



wwPDB EM Validation Summary Report ⓘ

Dec 31, 2024 – 08:44 PM EST

PDB ID : 8PJ1
EMDB ID : EMD-17696
Title : Structure of human 48S translation initiation complex in open codon scanning state (48S-1)
Authors : Petrychenko, V.; Yi, S.-H.; Liedtke, D.; Peng, B.Z.; Rodnina, M.V.; Fischer, N.
Deposited on : 2023-06-22
Resolution : 3.40 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:

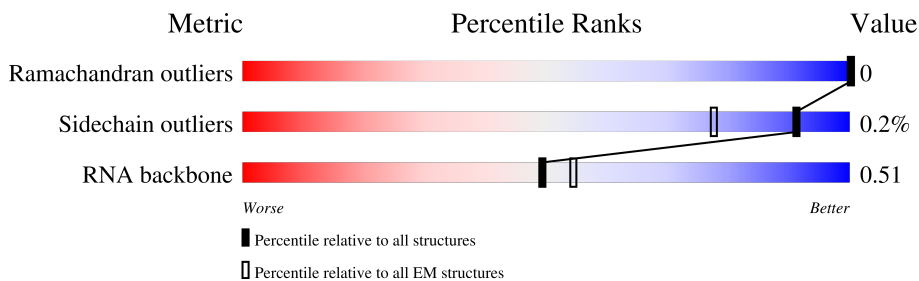
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, 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 3.40 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.



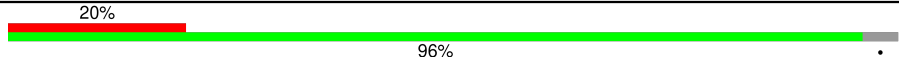
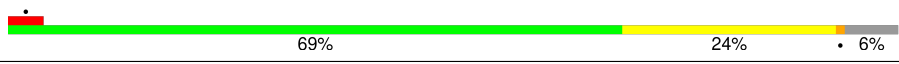
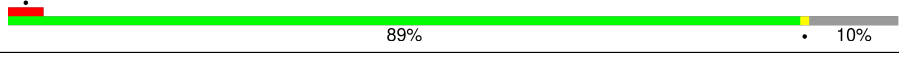
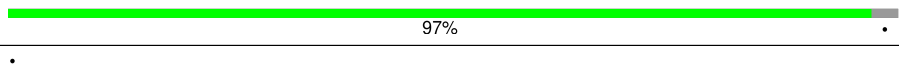
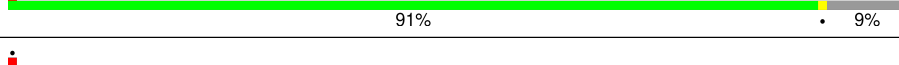
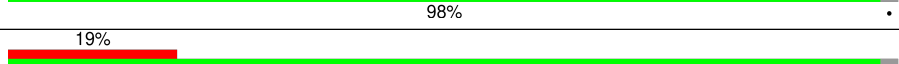
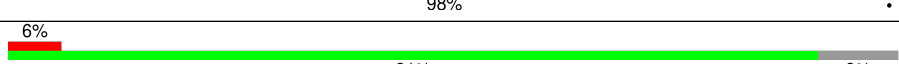
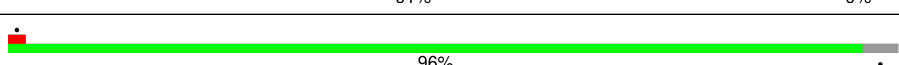
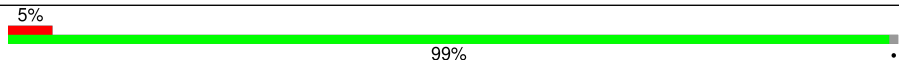
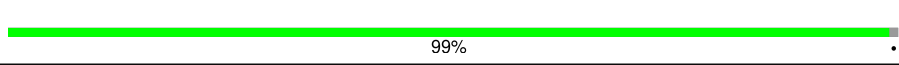
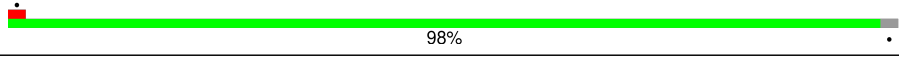
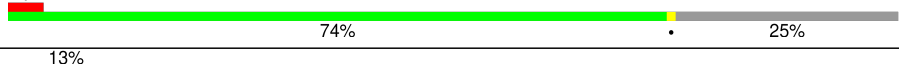
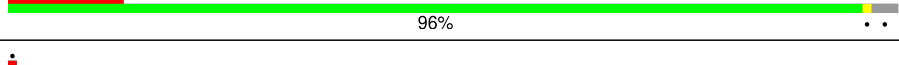

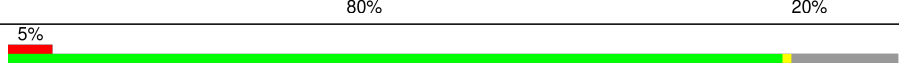

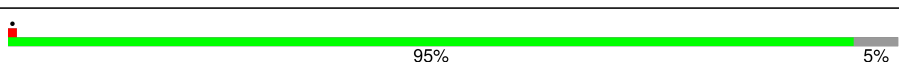
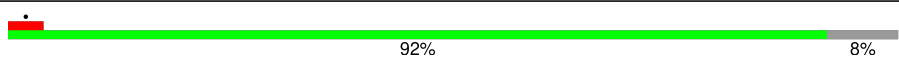
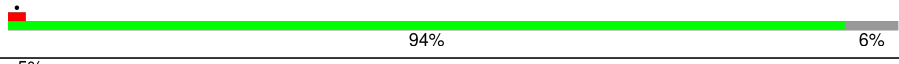
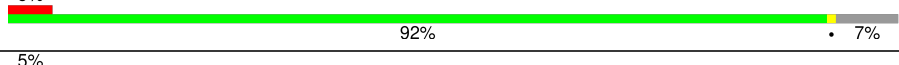
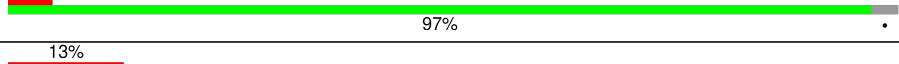
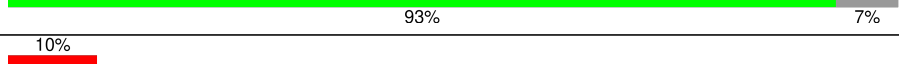



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	1	814	<p>72% 28%</p>
2	2	325	<p>94% 6%</p>
3	3	218	<p>96% 98%</p>
4	4	357	<p>62% 72% 28%</p>
5	5	564	<p>89% 92% 8%</p>
6	6	374	<p>84% 97%</p>
7	7	255	<p>13% 5% 13% 82%</p>
8	8	352	<p>75% 90% 10%</p>

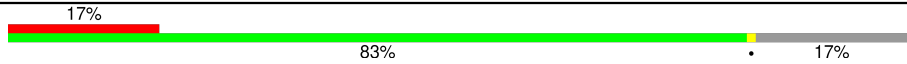
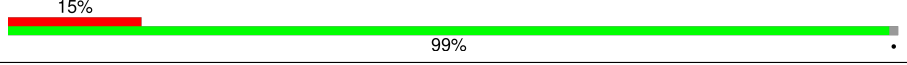
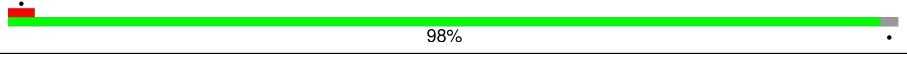
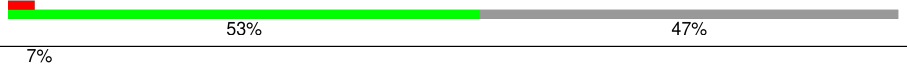
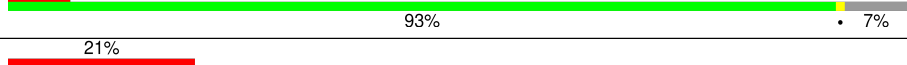
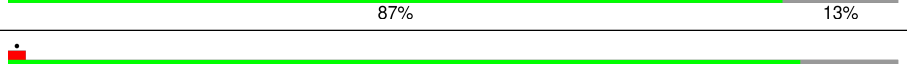

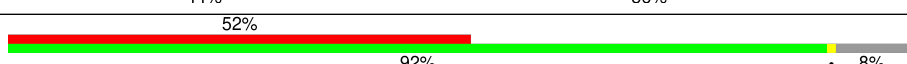
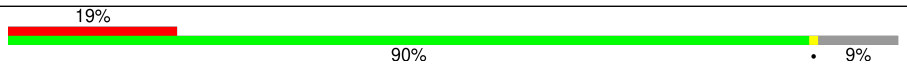

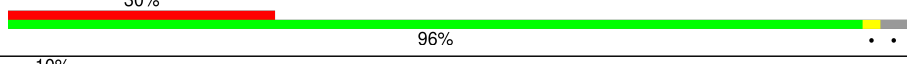
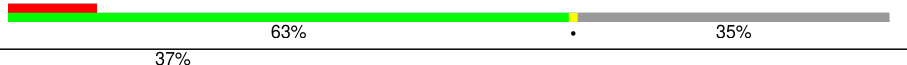
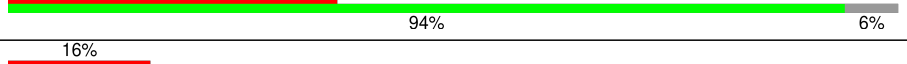

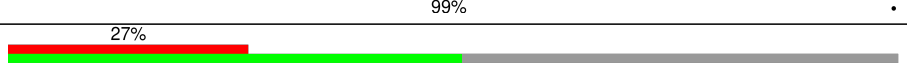






Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	9	25	
10	A	1869	
11	B	158	
12	C	263	
13	D	194	
14	E	143	
15	F	59	
16	G	194	
17	H	84	
18	I	151	
19	J	130	
20	K	83	
21	L	293	
22	M	135	
23	N	295	
24	O	264	
25	P	151	
26	Q	115	
27	R	208	
28	S	249	
29	T	133	
30	V	204	
31	Y	146	
32	Z	243	
33	a	165	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	b	145	
35	c	317	
36	d	145	
37	e	125	
38	f	152	
39	h	119	
40	i	56	
41	k	157	
42	m	132	
43	n	69	
44	o	320	
45	p	113	
46	q	144	
47	r	315	
48	s	333	
49	t	472	
50	u	1382	
51	v	445	
52	w	75	
53	x	548	
54	y	913	

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 119663 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 protein called Eukaryotic translation initiation factor 3 subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	588	3258	1986	633	634	5	0	0

- Molecule 2 is a protein called Eukaryotic translation initiation factor 3 subunit I.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	2	304	1493	885	304	304	0	0

- Molecule 3 is a protein called Eukaryotic translation initiation factor 3 subunit K.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	3	213	1057	631	213	213	0	0

- Molecule 4 is a protein called Eukaryotic translation initiation factor 3 subunit F.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	4	257	1272	757	257	258	0	0

- Molecule 5 is a protein called Eukaryotic translation initiation factor 3 subunit L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	5	520	4347	2814	721	793	19	0	0

- Molecule 6 is a protein called Eukaryotic translation initiation factor 3 subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	6	362	2196	1348	414	427	7	0	0

- Molecule 7 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	47	Total	C	N	O	P	0	0
			1003	453	199	304	47		

- Molecule 8 is a protein called Eukaryotic translation initiation factor 3 subunit H.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	8	317	Total	C	N	O	0	0
			1574	937	318	319		

- Molecule 9 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	9	24	Total	C	N	O	S	0	0
			230	139	62	26	3		

- Molecule 10 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	1754	Total	C	N	O	P	0	0
			37429	16718	6714	12244	1753		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1248	B8N	U	conflict	GB NR_046235.3

- Molecule 11 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	142	Total	C	N	O	S	0	0
			1166	743	218	199	6		

- Molecule 12 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	C	256	Total	C	N	O	S	0	0
			2035	1302	378	347	8		

- Molecule 13 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	177	Total	C	N	O	S	0	0
			1477	941	295	239	2		

- Molecule 14 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	E	140	Total	C	N	O	S	0	0
			1087	687	215	182	3		

- Molecule 15 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	F	58	Total	C	N	O	S	0	0
			459	284	100	74	1		

- Molecule 16 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	G	177	Total	C	N	O	S	0	0
			1430	917	260	252	1		

- Molecule 17 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	H	81	Total	C	N	O	S	0	0
			631	397	116	111	7		

- Molecule 18 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	I	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 19 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	J	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 20 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	K	81	Total	C	N	O	S	0	0
			617	380	114	118	5		

- Molecule 21 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	L	220	Total	C	N	O	S	0	0
			1707	1104	292	301	10		

- Molecule 22 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	M	131	Total	C	N	O	S	0	0
			1064	668	198	194	4		

- Molecule 23 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	N	207	Total	C	N	O	S	0	0
			1633	1040	288	297	8		

- Molecule 24 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	O	211	Total	C	N	O	S	0	0
			1715	1088	307	306	14		

- Molecule 25 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	P	133	Total	C	N	O	S	0	0
			997	610	196	185	6		

- Molecule 26 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Q	99	Total	C	N	O	S	0	0
			792	492	165	130	5		

- Molecule 27 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	R	198	Total	C	N	O	S	0	0
			1627	1021	322	279	5		

- Molecule 28 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	S	230	Total	C	N	O	S	0	0
			1862	1164	371	320	7		

- Molecule 29 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	T	125	Total	C	N	O	S	0	0
			1015	642	199	169	5		

- Molecule 30 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	V	189	Total	C	N	O	S	0	0
			1495	934	284	270	7		

- Molecule 31 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Y	141	Total	C	N	O	S	0	0
			1124	715	212	194	3		

- Molecule 32 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Z	227	Total	C	N	O	S	0	0
			1765	1125	317	315	8		

- Molecule 33 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	a	99	Total	C	N	O	S	0	0
			834	544	149	135	6		

- Molecule 34 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	b	121	Total	C	N	O	S	0	0
			989	628	185	169	7		

- Molecule 35 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	c	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 36 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	d	142	Total	C	N	O	S	0	0
			1105	692	213	197	3		

- Molecule 37 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	e	66	Total	C	N	O	S	0	0
			523	338	93	91	1		

