2	672	OMG	C5-C6-N1	2.30	118.01	113.95
1	2	905	OMG	C8-N7-C5	2.28	107.34	102.99
1	2	672	OMG	C8-N7-C5	2.27	107.32	102.99
1	2	843	4AC	N4-C4-N3	2.27	117.67	113.85
1	2	1061	OMG	C8-N7-C5	2.26	107.29	102.99
1	2	1018	OMG	C8-N7-C5	2.25	107.28	102.99
1	2	481	OMC	N4-C4-N3	2.25	121.91	117.97
1	2	337	OMG	C8-N7-C5	2.20	107.18	102.99
1	2	1477	4AC	O2-C2-N3	-2.19	118.78	122.33
1	2	399	OMG	C8-N7-C5	2.18	107.15	102.99
1	2	52	OMU	C1'-N1-C2	2.18	121.52	117.57
1	2	546	OMG	C8-N7-C5	2.18	107.14	102.99
1	2	538	OMC	O2-C2-N3	-2.10	118.91	122.33
30	4	54	5MU	C5M-C5-C6	-2.09	120.05	122.85
1	2	494	A2M	C4-C5-N7	-2.09	107.22	109.40
1	2	1344	OMU	O2-C2-N1	-2.06	120.04	122.79
1	2	399	OMG	O6-C6-C5	-2.05	120.36	124.37
1	2	1477	4AC	C1'-N1-C6	-2.04	116.40	120.84
1	2	1344	OMU	C1'-N1-C2	2.02	121.23	117.57
1	2	1475	MA6	N1-C6-N6	2.02	119.18	117.06

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	246	OMC	C3'-C4'-C5'-O5'
30	4	20	H2U	O4'-C1'-N1-C6
1	2	930	C4J	C4'-C5'-O5'-P
1	2	246	OMC	O4'-C4'-C5'-O5'
1	2	930	C4J	C3'-C4'-C5'-O5'
30	4	20	H2U	O4'-C1'-N1-C2
30	4	32	OMC	C1'-C2'-O2'-CM2
1	2	865	OMG	C3'-C4'-C5'-O5'
1	2	926	OMG	C3'-C2'-O2'-CM2
1	2	865	OMG	C4'-C5'-O5'-P
1	2	930	C4J	N3-C3-C31-C32

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Mol	Chain	Res	Type	Atoms
30	4	20	H2U	C4'-C5'-O5'-P
30	4	32	OMC	C3'-C2'-O2'-CM2
1	2	337	OMG	C4'-C5'-O5'-P
30	4	32	OMC	C2'-C1'-N1-C6
30	4	55	PSU	O4'-C1'-C5-C4
1	2	246	OMC	C2'-C1'-N1-C2
1	2	313	OMC	C2'-C1'-N1-C2
30	4	32	OMC	C2'-C1'-N1-C2
1	2	1477	4AC	C2'-C1'-N1-C2
1	2	865	OMG	O4'-C4'-C5'-O5'
1	2	1477	4AC	C2'-C1'-N1-C6

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 106 ligands modelled in this entry, 66 are monoatomic - leaving 40 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	$\# Z > 2$
36	SPM	2	1535	-	13,13,13	0.12	0	12,12,12	0.07	0
36	SPM	2	1515	-	13,13,13	0.08	0	12,12,12	0.12	0
36	SPM	2	1529	-	13,13,13	0.12	0	12,12,12	0.06	0
36	SPM	2	1537	-	13,13,13	0.13	0	12,12,12	0.11	0
36	SPM	2	1538	-	13,13,13	0.09	0	12,12,12	0.14	0
36	SPM	2	1510	-	13,13,13	0.08	0	12,12,12	0.17	0
36	SPM	2	1508	-	13,13,13	0.06	0	12,12,12	0.12	0
36	SPM	2	1519	-	13,13,13	0.10	0	12,12,12	0.08	0
36	SPM	2	1523	-	13,13,13	0.08	0	12,12,12	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	SPM	2	1518	-	13,13,13	0.07	0	12,12,12	0.14	0
36	SPM	2	1524	-	13,13,13	0.11	0	12,12,12	0.13	0
36	SPM	2	1532	-	13,13,13	0.11	0	12,12,12	0.06	0
36	SPM	2	1522	-	13,13,13	0.09	0	12,12,12	0.09	0
36	SPM	2	1536	-	13,13,13	0.12	0	12,12,12	0.08	0
39	GTP	5	102	34	26,34,34	1.13	2 (7%)	32,54,54	1.47	6 (18%)
36	SPM	2	1507	-	13,13,13	0.08	0	12,12,12	0.12	0
36	SPM	2	1530	-	13,13,13	0.09	0	12,12,12	0.12	0
36	SPM	2	1511	-	13,13,13	0.07	0	12,12,12	0.11	0
36	SPM	2	1513	-	13,13,13	0.09	0	12,12,12	0.19	0
36	SPM	2	1509	-	13,13,13	0.06	0	12,12,12	0.14	0
36	SPM	2	1539	-	13,13,13	0.09	0	12,12,12	0.12	0
36	SPM	2	1516	-	13,13,13	0.06	0	12,12,12	0.21	0
36	SPM	2	1521	-	13,13,13	0.12	0	12,12,12	0.07	0
36	SPM	2	1525	-	13,13,13	0.08	0	12,12,12	0.16	0
36	SPM	2	1514	-	13,13,13	0.10	0	12,12,12	0.09	0
36	SPM	2	1506	-	13,13,13	0.09	0	12,12,12	0.10	0
36	SPM	2	1528	-	13,13,13	0.11	0	12,12,12	0.09	0
36	SPM	2	1533	-	13,13,13	0.11	0	12,12,12	0.08	0
36	SPM	2	1517	-	13,13,13	0.07	0	12,12,12	0.18	0
36	SPM	2	1504	-	13,13,13	0.08	0	12,12,12	0.10	0
36	SPM	2	1502	-	13,13,13	0.11	0	12,12,12	0.06	0
36	SPM	2	1505	-	13,13,13	0.07	0	12,12,12	0.21	0
36	SPM	2	1534	-	13,13,13	0.12	0	12,12,12	0.07	0
36	SPM	2	1503	-	13,13,13	0.08	0	12,12,12	0.17	0
36	SPM	2	1531	-	13,13,13	0.09	0	12,12,12	0.09	0
36	SPM	2	1520	-	13,13,13	0.11	0	12,12,12	0.14	0
36	SPM	2	1526	-	13,13,13	0.11	0	12,12,12	0.11	0
36	SPM	2	1501	-	13,13,13	0.08	0	12,12,12	0.12	0
36	SPM	2	1527	-	13,13,13	0.09	0	12,12,12	0.08	0
36	SPM	2	1512	-	13,13,13	0.11	0	12,12,12	0.09	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
36	SPM	2	1535	-	-	5/11/11/11	-
36	SPM	2	1515	-	-	2/11/11/11	-
36	SPM	2	1529	-	-	6/11/11/11	-
36	SPM	2	1537	-	-	2/11/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	SPM	2	1538	-	-	5/11/11/11	-
36	SPM	2	1510	-	-	1/11/11/11	-
36	SPM	2	1508	-	-	2/11/11/11	-
36	SPM	2	1519	-	-	2/11/11/11	-
36	SPM	2	1523	-	-	4/11/11/11	-
36	SPM	2	1518	-	-	4/11/11/11	-
36	SPM	2	1524	-	-	3/11/11/11	-
36	SPM	2	1532	-	-	9/11/11/11	-
36	SPM	2	1522	-	-	2/11/11/11	-
36	SPM	2	1536	-	-	1/11/11/11	-
39	GTP	5	102	34	-	6/18/38/38	0/3/3/3
36	SPM	2	1507	-	-	4/11/11/11	-
36	SPM	2	1530	-	-	4/11/11/11	-
36	SPM	2	1511	-	-	2/11/11/11	-
36	SPM	2	1513	-	-	1/11/11/11	-
36	SPM	2	1509	-	-	2/11/11/11	-
36	SPM	2	1539	-	-	2/11/11/11	-
36	SPM	2	1516	-	-	0/11/11/11	-
36	SPM	2	1521	-	-	7/11/11/11	-
36	SPM	2	1525	-	-	1/11/11/11	-
36	SPM	2	1514	-	-	3/11/11/11	-
36	SPM	2	1506	-	-	4/11/11/11	-
36	SPM	2	1528	-	-	4/11/11/11	-
36	SPM	2	1533	-	-	1/11/11/11	-
36	SPM	2	1517	-	-	4/11/11/11	-
36	SPM	2	1504	-	-	2/11/11/11	-
36	SPM	2	1502	-	-	11/11/11/11	-
36	SPM	2	1505	-	-	4/11/11/11	-
36	SPM	2	1534	-	-	9/11/11/11	-
36	SPM	2	1503	-	-	3/11/11/11	-
36	SPM	2	1531	-	-	2/11/11/11	-
36	SPM	2	1520	-	-	4/11/11/11	-
36	SPM	2	1526	-	-	4/11/11/11	-
36	SPM	2	1501	-	-	2/11/11/11	-
36	SPM	2	1527	-	-	3/11/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	SPM	2	1512	-	-	3/11/11/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	5	102	GTP	C5-C6	-3.94	1.39	1.47
39	5	102	GTP	C2-N3	2.18	1.38	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	5	102	GTP	PB-O3B-PG	-3.30	121.50	132.83
39	5	102	GTP	PA-O3A-PB	-3.25	121.67	132.83
39	5	102	GTP	C5-C6-N1	3.17	119.55	113.95
39	5	102	GTP	C8-N7-C5	2.99	108.69	102.99
39	5	102	GTP	C2-N1-C6	-2.81	119.92	125.10
39	5	102	GTP	O6-C6-C5	-2.06	120.36	124.37

