wwPDB EM Validation Summary Report ⓘ

Dec 18, 2022 – 12:36 am GMT

PDB ID	:	6ZXF
EMDB ID	:	EMD-11519
Title	:	Cryo-EM structure of a late human pre-40S ribosomal subunit - State G
Authors	:	Ameismeier, M.; Zemp, I.; van den Heuvel, J.; Thoms, M.; Berninghausen, O.; Kutay, U.; Beckmann, R.
Deposited on	:	2020-07-29
Resolution	:	3.70 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:

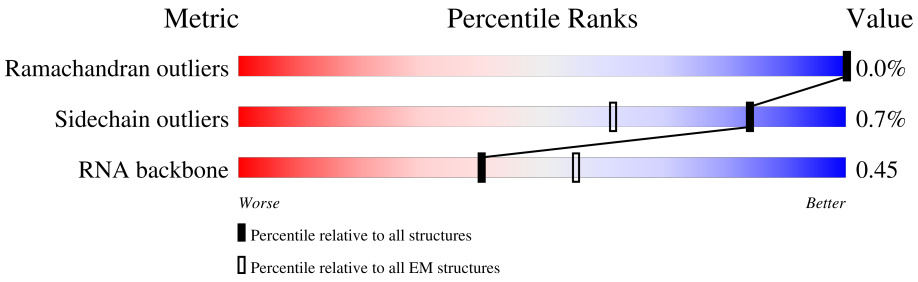
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.70 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	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 <=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	1874	61% 25% · 12%
2	A	295	73% 27%
3	B	264	· 80% 20%
4	C	293	73% 26%
5	E	263	97% ·
6	D	243	92% 8%
7	G	249	88% · 10%
8	H	194	92% · 8%

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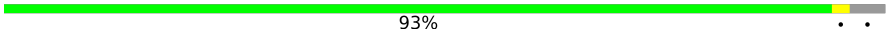
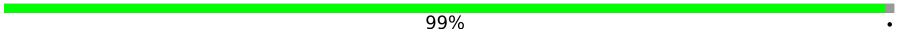
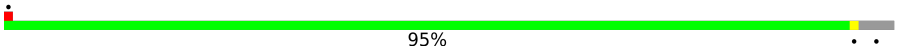
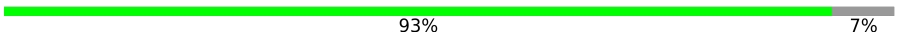
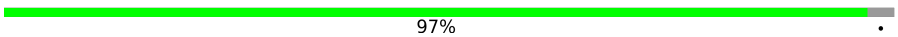
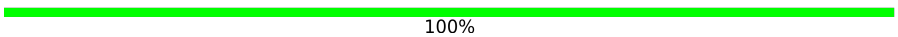
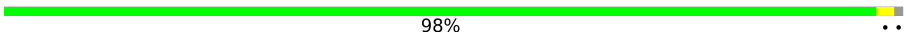
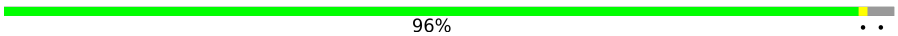
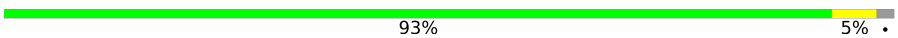
Mol	Chain	Length	Quality of chain
9	I	208	
10	J	194	
11	F	204	
12	L	158	
13	K	165	
14	N	151	
15	O	151	
16	M	132	
17	P	145	
18	R	135	
19	Q	146	
20	S	152	
21	T	145	
22	V	83	
23	W	130	
24	X	143	
25	Y	133	
26	U	119	
27	Z	125	
28	b	84	
29	c	69	
30	d	56	
31	e	59	
32	f	156	
33	g	317	

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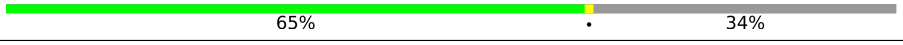
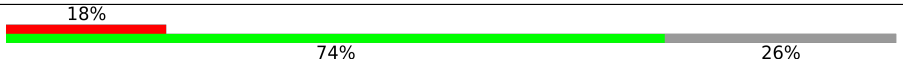
Mol	Chain	Length	Quality of chain
34	j	165	
35	z	568	
36	y	412	
37	k	583	

2 Entry composition (i)

There are 40 unique types of molecules in this entry. The entry contains 80133 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 pre-18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	1656	35367	15787	6366	11558	1656	0	0

- Molecule 2 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	216	1705	1083	299	315	8	0	0

- Molecule 3 is a protein called 40S ribosomal protein S3a.

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

- Molecule 4 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	216	1674	1085	287	292	10	0	0

- Molecule 5 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	255	2031	1299	377	347	8	0	0

- Molecule 6 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	D	224	1745	1112	314	312	7	0	0

- Molecule 7 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	223	Total	C	N	O	S	0	0
			1802	1128	358	309	7		

- Molecule 8 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	179	Total	C	N	O	S	0	0
			1446	927	264	254	1		

- Molecule 9 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	199	Total	C	N	O	S	0	0
			1638	1027	322	284	5		

- Molecule 10 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	176	Total	C	N	O	S	0	0
			1465	934	295	234	2		

- Molecule 11 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	184	Total	C	N	O	S	0	0
			1461	914	276	264	7		

- Molecule 12 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	136	Total	C	N	O	S	0	0
			1127	719	212	190	6		

- Molecule 13 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	95	Total	C	N	O	S	0	0
			799	524	139	130	6		

- Molecule 14 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 15 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	126	Total	C	N	O	S	0	0
			947	580	188	173	6		

- Molecule 16 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	108	Total	C	N	O	S	0	0
			837	530	147	153	7		

- Molecule 17 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	131	Total	C	N	O	S	0	0
			1072	682	201	182	7		

- Molecule 18 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	121	Total	C	N	O	S	0	0
			983	617	183	180	3		

- Molecule 19 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Q	140	Total	C	N	O	S	0	0
			1116	710	211	192	3		

- Molecule 20 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	141	Total	C	N	O	S	0	0
			1162	731	232	198	1		

- Molecule 21 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	141	Total	C	N	O	S	0	0
			1094	685	210	196	3		

- Molecule 22 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 23 is a protein called 40S ribosomal protein S15a.

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

- Molecule 24 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	139	Total	C	N	O	S	0	0
			1080	682	214	181	3		

- Molecule 25 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	122	Total	C	N	O	S	0	0
			987	624	193	165	5		

- Molecule 26 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	U	98	Total	C	N	O	S	0	0
			774	486	145	139	4		

- Molecule 27 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	70	Total	C	N	O	S	0	0
			557	358	101	97	1		

- Molecule 28 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	77	Total	C	N	O	S	0	0
			611	386	113	107	5		

- Molecule 29 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	61	Total	C	N	O	S	0	0
			479	292	95	90	2		

- Molecule 30 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	55	Total	C	N	O	S	0	0
			458	286	94	73	5		

- Molecule 31 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	50	Total	C	N	O	S	0	0
			398	244	90	63	1		

- Molecule 32 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	57	Total	C	N	O	S	0	0
			465	295	89	74	7		

- Molecule 33 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	295	Total	C	N	O	S	0	0
			2306	1460	403	431	12		

- Molecule 34 is a protein called Probable RNA-binding protein EIF1AD.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	j	115	Total	C	N	O	S	0	0
			928	590	166	170	2		

- Molecule 35 is a protein called Serine/threonine-protein kinase RIO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	z	373	Total	C	N	O	S	0	0
			3041	1911	553	555	22		

- Molecule 36 is a protein called RNA-binding protein NOB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	y	233	Total	C	N	O	S	0	0
			1838	1167	335	327	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
y	10	ASN	ASP	conflict	UNP Q9ULX3

- Molecule 37 is a protein called Leucine-rich repeat-containing protein 47.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	k	430	Total	C	N	O	0	0
			2117	1257	430	430		

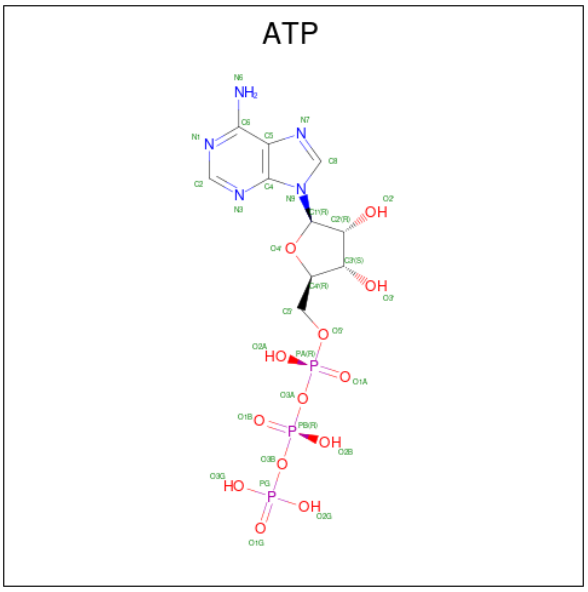
- Molecule 38 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
38	d	1	Total	Zn	0
			1	1	
38	f	1	Total	Zn	0
			1	1	
38	y	1	Total	Zn	0
			1	1	

- Molecule 39 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
39	z	2	Total	Mg	0
			2	2	

- Molecule 40 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



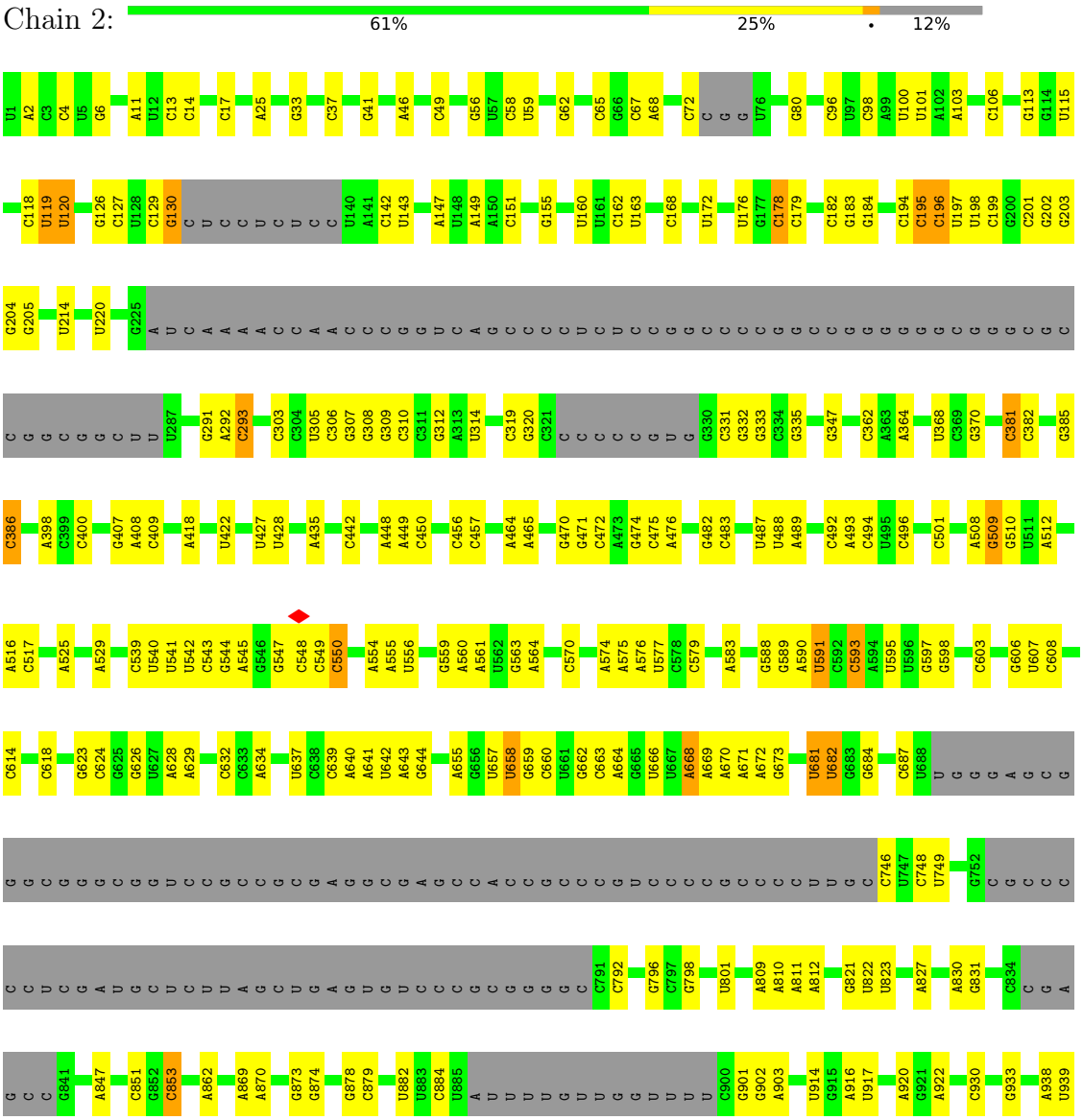
Mol	Chain	Residues	Atoms					AltConf
40	z	1	Total	C	N	O	P	0
			31	10	5	13	3	