- Molecule 38 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	f	142	Total	C	N	O	S	0	0
			1176	737	239	199	1		

- Molecule 39 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	h	103	Total	C	N	O	S	0	0
			817	511	155	147	4		

- Molecule 40 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	i	50	Total	C	N	O	S	0	0
			419	262	85	67	5		

- Molecule 41 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	k	69	559	352	104	96	7	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	87	ALA	-	insertion	UNP P62979

- Molecule 42 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	m	122	950	596	168	177	9	0	0

- Molecule 43 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	n	63	498	302	101	93	2	0	0

- Molecule 44 is a protein called Eukaryotic translation initiation factor 3 subunit G.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
44	o	77	616	389	111	116	0	0

- Molecule 45 is a protein called Eukaryotic translation initiation factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	p	110	830	524	150	154	2	0	0

- Molecule 46 is a protein called Eukaryotic translation initiation factor 1A, X-chromosomal.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	q	93	754	476	137	137	4	0	0

- Molecule 47 is a protein called Eukaryotic translation initiation factor 2 subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	r	296	2138	1342	384	404	8	0	0

- Molecule 48 is a protein called Eukaryotic translation initiation factor 2 subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	s	159	1275	804	236	226	9	0	0

- Molecule 49 is a protein called Eukaryotic translation initiation factor 2 subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	t	472	3586	2272	628	668	18	0	0

- Molecule 50 is a protein called Eukaryotic translation initiation factor 3 subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	u	706	5383	3379	982	999	23	1	0

- Molecule 51 is a protein called Eukaryotic translation initiation factor 3 subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	v	405	2740	1720	498	510	12	0	0

- Molecule 52 is a RNA chain called Initiator Met-tRNA-i.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
52	w	75	1604	717	298	515	74	0	0

- Molecule 53 is a protein called Eukaryotic translation initiation factor 3 subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	x	423	2842	1752	523	557	10	0	0

- Molecule 54 is a protein called Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	y	731	5657	3547	1018	1057	35	0	0

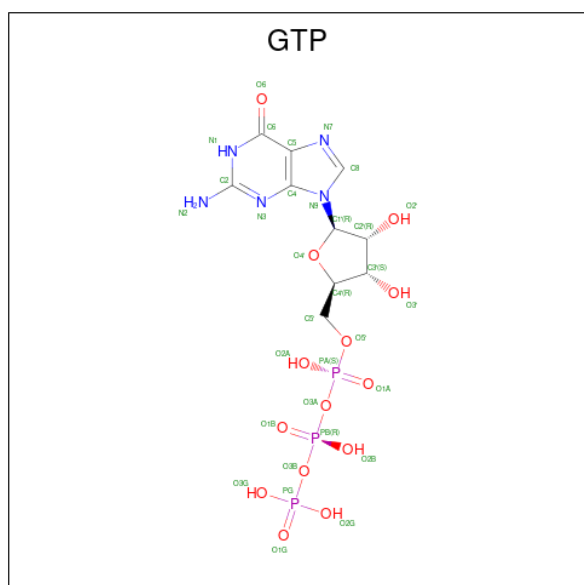
- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
55	A	88	Total	Mg	0
			88	88	
55	f	1	Total	Mg	0
			1	1	
55	t	1	Total	Mg	0
			1	1	

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

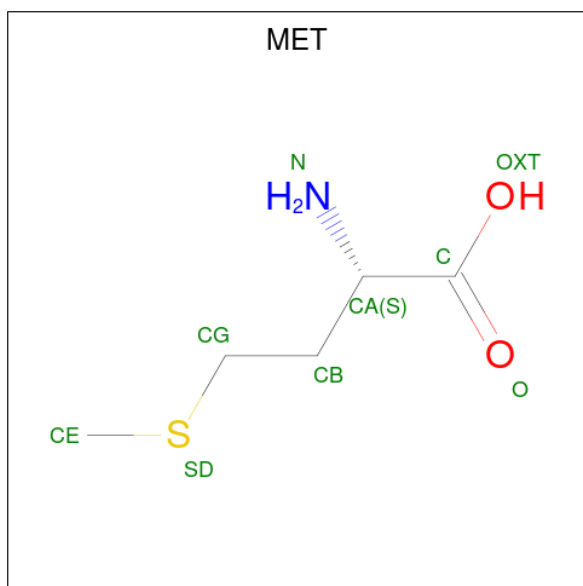
Mol	Chain	Residues	Atoms		AltConf
56	Q	1	Total	Zn	0
			1	1	
56	k	1	Total	Zn	0
			1	1	
56	s	1	Total	Zn	0
			1	1	

- Molecule 57 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

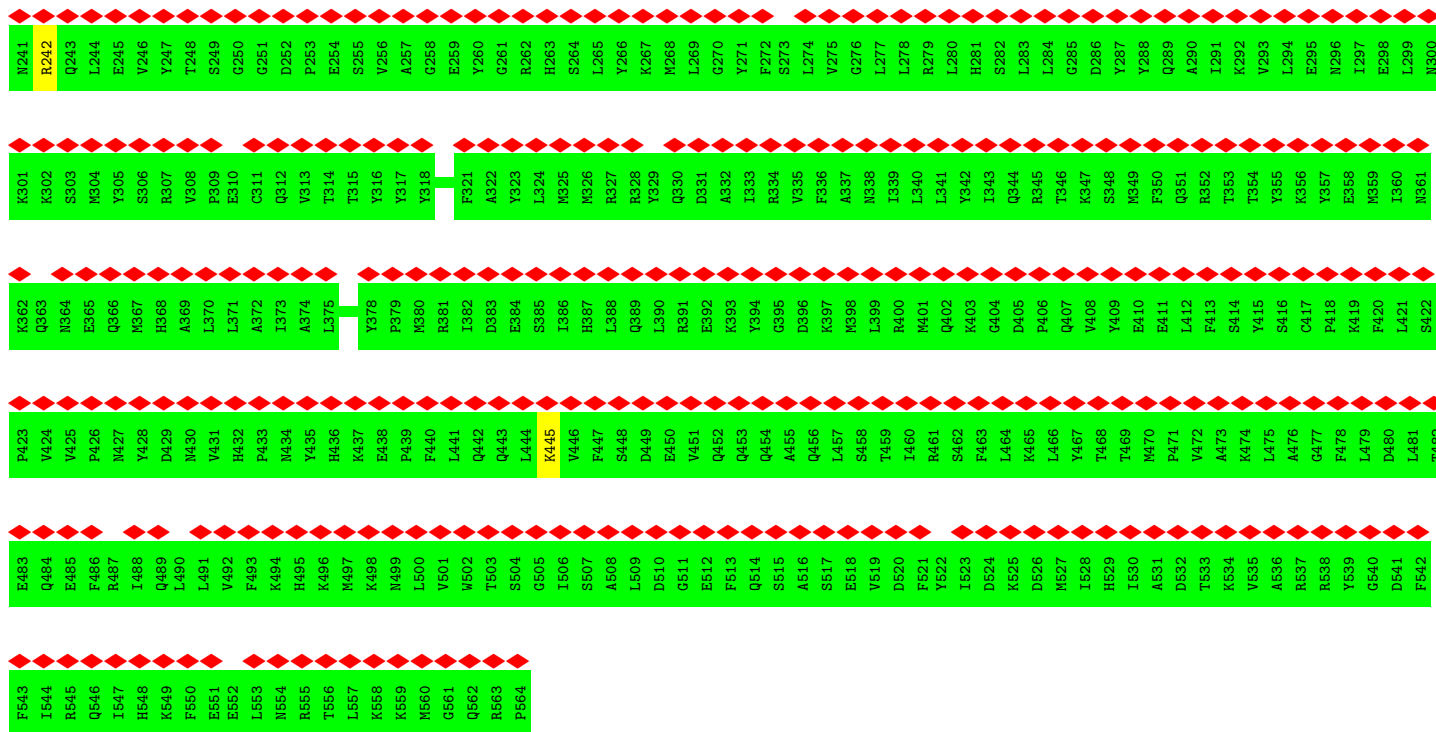


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
57	t	1	32	10	5	14	3	0

- Molecule 58 is METHIONINE (three-letter code: MET) (formula: C₅H₁₁NO₂S).

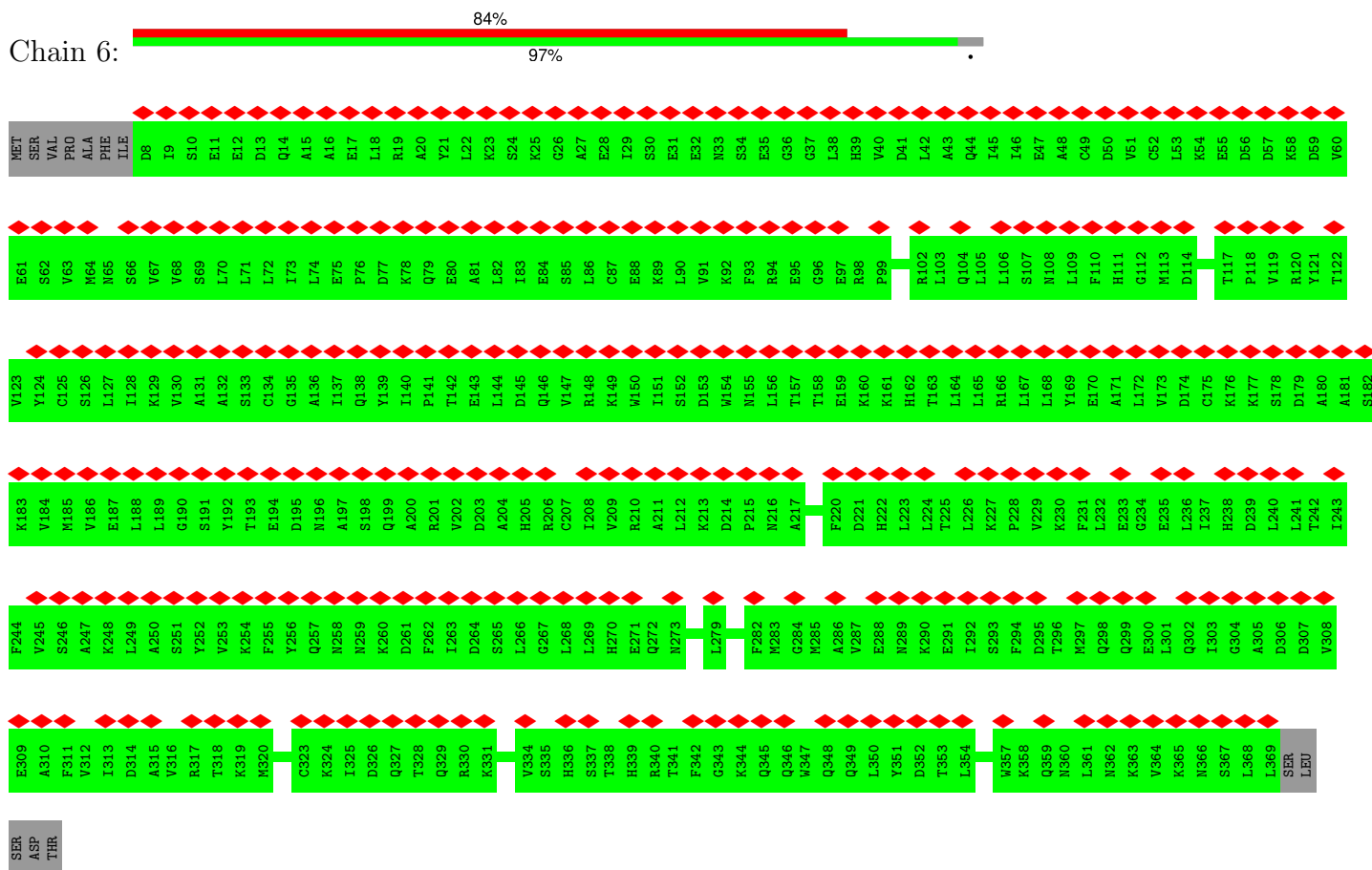


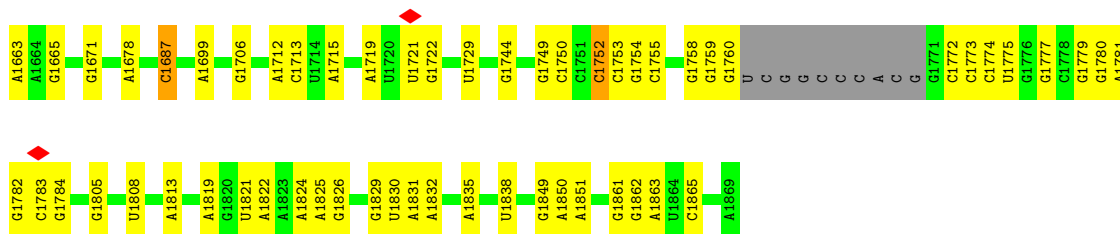
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
58	w	1	8	5	1	1	1	0



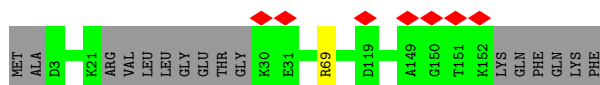
● Molecule 6: Eukaryotic translation initiation factor 3 subunit M

Chain 6:

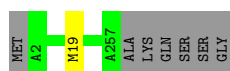




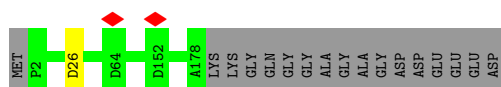
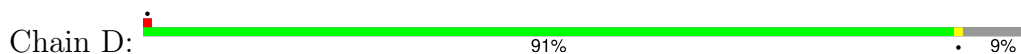
- Molecule 11: 40S ribosomal protein S11



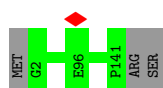
- Molecule 12: 40S ribosomal protein S4, X isoform



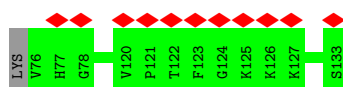
- Molecule 13: 40S ribosomal protein S9



- Molecule 14: 40S ribosomal protein S23

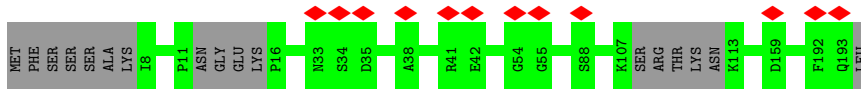


- Molecule 15: 40S ribosomal protein S30

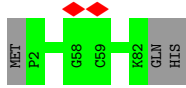


- Molecule 16: 40S ribosomal protein S7

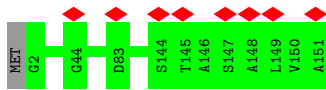




- Molecule 17: 40S ribosomal protein S27



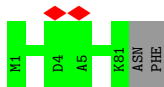
- Molecule 18: 40S ribosomal protein S13