There are no chirality outliers.

All (140) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	2	1509	SPM	C12-C11-N10-C9
36	2	1520	SPM	C12-C11-N10-C9
36	2	1524	SPM	C3-C4-N5-C6
36	2	1525	SPM	C3-C4-N5-C6
36	2	1533	SPM	C7-C6-N5-C4
39	5	102	GTP	C5'-O5'-PA-O1A
36	2	1502	SPM	N5-C6-C7-C8
36	2	1507	SPM	C7-C8-C9-N10
36	2	1521	SPM	C7-C8-C9-N10
36	2	1528	SPM	C3-C4-N5-C6
36	2	1529	SPM	N5-C6-C7-C8
39	5	102	GTP	C3'-C4'-C5'-O5'
36	2	1517	SPM	N10-C11-C12-C13
36	2	1532	SPM	N5-C6-C7-C8
36	2	1532	SPM	C7-C8-C9-N10
36	2	1502	SPM	C7-C8-C9-N10
36	2	1502	SPM	N10-C11-C12-C13
36	2	1521	SPM	N5-C6-C7-C8
36	2	1532	SPM	N10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
36	2	1501	SPM	C8-C9-N10-C11
36	2	1503	SPM	C8-C9-N10-C11
36	2	1512	SPM	C7-C6-N5-C4
36	2	1517	SPM	C3-C4-N5-C6
36	2	1519	SPM	C8-C9-N10-C11
36	2	1520	SPM	C8-C9-N10-C11
36	2	1522	SPM	C8-C9-N10-C11
36	2	1523	SPM	C7-C6-N5-C4
36	2	1535	SPM	C3-C4-N5-C6
39	5	102	GTP	O4'-C4'-C5'-O5'
36	2	1529	SPM	C2-C3-C4-N5
36	2	1502	SPM	C3-C4-N5-C6
36	2	1506	SPM	C3-C4-N5-C6
36	2	1507	SPM	C12-C11-N10-C9
36	2	1514	SPM	C8-C9-N10-C11
36	2	1517	SPM	C8-C9-N10-C11
36	2	1518	SPM	C3-C4-N5-C6
36	2	1520	SPM	C3-C4-N5-C6
36	2	1521	SPM	C7-C6-N5-C4
36	2	1522	SPM	C7-C6-N5-C4
36	2	1524	SPM	C8-C9-N10-C11
36	2	1527	SPM	C8-C9-N10-C11
36	2	1538	SPM	C8-C9-N10-C11
36	2	1529	SPM	C6-C7-C8-C9
36	2	1518	SPM	C7-C6-N5-C4
36	2	1521	SPM	C3-C4-N5-C6
36	2	1536	SPM	C3-C4-N5-C6
36	2	1534	SPM	C6-C7-C8-C9
36	2	1532	SPM	C6-C7-C8-C9
36	2	1521	SPM	C6-C7-C8-C9
36	2	1502	SPM	C2-C3-C4-N5
36	2	1512	SPM	C12-C11-N10-C9
36	2	1515	SPM	C8-C9-N10-C11
36	2	1527	SPM	C12-C11-N10-C9
36	2	1528	SPM	C7-C6-N5-C4
36	2	1528	SPM	C8-C9-N10-C11
36	2	1530	SPM	C3-C4-N5-C6
36	2	1531	SPM	C7-C6-N5-C4
36	2	1539	SPM	C3-C4-N5-C6
36	2	1523	SPM	C6-C7-C8-C9
36	2	1502	SPM	C11-C12-C13-N14
36	2	1521	SPM	C11-C12-C13-N14

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Mol	Chain	Res	Type	Atoms
36	2	1523	SPM	C11-C12-C13-N14
36	2	1502	SPM	C8-C9-N10-C11
36	2	1506	SPM	C12-C11-N10-C9
36	2	1535	SPM	C6-C7-C8-C9
36	2	1514	SPM	C3-C4-N5-C6
36	2	1532	SPM	C7-C6-N5-C4
36	2	1508	SPM	C3-C4-N5-C6
36	2	1529	SPM	C7-C6-N5-C4
36	2	1534	SPM	C7-C8-C9-N10
36	2	1502	SPM	C7-C6-N5-C4
36	2	1505	SPM	C12-C11-N10-C9
36	2	1509	SPM	C8-C9-N10-C11
36	2	1511	SPM	C12-C11-N10-C9
36	2	1512	SPM	C3-C4-N5-C6
36	2	1518	SPM	C8-C9-N10-C11
36	2	1526	SPM	C8-C9-N10-C11
36	2	1534	SPM	C7-C6-N5-C4
36	2	1538	SPM	C3-C4-N5-C6
36	2	1521	SPM	N1-C2-C3-C4
36	2	1529	SPM	N1-C2-C3-C4
36	2	1532	SPM	N1-C2-C3-C4
36	2	1534	SPM	C11-C12-C13-N14
39	5	102	GTP	C5'-O5'-PA-O3A
36	2	1514	SPM	C12-C11-N10-C9
36	2	1534	SPM	C12-C11-N10-C9
39	5	102	GTP	C5'-O5'-PA-O2A
36	2	1503	SPM	C12-C11-N10-C9
36	2	1507	SPM	C8-C9-N10-C11
36	2	1528	SPM	C12-C11-N10-C9
36	2	1530	SPM	C7-C6-N5-C4
36	2	1531	SPM	C8-C9-N10-C11
36	2	1535	SPM	C12-C11-N10-C9
36	2	1532	SPM	C2-C3-C4-N5
36	2	1524	SPM	C7-C6-N5-C4
36	2	1505	SPM	C7-C6-N5-C4
36	2	1510	SPM	C3-C4-N5-C6
36	2	1513	SPM	C8-C9-N10-C11
36	2	1535	SPM	N10-C11-C12-C13
36	2	1508	SPM	C12-C11-N10-C9
36	2	1517	SPM	C7-C6-N5-C4
36	2	1527	SPM	C3-C4-N5-C6
36	2	1537	SPM	C7-C6-N5-C4

