



wwPDB EM Validation Summary 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 wwPDB EM Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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

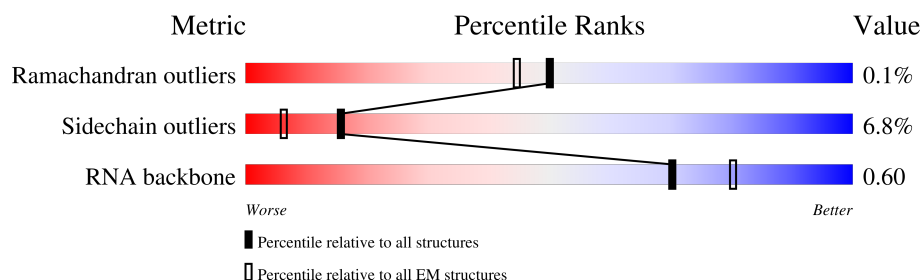
1 Overall quality at a glance

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.



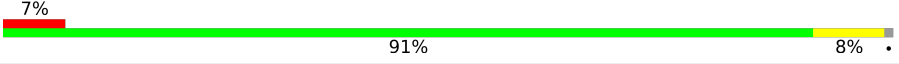
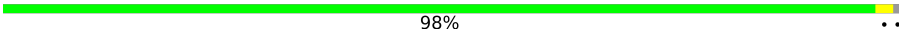


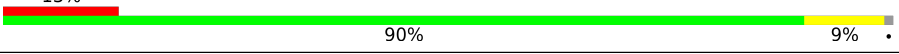
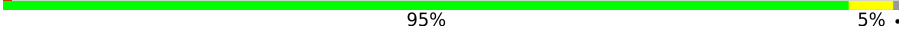
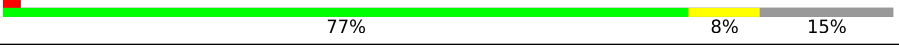


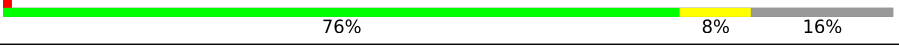


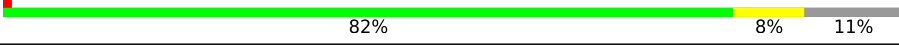





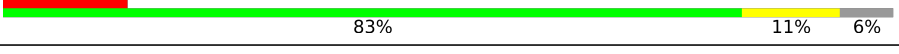


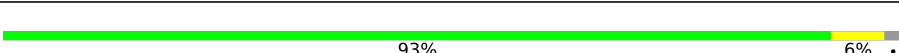
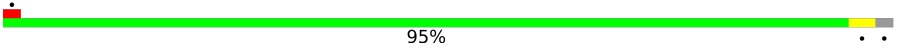


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	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		

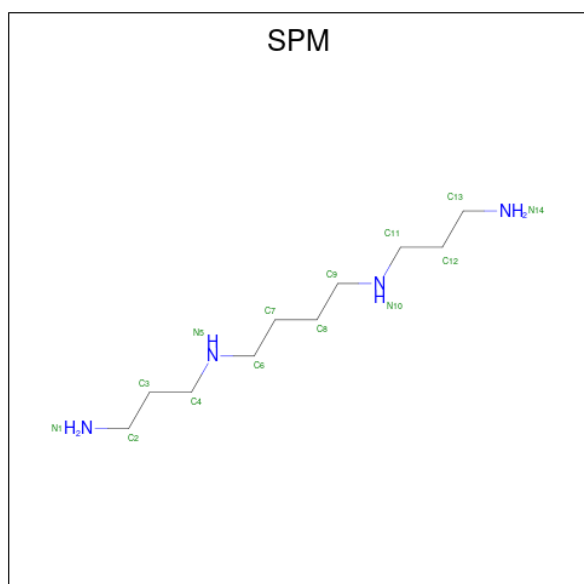
- Molecule 34 is a RNA chain called mRNA Ss-aIF2beta.

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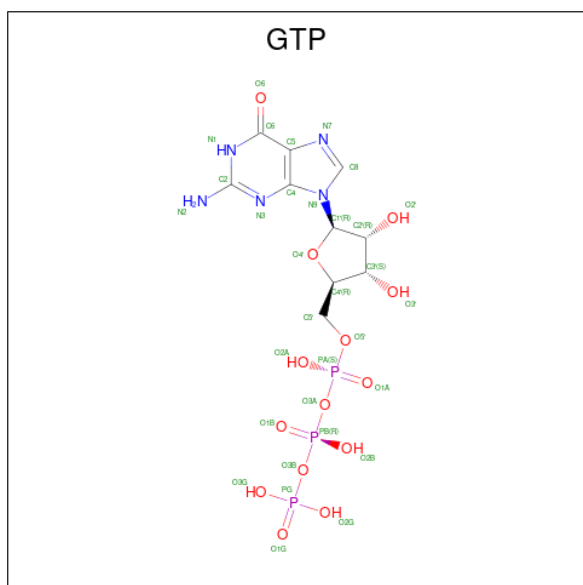
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Mol	Chain	Residues	Atoms		AltConf
37	R	1	Total	Mg	0
			1	1	
37	5	1	Total	Mg	0
			1	1	

- 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	

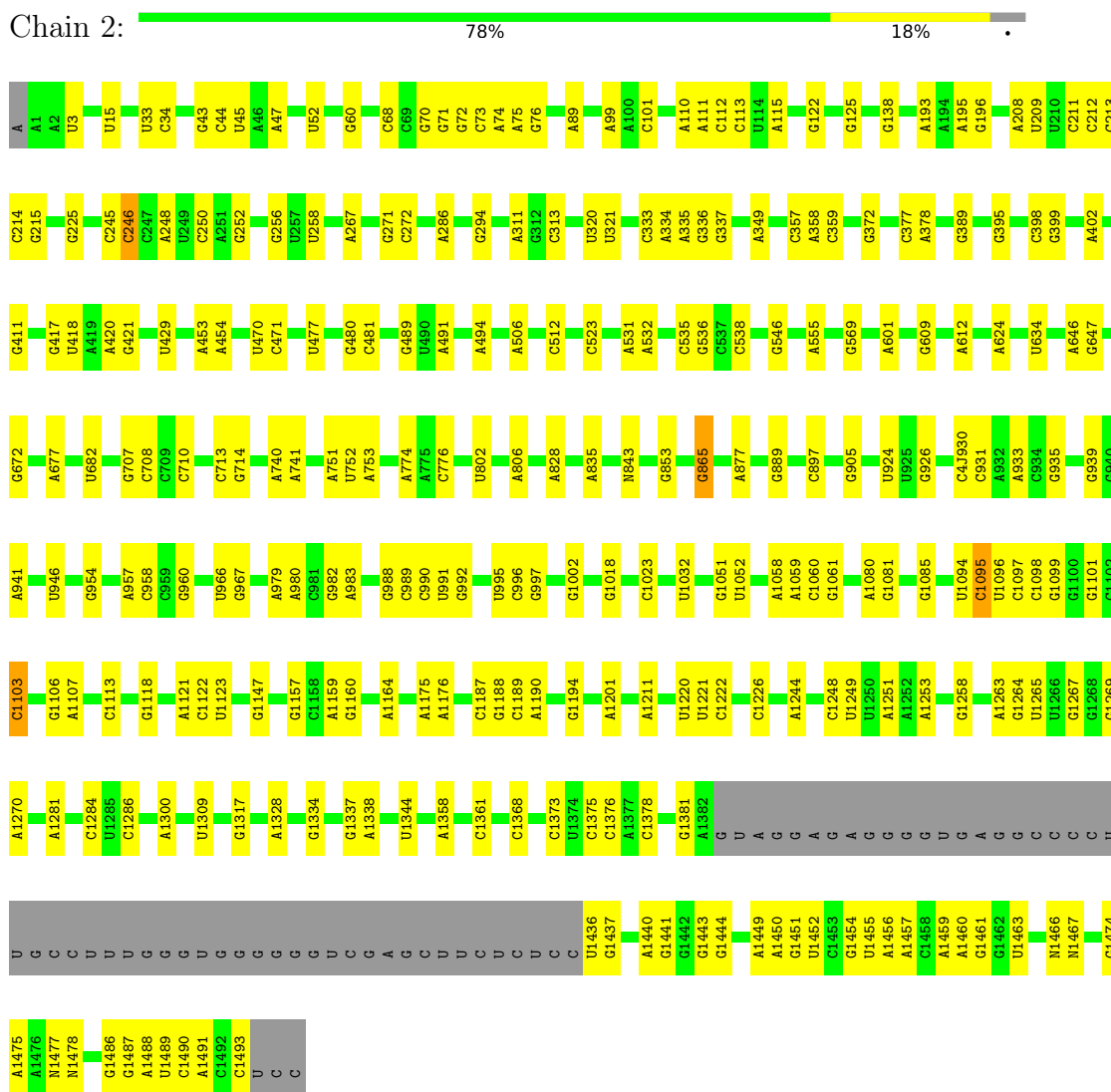
- Molecule 40 is water.