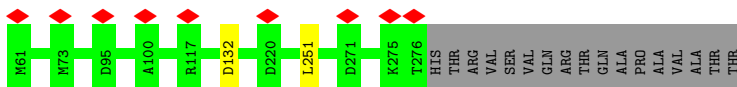
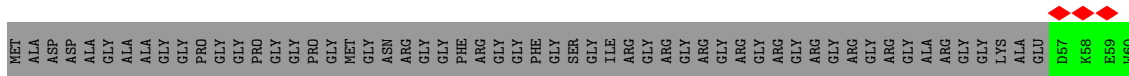
- Molecule 19: 40S ribosomal protein S15a



- Molecule 20: 40S ribosomal protein S21

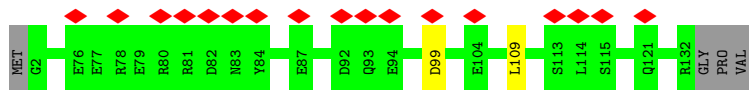


- Molecule 21: 40S ribosomal protein S2

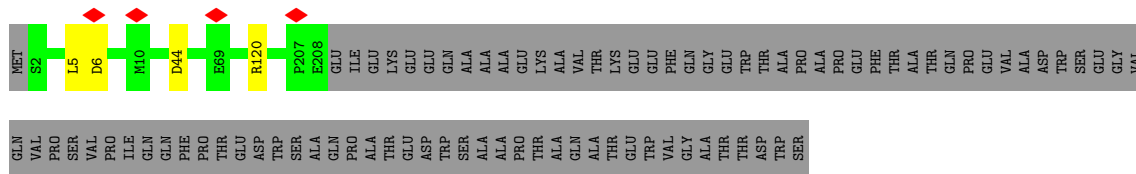


- Molecule 22: 40S ribosomal protein S17

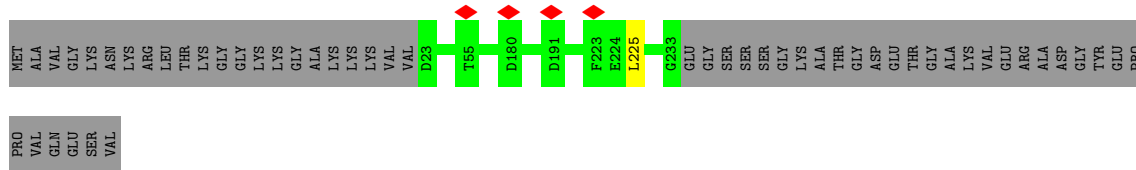




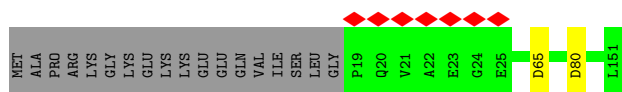
• Molecule 23: 40S ribosomal protein SA



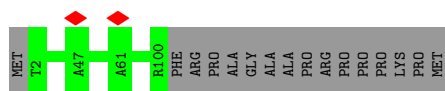
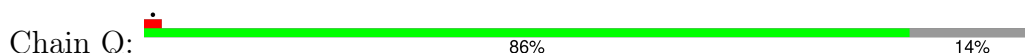
• Molecule 24: 40S ribosomal protein S3a



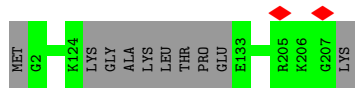
• Molecule 25: 40S ribosomal protein S14



• Molecule 26: 40S ribosomal protein S26

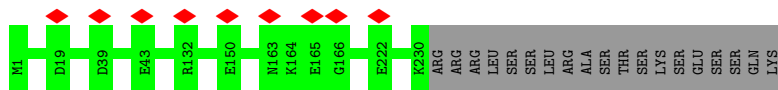


• Molecule 27: 40S ribosomal protein S8

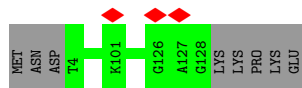


• Molecule 28: 40S ribosomal protein S6

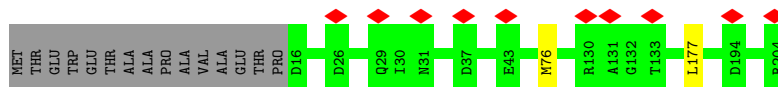
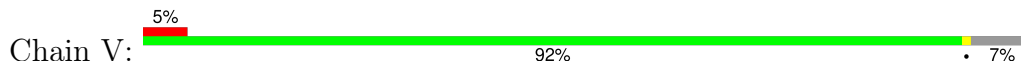




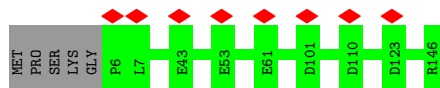
• Molecule 29: 40S ribosomal protein S24



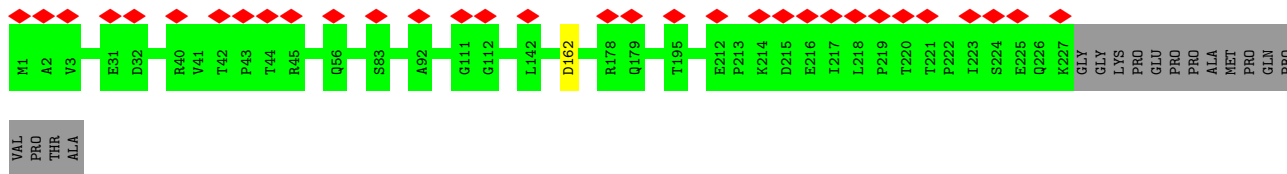
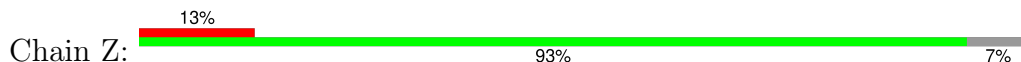
• Molecule 30: 40S ribosomal protein S5



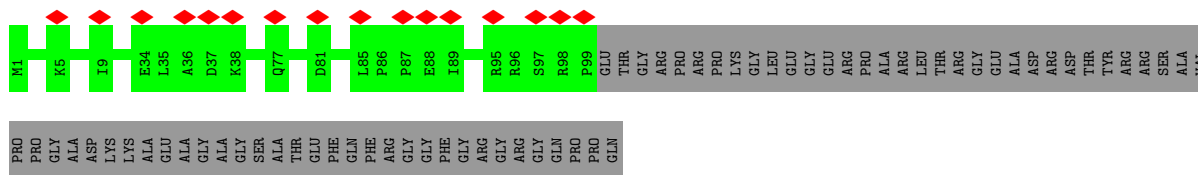
• Molecule 31: 40S ribosomal protein S16



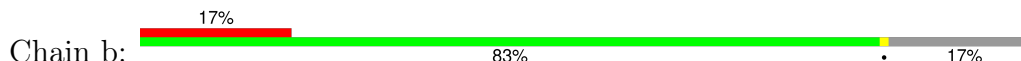
• Molecule 32: 40S ribosomal protein S3

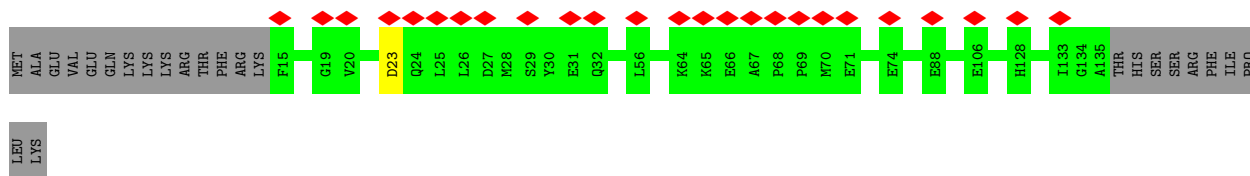


• Molecule 33: 40S ribosomal protein S10

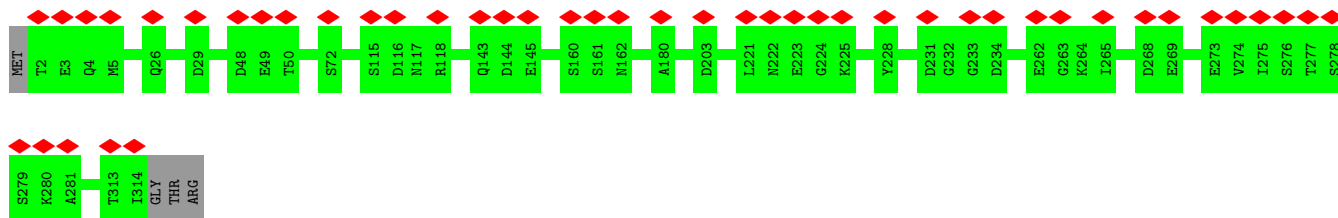


• Molecule 34: 40S ribosomal protein S15

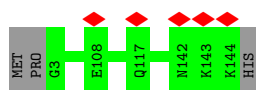




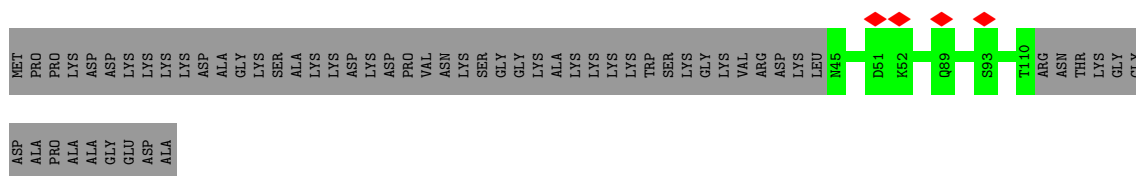
- Molecule 35: Receptor of activated protein C kinase 1



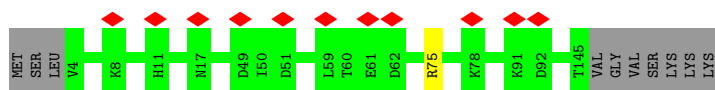
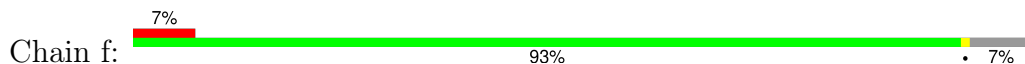
- Molecule 36: 40S ribosomal protein S19



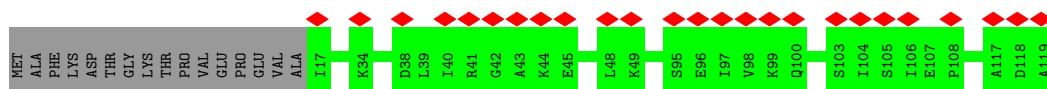
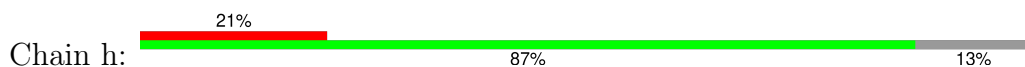
- Molecule 37: 40S ribosomal protein S25