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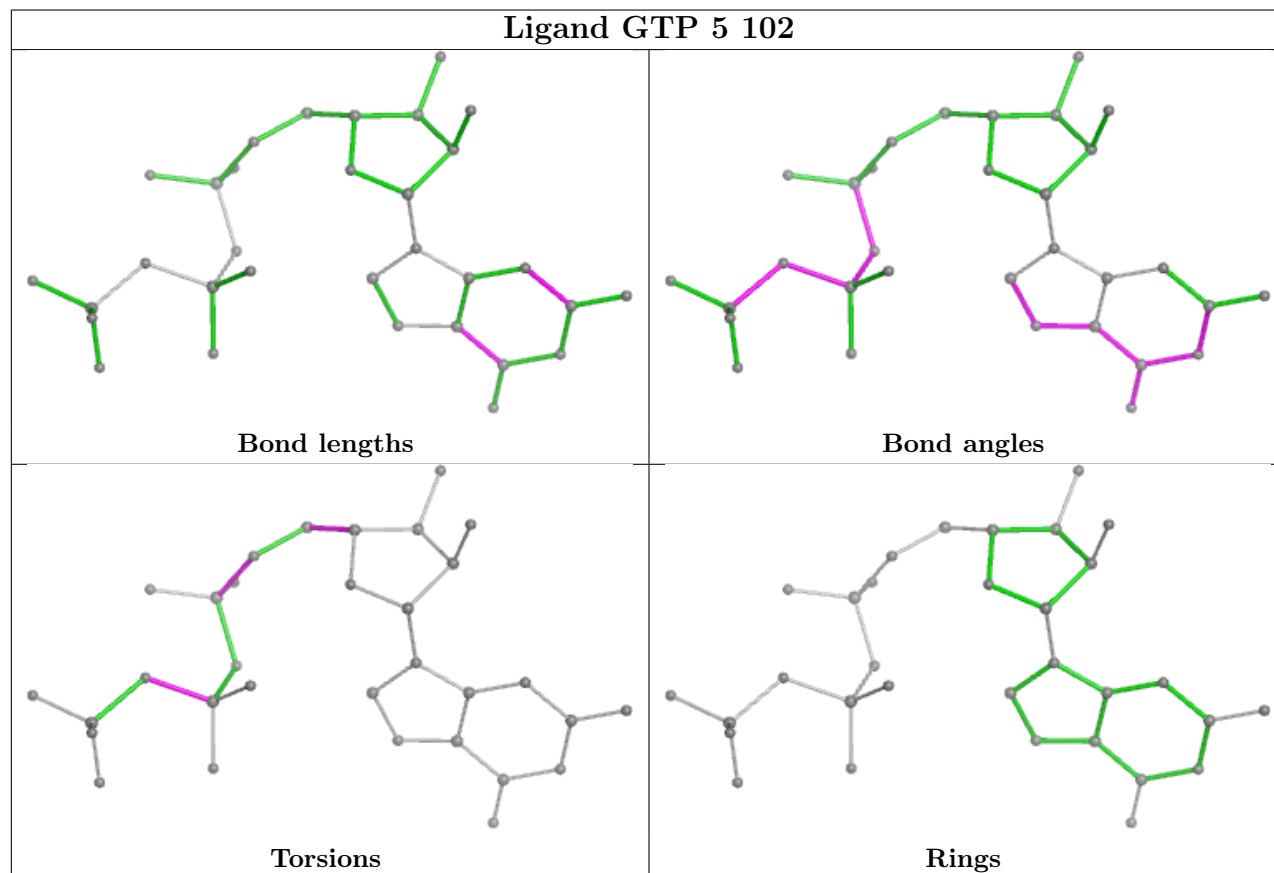
Mol	Chain	Res	Type	Atoms
36	2	1538	SPM	C12-C11-N10-C9
36	2	1534	SPM	C2-C3-C4-N5
36	2	1526	SPM	C3-C4-N5-C6
36	2	1539	SPM	C7-C6-N5-C4
36	2	1502	SPM	N1-C2-C3-C4
36	2	1532	SPM	C11-C12-C13-N14
36	2	1534	SPM	N1-C2-C3-C4
36	2	1503	SPM	C3-C4-N5-C6
36	2	1506	SPM	C8-C9-N10-C11
36	2	1511	SPM	C3-C4-N5-C6
36	2	1530	SPM	C8-C9-N10-C11
36	2	1532	SPM	C3-C4-N5-C6
36	2	1534	SPM	C3-C4-N5-C6
36	2	1505	SPM	C8-C9-N10-C11
36	2	1515	SPM	C7-C6-N5-C4
36	2	1526	SPM	C12-C11-N10-C9
36	2	1535	SPM	C8-C9-N10-C11
36	2	1505	SPM	C7-C8-C9-N10
36	2	1506	SPM	C6-C7-C8-C9
36	2	1502	SPM	C6-C7-C8-C9
36	2	1501	SPM	C12-C11-N10-C9
36	2	1537	SPM	C12-C11-N10-C9
36	2	1538	SPM	C6-C7-C8-C9
36	2	1504	SPM	C8-C9-N10-C11
36	2	1507	SPM	C3-C4-N5-C6
36	2	1519	SPM	C3-C4-N5-C6
36	2	1526	SPM	C7-C6-N5-C4
36	2	1529	SPM	C8-C9-N10-C11
36	2	1530	SPM	C12-C11-N10-C9
36	2	1518	SPM	C6-C7-C8-C9
39	5	102	GTP	PG-O3B-PB-O2B
36	2	1520	SPM	C6-C7-C8-C9
36	2	1502	SPM	C12-C11-N10-C9
36	2	1523	SPM	C8-C9-N10-C11
36	2	1534	SPM	C8-C9-N10-C11
36	2	1504	SPM	C6-C7-C8-C9
36	2	1538	SPM	N5-C6-C7-C8

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

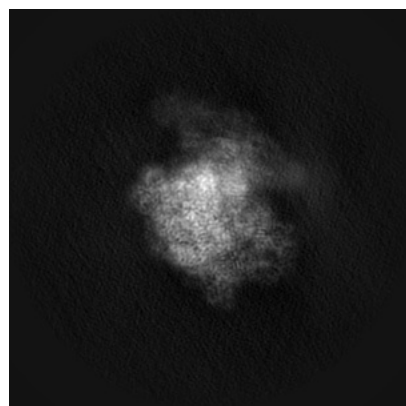
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50724. These allow visual inspection of the internal detail of the map and identification of artifacts.

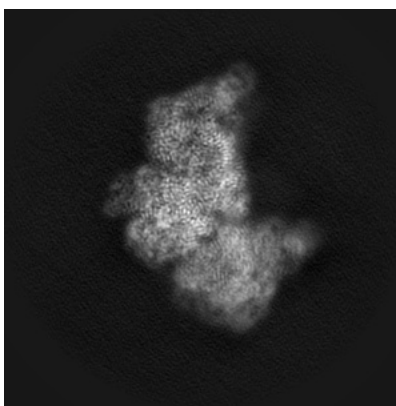
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

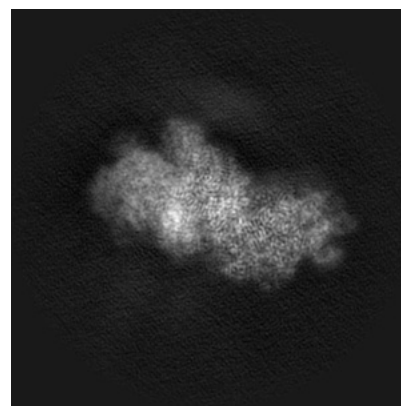
6.1.1 Primary map



X

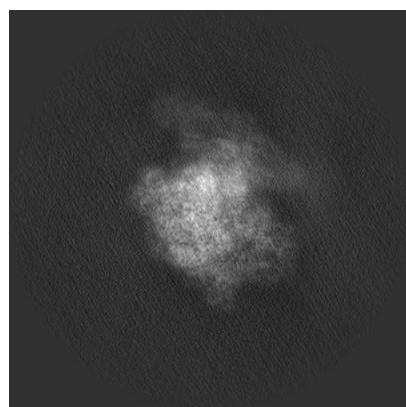


Y

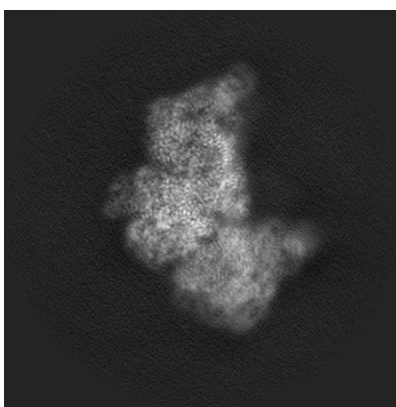


Z

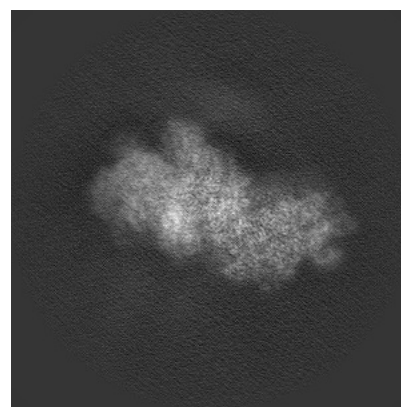
6.1.2 Raw map



X



Y

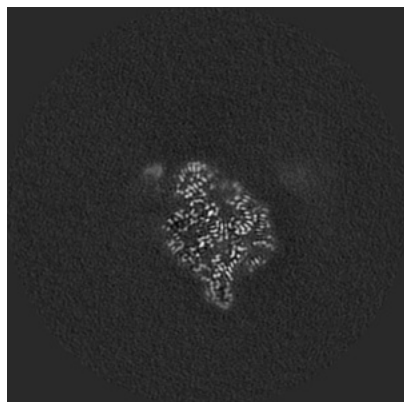


Z

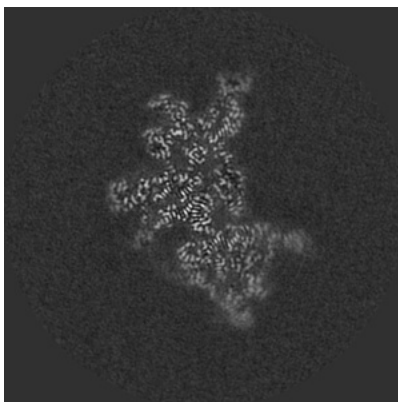
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