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

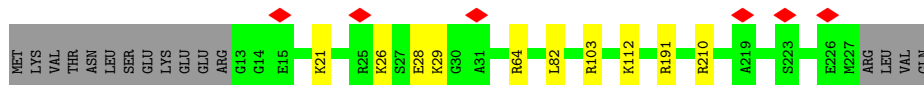
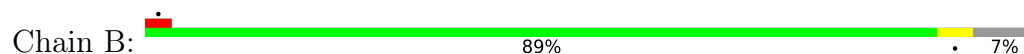
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

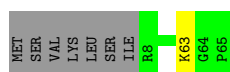
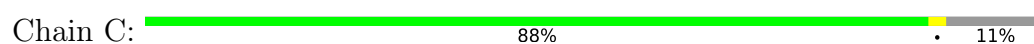




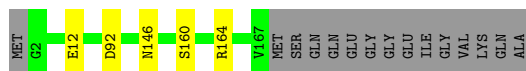
- Molecule 3: Small ribosomal subunit protein uS2



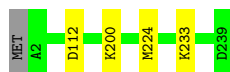
- Molecule 4: Small zinc finger protein HVO-2753-like zinc-binding pocket domain-containing protein



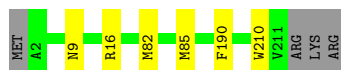
- Molecule 5: Small ribosomal subunit protein uS4



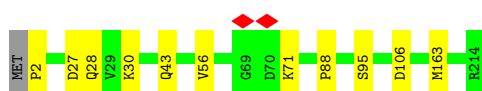
- Molecule 6: Small ribosomal subunit protein eS4



- Molecule 7: Small ribosomal subunit protein uS5



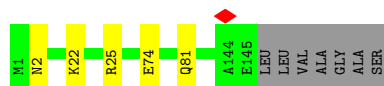
- Molecule 8: Small ribosomal subunit protein eS6



- Molecule 9: Small ribosomal subunit protein uS7

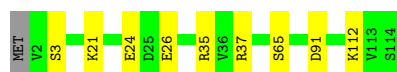
- Molecule 16: Small ribosomal subunit protein uS15

Chain Q:  92% 5%




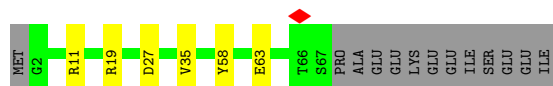
- Molecule 17: Small ribosomal subunit protein uS17

Chain R:  91% 8%




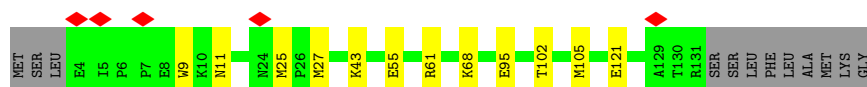
- Molecule 18: Small ribosomal subunit protein eS17

Chain S:  76% 8% 16%




- Molecule 19: Small ribosomal subunit protein uS19

Chain T:  83% 9% 9%




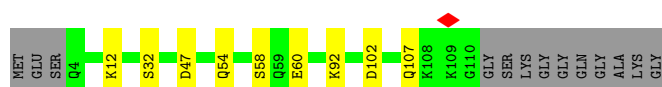
- Molecule 20: Small ribosomal subunit protein eS19

Chain U:  89% 8%




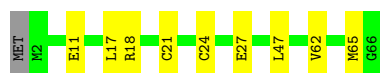
- Molecule 21: Small ribosomal subunit protein eS24

Chain V:  82% 8% 11%



- Molecule 22: Small ribosomal subunit protein eS27

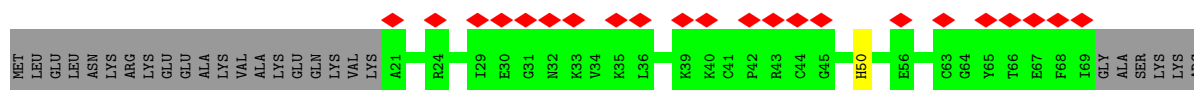
Chain W:  85% 14%



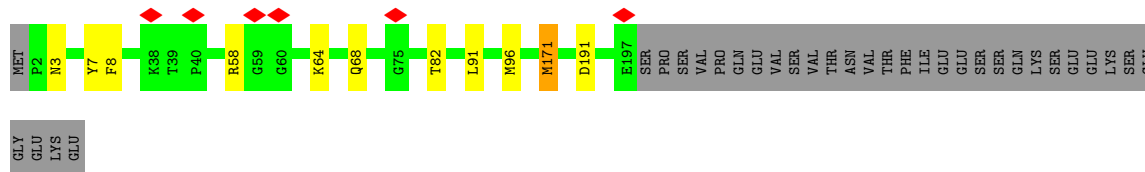
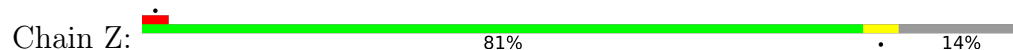
- Molecule 23: Small ribosomal subunit protein eS28



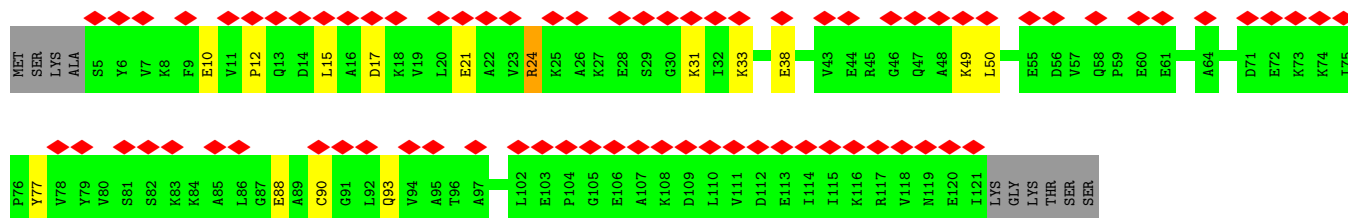
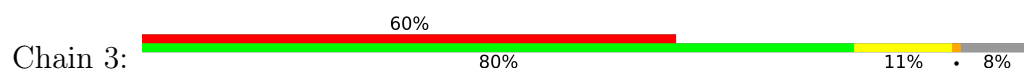
- Molecule 24: Small ribosomal subunit protein eS31



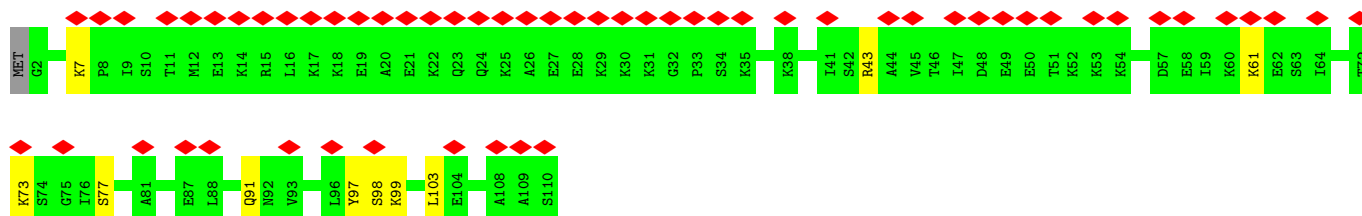
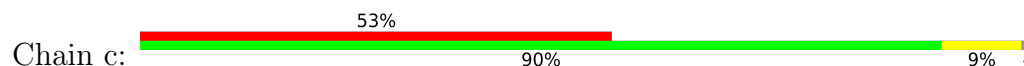
- Molecule 25: Small ribosomal subunit protein uS3



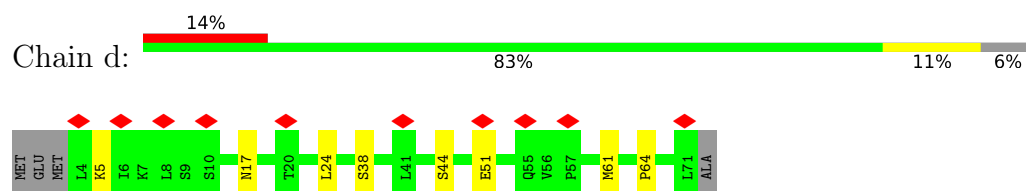
- Molecule 26: Large ribosomal subunit protein eL8