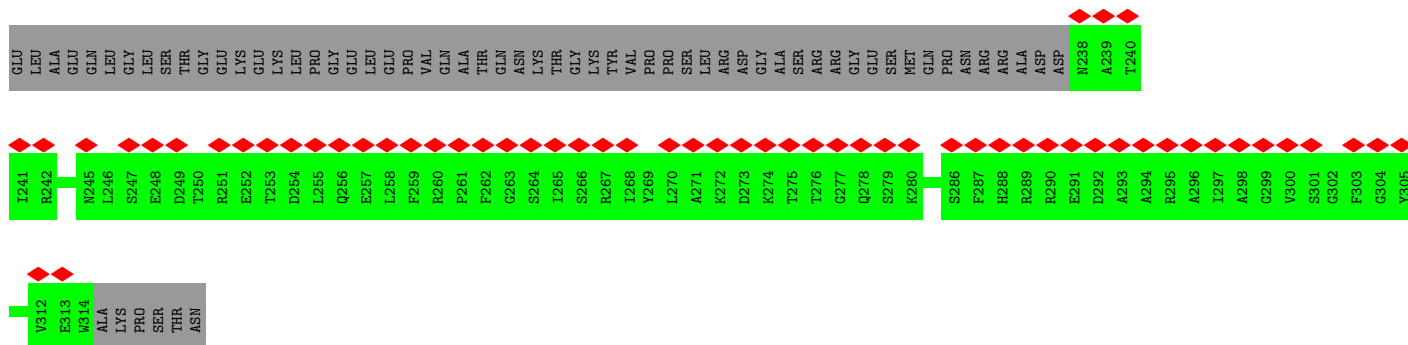


- Molecule 38: 40S ribosomal protein S18

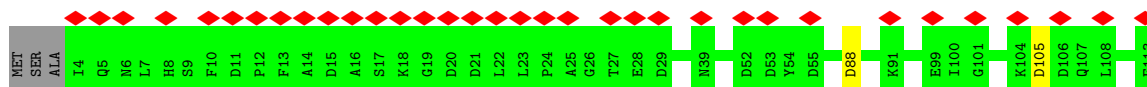


- Molecule 39: 40S ribosomal protein S20

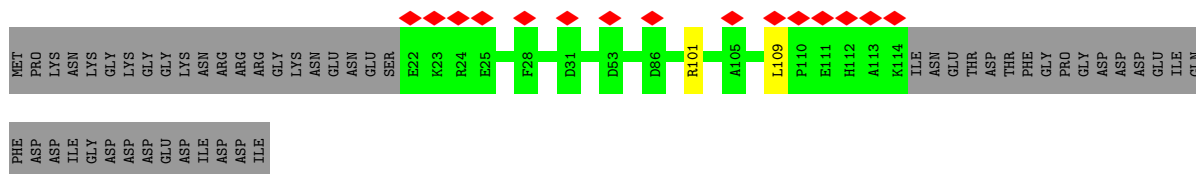




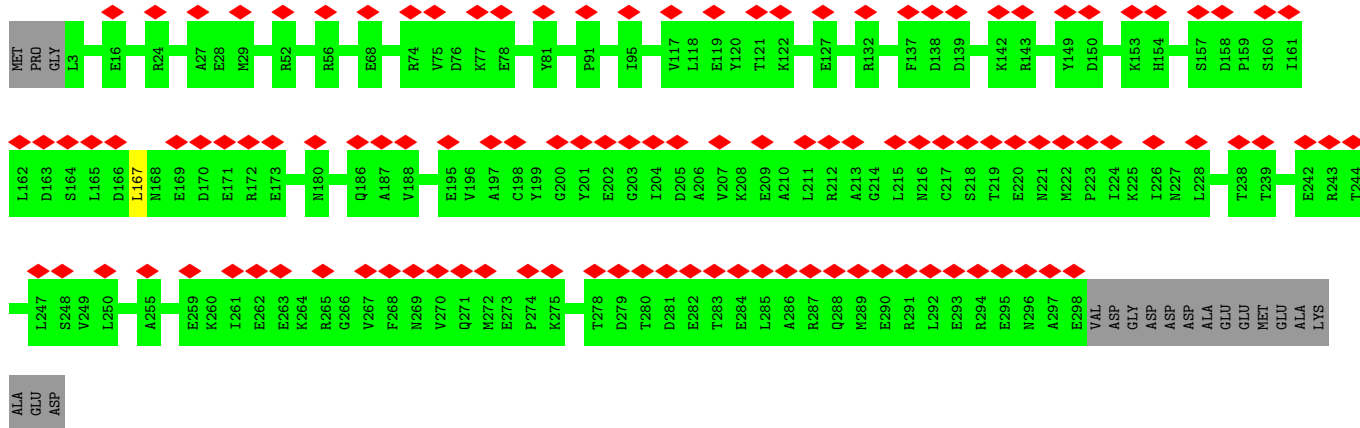
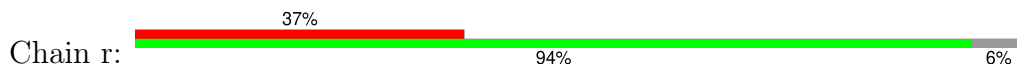
• Molecule 45: Eukaryotic translation initiation factor 1



• Molecule 46: Eukaryotic translation initiation factor 1A, X-chromosomal



• Molecule 47: Eukaryotic translation initiation factor 2 subunit 1



• Molecule 48: Eukaryotic translation initiation factor 2 subunit 2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	92749	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	24.146	Depositor
Minimum map value	-8.937	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4	Depositor
Map size (Å)	417.74402, 417.74402, 417.74402	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.96700007, 0.96700007, 0.96700007	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: OMG, PSU, OMU, 6MZ, GTP, UR3, A2M, ZN, MA6, 5MC, 5MU, JMH, MG, B8N, OMC

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	1	0.26	0/3279	0.52	0/4534
2	2	0.24	0/1491	0.47	0/2068
3	3	0.23	0/1055	0.37	0/1469
4	4	0.24	0/1269	0.40	0/1762
5	5	0.25	0/4458	0.50	0/6027
6	6	0.25	0/2212	0.48	0/3034
7	7	0.21	0/1126	0.78	1/1750 (0.1%)
8	8	0.24	0/1572	0.42	0/2187
9	9	0.28	0/231	0.74	0/294
10	A	0.37	0/41130	0.96	118/64100 (0.2%)
11	B	0.32	0/1186	0.59	0/1585
12	C	0.30	0/2077	0.62	2/2796 (0.1%)
13	D	0.30	0/1502	0.61	1/2008 (0.0%)
14	E	0.29	0/1105	0.54	0/1476
15	F	0.25	0/465	0.58	0/612
16	G	0.28	0/1451	0.56	0/1942
17	H	0.30	0/644	0.57	0/864
18	I	0.29	0/1232	0.54	0/1656
19	J	0.30	0/1051	0.59	0/1406
20	K	0.29	0/623	0.57	0/833
21	L	0.32	0/1743	0.62	2/2354 (0.1%)
22	M	0.34	0/1078	0.70	2/1447 (0.1%)
23	N	0.30	0/1670	0.63	3/2271 (0.1%)
24	O	0.30	0/1742	0.61	1/2330 (0.0%)
25	P	0.32	0/1010	0.72	2/1353 (0.1%)
26	Q	0.32	0/805	0.62	0/1079
27	R	0.29	0/1654	0.57	0/2203
28	S	0.29	0/1885	0.59	0/2510
29	T	0.29	0/1032	0.57	0/1371
30	V	0.28	0/1516	0.61	2/2037 (0.1%)
31	Y	0.30	0/1142	0.62	0/1528
32	Z	0.29	0/1793	0.59	1/2414 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	a	0.29	0/859	0.53	0/1159
34	b	0.29	0/1008	0.62	1/1348 (0.1%)
35	c	0.26	0/2493	0.57	0/3394
36	d	0.27	0/1123	0.56	0/1504
37	e	0.26	0/529	0.58	0/712
38	f	0.27	0/1194	0.61	0/1599
39	h	0.30	0/827	0.66	0/1110
40	i	0.28	0/429	0.62	0/568
41	k	0.31	0/571	0.64	0/760
42	m	0.26	0/960	0.57	1/1286 (0.1%)
43	n	0.31	0/500	0.74	0/669
44	o	0.26	0/628	0.59	0/846
45	p	0.30	0/843	0.70	2/1134 (0.2%)
46	q	0.30	0/764	0.70	1/1020 (0.1%)
47	r	0.27	0/2167	0.55	1/2943 (0.0%)
48	s	0.31	0/1295	0.65	0/1739
49	t	0.28	0/3644	0.60	1/4929 (0.0%)
50	u	0.26	0/5475	0.55	1/7432 (0.0%)
51	v	0.26	0/2778	0.54	0/3797
52	w	0.37	0/1795	1.13	15/2798 (0.5%)
53	x	0.26	0/2885	0.55	0/3940
54	y	0.27	0/5744	0.56	0/7761
All	All	0.31	0/124740	0.75	158/177748 (0.1%)

There are no bond length outliers.

The worst 5 of 158 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1453	C	C2-N1-C1'	10.83	130.71	118.80
10	A	1453	C	N1-C2-O2	10.79	125.37	118.90
10	A	1115	U	C2-N1-C1'	8.89	128.37	117.70
10	A	888	U	C2-N1-C1'	8.70	128.14	117.70
10	A	501	C	C2-N1-C1'	8.63	128.29	118.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	584/814 (72%)	541 (93%)	43 (7%)	0	100	100
2	2	300/325 (92%)	296 (99%)	4 (1%)	0	100	100
3	3	209/218 (96%)	197 (94%)	12 (6%)	0	100	100
4	4	251/357 (70%)	240 (96%)	11 (4%)	0	100	100
5	5	518/564 (92%)	508 (98%)	10 (2%)	0	100	100
6	6	360/374 (96%)	347 (96%)	13 (4%)	0	100	100
8	8	313/352 (89%)	293 (94%)	20 (6%)	0	100	100
9	9	22/25 (88%)	22 (100%)	0	0	100	100
11	B	138/158 (87%)	135 (98%)	3 (2%)	0	100	100
12	C	254/263 (97%)	248 (98%)	6 (2%)	0	100	100
13	D	175/194 (90%)	172 (98%)	3 (2%)	0	100	100
14	E	138/143 (96%)	133 (96%)	5 (4%)	0	100	100
15	F	56/59 (95%)	48 (86%)	8 (14%)	0	100	100
16	G	171/194 (88%)	164 (96%)	7 (4%)	0	100	100
17	H	79/84 (94%)	75 (95%)	4 (5%)	0	100	100
18	I	148/151 (98%)	148 (100%)	0	0	100	100
19	J	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
20	K	79/83 (95%)	73 (92%)	6 (8%)	0	100	100
21	L	218/293 (74%)	212 (97%)	6 (3%)	0	100	100
22	M	129/135 (96%)	125 (97%)	4 (3%)	0	100	100
23	N	205/295 (70%)	196 (96%)	9 (4%)	0	100	100
24	O	209/264 (79%)	202 (97%)	7 (3%)	0	100	100
25	P	131/151 (87%)	121 (92%)	10 (8%)	0	100	100
26	Q	97/115 (84%)	95 (98%)	2 (2%)	0	100	100
27	R	194/208 (93%)	189 (97%)	5 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	S	228/249 (92%)	223 (98%)	5 (2%)	0	100	100
29	T	123/133 (92%)	123 (100%)	0	0	100	100
30	V	187/204 (92%)	174 (93%)	13 (7%)	0	100	100
31	Y	139/146 (95%)	134 (96%)	5 (4%)	0	100	100
32	Z	225/243 (93%)	219 (97%)	6 (3%)	0	100	100
33	a	97/165 (59%)	90 (93%)	7 (7%)	0	100	100
34	b	119/145 (82%)	117 (98%)	2 (2%)	0	100	100
35	c	311/317 (98%)	292 (94%)	19 (6%)	0	100	100
36	d	140/145 (97%)	138 (99%)	2 (1%)	0	100	100
37	e	64/125 (51%)	63 (98%)	1 (2%)	0	100	100
38	f	140/152 (92%)	134 (96%)	6 (4%)	0	100	100
39	h	101/119 (85%)	97 (96%)	4 (4%)	0	100	100
40	i	48/56 (86%)	46 (96%)	2 (4%)	0	100	100
41	k	67/157 (43%)	55 (82%)	12 (18%)	0	100	100
42	m	120/132 (91%)	116 (97%)	4 (3%)	0	100	100
43	n	61/69 (88%)	55 (90%)	6 (10%)	0	100	100
44	o	75/320 (23%)	70 (93%)	5 (7%)	0	100	100
45	p	108/113 (96%)	96 (89%)	12 (11%)	0	100	100
46	q	91/144 (63%)	87 (96%)	4 (4%)	0	100	100
47	r	294/315 (93%)	276 (94%)	18 (6%)	0	100	100
48	s	157/333 (47%)	138 (88%)	19 (12%)	0	100	100
49	t	470/472 (100%)	431 (92%)	39 (8%)	0	100	100
50	u	705/1382 (51%)	672 (95%)	33 (5%)	0	100	100
51	v	403/445 (91%)	377 (94%)	26 (6%)	0	100	100
53	x	417/548 (76%)	396 (95%)	21 (5%)	0	100	100
54	y	725/913 (79%)	697 (96%)	28 (4%)	0	100	100
All	All	10720/13491 (80%)	10218 (95%)	502 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	
1	1	97/702 (14%)	96 (99%)	1 (1%)	73	83
5	5	477/515 (93%)	475 (100%)	2 (0%)	89	93
6	6	112/335 (33%)	112 (100%)	0	100	100
8	8	1/310 (0%)	1 (100%)	0	100	100
9	9	23/24 (96%)	23 (100%)	0	100	100
11	B	129/142 (91%)	128 (99%)	1 (1%)	79	87
12	C	220/225 (98%)	220 (100%)	0	100	100
13	D	158/168 (94%)	158 (100%)	0	100	100
14	E	112/115 (97%)	112 (100%)	0	100	100
15	F	47/48 (98%)	47 (100%)	0	100	100
16	G	159/174 (91%)	159 (100%)	0	100	100
17	H	73/76 (96%)	73 (100%)	0	100	100
18	I	130/131 (99%)	130 (100%)	0	100	100
19	J	112/113 (99%)	112 (100%)	0	100	100
20	K	65/67 (97%)	65 (100%)	0	100	100
21	L	186/225 (83%)	186 (100%)	0	100	100
22	M	119/122 (98%)	119 (100%)	0	100	100
23	N	173/243 (71%)	172 (99%)	1 (1%)	84	90
24	O	192/231 (83%)	192 (100%)	0	100	100
25	P	104/119 (87%)	104 (100%)	0	100	100
26	Q	86/98 (88%)	86 (100%)	0	100	100
27	R	172/180 (96%)	172 (100%)	0	100	100
28	S	200/218 (92%)	200 (100%)	0	100	100
29	T	107/115 (93%)	107 (100%)	0	100	100
30	V	159/170 (94%)	159 (100%)	0	100	100
31	Y	117/121 (97%)	117 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	Z	190/202 (94%)	190 (100%)	0	100	100
33	a	90/136 (66%)	90 (100%)	0	100	100
34	b	107/130 (82%)	107 (100%)	0	100	100
35	c	272/275 (99%)	272 (100%)	0	100	100
36	d	112/115 (97%)	112 (100%)	0	100	100
37	e	58/103 (56%)	58 (100%)	0	100	100
38	f	123/132 (93%)	122 (99%)	1 (1%)	79	87
39	h	94/107 (88%)	94 (100%)	0	100	100
40	i	44/49 (90%)	44 (100%)	0	100	100
41	k	61/140 (44%)	61 (100%)	0	100	100
42	m	104/108 (96%)	104 (100%)	0	100	100
43	n	56/62 (90%)	55 (98%)	1 (2%)	54	73
44	o	64/277 (23%)	64 (100%)	0	100	100
45	p	79/96 (82%)	79 (100%)	0	100	100
46	q	79/123 (64%)	78 (99%)	1 (1%)	65	78
47	r	190/280 (68%)	190 (100%)	0	100	100
48	s	142/304 (47%)	142 (100%)	0	100	100
49	t	397/397 (100%)	395 (100%)	2 (0%)	86	91
50	u	528/1259 (42%)	526 (100%)	2 (0%)	89	93
51	v	206/406 (51%)	205 (100%)	1 (0%)	86	91
53	x	207/494 (42%)	207 (100%)	0	100	100
54	y	569/811 (70%)	568 (100%)	1 (0%)	92	96
All	All	7302/10993 (66%)	7288 (100%)	14 (0%)	91	96

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
46	q	101	ARG
49	t	324	GLU
54	y	347	ARG
50	u	520	ARG
51	v	414	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
53	x	322	ASN
54	y	819	HIS
45	p	111	HIS
49	t	169	GLN
50	u	110	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	1741/1869 (93%)	410 (23%)	8 (0%)
52	w	74/75 (98%)	28 (37%)	0
7	7	46/255 (18%)	34 (73%)	4 (8%)
All	All	1861/2199 (84%)	472 (25%)	12 (0%)

5 of 472 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	7	-27	A
7	7	-26	C
7	7	-23	C
7	7	-22	A
7	7	-21	A