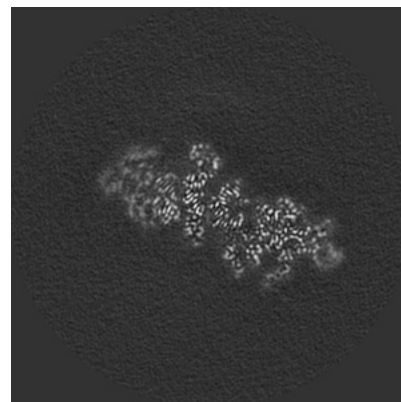
6.2.1 Primary map



X Index: 258

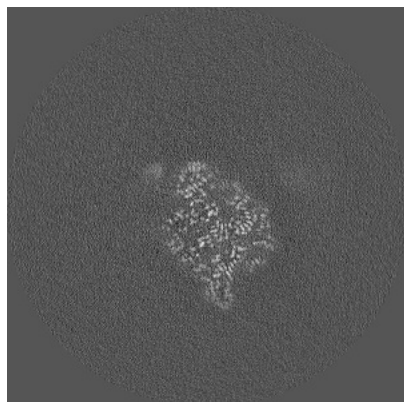


Y Index: 258

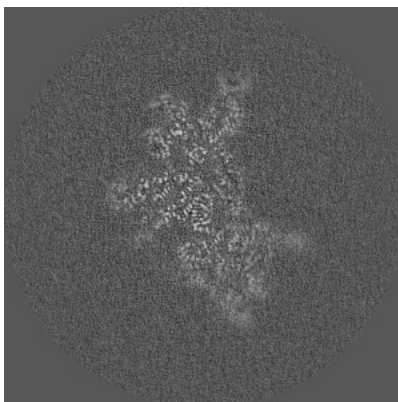


Z Index: 258

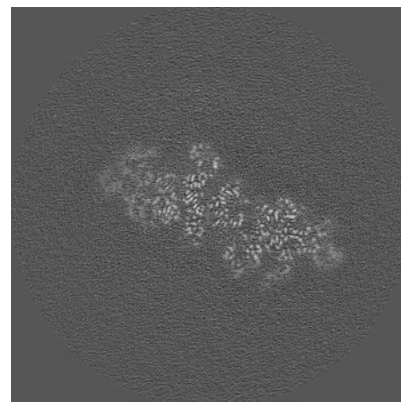
6.2.2 Raw map



X Index: 258



Y Index: 258

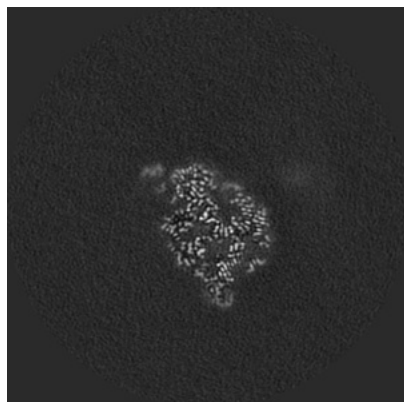


Z Index: 258

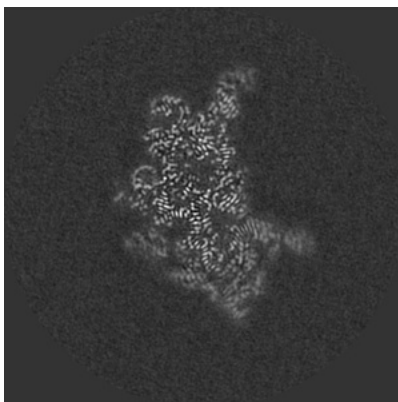
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

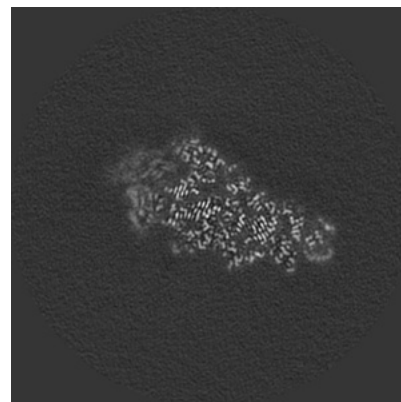
6.3.1 Primary map



X Index: 261

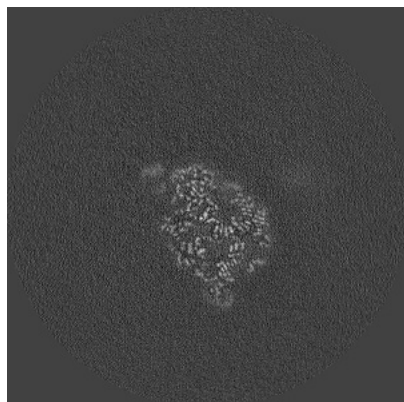


Y Index: 251

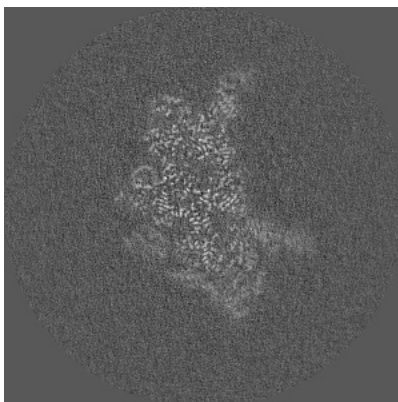


Z Index: 244

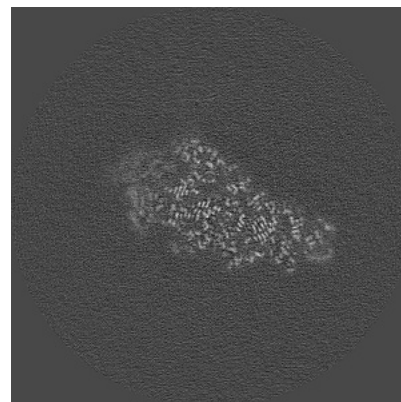
6.3.2 Raw map



X Index: 261



Y Index: 251

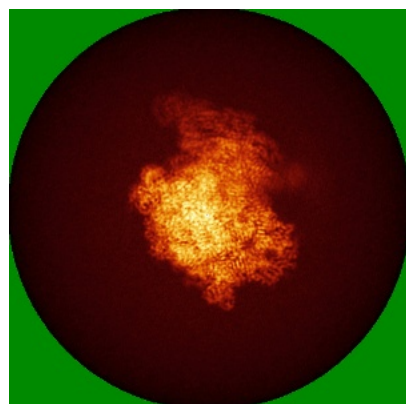


Z Index: 244

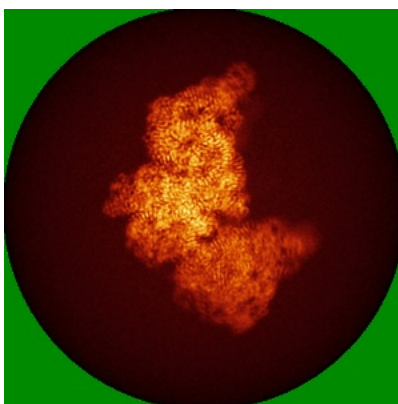
The images above show the largest variance slices of the map in three orthogonal directions.