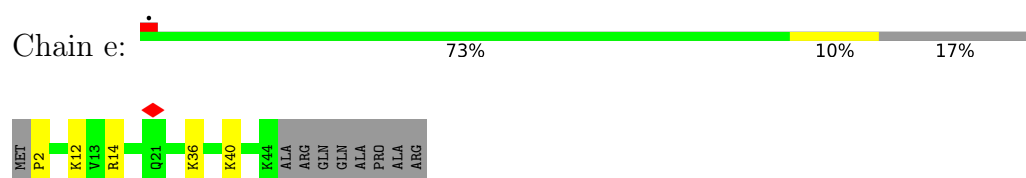
- Molecule 27: Small ribosomal subunit protein eS25



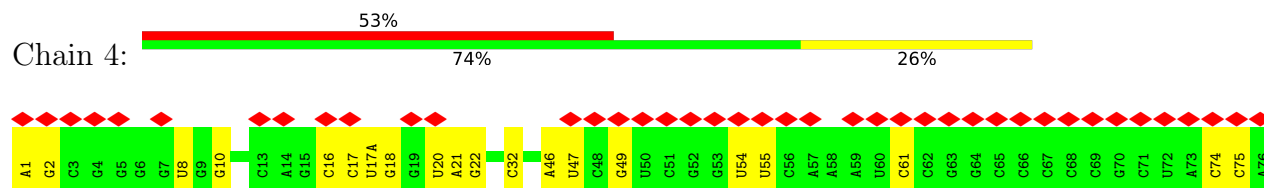
- Molecule 28: VapB-type antitoxin



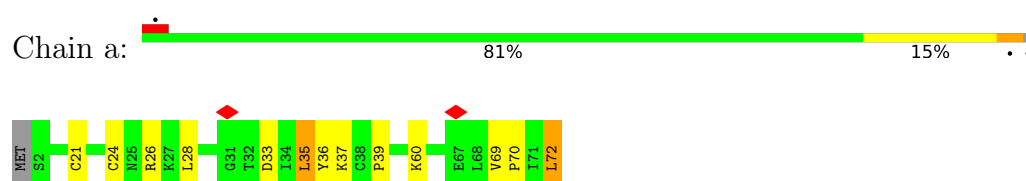
- Molecule 29: LSU ribosomal protein S30E (Rps30E)



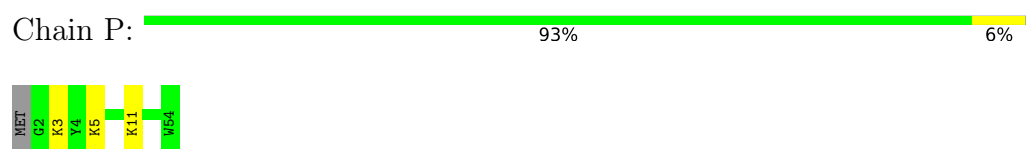
- Molecule 30: tRNA met initiator



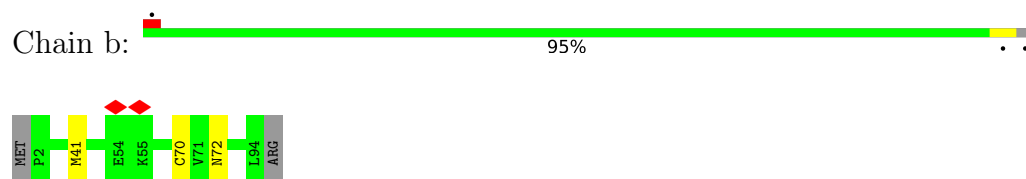
- Molecule 31: aS34



- 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% ...



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%)

The worst 5 of 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

The worst 5 of 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

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

5 of 236 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	R	65	SER
31	a	35	LEU
20	U	121	LYS
31	a	26	ARG
27	c	43	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
18	S	31	ASN
21	V	22	GLN
31	a	25	ASN
20	U	150	ASN
24	Y	50	HIS

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%)

5 of 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

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 [i](#)

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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
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

The worst 5 of 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
1	2	1061	OMG	C6-N1	-3.00	1.33	1.37

The worst 5 of 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

There are no chirality outliers.

5 of 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'

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
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	-
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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

The worst 5 of 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

There are no chirality outliers.

5 of 140 torsion outliers are listed below:

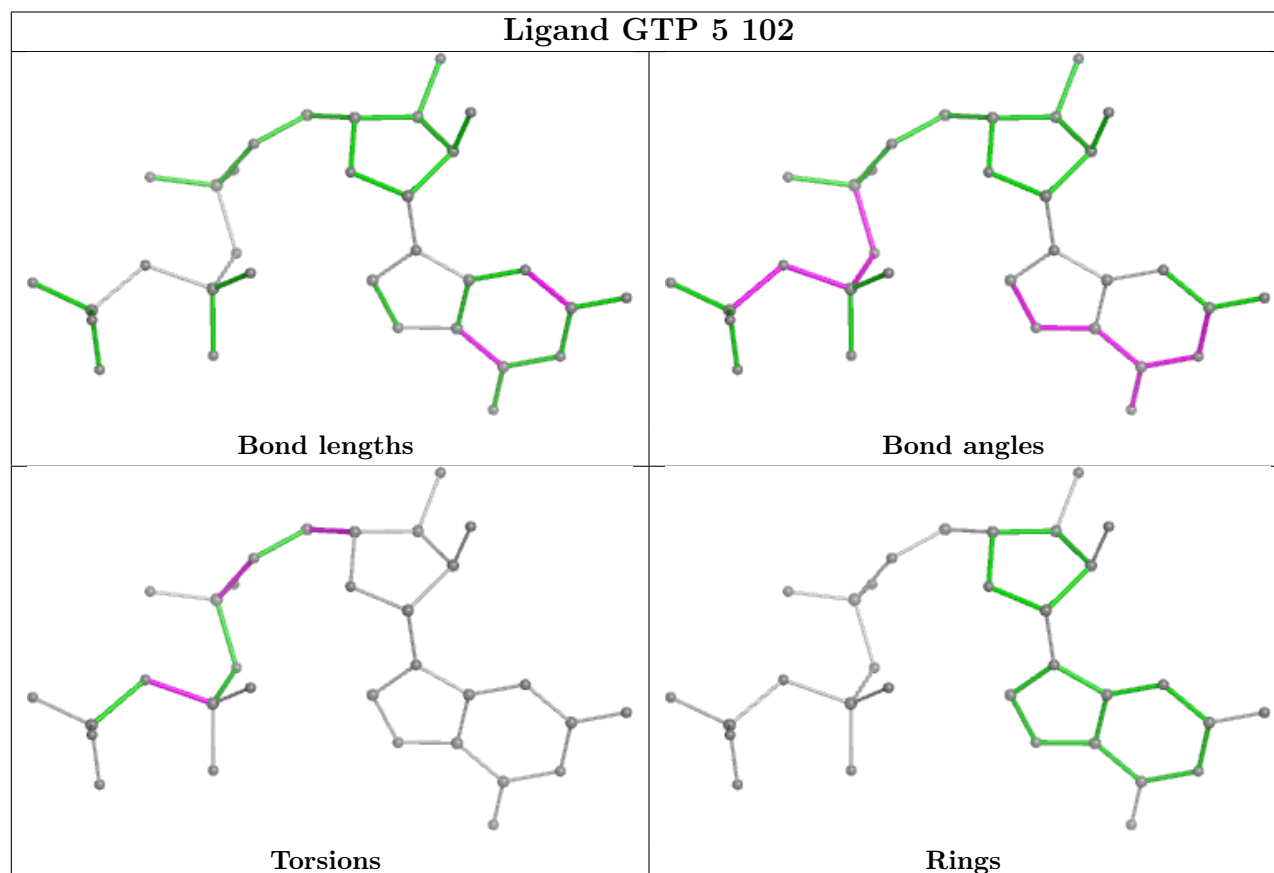
Mol	Chain	Res	Type	Atoms
36	2	1509	SPM	C12-C11-N10-C9
36	2	1520	SPM	C12-C11-N10-C9
36	2	1524	SPM	C3-C4-N5-C6
36	2	1525	SPM	C3-C4-N5-C6
36	2	1533	SPM	C7-C6-N5-C4

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.

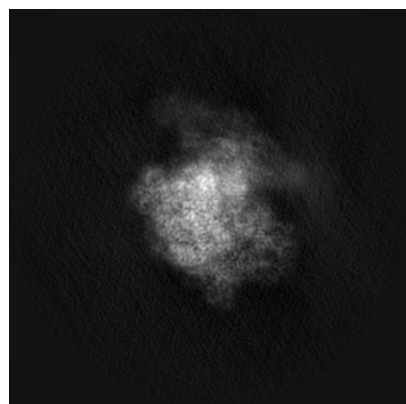
6 Map visualisation [i](#)

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.