5 of 12 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
10	A	606	G
10	A	688	U
10	A	1600	G
10	A	731	G
7	7	-4	A

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

29 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
10	OMG	A	683	10	19,26,27	1.18	2 (10%)	21,38,41	0.88	1 (4%)
10	A2M	A	668	55,10	18,25,26	4.55	9 (50%)	20,36,39	4.28	7 (35%)
10	OMU	A	116	10	19,22,23	3.03	6 (31%)	25,31,34	1.75	5 (20%)
10	MA6	A	1850	10	19,26,27	1.91	3 (15%)	18,38,41	3.23	3 (16%)
10	OMC	A	517	10	19,22,23	0.53	0	25,31,34	0.65	0
10	JMH	A	1219	55,10	18,22,23	2.91	5 (27%)	23,32,35	1.50	3 (13%)
10	5MU	A	814	10	19,22,23	0.46	0	27,32,35	1.37	4 (14%)
10	A2M	A	1031	10	18,25,26	4.67	8 (44%)	20,36,39	4.12	6 (30%)
10	PSU	A	823	10	18,21,22	1.14	1 (5%)	21,30,33	1.85	4 (19%)
10	A2M	A	27	55,10	18,25,26	4.64	8 (44%)	20,36,39	4.02	6 (30%)
10	OMC	A	174	55,10	19,22,23	0.54	0	25,31,34	0.70	0
10	OMG	A	509	55,10	19,26,27	1.18	2 (10%)	21,38,41	0.85	1 (4%)
10	5MC	A	1374	10	19,22,23	0.57	0	26,32,35	0.72	0
10	PSU	A	1243	10	18,21,22	1.14	1 (5%)	21,30,33	1.91	4 (19%)
10	PSU	A	119	10	18,21,22	1.00	1 (5%)	21,30,33	1.73	4 (19%)
10	A2M	A	159	10	18,25,26	4.65	8 (44%)	20,36,39	4.09	6 (30%)
10	OMG	A	644	10	19,26,27	1.19	2 (10%)	21,38,41	0.79	1 (4%)
10	6MZ	A	1832	55,10	17,25,26	1.44	1 (5%)	15,36,39	2.96	5 (33%)
10	UR3	A	1830	10	19,22,23	2.84	8 (42%)	26,32,35	1.76	4 (15%)
10	PSU	A	1081	10	18,21,22	1.05	1 (5%)	21,30,33	1.84	5 (23%)
10	OMU	A	121	10	19,22,23	3.01	6 (31%)	25,31,34	1.78	5 (20%)
10	A2M	A	1678	10	18,25,26	4.70	9 (50%)	20,36,39	4.31	6 (30%)
10	OMC	A	1703	10	19,22,23	0.53	0	25,31,34	0.69	0
10	PSU	A	822	10	18,21,22	1.09	1 (5%)	21,30,33	1.85	5 (23%)
10	PSU	A	612	10	18,21,22	1.03	1 (5%)	21,30,33	1.87	5 (23%)
10	A2M	A	484	10	18,25,26	4.53	9 (50%)	20,36,39	3.95	6 (30%)
10	B8N	A	1248	10	25,29,30	3.40	9 (36%)	28,42,45	1.98	7 (25%)
10	MA6	A	1851	10	19,26,27	1.89	2 (10%)	18,38,41	3.22	3 (16%)
10	A2M	A	166	10	18,25,26	4.70	8 (44%)	20,36,39	4.19	8 (40%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	OMG	A	683	10	-	2/5/27/28	0/3/3/3
10	A2M	A	668	55,10	-	2/5/27/28	0/3/3/3
10	OMU	A	116	10	-	1/9/27/28	0/2/2/2
10	MA6	A	1850	10	-	1/7/29/30	0/3/3/3
10	OMC	A	517	10	-	2/9/27/28	0/2/2/2
10	JMH	A	1219	55,10	-	1/7/25/26	0/2/2/2
10	5MU	A	814	10	-	1/7/25/26	0/2/2/2
10	A2M	A	1031	10	-	1/5/27/28	0/3/3/3
10	PSU	A	823	10	-	0/7/25/26	0/2/2/2
10	A2M	A	27	55,10	-	2/5/27/28	0/3/3/3
10	OMC	A	174	55,10	-	0/9/27/28	0/2/2/2
10	OMG	A	509	55,10	-	1/5/27/28	0/3/3/3
10	5MC	A	1374	10	-	0/7/25/26	0/2/2/2
10	PSU	A	1243	10	-	2/7/25/26	0/2/2/2
10	PSU	A	119	10	-	1/7/25/26	0/2/2/2
10	A2M	A	159	10	-	2/5/27/28	0/3/3/3
10	OMG	A	644	10	-	3/5/27/28	0/3/3/3
10	6MZ	A	1832	55,10	-	0/5/27/28	0/3/3/3
10	UR3	A	1830	10	-	2/7/25/26	0/2/2/2
10	PSU	A	1081	10	-	1/7/25/26	0/2/2/2
10	OMU	A	121	10	-	0/9/27/28	0/2/2/2
10	A2M	A	1678	10	-	1/5/27/28	0/3/3/3
10	OMC	A	1703	10	-	0/9/27/28	0/2/2/2
10	PSU	A	822	10	-	2/7/25/26	0/2/2/2
10	PSU	A	612	10	-	0/7/25/26	0/2/2/2
10	A2M	A	484	10	-	0/5/27/28	0/3/3/3
10	B8N	A	1248	10	-	9/16/34/35	0/2/2/2
10	MA6	A	1851	10	-	3/7/29/30	0/3/3/3
10	A2M	A	166	10	-	1/5/27/28	0/3/3/3

The worst 5 of 111 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	166	A2M	C3'-C2'	-13.15	1.24	1.53
10	A	1678	A2M	C3'-C2'	-13.09	1.24	1.53
10	A	1031	A2M	C3'-C2'	-13.07	1.24	1.53
10	A	27	A2M	C3'-C2'	-12.97	1.24	1.53
10	A	159	A2M	C3'-C2'	-12.89	1.24	1.53

The worst 5 of 114 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1851	MA6	N1-C6-N6	-11.28	103.80	116.83
10	A	1850	MA6	N1-C6-N6	-11.20	103.89	116.83
10	A	1678	A2M	C1'-N9-C4	10.87	145.74	126.64
10	A	159	A2M	C1'-N9-C4	10.65	145.35	126.64
10	A	484	A2M	C1'-N9-C4	10.59	145.24	126.64

There are no chirality outliers.

5 of 41 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	27	A2M	C1'-C2'-O2'-CM'
10	A	116	OMU	C1'-C2'-O2'-CM2
10	A	159	A2M	C1'-C2'-O2'-CM'
10	A	668	A2M	O4'-C4'-C5'-O5'
10	A	668	A2M	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 95 ligands modelled in this entry, 93 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
58	MET	w	101	-	6,7,8	0.66	0	2,7,9	0.53	0
57	GTP	t	501	55	29,34,34	1.25	2 (6%)	35,54,54	1.25	4 (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
58	MET	w	101	-	-	1/5/6/8	-
57	GTP	t	501	55	-	7/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	t	501	GTP	C5-C6	-4.08	1.39	1.47
57	t	501	GTP	C2-N3	2.19	1.38	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	t	501	GTP	C8-N7-C5	3.70	108.84	102.55
57	t	501	GTP	C2-N1-C6	-2.97	119.67	125.11
57	t	501	GTP	C5-C6-N1	2.88	119.57	114.07
57	t	501	GTP	O6-C6-C5	-2.06	120.24	124.32

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

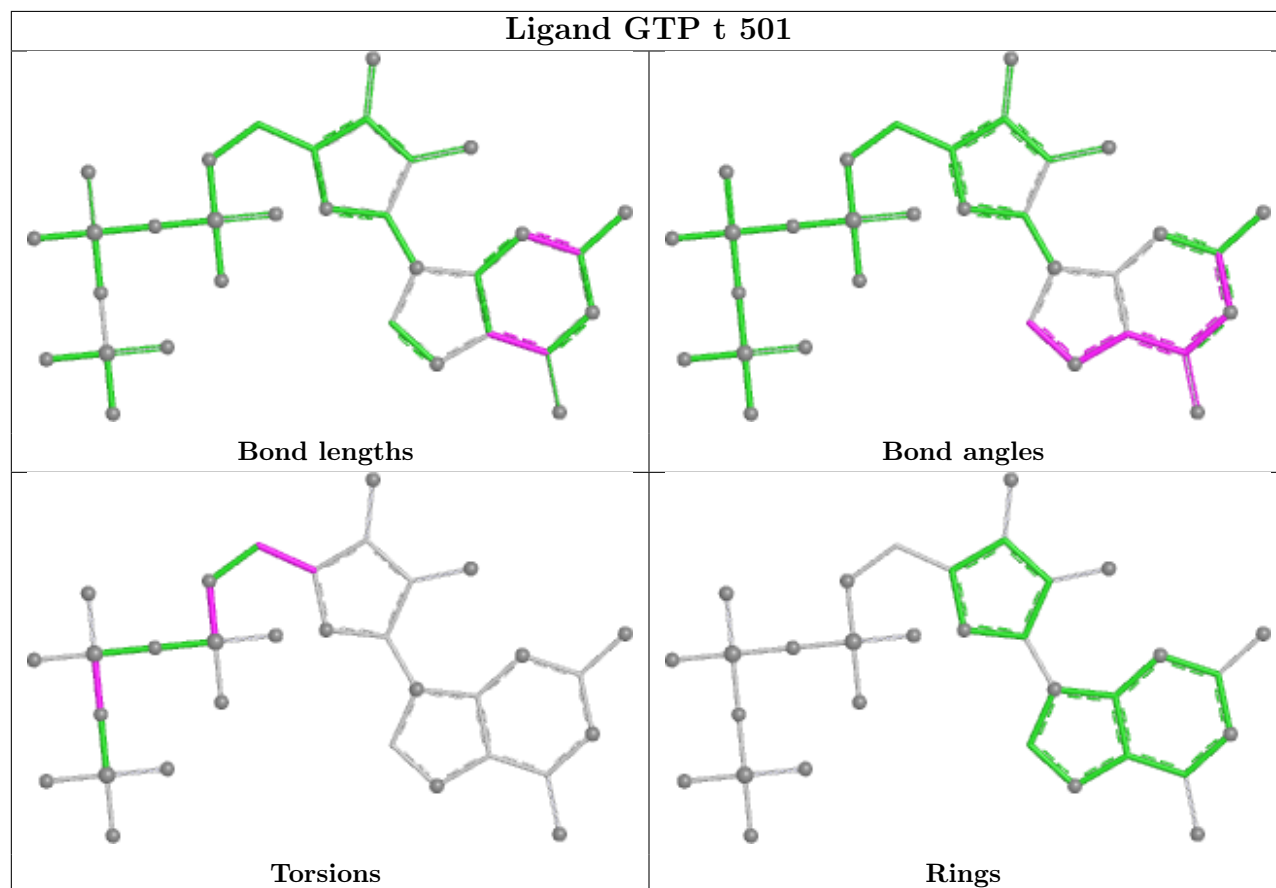
Mol	Chain	Res	Type	Atoms
57	t	501	GTP	C5'-O5'-PA-O3A
57	t	501	GTP	C5'-O5'-PA-O1A
57	t	501	GTP	C5'-O5'-PA-O2A
58	w	101	MET	O-C-CA-CB
57	t	501	GTP	C3'-C4'-C5'-O5'

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.

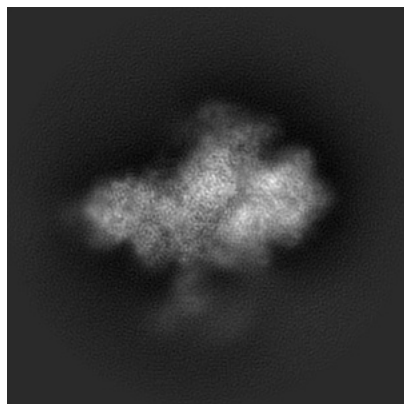
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17696. These allow visual inspection of the internal detail of the map and identification of artifacts.

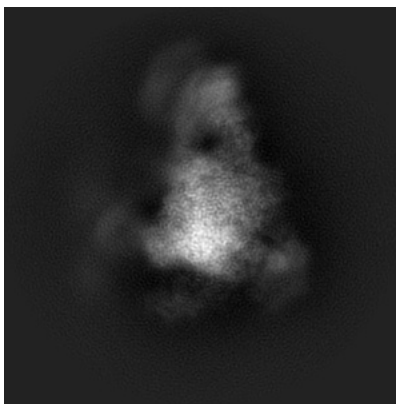
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

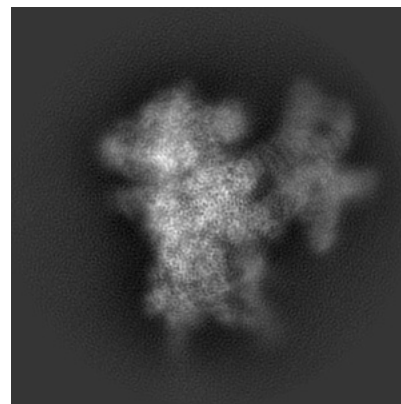
6.1.1 Primary map



X

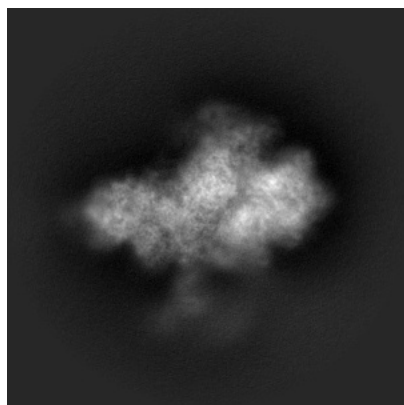


Y

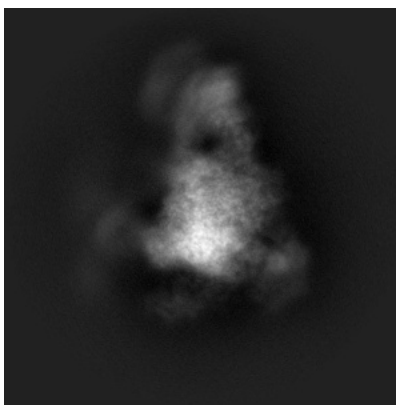


Z

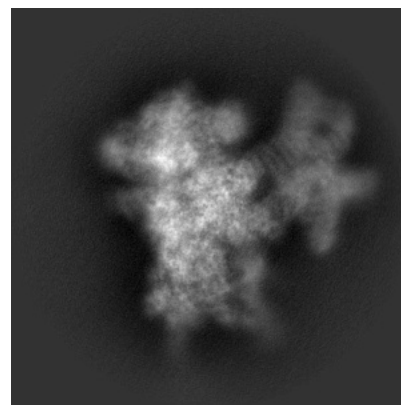
6.1.2 Raw map



X



Y

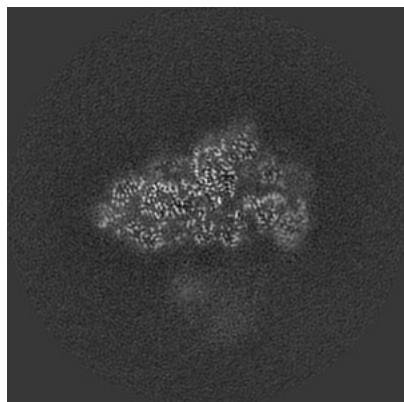


Z

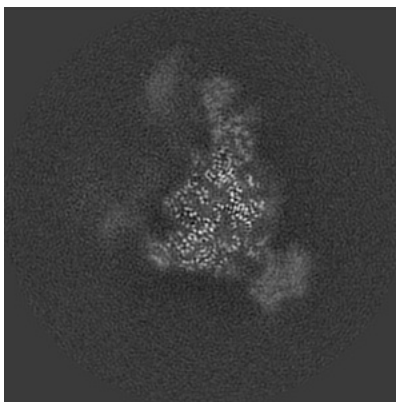
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