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

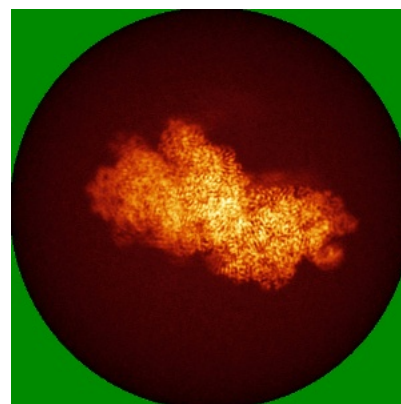
6.4.1 Primary map



X

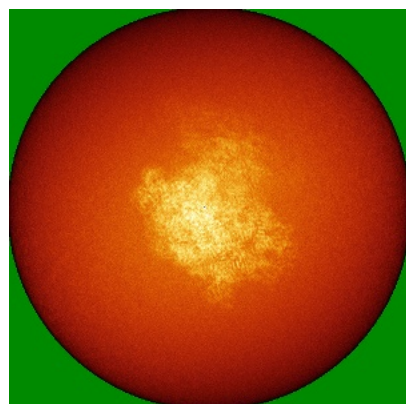


Y

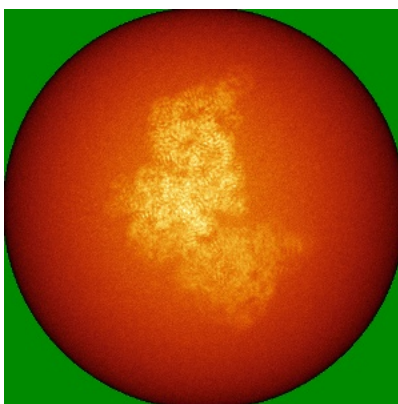


Z

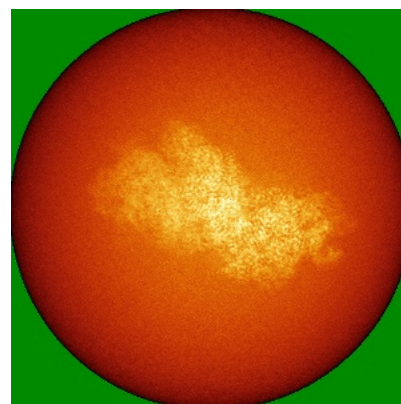
6.4.2 Raw map



X



Y

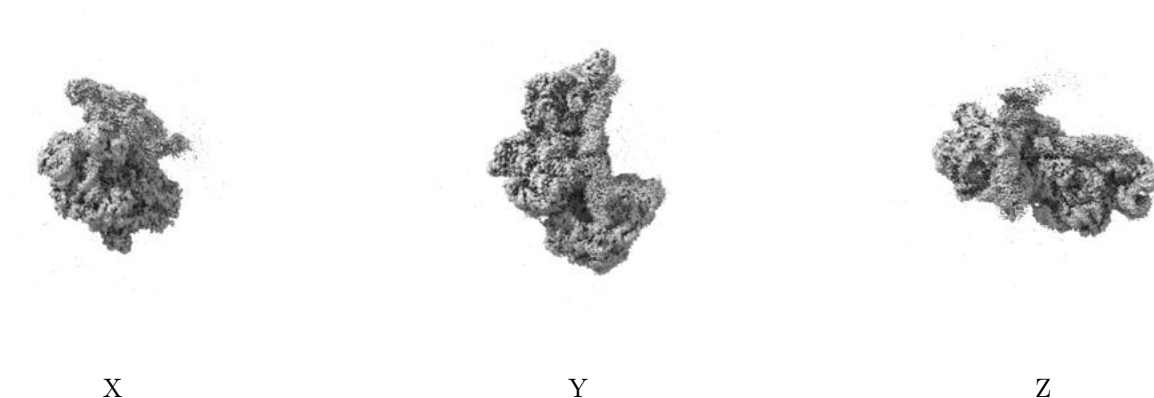


Z

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

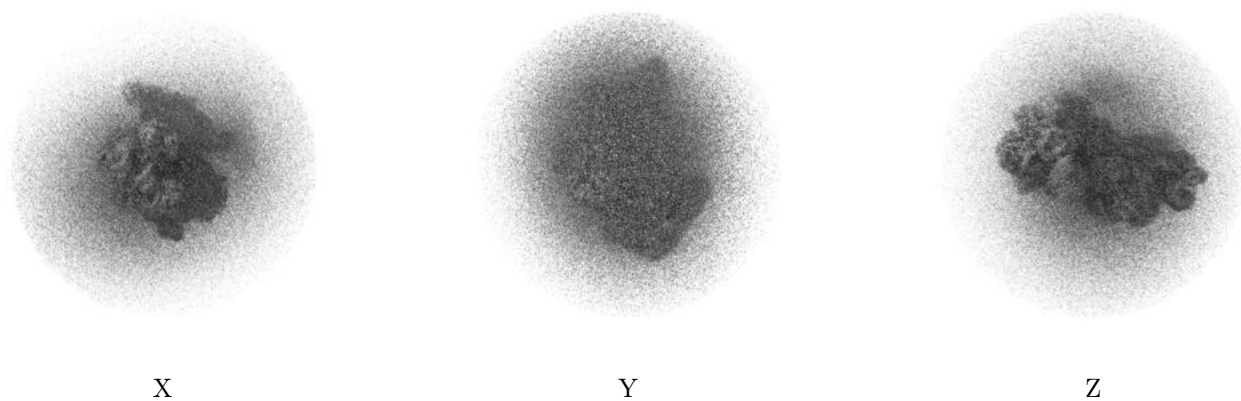
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0045. 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.

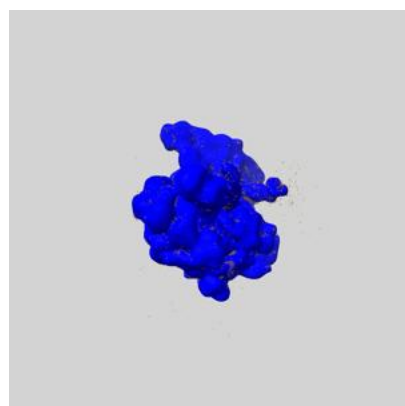
6.6 Mask visualisation [i](#)

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

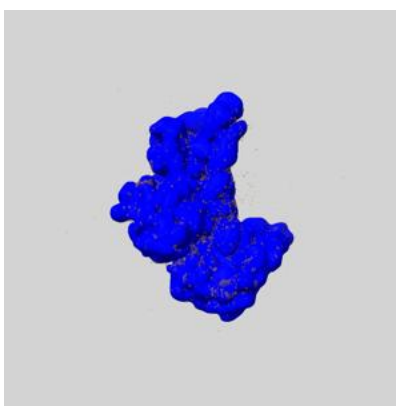
A mask typically either:

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

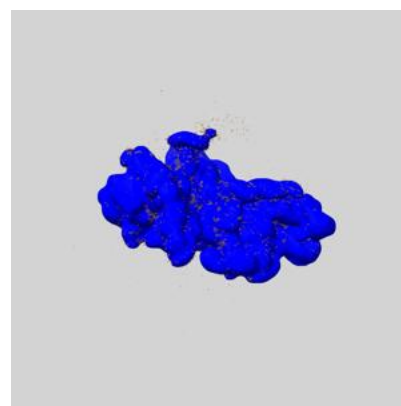
6.6.1 emd_50724_msk_1.map [i](#)