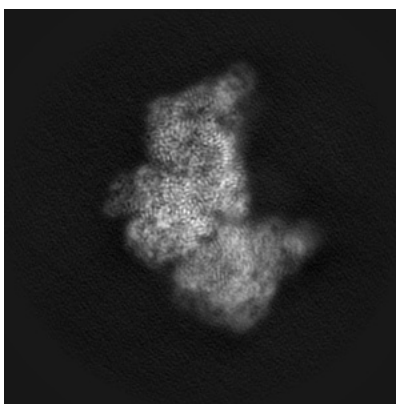
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

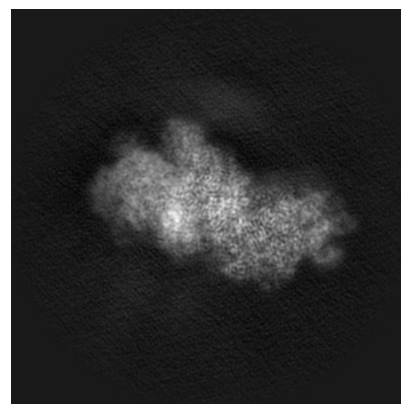
6.1.1 Primary map



X

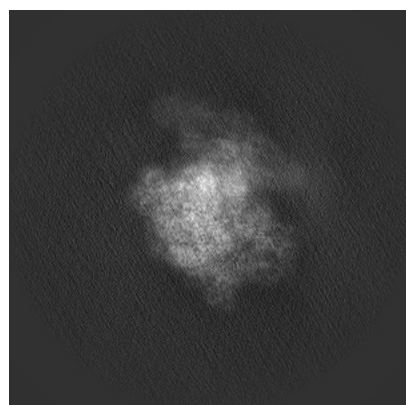


Y

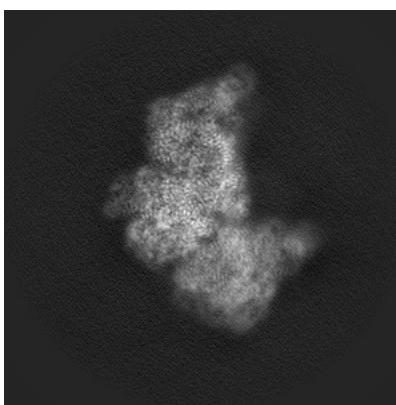


Z

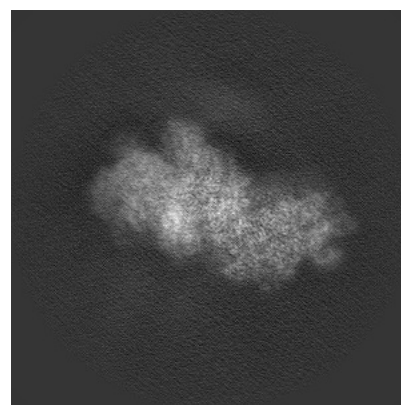
6.1.2 Raw map



X



Y

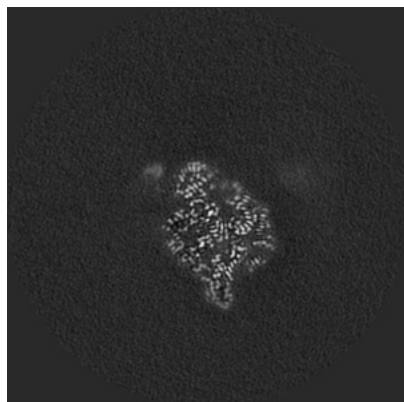


Z

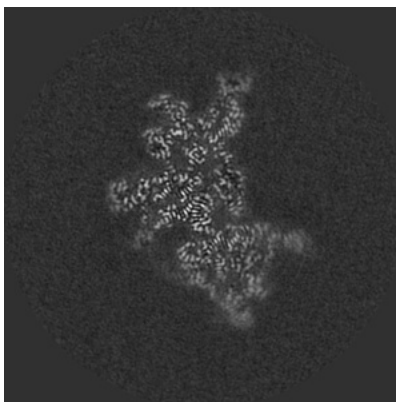
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

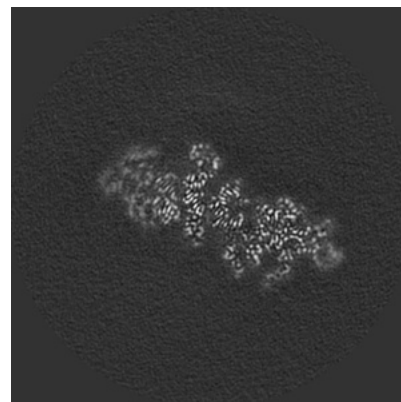
6.2.1 Primary map



X Index: 258

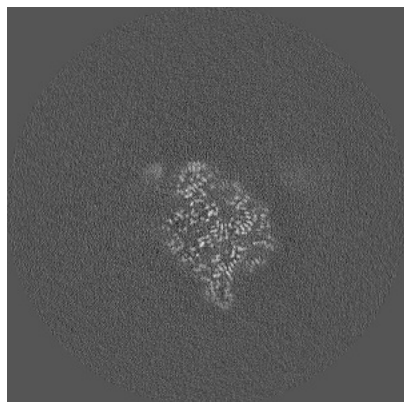


Y Index: 258

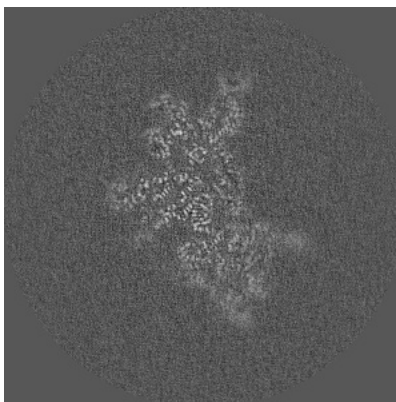


Z Index: 258

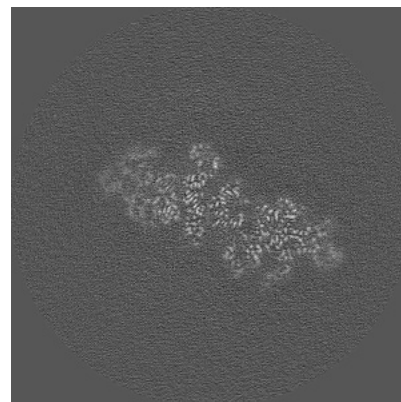
6.2.2 Raw map



X Index: 258



Y Index: 258

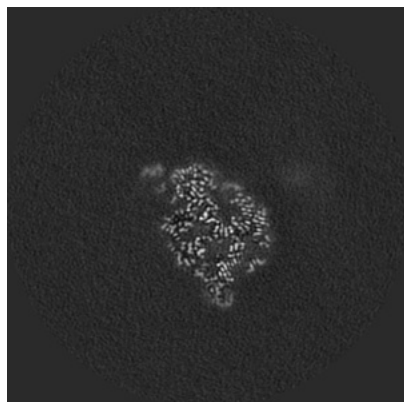


Z Index: 258

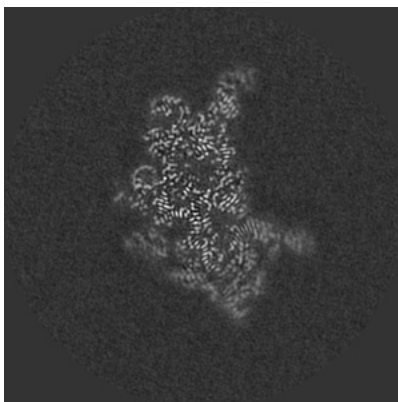
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