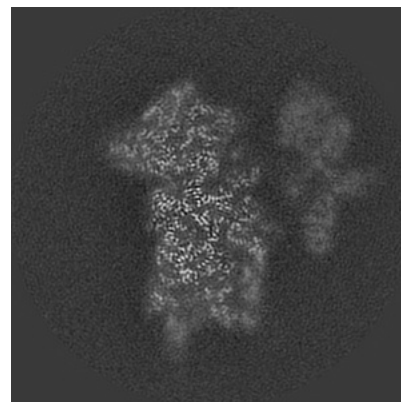
6.2.1 Primary map



X Index: 216

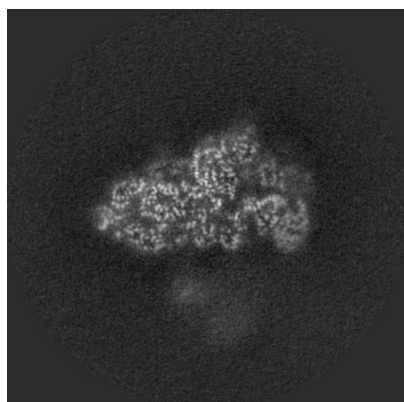


Y Index: 216

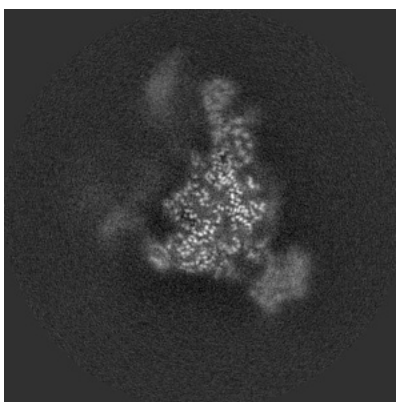


Z Index: 216

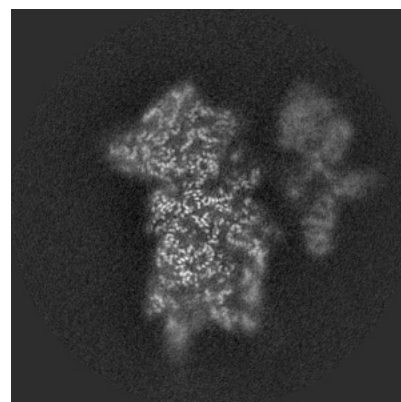
6.2.2 Raw map



X Index: 180



Y Index: 180

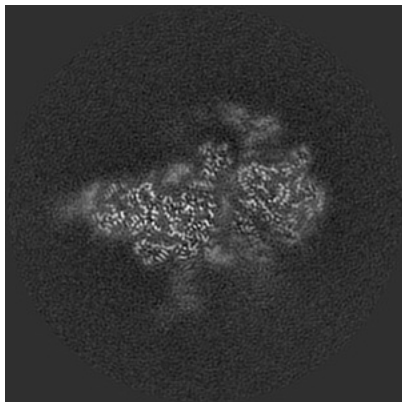


Z Index: 180

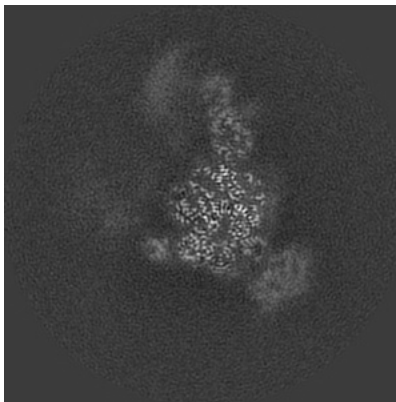
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

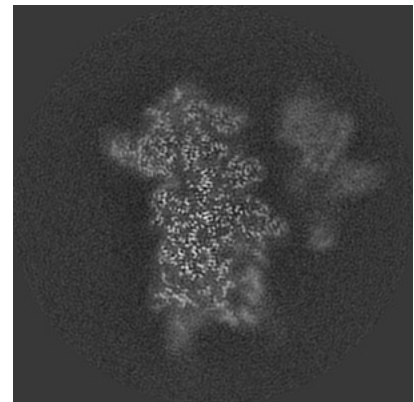
6.3.1 Primary map



X Index: 175

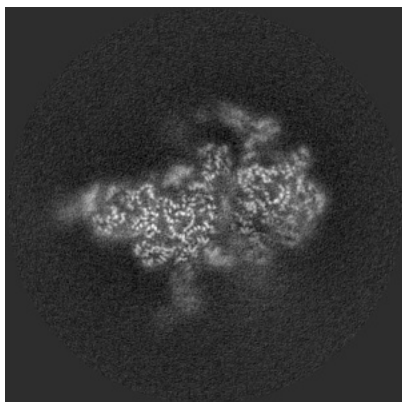


Y Index: 221

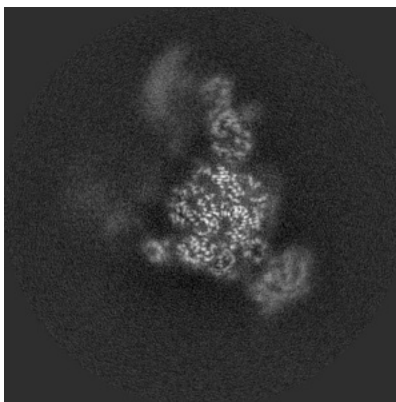


Z Index: 210

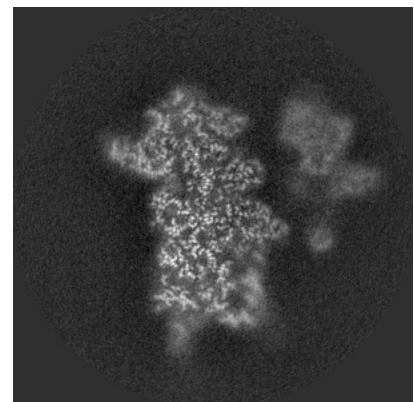
6.3.2 Raw map



X Index: 145



Y Index: 185

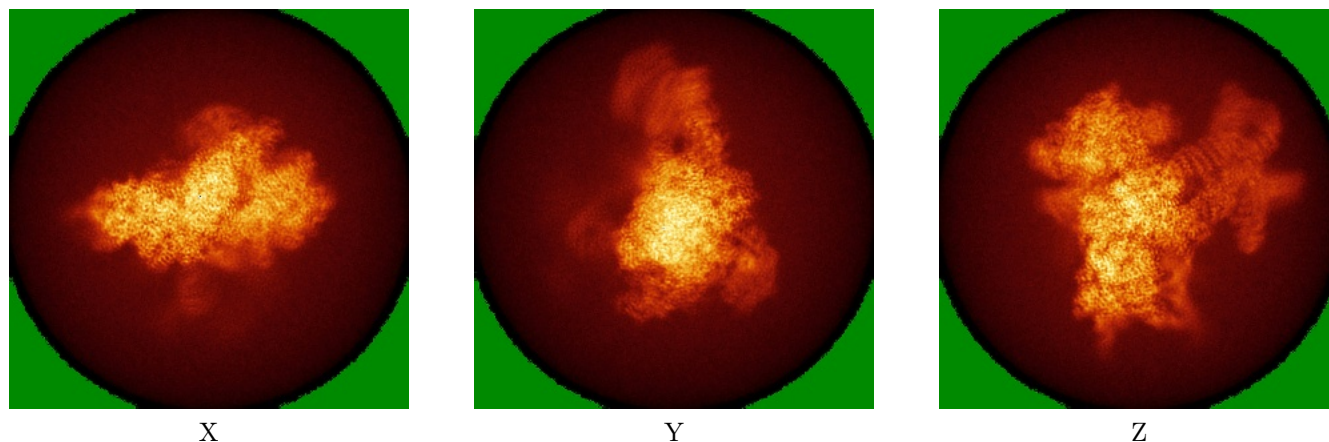


Z Index: 174

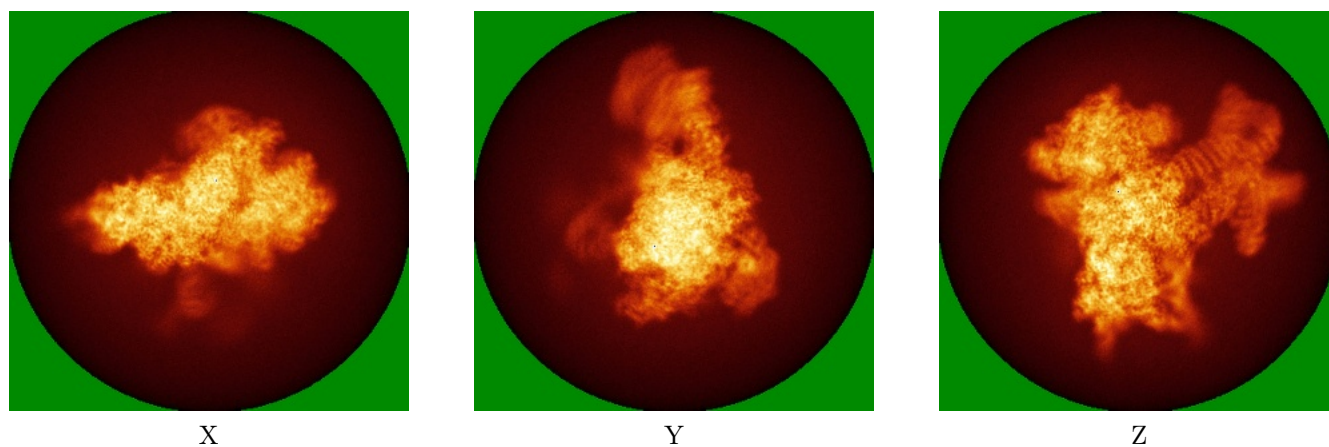
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



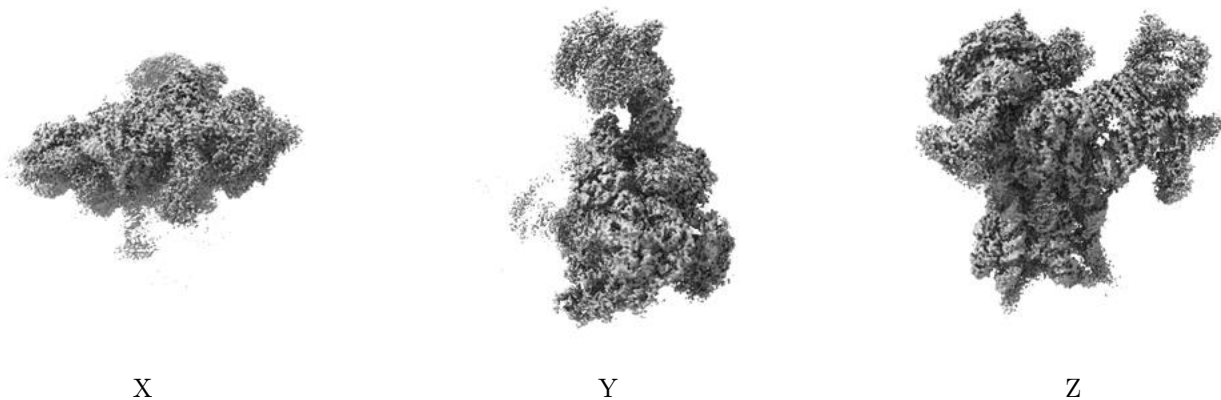
6.4.2 Raw map



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.

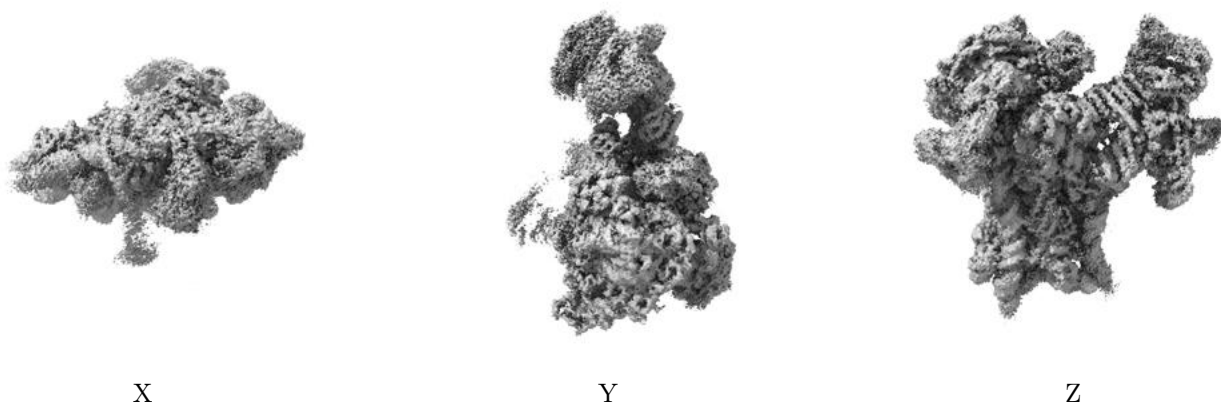
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 4.0. 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.