X



Y

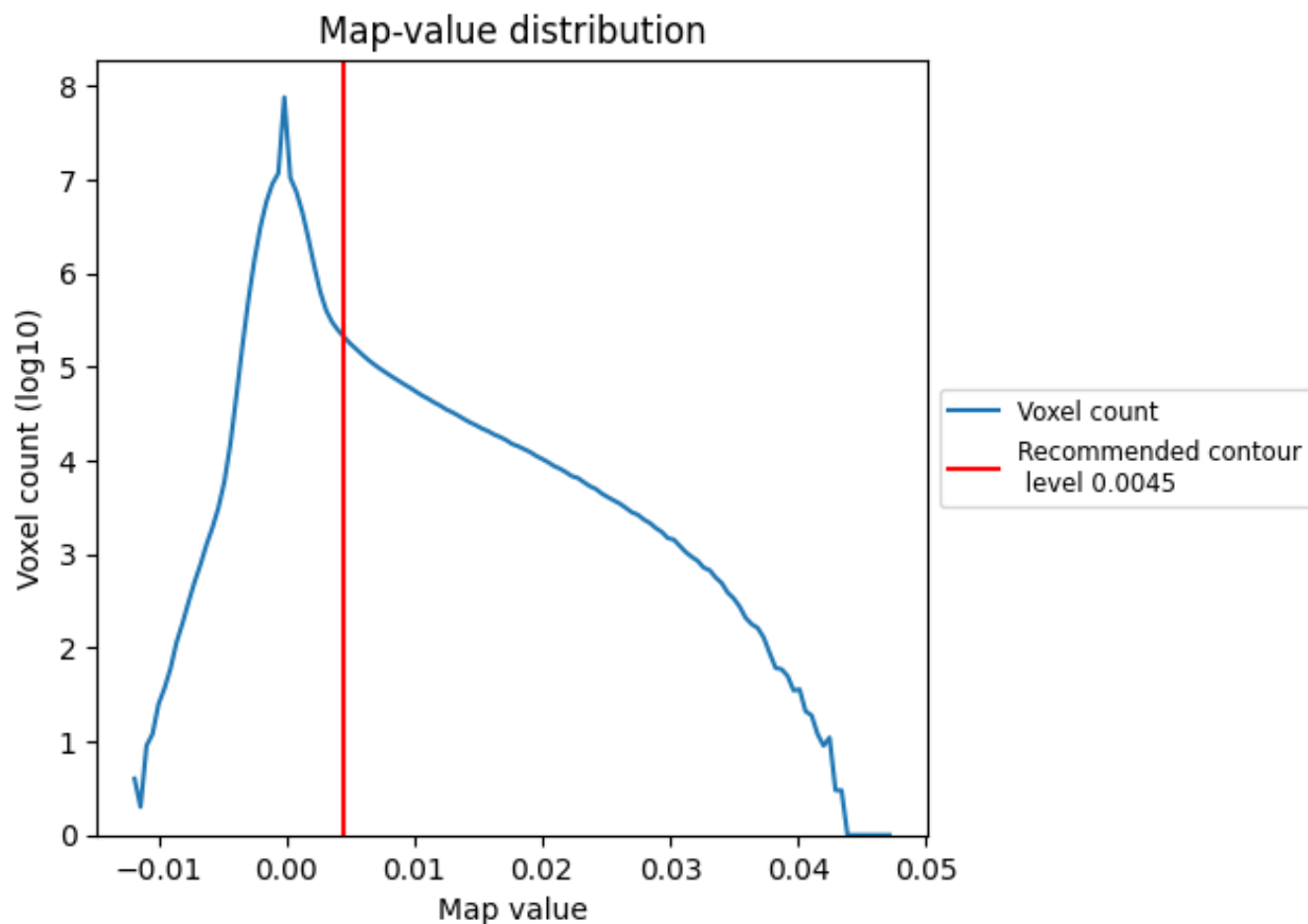


Z

7 Map analysis [i](#)

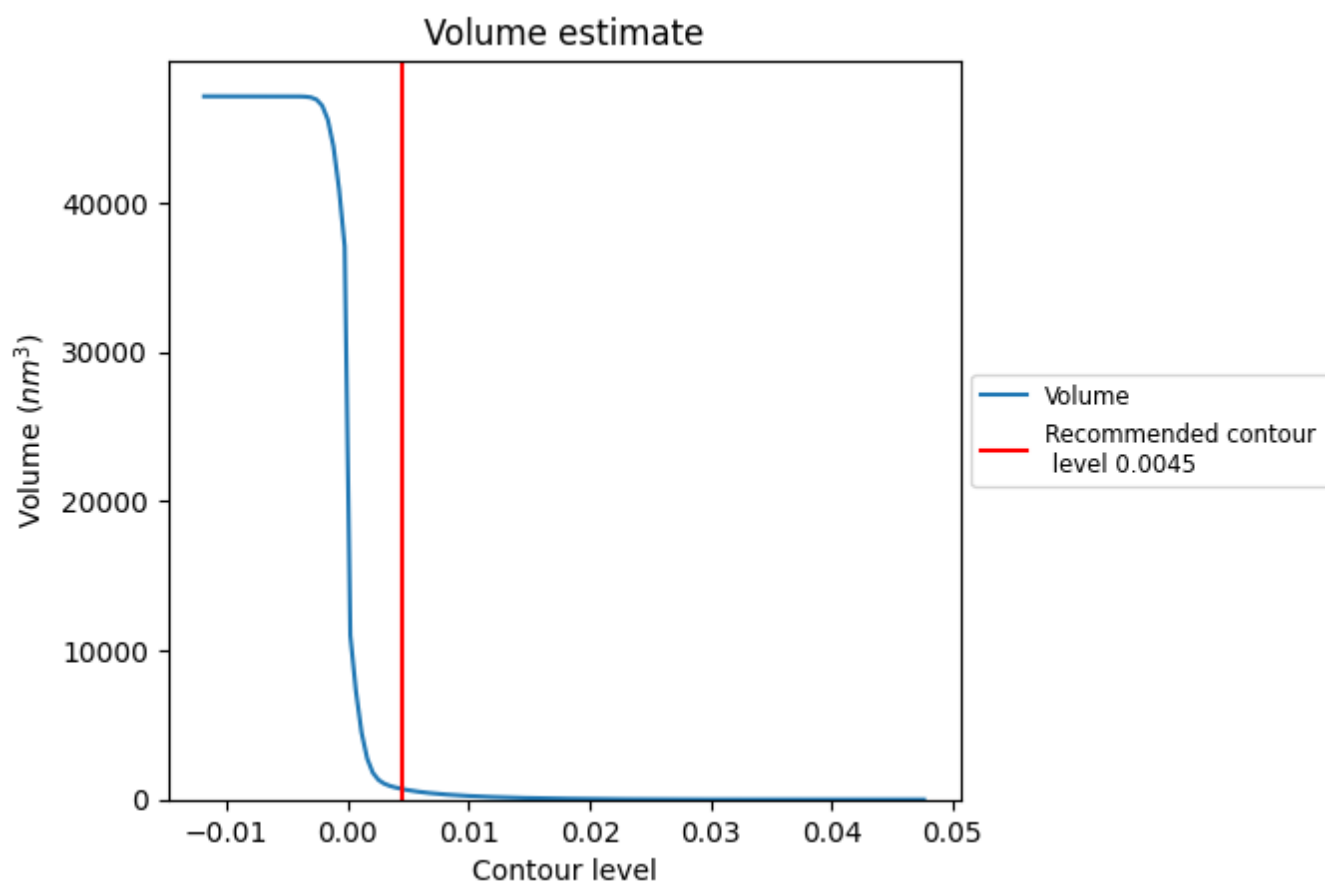
This section contains the results of statistical analysis of the map.

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.