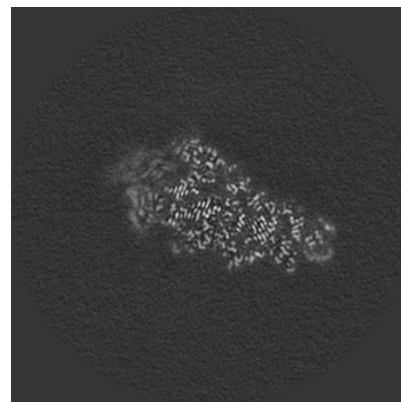
6.3.1 Primary map



X Index: 261

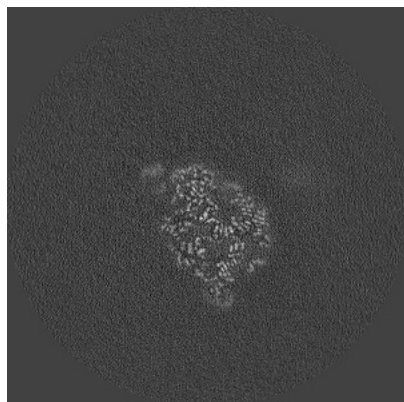


Y Index: 251

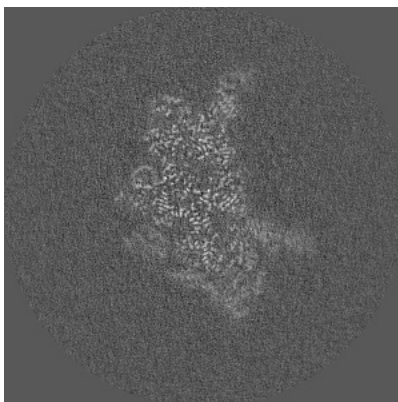


Z Index: 244

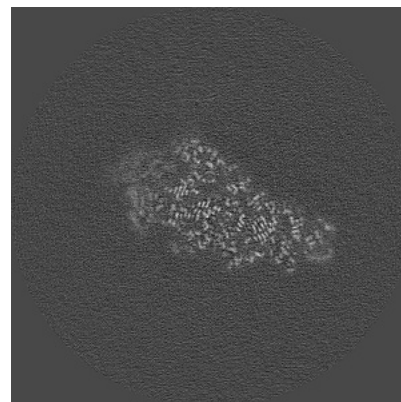
6.3.2 Raw map



X Index: 261



Y Index: 251

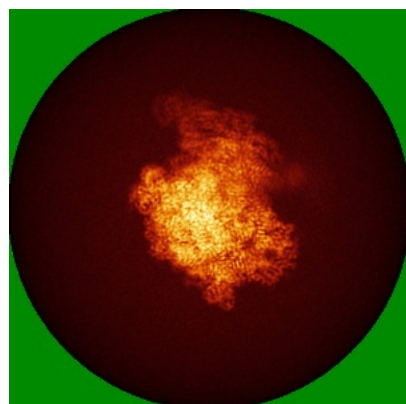


Z Index: 244

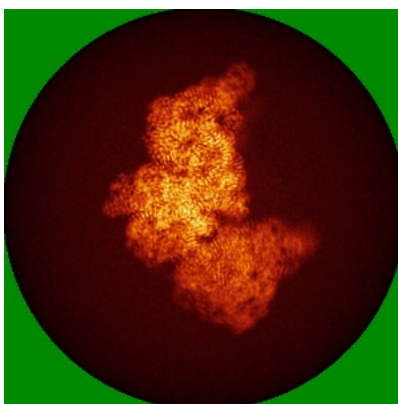
The images above show the largest variance slices of the map in three orthogonal directions.

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

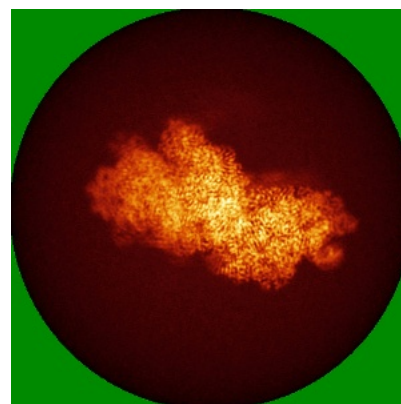
6.4.1 Primary map



X

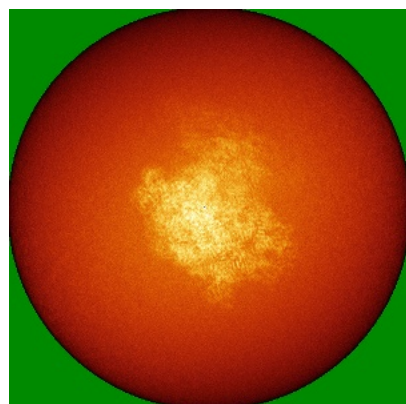


Y

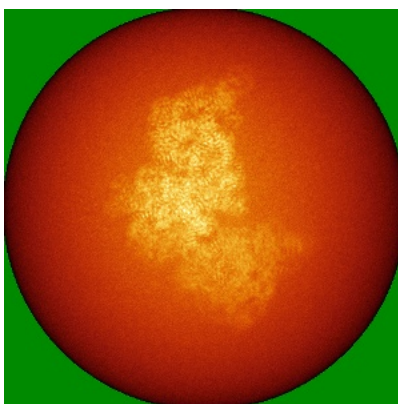


Z

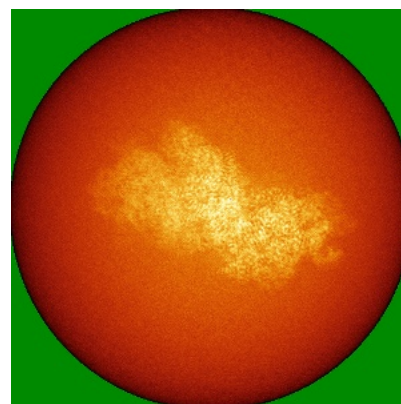
6.4.2 Raw map



X



Y

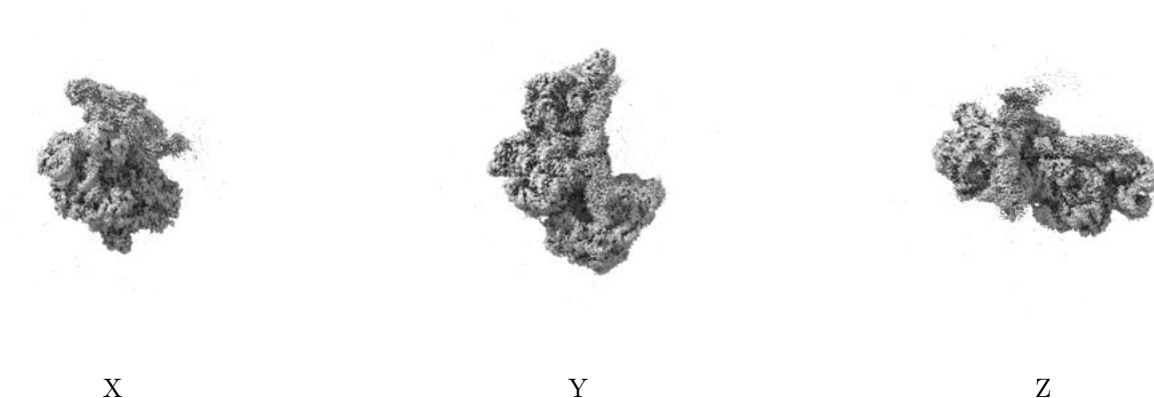


Z

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.

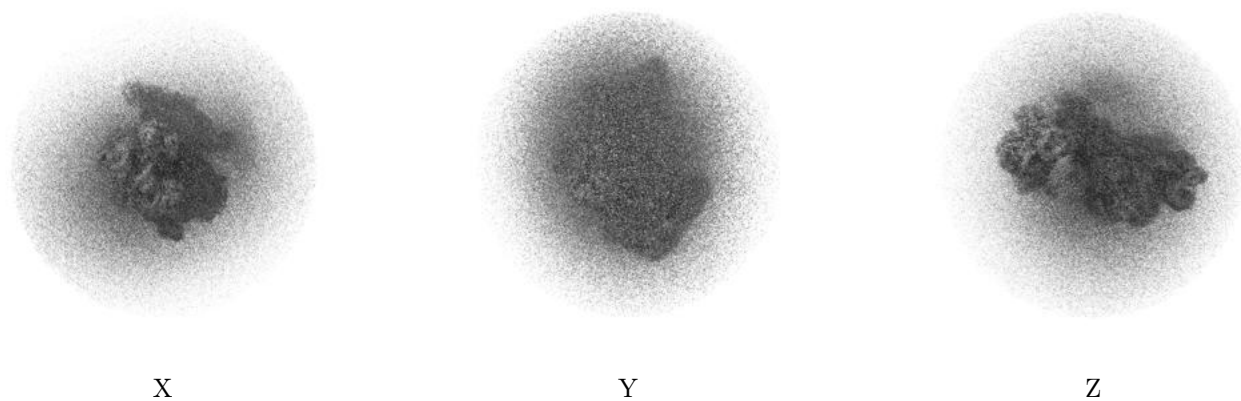
6.5 Orthogonal surface views [i](#)

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.