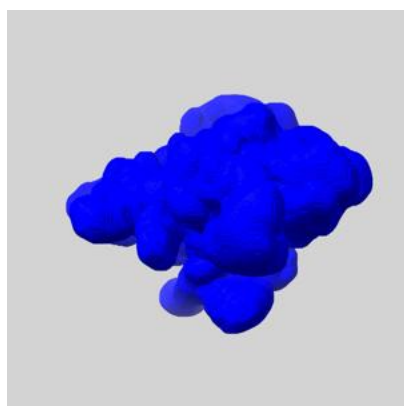
6.6 Mask visualisation [i](#)

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

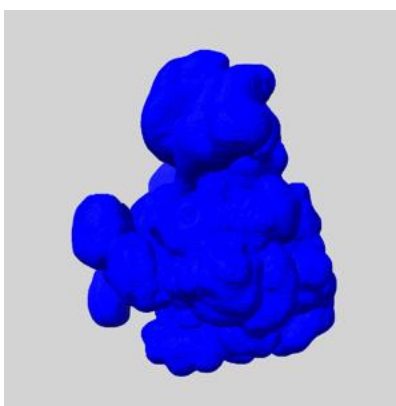
A mask typically either:

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

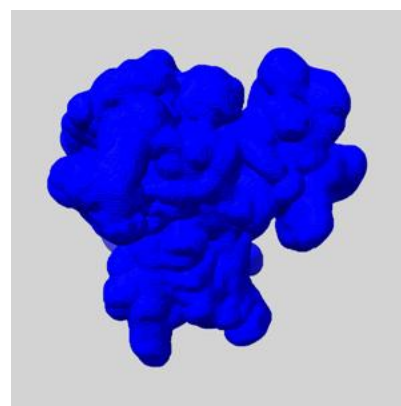
6.6.1 emd_17696_msk_1.map [i](#)



X



Y

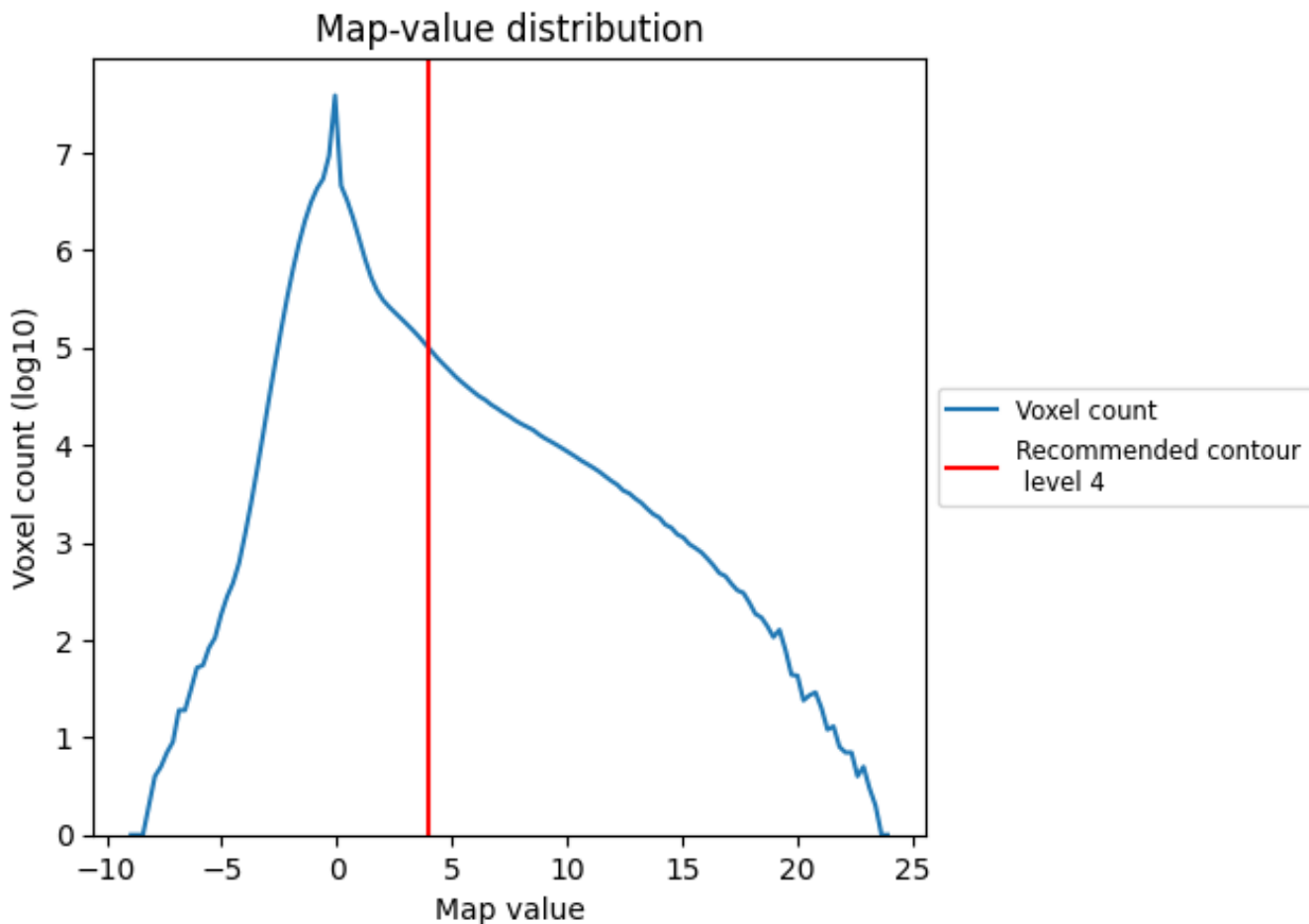


Z

7 Map analysis [i](#)

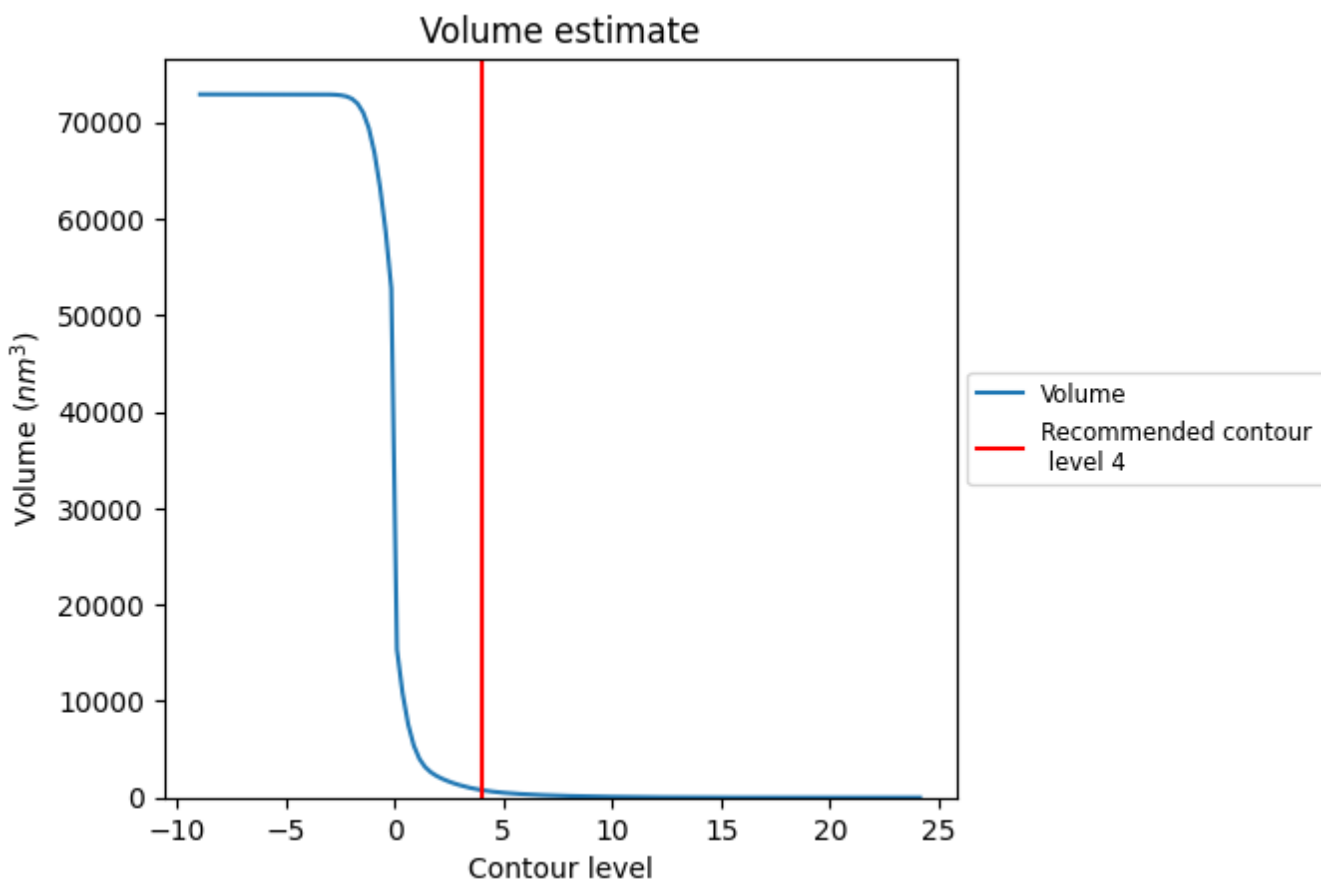
This section contains the results of statistical analysis of the map.

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.

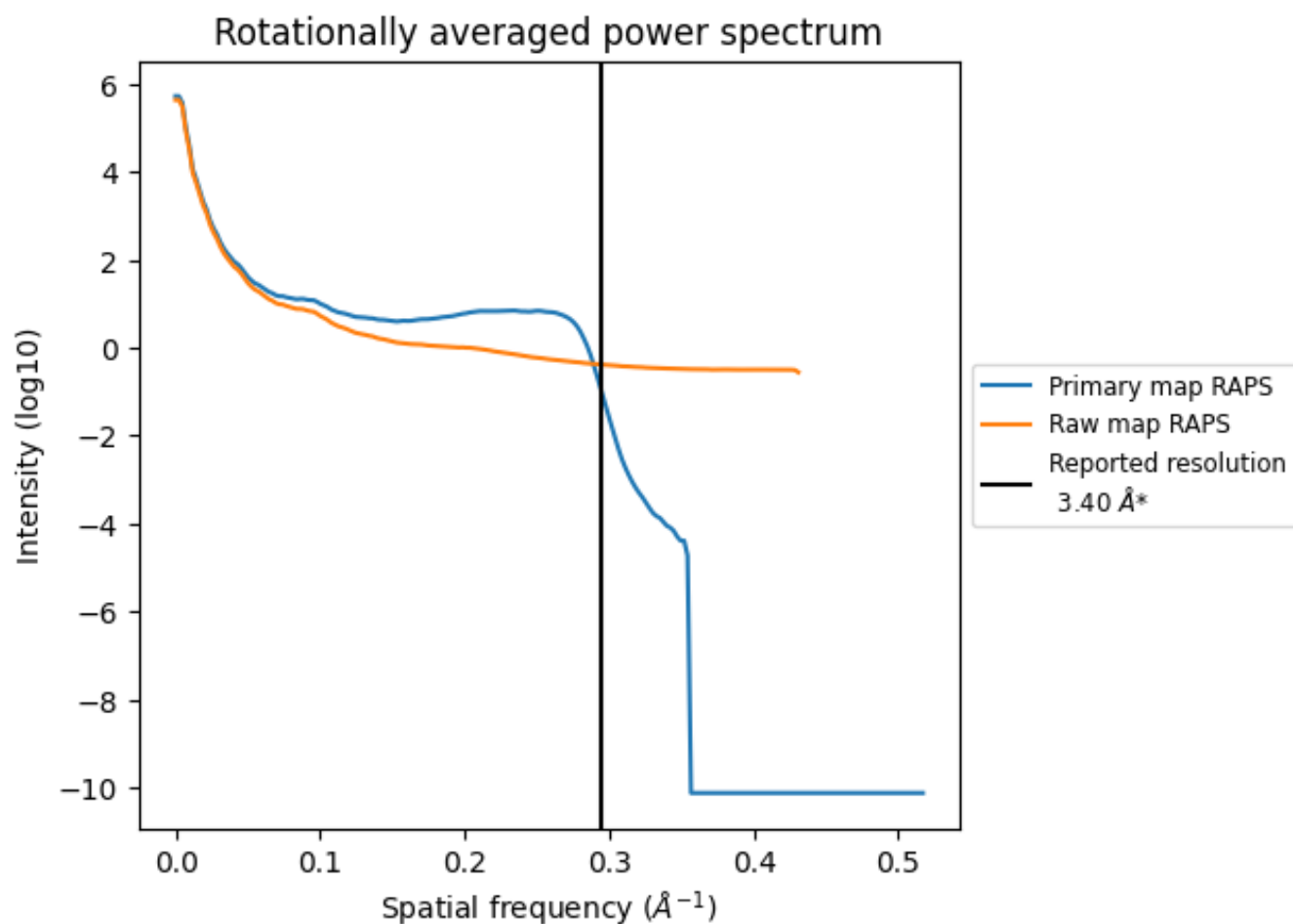
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 777 nm³; this corresponds to an approximate mass of 702 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