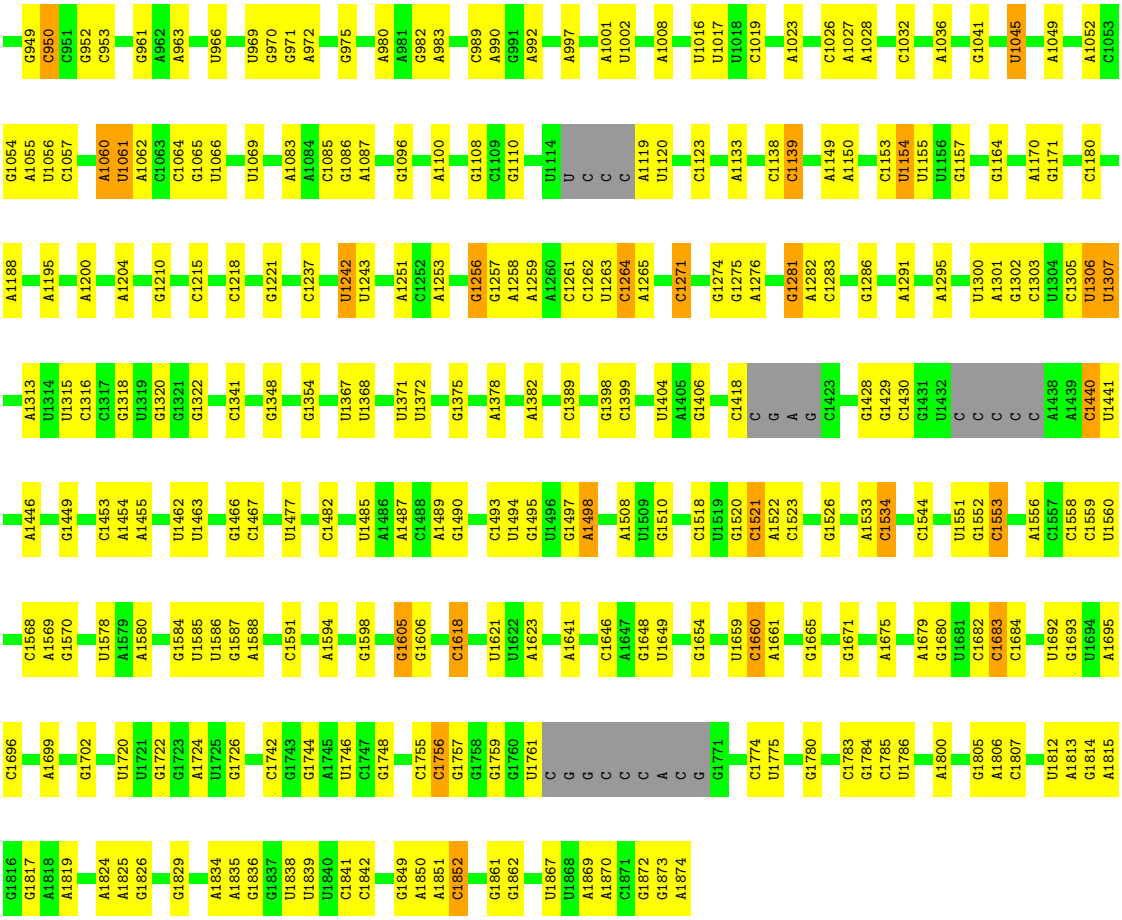
3 Residue-property plots (i)

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: pre-18S ribosomal RNA

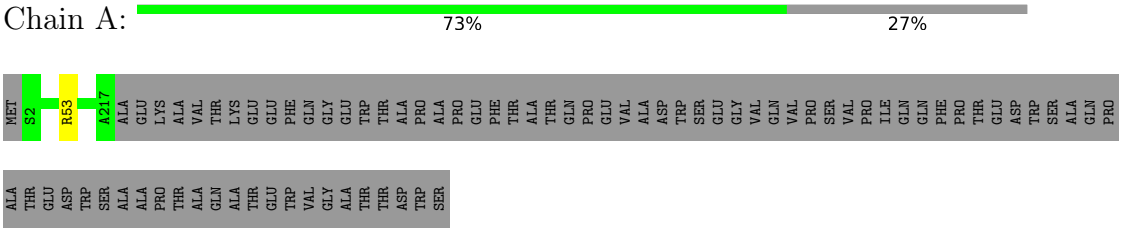
Chain 2:





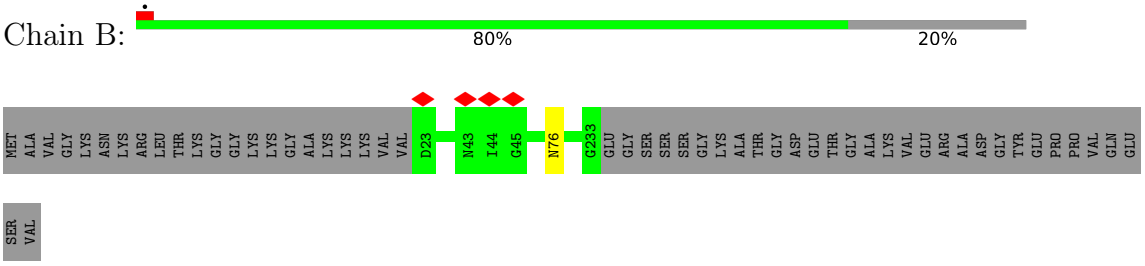
• Molecule 2: 40S ribosomal protein SA

Chain A:



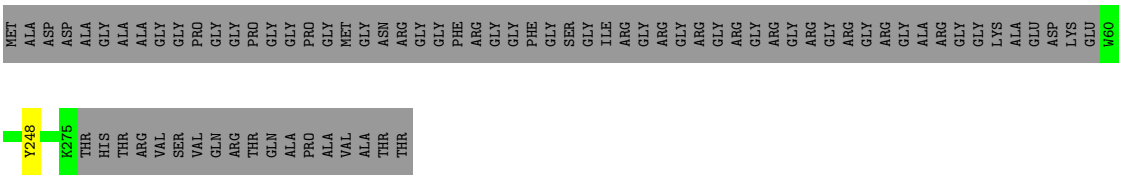
• Molecule 3: 40S ribosomal protein S3a

Chain B:



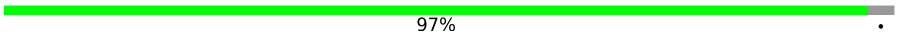
• Molecule 4: 40S ribosomal protein S2

Chain C:



• Molecule 5: 40S ribosomal protein S4, X isoform

Chain E:

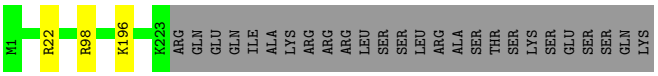


• Molecule 6: 40S ribosomal protein S3

Chain D:

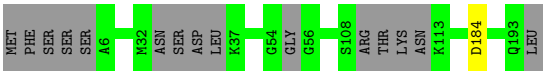
• Molecule 7: 40S ribosomal protein S6

Chain G:



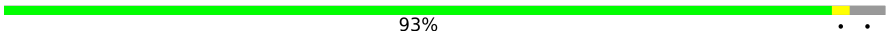
• Molecule 8: 40S ribosomal protein S7

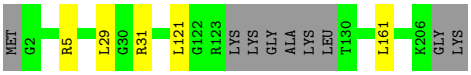
Chain H:



• Molecule 9: 40S ribosomal protein S8

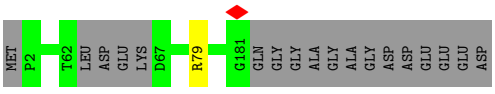
Chain I:





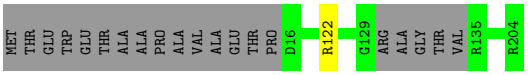
• Molecule 10: 40S ribosomal protein S9

Chain J:



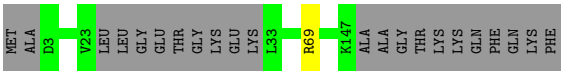
• Molecule 11: 40S ribosomal protein S5

Chain F:



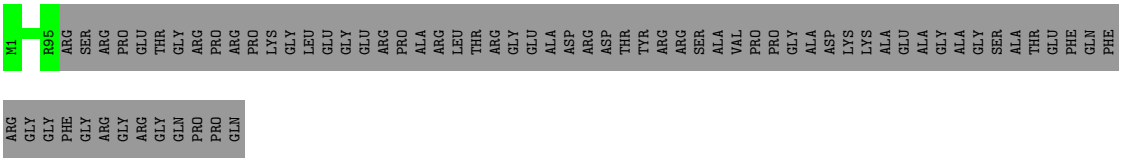
• Molecule 12: 40S ribosomal protein S11

Chain L:



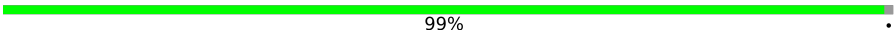
• Molecule 13: 40S ribosomal protein S10

Chain K:



• Molecule 14: 40S ribosomal protein S13

Chain N:

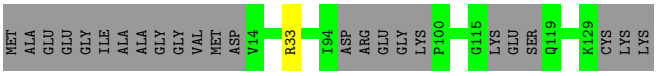


• Molecule 15: 40S ribosomal protein S14

Chain O:

• Molecule 16: 40S ribosomal protein S12

Chain M:

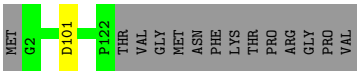


• Molecule 17: 40S ribosomal protein S15

Chain P:

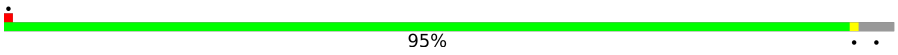
• Molecule 18: 40S ribosomal protein S17

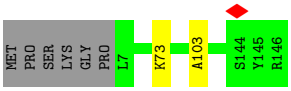
Chain R:



• Molecule 19: 40S ribosomal protein S16

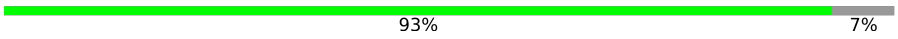
Chain Q:

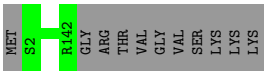




• Molecule 20: 40S ribosomal protein S18

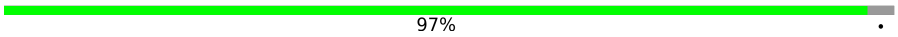
Chain S:

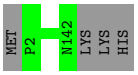




• Molecule 21: 40S ribosomal protein S19

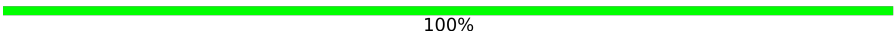
Chain T:





• Molecule 22: 40S ribosomal protein S21

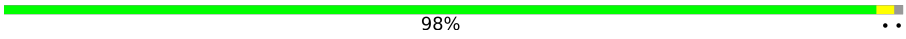
Chain V:

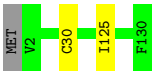


There are no outlier residues recorded for this chain.