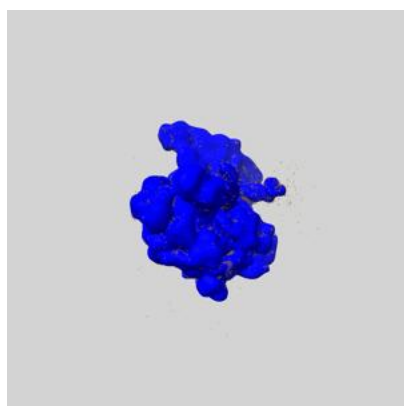
6.6 Mask visualisation [i](#)

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

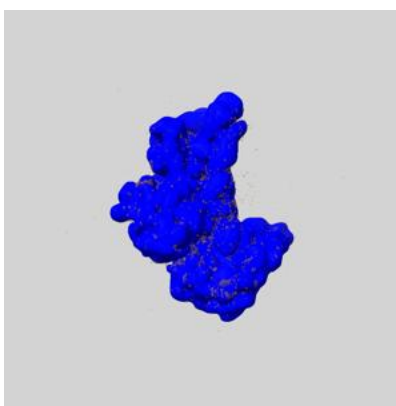
A mask typically either:

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

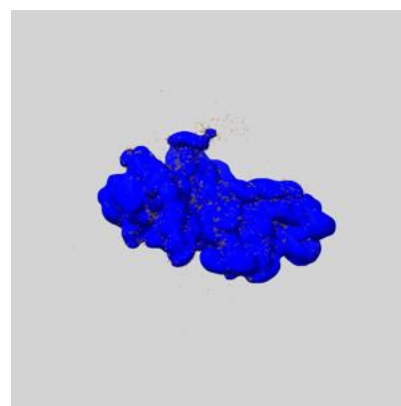
6.6.1 emd_50724_msk_1.map [i](#)



X



Y

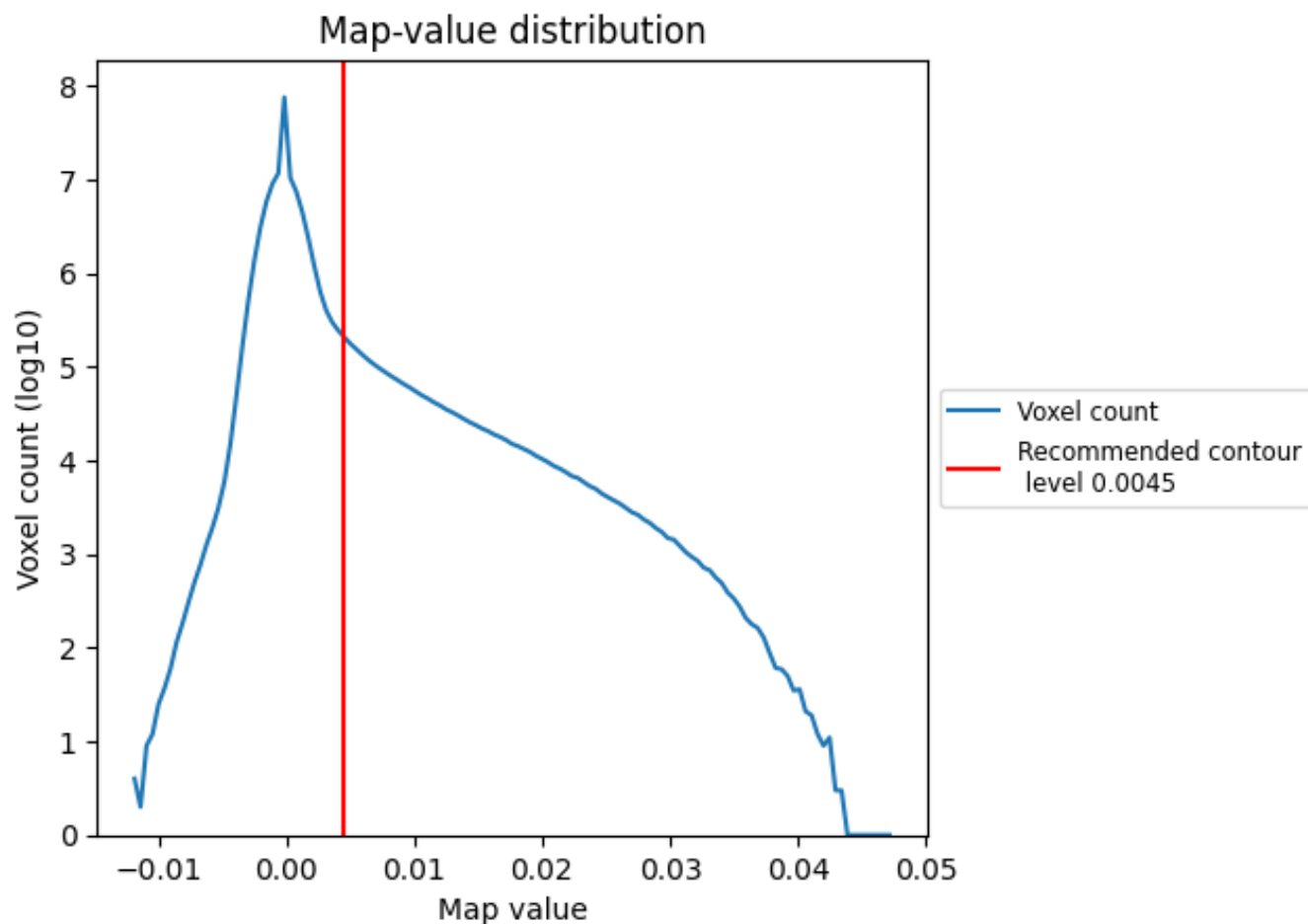


Z

7 Map analysis [i](#)

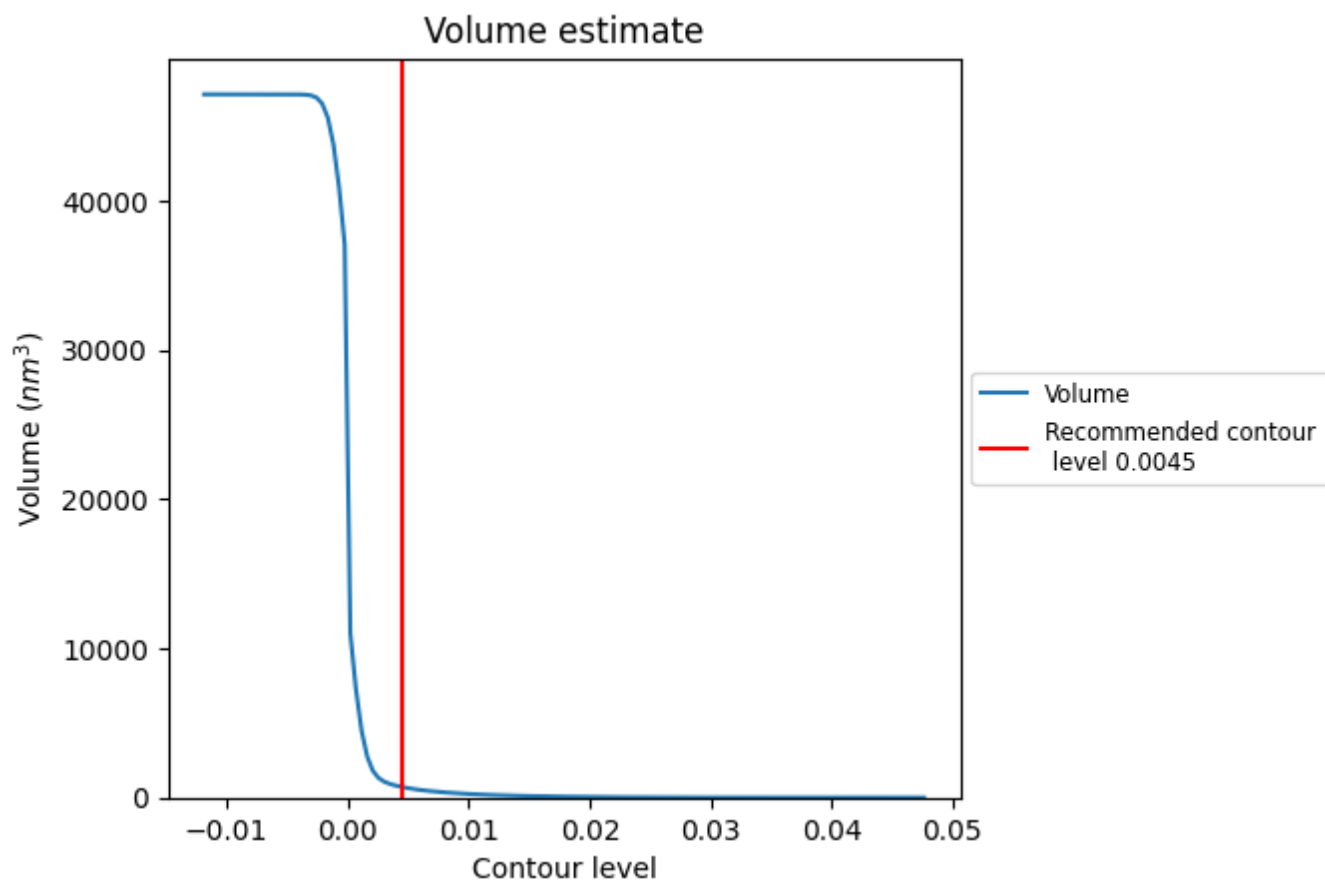
This section contains the results of statistical analysis of the map.