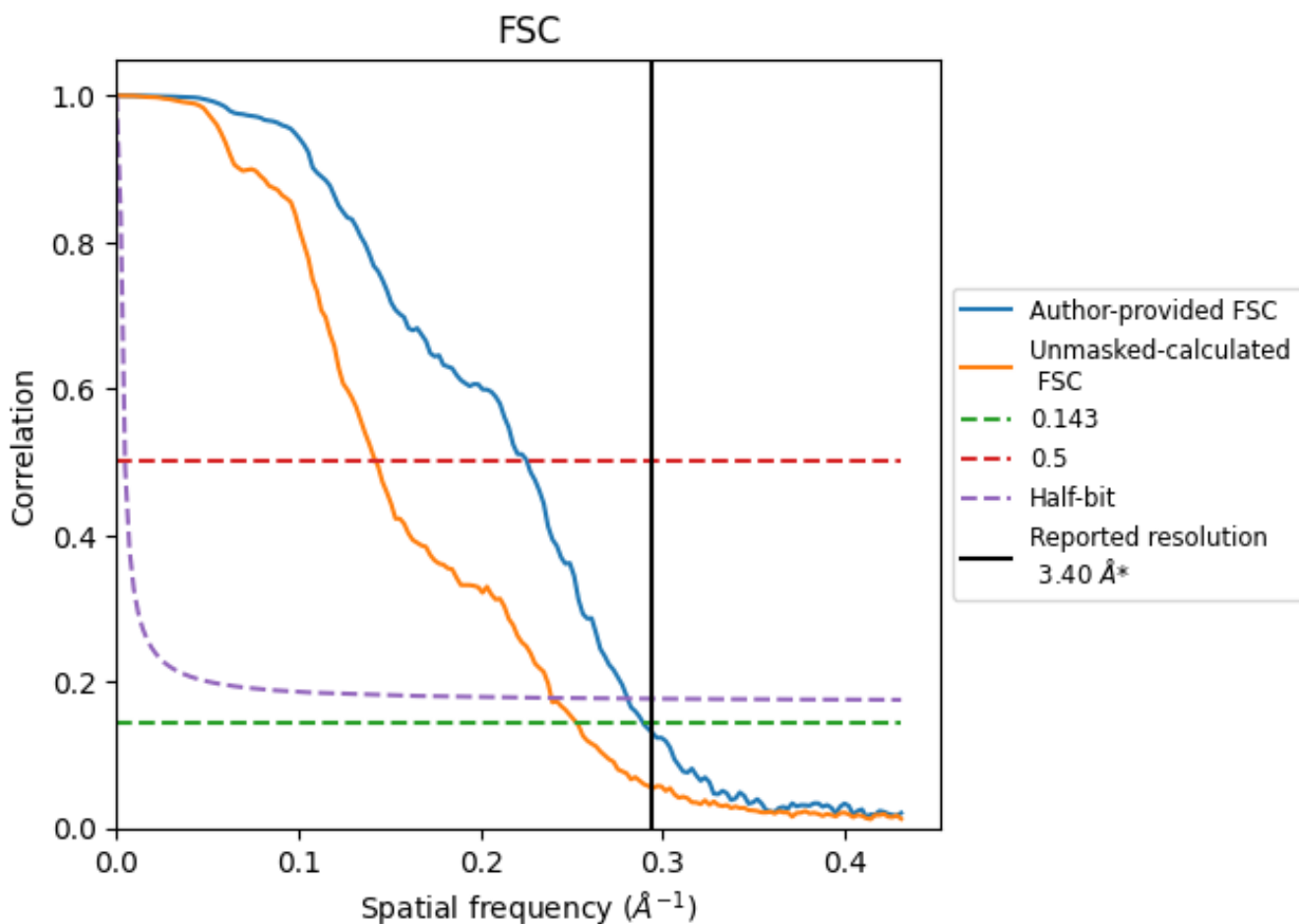


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294\AA^{-1}

8.2 Resolution estimates [i](#)

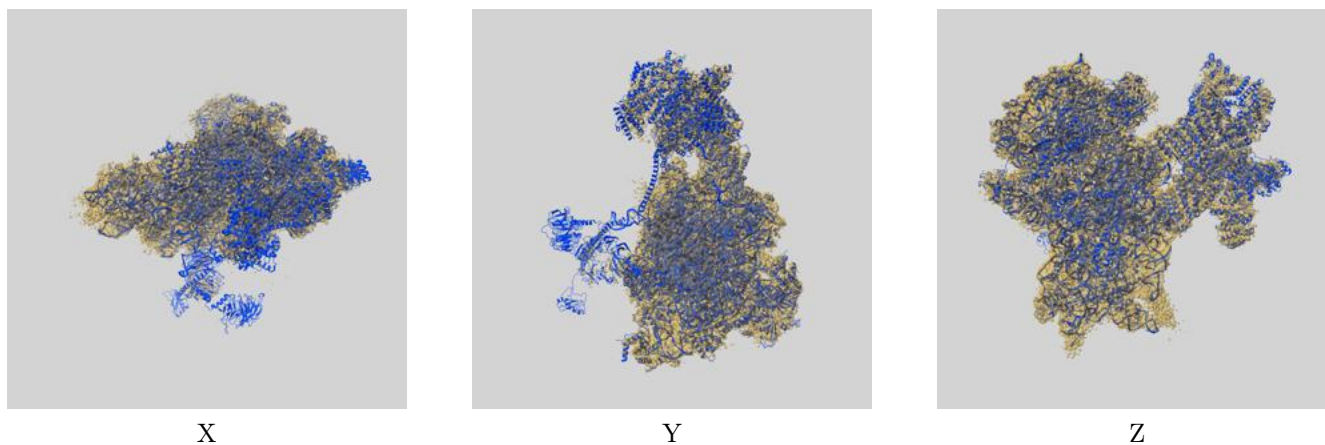
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.46	4.43	3.56
Unmasked-calculated*	3.96	7.02	4.19

*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 3.96 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

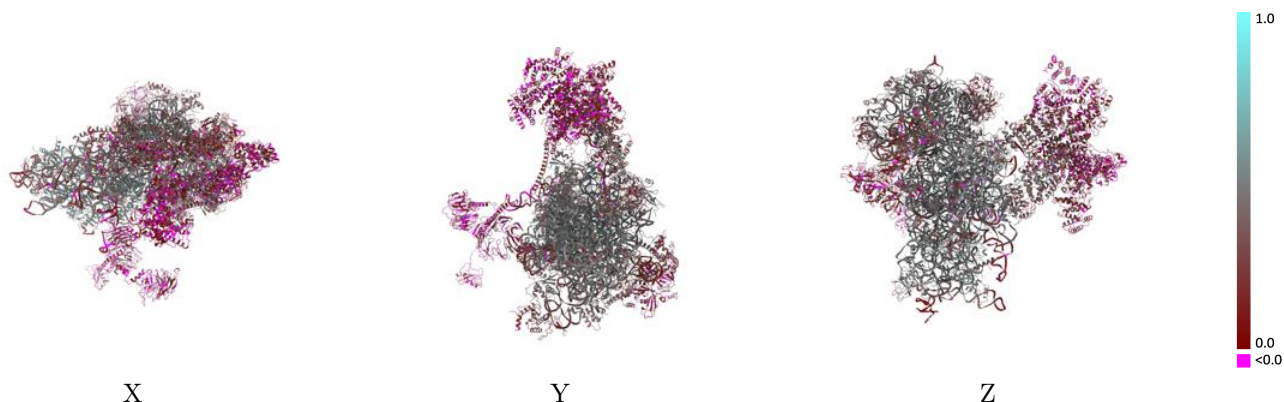
This section contains information regarding the fit between EMDB map EMD-17696 and PDB model 8PJ1. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



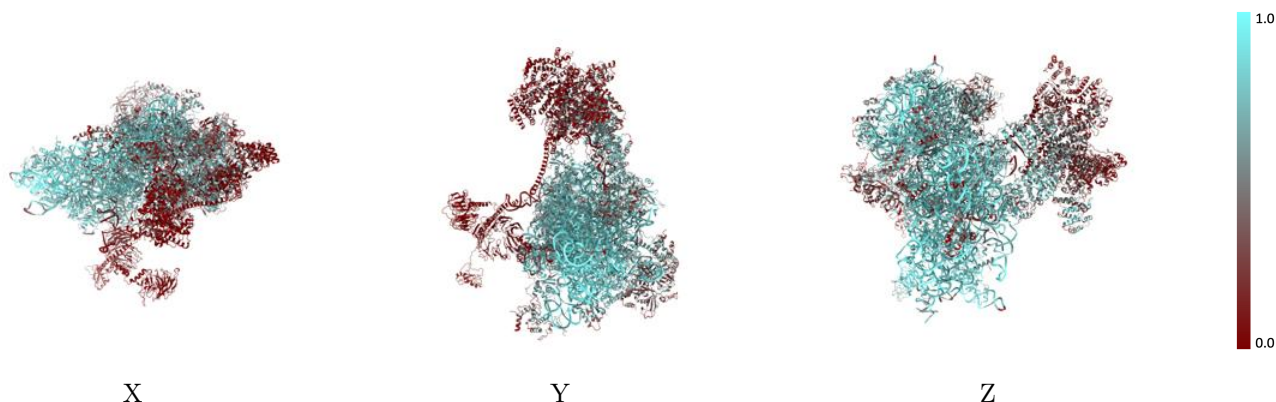
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



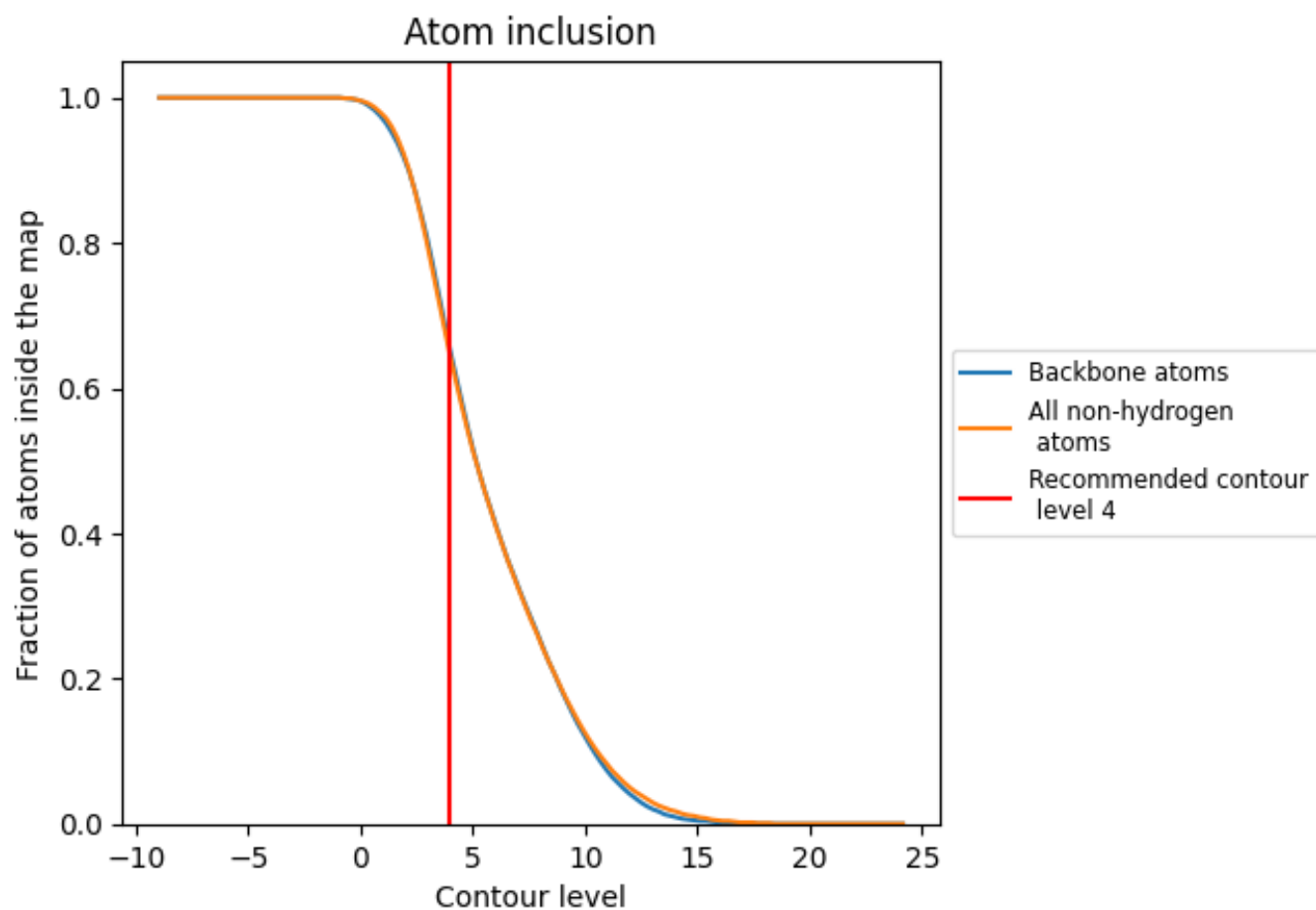
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 64% 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 (4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6440	 0.3680
1	 0.0360	 0.1280
2	 0.0010	 0.1030
3	 0.0860	 0.0960
4	 0.1970	 0.1250
5	 0.0910	 0.0960
6	 0.2010	 0.1480
7	 0.2940	 0.2100
8	 0.2170	 0.1350
9	 0.6790	 0.4710
A	 0.9040	 0.4360
B	 0.8380	 0.5120
C	 0.8510	 0.5170
D	 0.8220	 0.5000
E	 0.8480	 0.5240
F	 0.7070	 0.4540
G	 0.7250	 0.4520
H	 0.7820	 0.4910
I	 0.8020	 0.4990
J	 0.8410	 0.5180
K	 0.7740	 0.4930
L	 0.7640	 0.4920
M	 0.6780	 0.4520
N	 0.7880	 0.4960
O	 0.7900	 0.4840
P	 0.7840	 0.4810
Q	 0.8440	 0.5230
R	 0.8540	 0.4880
S	 0.8060	 0.4460
T	 0.8690	 0.5030
V	 0.7300	 0.4670
Y	 0.7770	 0.4750
Z	 0.6300	 0.4460
a	 0.6600	 0.4140
b	 0.6490	 0.4180



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
c	 0.6500	 0.4070
d	 0.7950	 0.4590
e	 0.6990	 0.4350
f	 0.7070	 0.4220
h	 0.6220	 0.4380
i	 0.8530	 0.4940
k	 0.4480	 0.2430
m	 0.3430	 0.2390
n	 0.5900	 0.4560
o	 0.2420	 0.2490
p	 0.5620	 0.4100
q	 0.6710	 0.4500
r	 0.5010	 0.3140
s	 0.4910	 0.3350
t	 0.3330	 0.1900
u	 0.4040	 0.2780
v	 0.3690	 0.1990
w	 0.8210	 0.2820
x	 0.4000	 0.3140
y	 0.4760	 0.3240