• Molecule 23: 40S ribosomal protein S15a

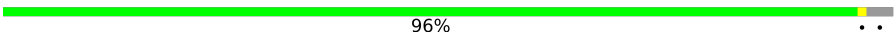
Chain W:





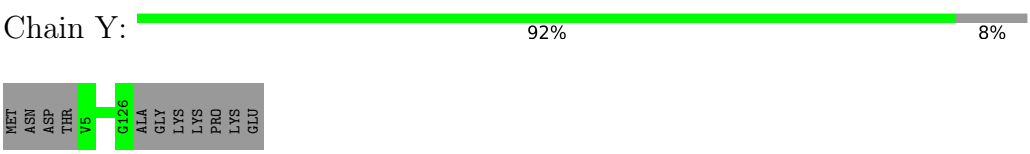
• Molecule 24: 40S ribosomal protein S23

Chain X:



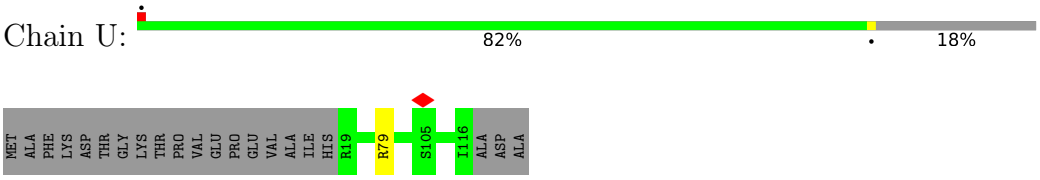
• Molecule 25: 40S ribosomal protein S24

Chain Y:



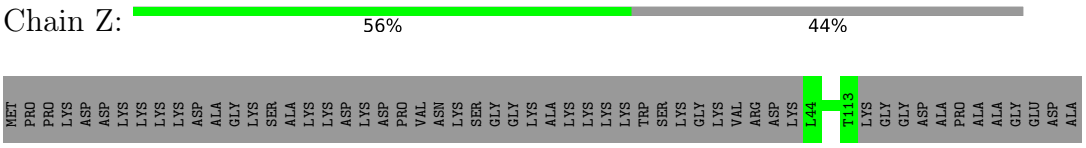
• Molecule 26: 40S ribosomal protein S20

Chain U:



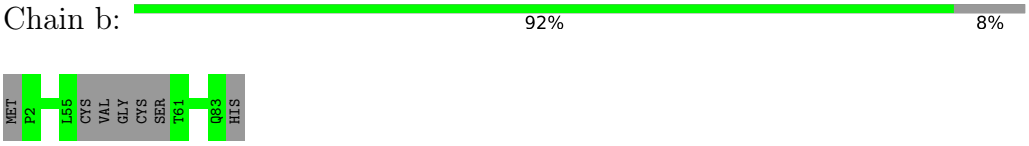
• Molecule 27: 40S ribosomal protein S25

Chain Z:



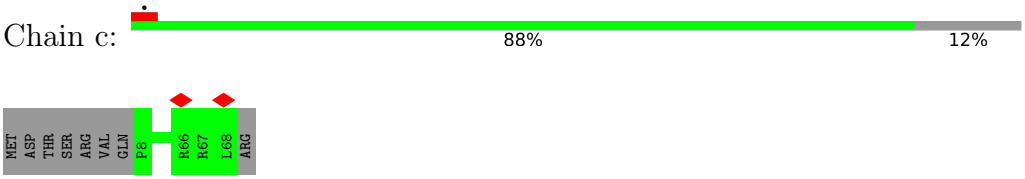
• Molecule 28: 40S ribosomal protein S27

Chain b:



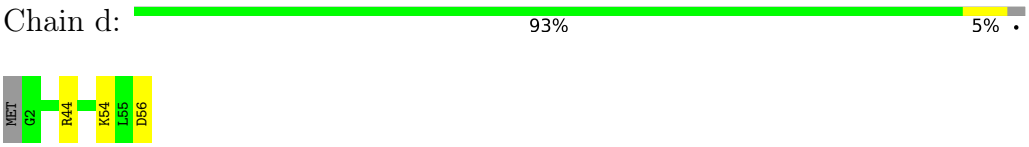
• Molecule 29: 40S ribosomal protein S28

Chain c:



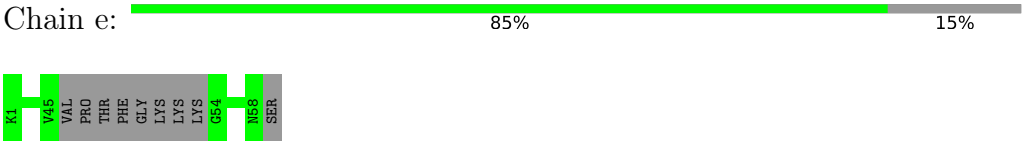
• Molecule 30: 40S ribosomal protein S29

Chain d:



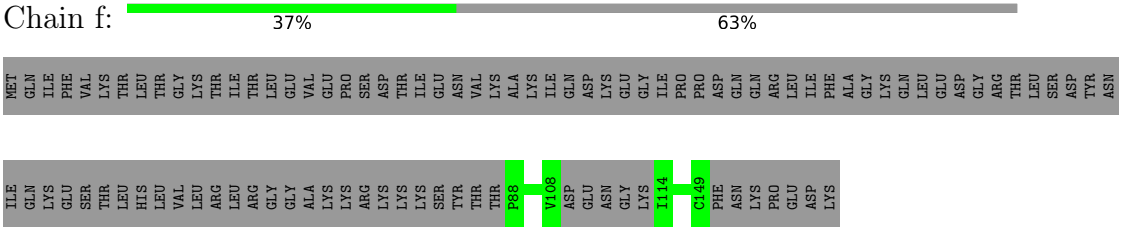
• Molecule 31: 40S ribosomal protein S30

Chain e:



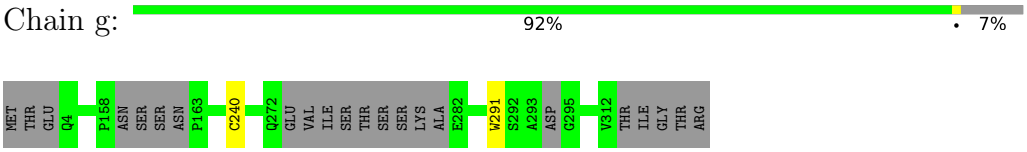
• Molecule 32: Ubiquitin-40S ribosomal protein S27a

Chain f:



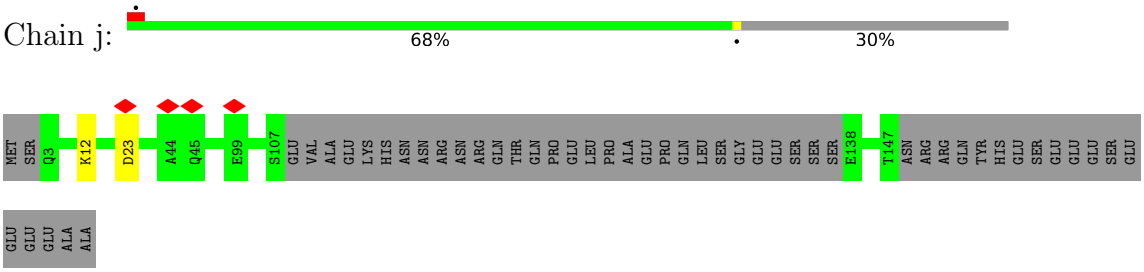
• Molecule 33: Receptor of activated protein C kinase 1

Chain g:



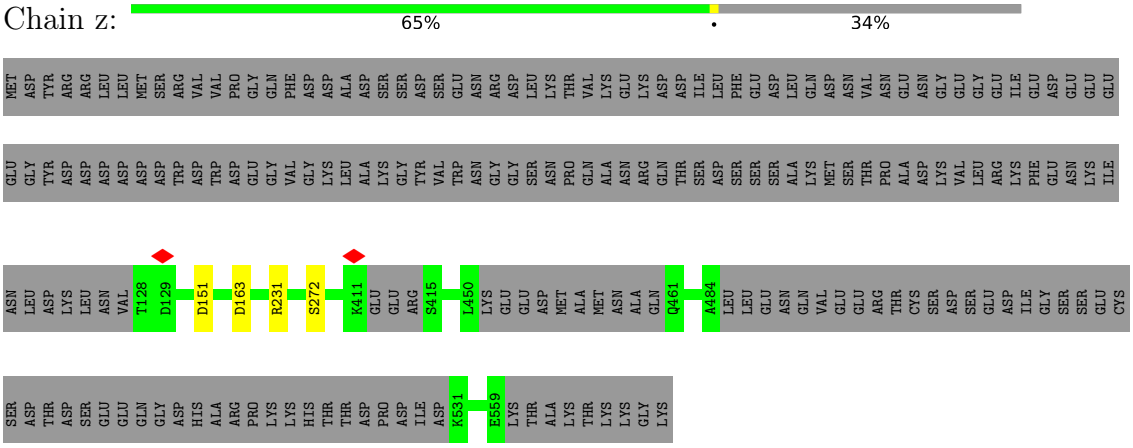
• Molecule 34: Probable RNA-binding protein EIF1AD

Chain j:



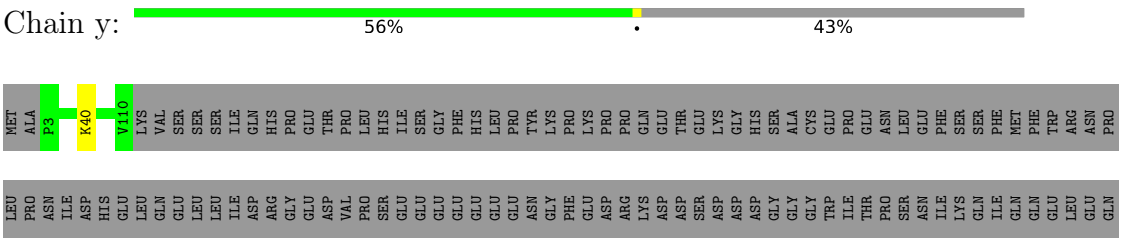
• Molecule 35: Serine/threonine-protein kinase RIO1