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.

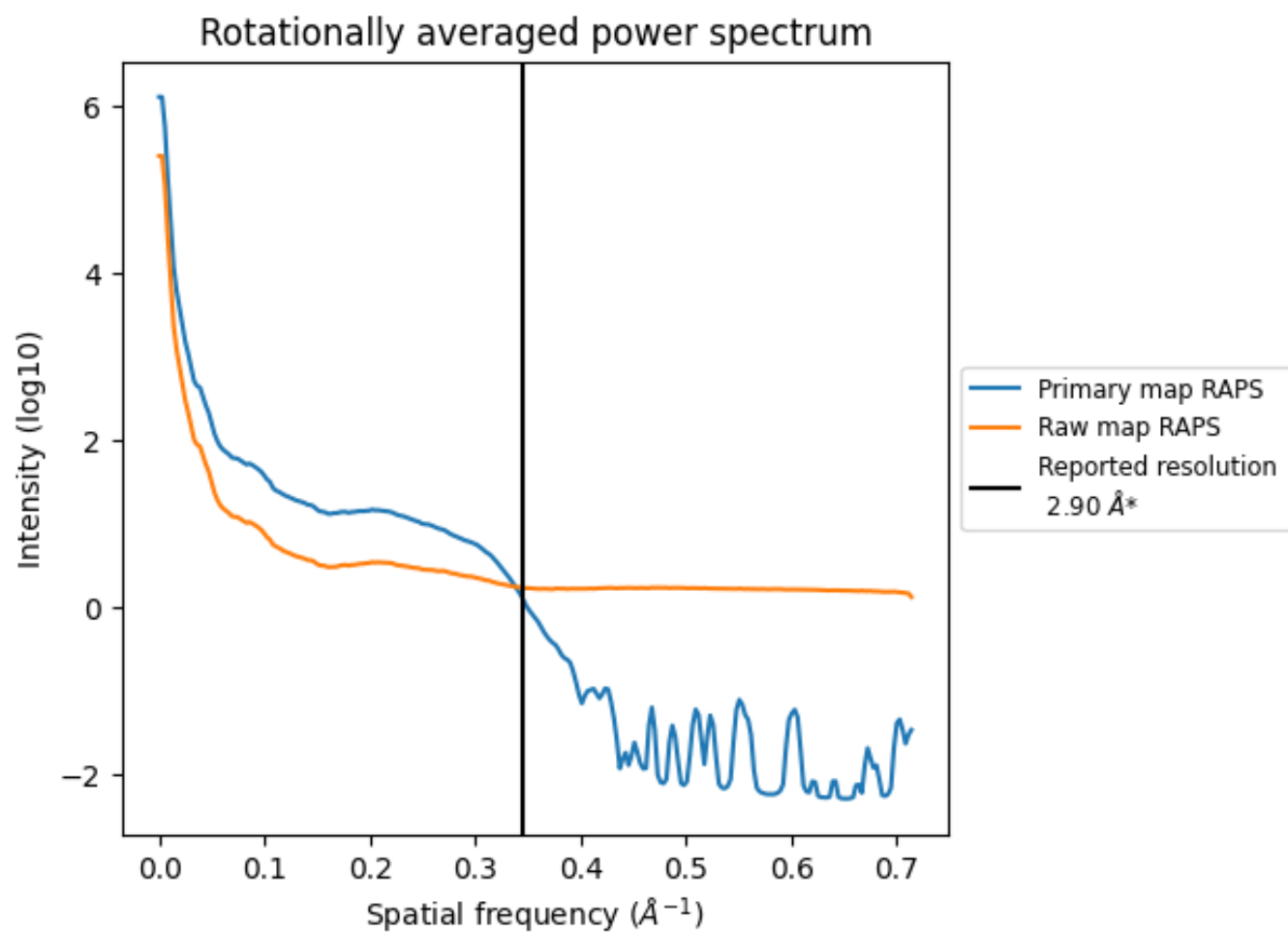
7.2 Volume estimate [i](#)



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 ⓘ

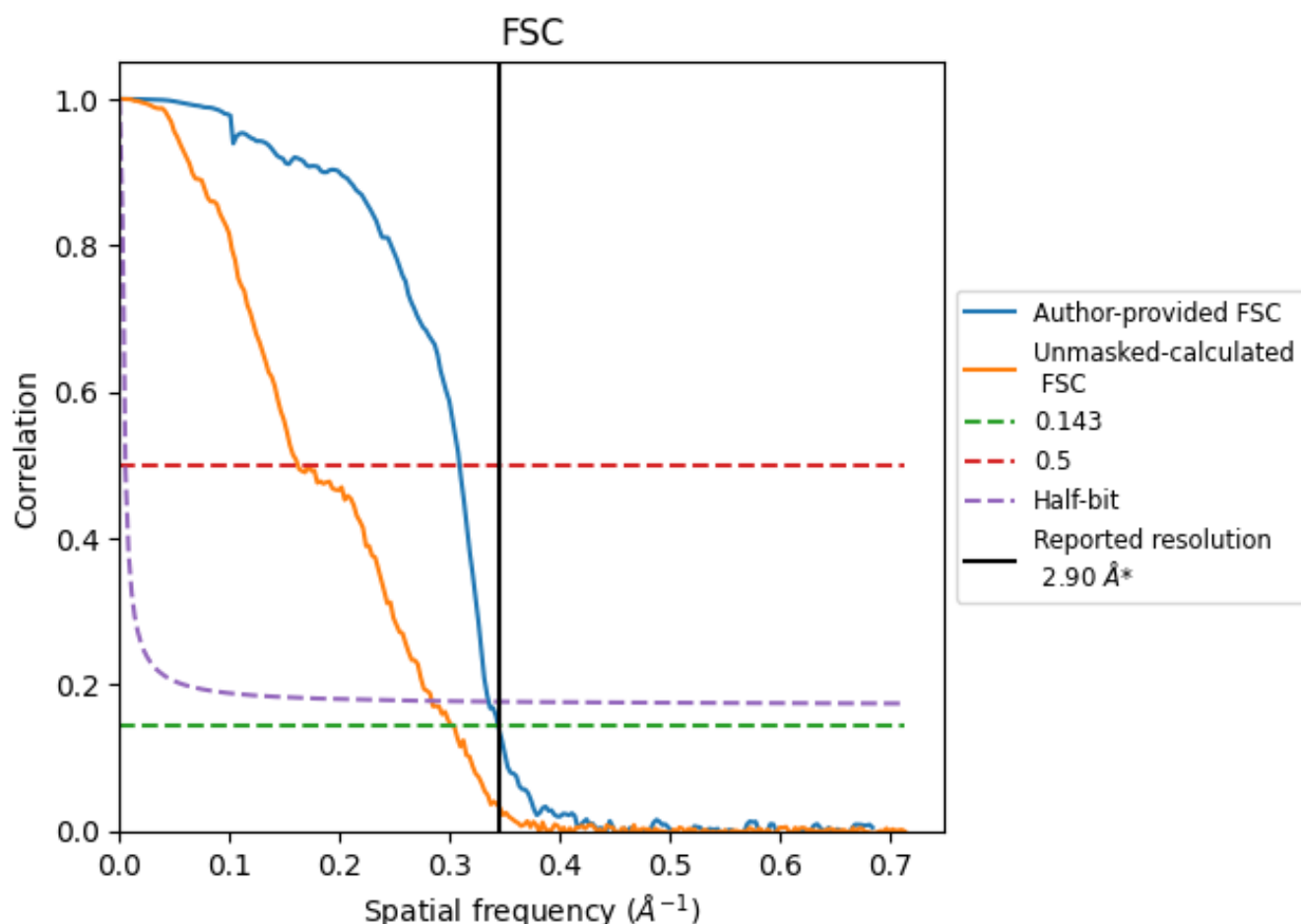


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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](#)