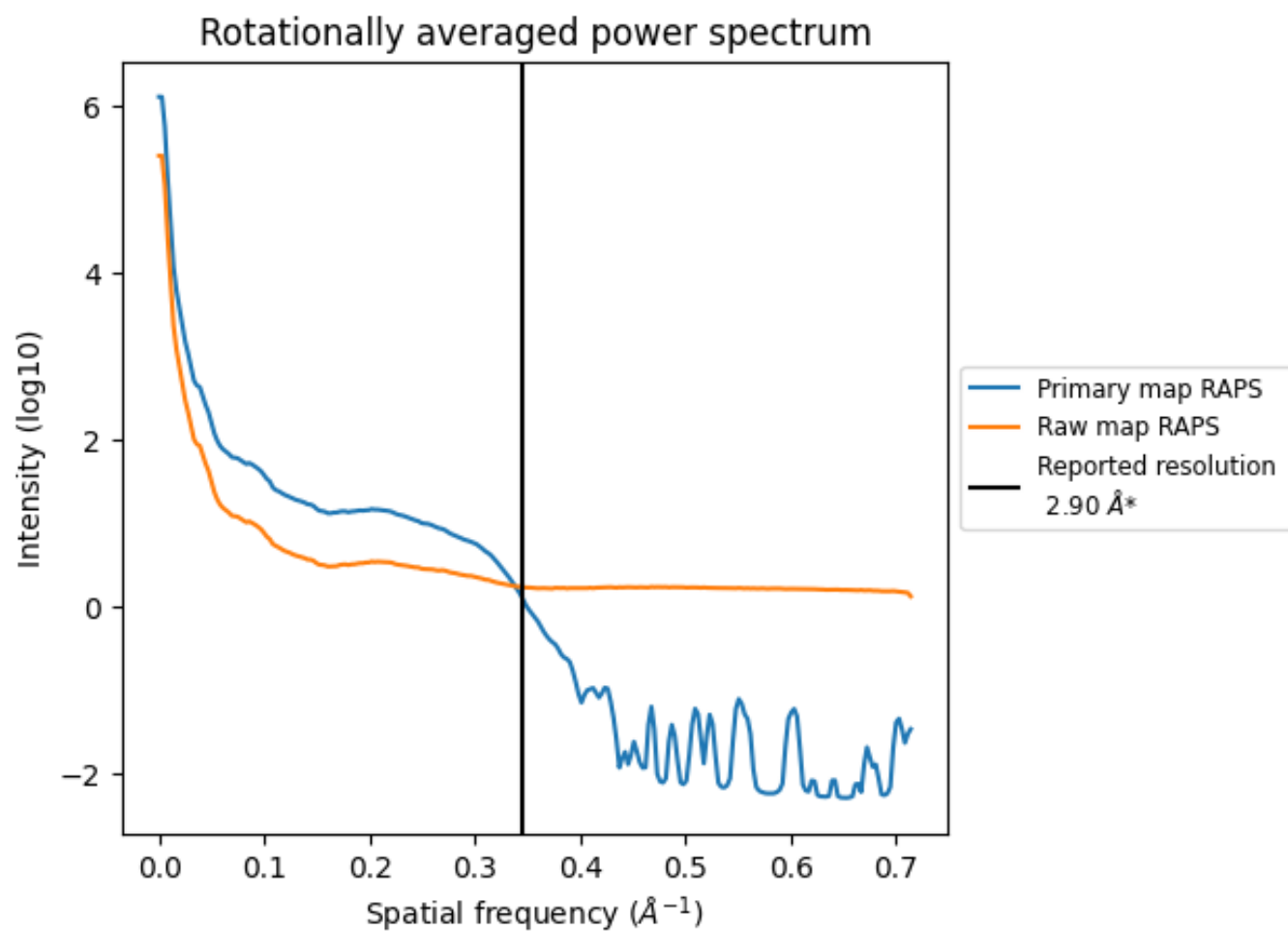
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 709 nm³; this corresponds to an approximate mass of 640 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 ⓘ

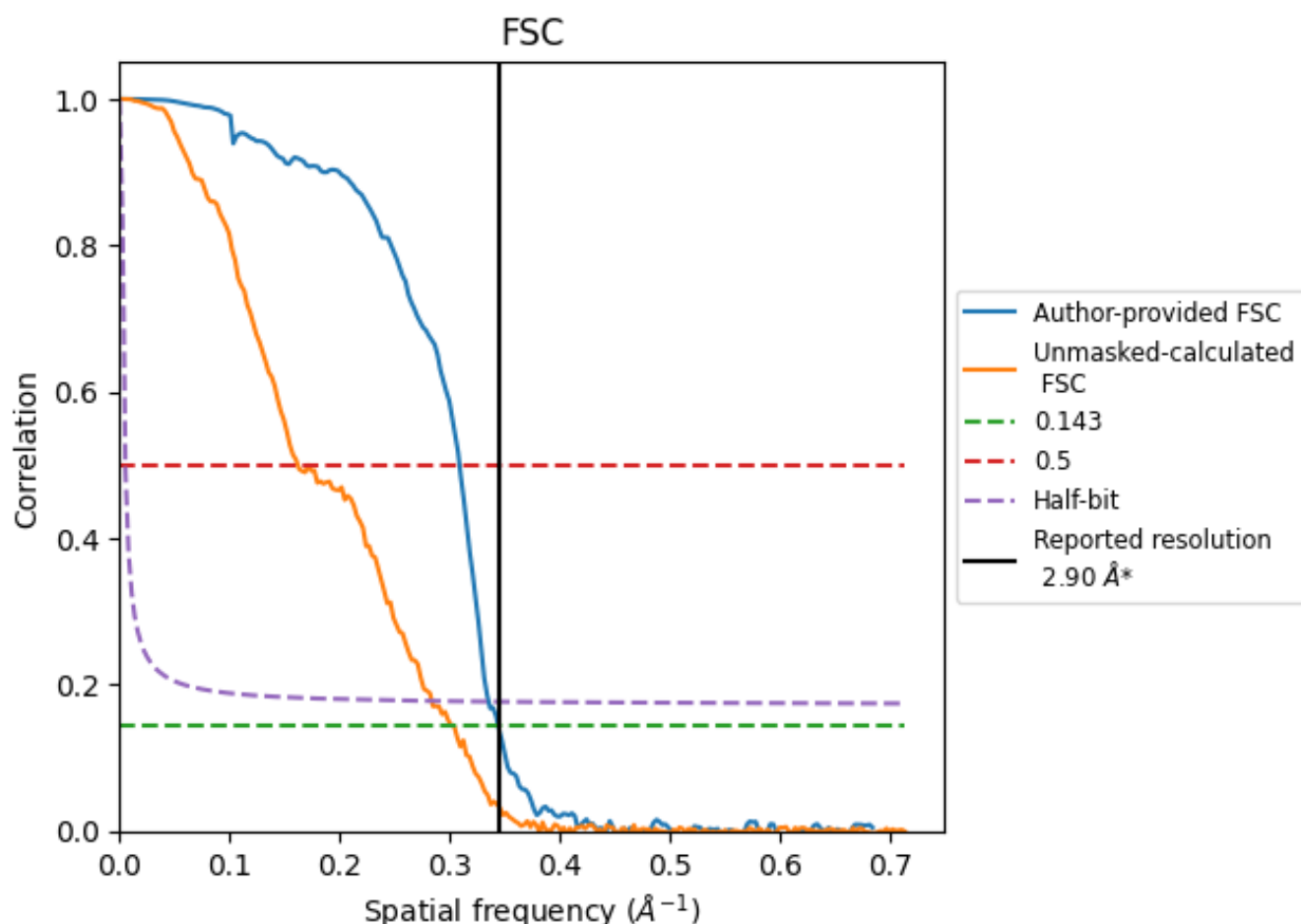


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

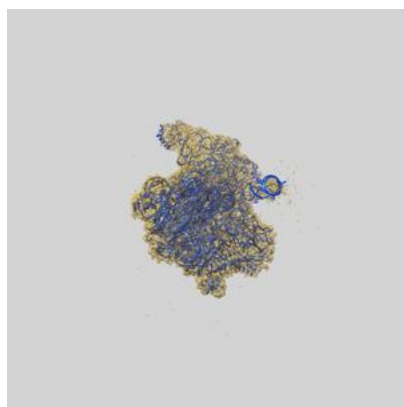
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.90	3.23	2.98
Unmasked-calculated*	3.29	6.17	3.52

*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 3.29 differs from the reported value 2.9 by more than 10 %

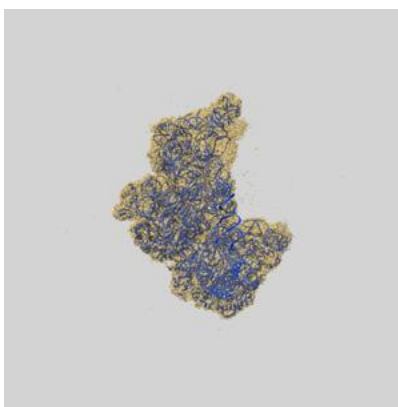
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-50724 and PDB model 9FS6. Per-residue inclusion information can be found in section [3](#) on page [15](#).