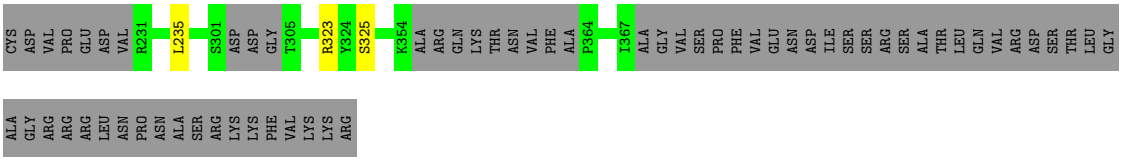
Chain z:



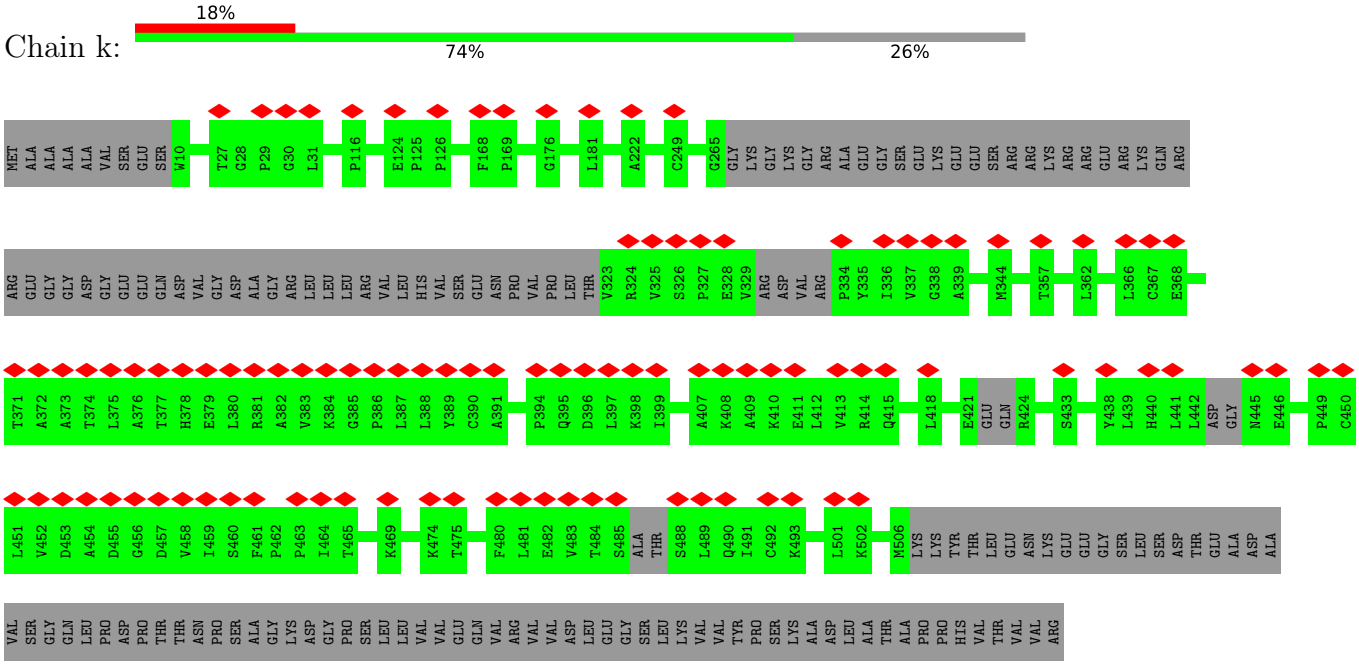
• Molecule 36: RNA-binding protein NOB1

Chain y:





• Molecule 37: Leucine-rich repeat-containing protein 47



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	140612	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 ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.340	Depositor
Minimum map value	-0.135	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	390.24, 390.24, 390.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.084, 1.084, 1.084	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: ATP, ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	2	1.14	13/39549 (0.0%)	1.18	233/61629 (0.4%)
2	A	0.55	0/1742	0.55	0/2367
3	B	0.49	0/1742	0.60	0/2330
4	C	0.62	0/1710	0.59	0/2310
5	E	0.47	0/2073	0.55	0/2791
6	D	0.48	0/1773	0.55	0/2387
7	G	0.39	0/1825	0.54	0/2431
8	H	0.41	0/1466	0.51	0/1959
9	I	0.48	0/1666	0.56	0/2223
10	J	0.47	0/1489	0.54	0/1987
11	F	0.48	0/1481	0.54	0/1988
12	L	0.62	0/1147	0.56	0/1535
13	K	0.51	0/823	0.53	0/1111
14	N	0.48	0/1226	0.52	0/1649
15	O	0.46	0/959	0.58	0/1286
16	M	0.33	0/845	0.52	0/1134
17	P	0.44	0/1094	0.54	0/1464
18	R	0.47	0/995	0.55	0/1335
19	Q	0.54	0/1133	0.58	0/1517
20	S	0.43	0/1180	0.53	0/1582
21	T	0.45	0/1113	0.52	0/1493
22	V	0.49	0/643	0.56	0/860
23	W	0.56	0/1051	0.59	0/1406
24	X	0.53	0/1097	0.56	0/1464
25	Y	0.40	0/1004	0.51	0/1337
26	U	0.49	0/783	0.56	0/1052
27	Z	0.36	0/563	0.54	0/758
28	b	0.48	0/623	0.55	0/834
29	c	0.46	0/481	0.60	0/643
30	d	0.64	0/469	0.65	0/623
31	e	0.43	0/401	0.53	0/526
32	f	0.37	0/474	0.53	0/626

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	g	0.44	0/2360	0.58	0/3207
34	j	0.40	0/946	0.59	1/1274 (0.1%)
35	z	0.52	0/3088	0.59	0/4134
36	y	0.49	1/1874 (0.1%)	0.57	0/2531
37	k	0.27	0/2111	0.50	0/2926
All	All	0.85	14/84999 (0.0%)	0.93	234/122709 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
19	Q	0	1
35	z	0	1
All	All	0	2

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	13	C	N1-C6	-6.29	1.33	1.37
1	2	1522	A	N9-C4	-5.75	1.34	1.37
1	2	668	A	N3-C4	-5.70	1.31	1.34
1	2	1498	A	N9-C4	-5.59	1.34	1.37
1	2	1100	A	N9-C4	-5.41	1.34	1.37

The worst 5 of 234 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	501	C	C2-N1-C1'	13.33	133.46	118.80
1	2	501	C	N1-C2-O2	12.59	126.45	118.90
1	2	1016	U	N3-C2-O2	-10.87	114.59	122.20
1	2	851	C	N1-C2-O2	10.53	125.22	118.90
1	2	501	C	C6-N1-C1'	-10.40	108.32	120.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	Q	103	ALA	Peptide
35	z	272	SER	Peptide

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	214/295 (72%)	199 (93%)	15 (7%)	0	100	100
3	B	209/264 (79%)	194 (93%)	15 (7%)	0	100	100
4	C	214/293 (73%)	198 (92%)	16 (8%)	0	100	100
5	E	253/263 (96%)	232 (92%)	21 (8%)	0	100	100
6	D	222/243 (91%)	211 (95%)	11 (5%)	0	100	100
7	G	221/249 (89%)	203 (92%)	18 (8%)	0	100	100
8	H	171/194 (88%)	165 (96%)	6 (4%)	0	100	100
9	I	195/208 (94%)	181 (93%)	14 (7%)	0	100	100
10	J	172/194 (89%)	159 (92%)	13 (8%)	0	100	100
11	F	180/204 (88%)	170 (94%)	10 (6%)	0	100	100
12	L	132/158 (84%)	128 (97%)	4 (3%)	0	100	100
13	K	93/165 (56%)	92 (99%)	1 (1%)	0	100	100
14	N	147/151 (97%)	140 (95%)	7 (5%)	0	100	100
15	O	124/151 (82%)	113 (91%)	11 (9%)	0	100	100
16	M	102/132 (77%)	97 (95%)	5 (5%)	0	100	100
17	P	129/145 (89%)	117 (91%)	12 (9%)	0	100	100
18	R	119/135 (88%)	110 (92%)	9 (8%)	0	100	100
19	Q	138/146 (94%)	124 (90%)	14 (10%)	0	100	100
20	S	139/152 (91%)	128 (92%)	11 (8%)	0	100	100
21	T	139/145 (96%)	135 (97%)	4 (3%)	0	100	100
22	V	81/83 (98%)	77 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
23	W	127/130 (98%)	114 (90%)	13 (10%)	0	100 100
24	X	137/143 (96%)	128 (93%)	8 (6%)	1 (1%)	22 59
25	Y	120/133 (90%)	113 (94%)	7 (6%)	0	100 100
26	U	96/119 (81%)	90 (94%)	6 (6%)	0	100 100
27	Z	68/125 (54%)	63 (93%)	5 (7%)	0	100 100
28	b	73/84 (87%)	67 (92%)	6 (8%)	0	100 100
29	c	59/69 (86%)	53 (90%)	6 (10%)	0	100 100
30	d	53/56 (95%)	44 (83%)	9 (17%)	0	100 100
31	e	46/59 (78%)	43 (94%)	3 (6%)	0	100 100
32	f	53/156 (34%)	46 (87%)	7 (13%)	0	100 100
33	g	287/317 (90%)	256 (89%)	31 (11%)	0	100 100
34	j	111/165 (67%)	98 (88%)	13 (12%)	0	100 100
35	z	365/568 (64%)	318 (87%)	47 (13%)	0	100 100
36	y	225/412 (55%)	187 (83%)	37 (16%)	1 (0%)	34 69
37	k	418/583 (72%)	359 (86%)	59 (14%)	0	100 100
All	All	5632/7089 (79%)	5152 (92%)	478 (8%)	2 (0%)	100 100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
36	y	40	LYS
24	X	86	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	A	180/243 (74%)	179 (99%)	1 (1%)	86 93
3	B	192/231 (83%)	191 (100%)	1 (0%)	88 94
4	C	182/225 (81%)	181 (100%)	1 (0%)	88 94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	220/225 (98%)	220 (100%)	0	100	100
6	D	188/202 (93%)	188 (100%)	0	100	100
7	G	194/218 (89%)	191 (98%)	3 (2%)	65	81
8	H	160/174 (92%)	159 (99%)	1 (1%)	86	93
9	I	174/180 (97%)	169 (97%)	5 (3%)	42	66
10	J	156/168 (93%)	155 (99%)	1 (1%)	86	93
11	F	156/170 (92%)	155 (99%)	1 (1%)	86	93
12	L	126/142 (89%)	125 (99%)	1 (1%)	81	89
13	K	86/136 (63%)	86 (100%)	0	100	100
14	N	130/131 (99%)	130 (100%)	0	100	100
15	O	99/119 (83%)	99 (100%)	0	100	100
16	M	91/108 (84%)	90 (99%)	1 (1%)	73	85
17	P	117/130 (90%)	117 (100%)	0	100	100
18	R	109/122 (89%)	108 (99%)	1 (1%)	78	88
19	Q	116/121 (96%)	115 (99%)	1 (1%)	78	88
20	S	122/132 (92%)	122 (100%)	0	100	100
21	T	111/115 (96%)	111 (100%)	0	100	100
22	V	67/67 (100%)	67 (100%)	0	100	100
23	W	112/113 (99%)	110 (98%)	2 (2%)	59	77
24	X	111/115 (96%)	110 (99%)	1 (1%)	78	88
25	Y	103/115 (90%)	103 (100%)	0	100	100
26	U	90/107 (84%)	89 (99%)	1 (1%)	73	85
27	Z	62/103 (60%)	62 (100%)	0	100	100
28	b	70/76 (92%)	70 (100%)	0	100	100
29	c	54/62 (87%)	54 (100%)	0	100	100
30	d	48/49 (98%)	45 (94%)	3 (6%)	18	49
31	e	40/48 (83%)	40 (100%)	0	100	100
32	f	51/140 (36%)	51 (100%)	0	100	100
33	g	255/275 (93%)	253 (99%)	2 (1%)	81	89
34	j	102/150 (68%)	101 (99%)	1 (1%)	76	86
35	z	336/512 (66%)	333 (99%)	3 (1%)	78	88

Continued on next page...