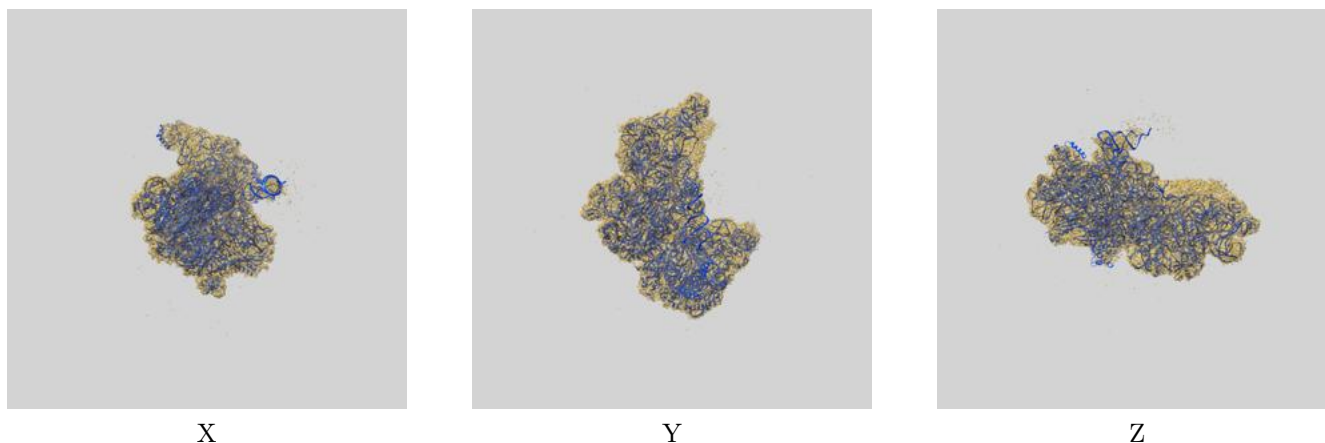
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.90	3.23	2.98
Unmasked-calculated*	3.29	6.17	3.52

*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](#)

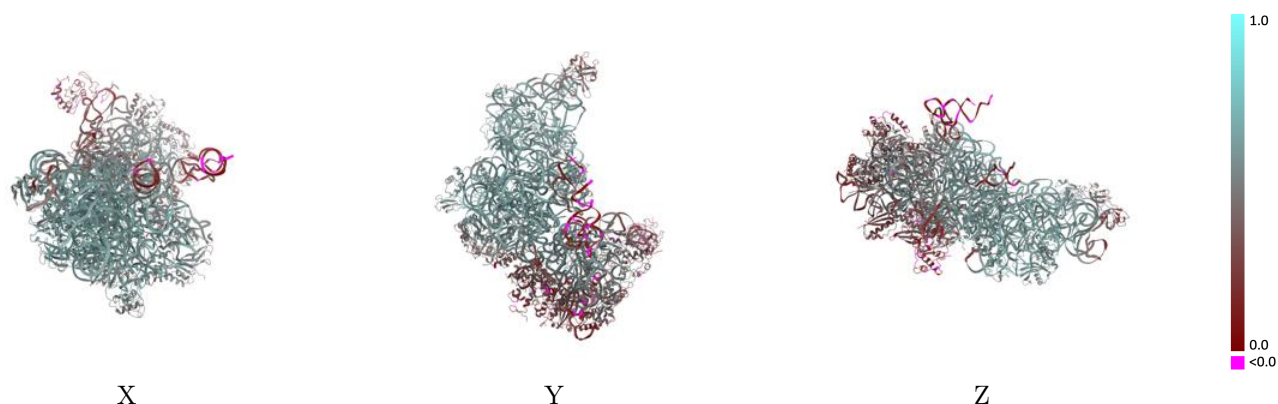
This section contains information regarding the fit between EMDB map EMD-50724 and PDB model 9FS6. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

9.1 Map-model overlay [i](#)



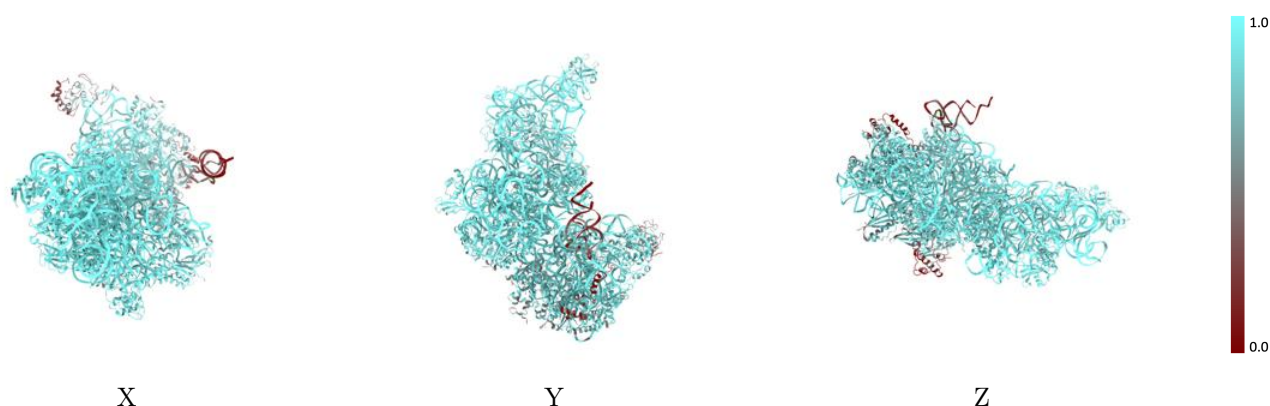
The images above show the 3D surface view of the map at the recommended contour level 0.0045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



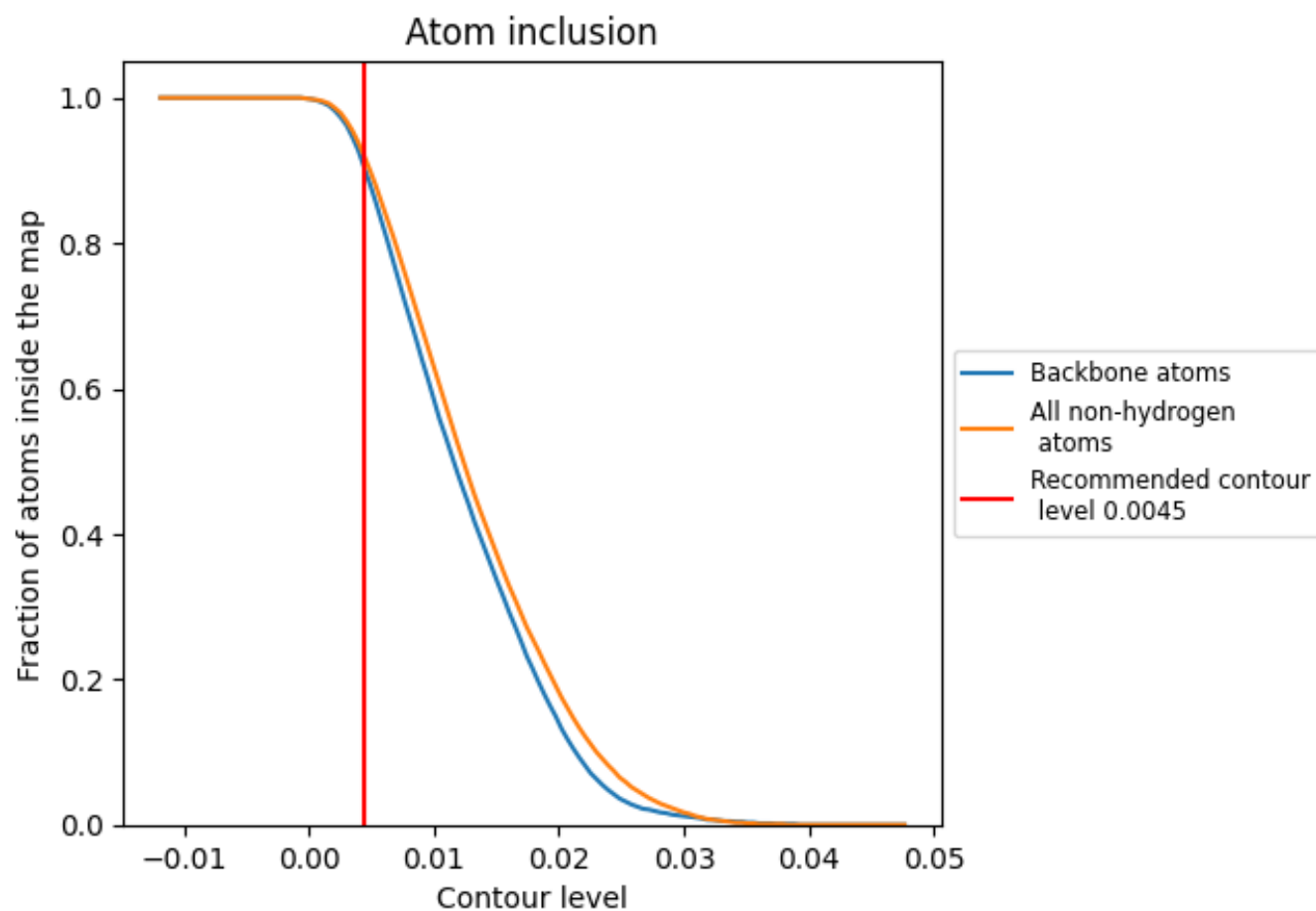
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