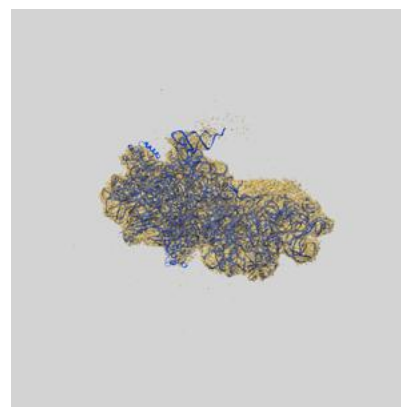
9.1 Map-model overlay [i](#)



X



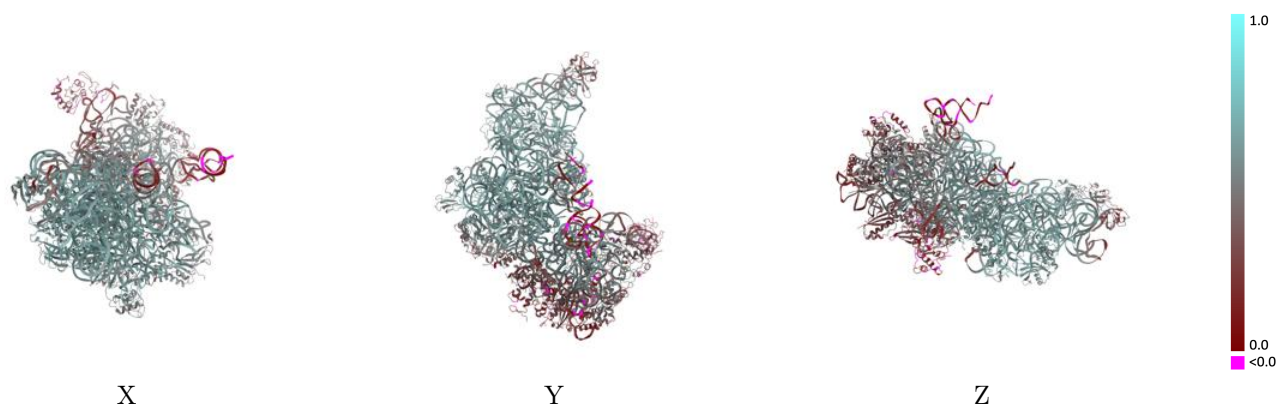
Y



Z

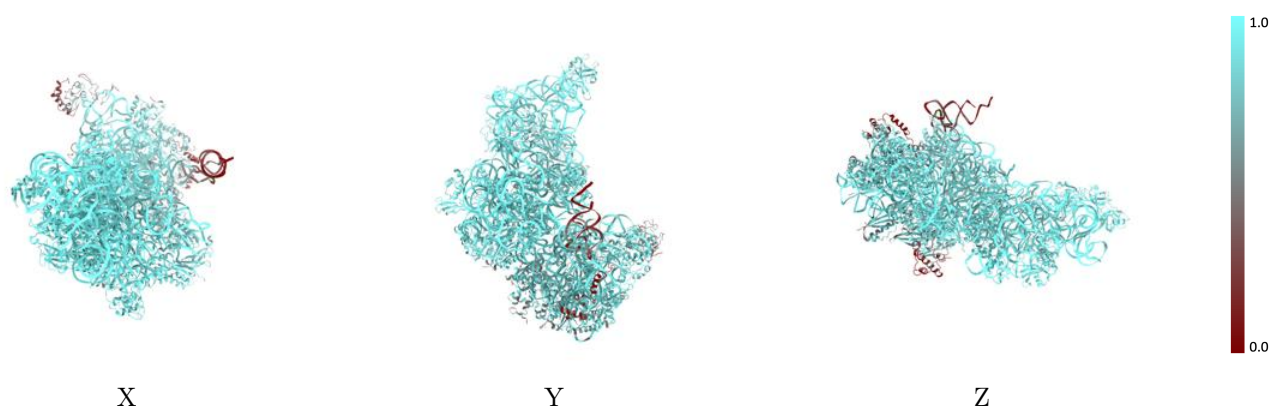
The images above show the 3D surface view of the map at the recommended contour level 0.0045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



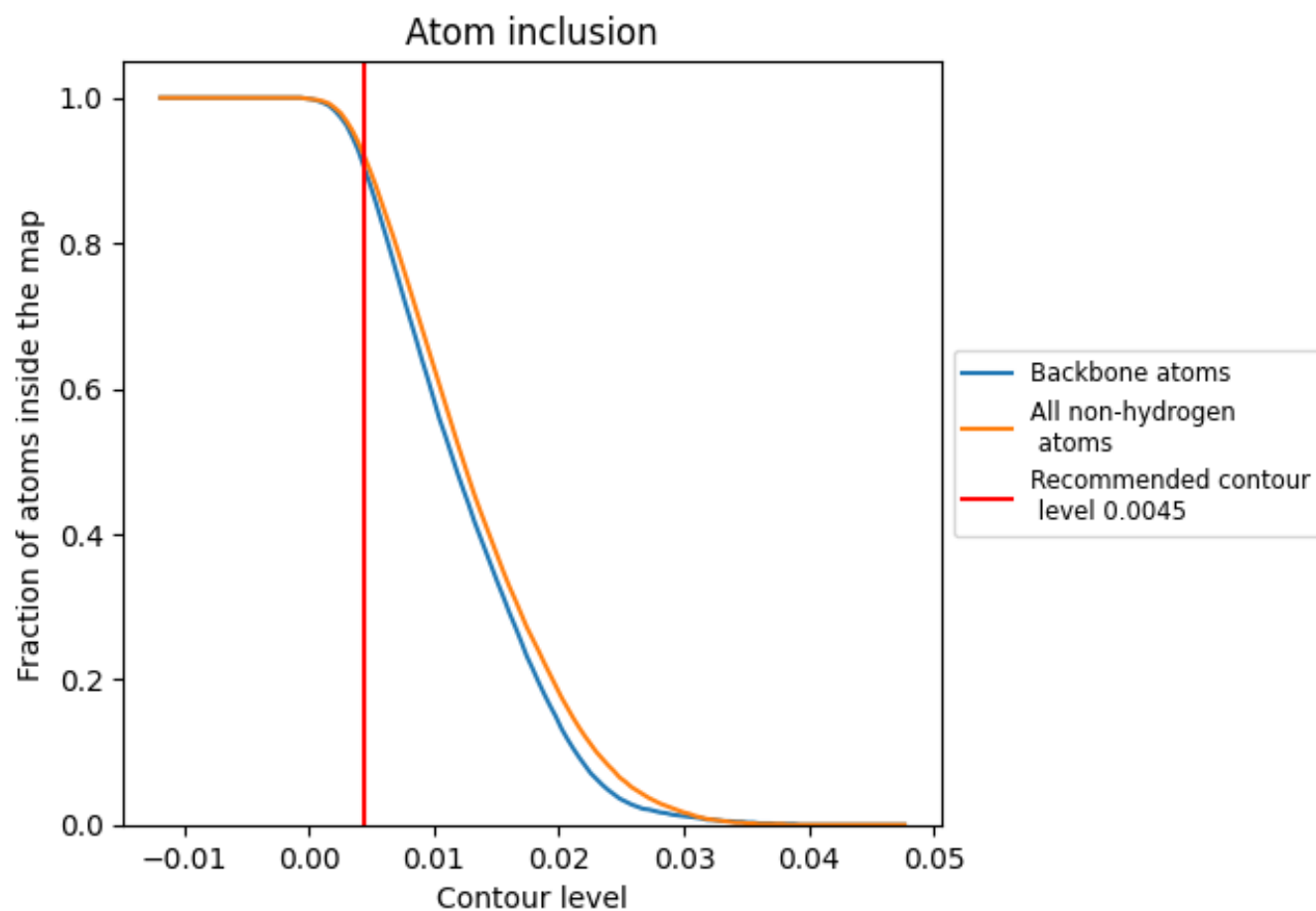
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0045).









































































9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9170	 0.5020
2	 0.9890	 0.5630
3	 0.3250	 0.1480
4	 0.4510	 0.1940
5	 1.0000	 0.5780
A	 0.9260	 0.5060
B	 0.8830	 0.4540
C	 0.9510	 0.5540
D	 0.9700	 0.5900
E	 0.9760	 0.5940
F	 0.9640	 0.5880
G	 0.8990	 0.4210
H	 0.7870	 0.3100
I	 0.9840	 0.6110
J	 0.9660	 0.5680
K	 0.8760	 0.3820
L	 0.7920	 0.3470
M	 0.9120	 0.4910
N	 0.9770	 0.5820
O	 0.8730	 0.4350
P	 0.9810	 0.5110
Q	 0.9540	 0.5440
R	 0.9780	 0.6050
S	 0.8930	 0.3790
T	 0.8490	 0.3970
U	 0.8890	 0.3900
V	 0.9400	 0.5490
W	 0.9530	 0.5480
X	 0.7360	 0.2790
Y	 0.4130	 0.1340
Z	 0.8910	 0.4320
a	 0.8710	 0.3610
b	 0.9090	 0.5140
c	 0.3830	 0.2050
d	 0.7300	 0.2360
e	 0.8370	 0.5300