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
36	y	201/367 (55%)	199 (99%)	2 (1%)	76 86
All	All	4611/5591 (82%)	4578 (99%)	33 (1%)	84 91

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
35	z	151	ASP
35	z	163	ASP
36	y	323	ARG
10	J	79	ARG
9	I	161	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 73 such sidechains are listed below:

Mol	Chain	Res	Type
30	d	45	GLN
36	y	287	HIS
31	e	58	ASN
35	z	363	ASN
9	I	155	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1644/1874 (87%)	427 (25%)	19 (1%)

5 of 427 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	11	A
1	2	14	C
1	2	17	C
1	2	25	A

5 of 19 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	1679	A

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Mol	Chain	Res	Type
1	2	1850	A
1	2	1872	G
1	2	1814	G
1	2	1060	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 5 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
40	ATP	z	603	39	26,33,33	0.99	1 (3%)	31,52,52	1.60	5 (16%)

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
40	ATP	z	603	39	-	2/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	z	603	ATP	C5-C4	2.10	1.46	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	z	603	ATP	PA-O3A-PB	-5.16	115.12	132.83
40	z	603	ATP	C3'-C2'-C1'	3.19	105.78	100.98
40	z	603	ATP	PB-O3B-PG	-2.82	123.14	132.83
40	z	603	ATP	N3-C2-N1	-2.75	124.38	128.68
40	z	603	ATP	C4-C5-N7	-2.26	107.04	109.40

There are no chirality outliers.

All (2) torsion outliers are listed below:

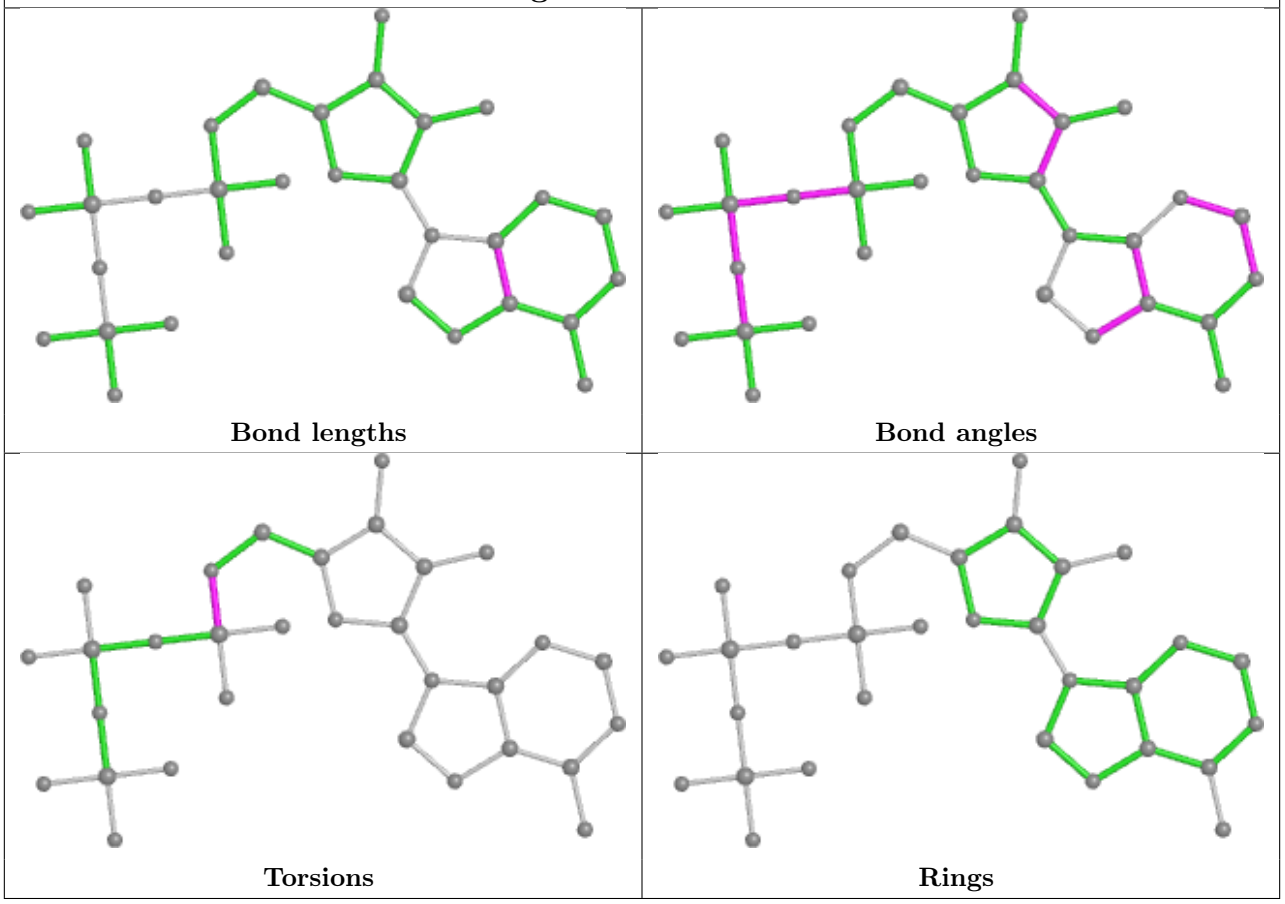
Mol	Chain	Res	Type	Atoms
40	z	603	ATP	C5'-O5'-PA-O3A
40	z	603	ATP	C5'-O5'-PA-O1A

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 then 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.

Ligand ATP z 603



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.

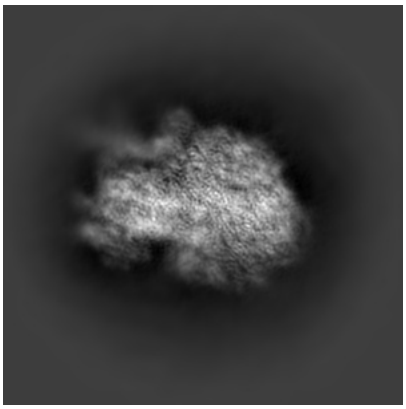
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11519. These allow visual inspection of the internal detail of the map and identification of artifacts.

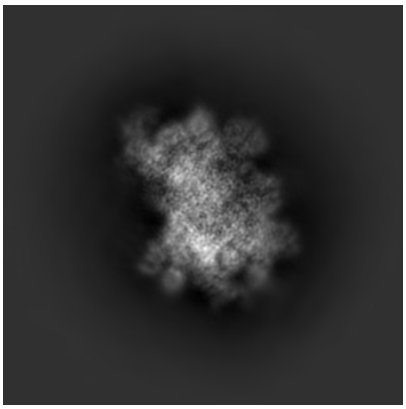
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

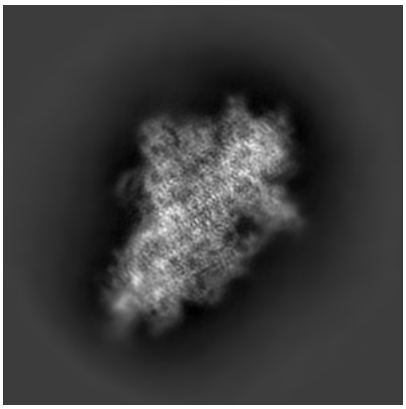
6.1.1 Primary map



X

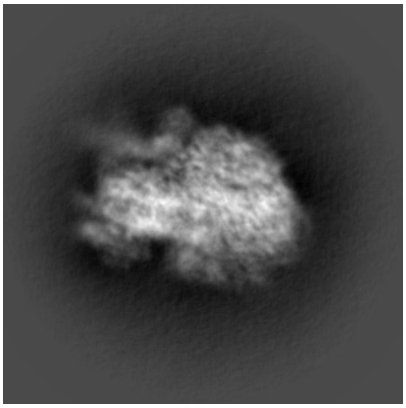


Y

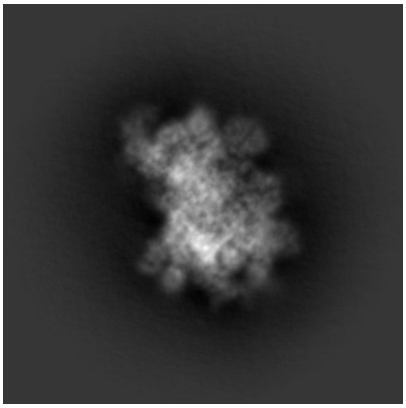


Z

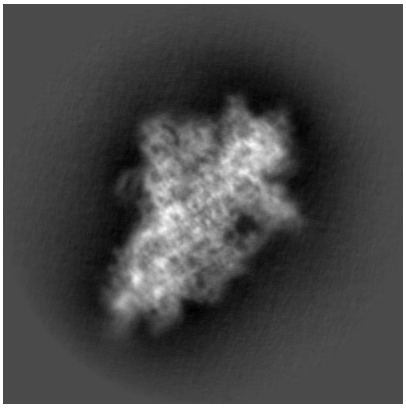
6.1.2 Raw map



X



Y

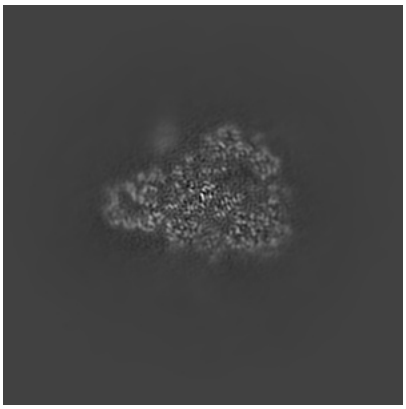


Z

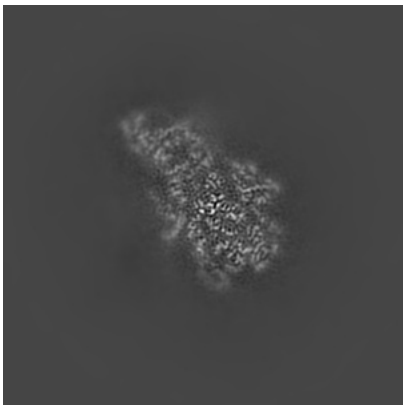
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

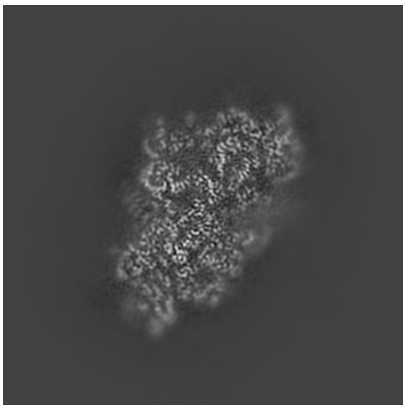
6.2.1 Primary map



X Index: 180

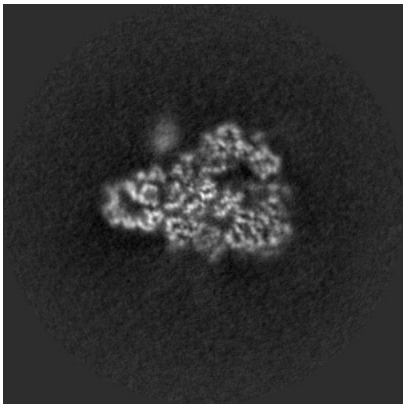


Y Index: 180

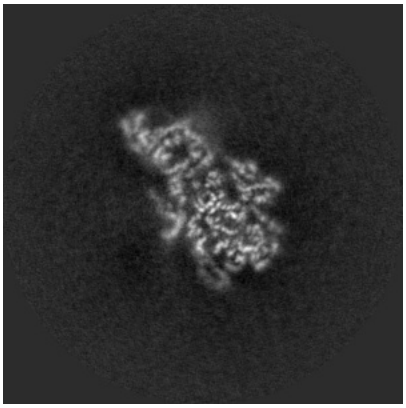


Z Index: 180

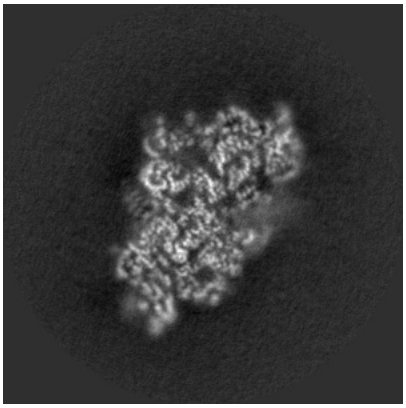
6.2.2 Raw map



X Index: 180



Y Index: 180

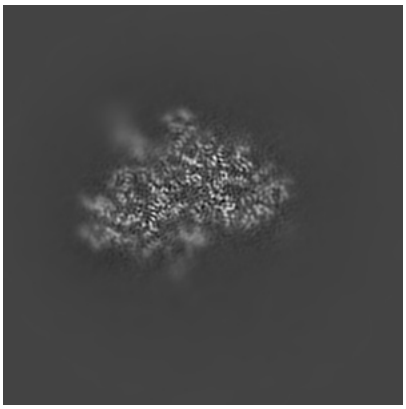


Z Index: 180

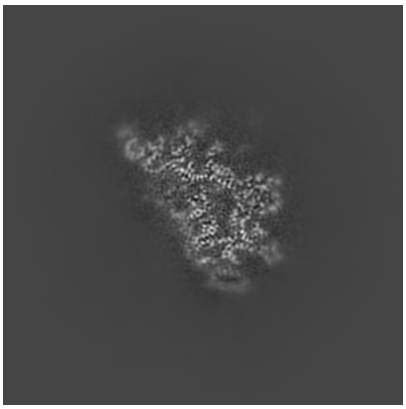
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

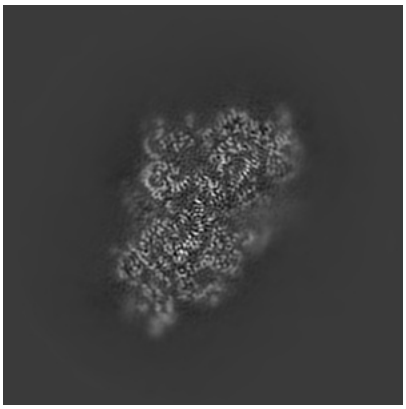
6.3.1 Primary map



X Index: 150

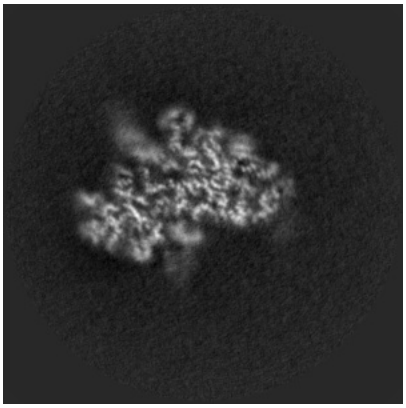


Y Index: 198

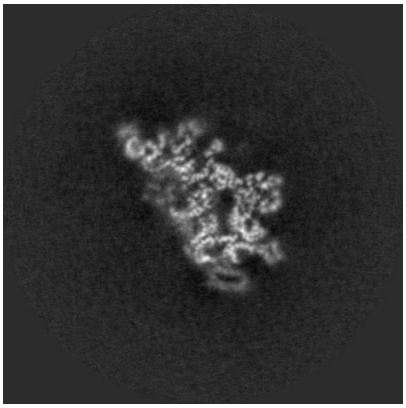


Z Index: 181

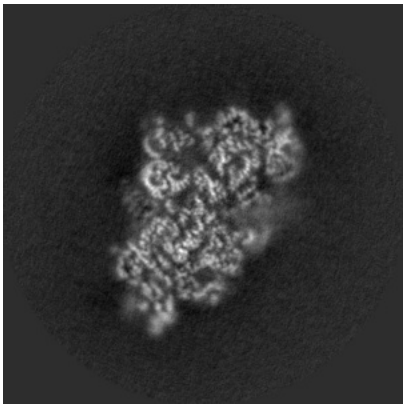
6.3.2 Raw map



X Index: 145



Y Index: 197

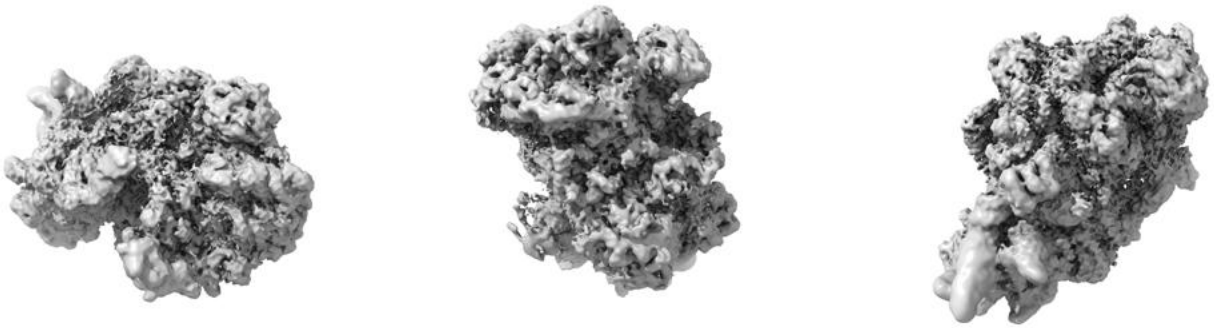


Z Index: 181

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

6.4 Orthogonal surface views (i)

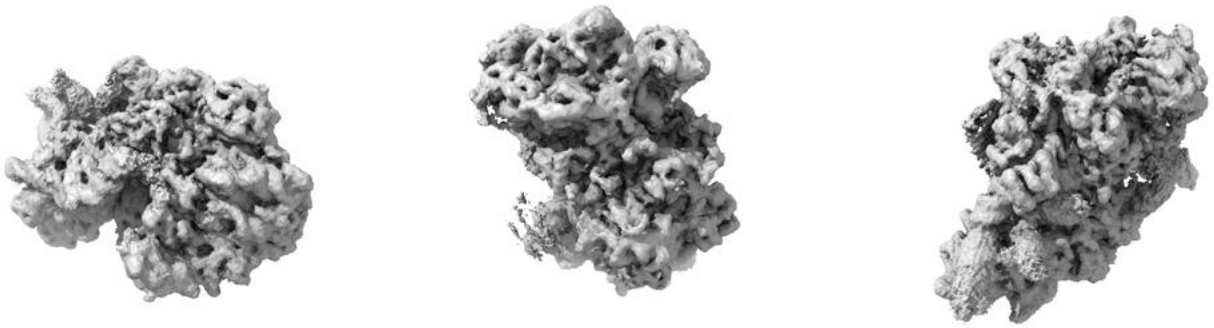
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

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

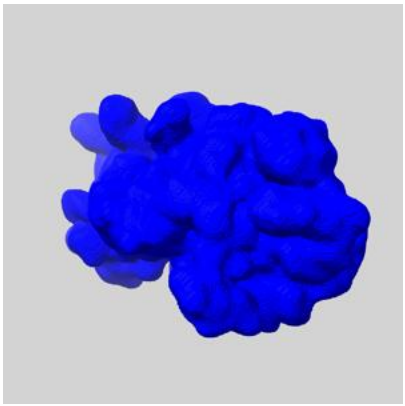
6.5 Mask visualisation

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

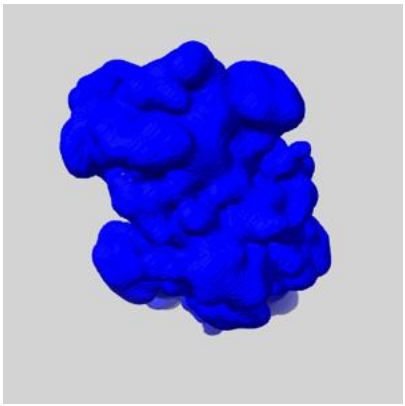
A mask typically either:

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

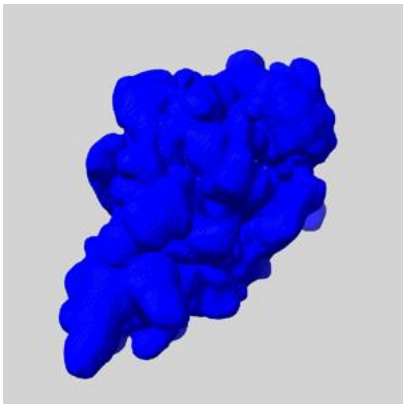
6.5.1 emd_11519_msk_1.map



X



Y

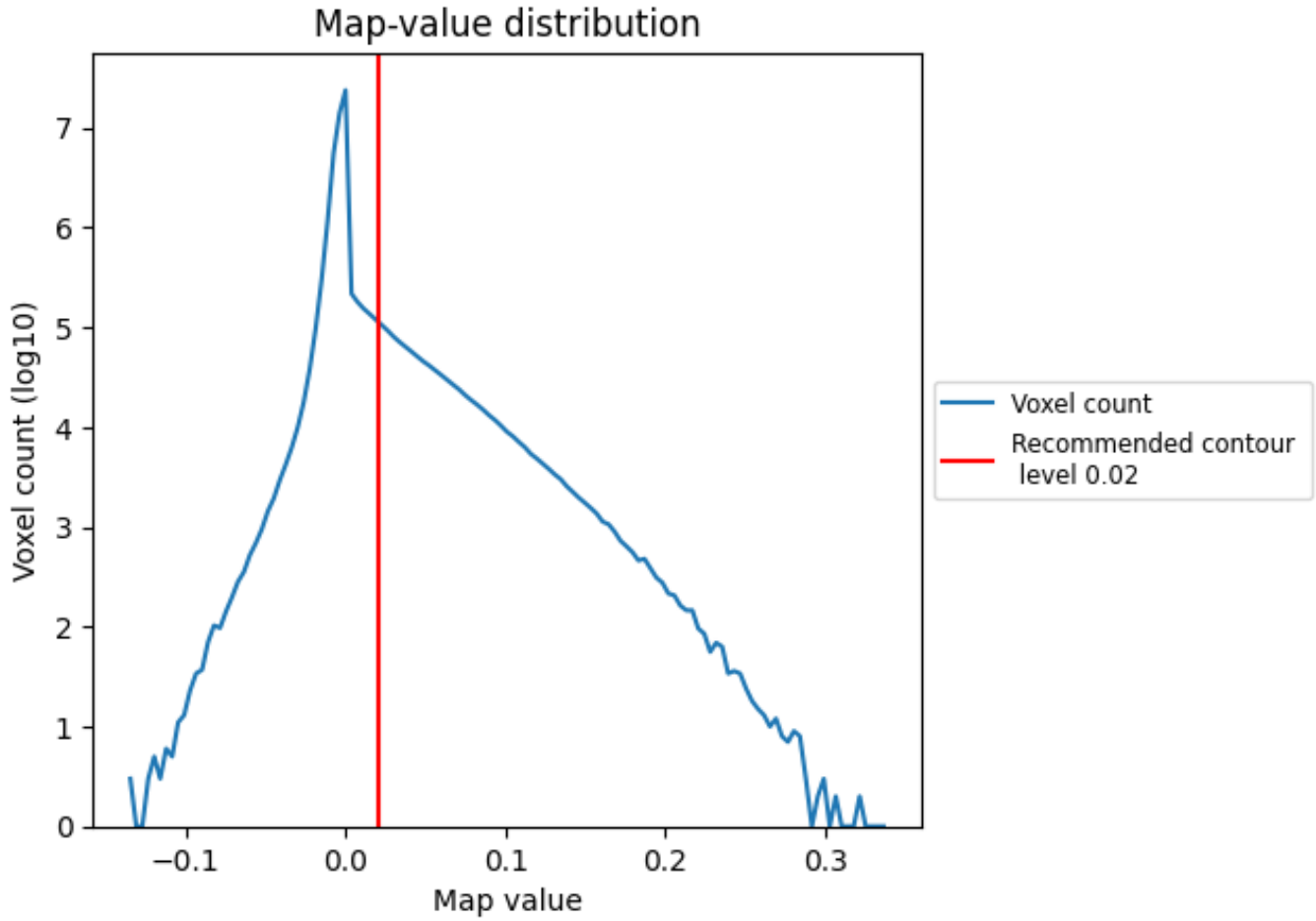


Z

7 Map analysis

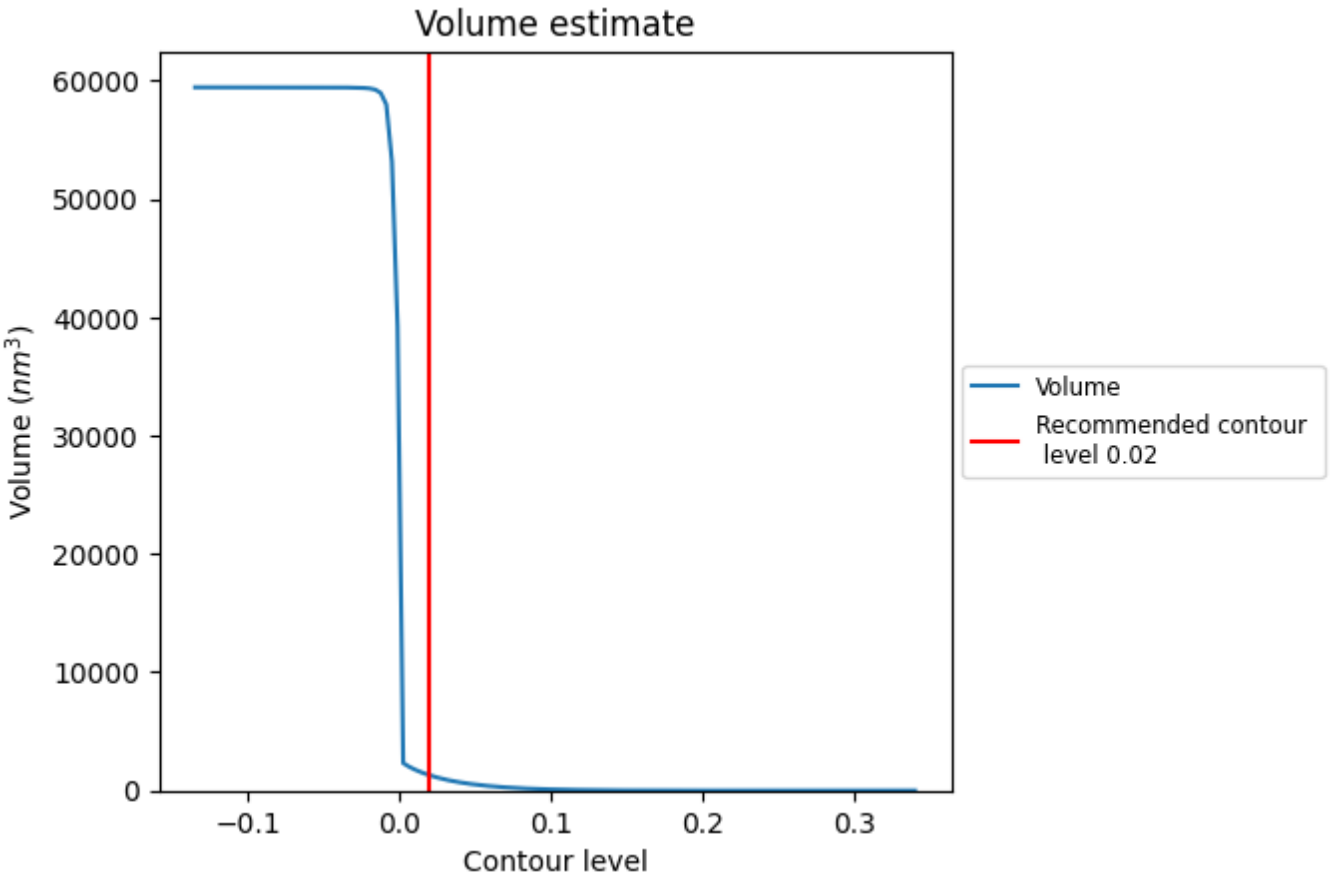
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

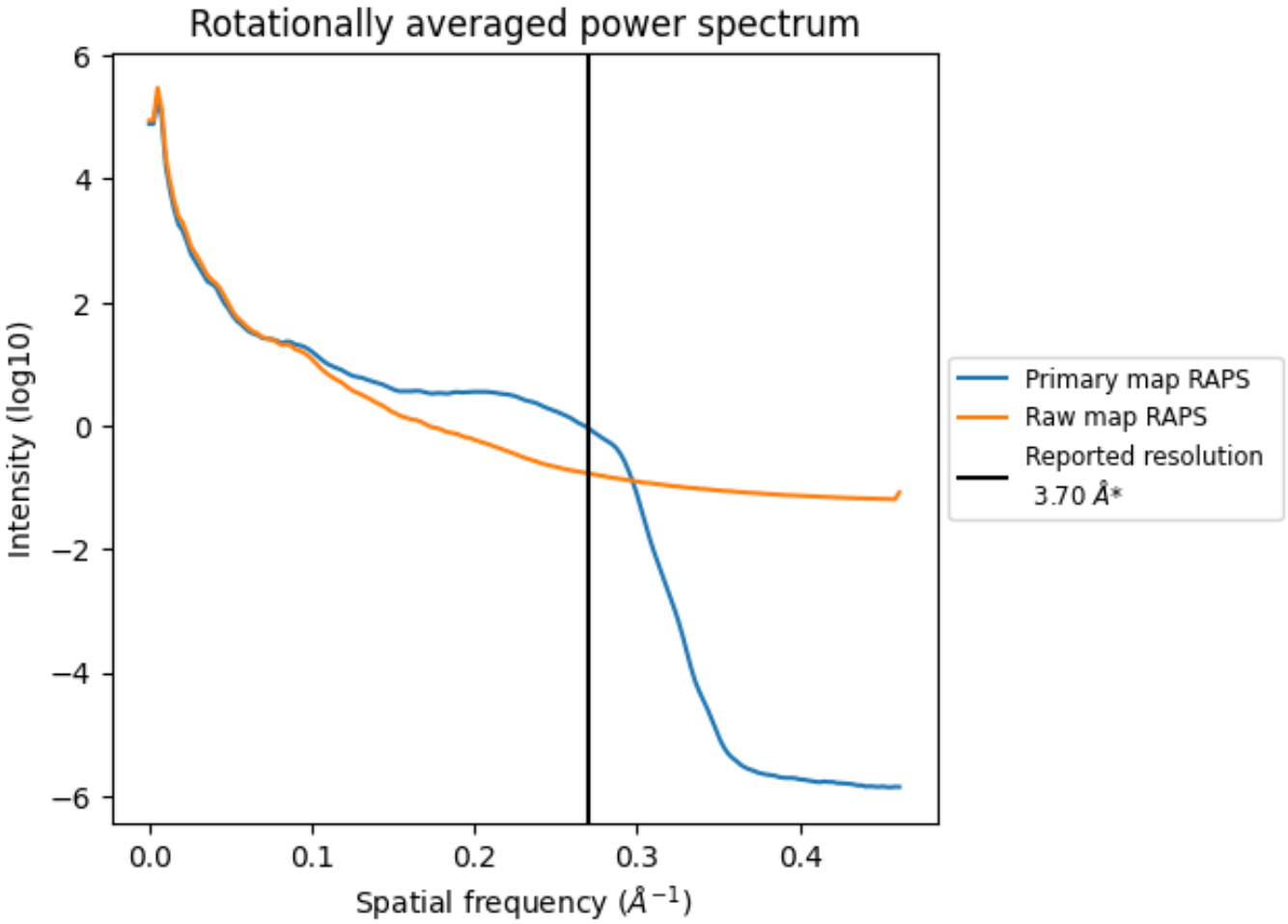
7.2 Volume estimate (i)



The volume at the recommended contour level is 1298 nm^3; this corresponds to an approximate mass of 1173 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)

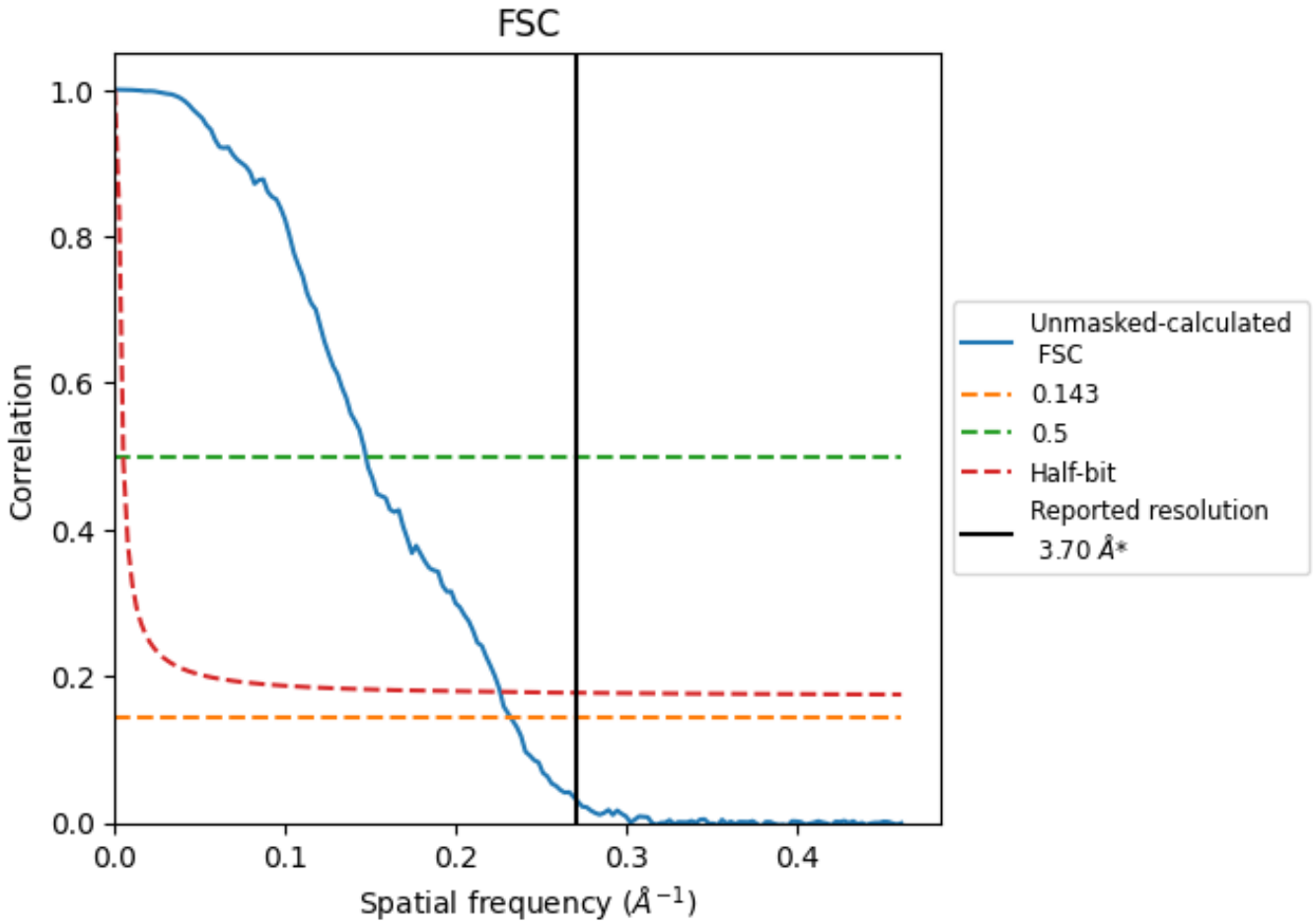


*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8.2 Resolution estimates (i)

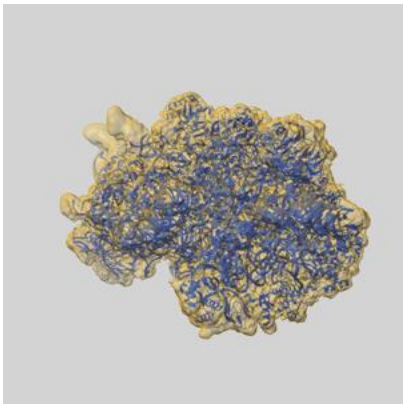
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.30	6.79	4.42

*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 4.30 differs from the reported value 3.7 by more than 10 %

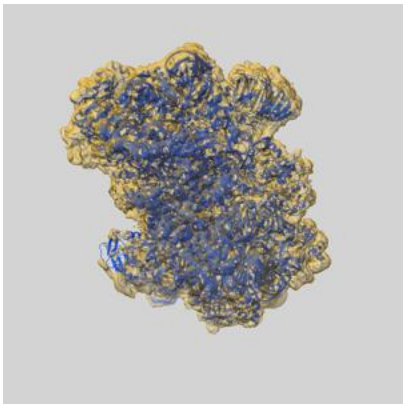
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11519 and PDB model 6ZXF. Per-residue inclusion information can be found in section 3 on page 12.

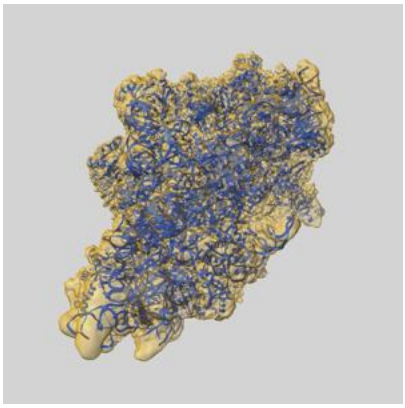
9.1 Map-model overlay



X



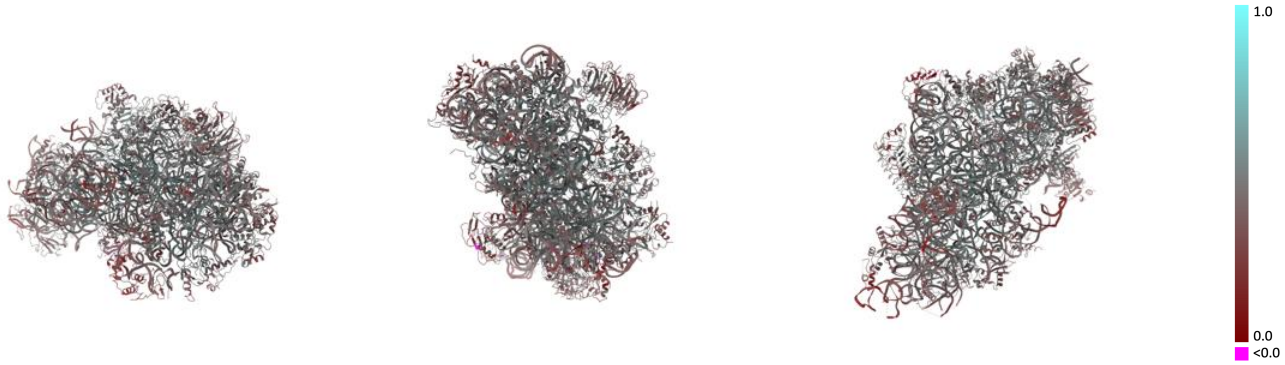
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

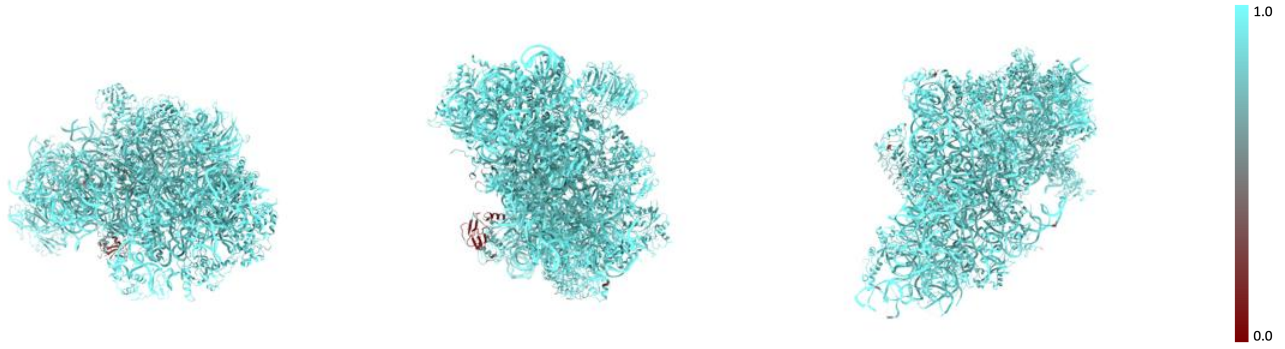
9.2 Q-score mapped to coordinate model



X Y Z

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.

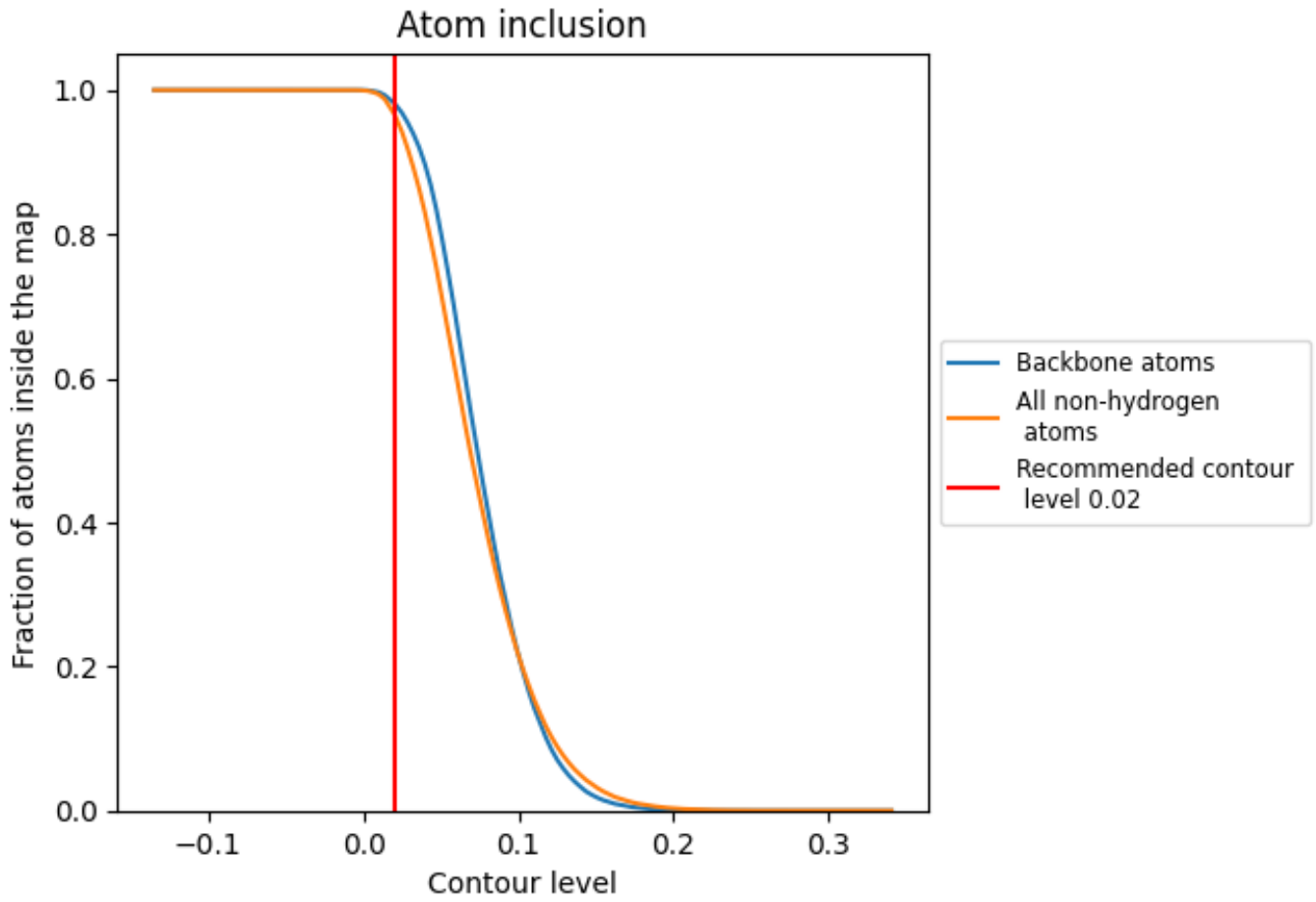
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 97% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9665	0.4370
2	0.9944	0.4450
A	0.9657	0.4650
B	0.9341	0.3750
C	0.9507	0.4750
D	0.9606	0.4460
E	0.9576	0.4510
F	0.9606	0.4670
G	0.9633	0.3710
H	0.9584	0.3880
I	0.9639	0.4110
J	0.9516	0.4090
K	0.9731	0.4240
L	0.9597	0.4910
M	0.9576	0.2680
N	0.9614	0.4650
O	0.9564	0.4470
P	0.9721	0.4350
Q	0.9593	0.4700
R	0.9560	0.4430
S	0.9545	0.4160
T	0.9662	0.4600
U	0.9629	0.4410
V	0.9614	0.4700
W	0.9663	0.5000
X	0.9782	0.4980
Y	0.9781	0.4030
Z	0.9449	0.3820
b	0.9750	0.4740
c	0.9328	0.4620
d	0.9819	0.5090
e	0.9791	0.4410
f	0.9867	0.3310
g	0.9686	0.3990
j	0.8452	0.4290

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Chain	Atom inclusion	Q-score
k	0.7000	0.3540
y	0.9582	0.4540
z	0.9314	0.4480