



wwPDB EM Validation Summary Report ⓘ

Jun 20, 2026 – 10:06 pm BST

PDB ID : 8R6F / pdb_00008r6f
EMDB ID : EMD-18951
Title : CryoEM structure of wheat 40S ribosomal subunit, body domain
Authors : Kravchenko, O.V.; Baymukhametov, T.N.; Afonina, Z.A.; Vasilenko, K.S.
Deposited on : 2023-11-22
Resolution : 2.34 Å(reported)
Based on initial model : 7qix

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:

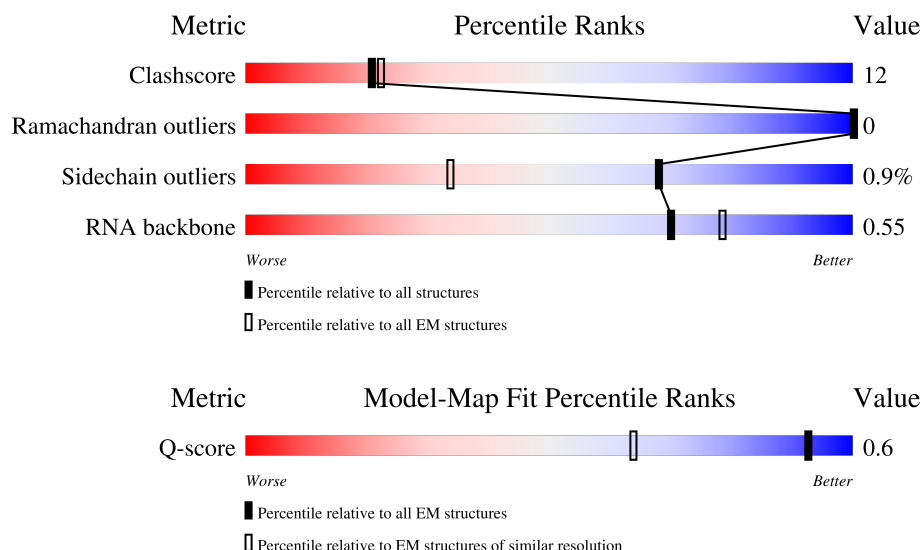
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.34 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.



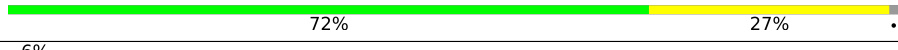
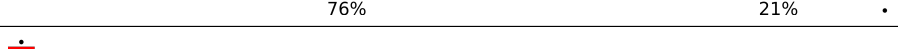
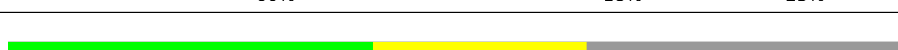
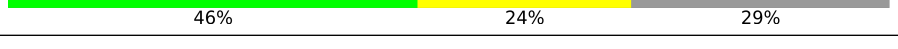
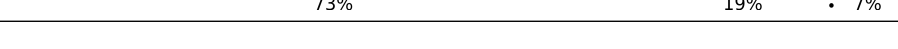
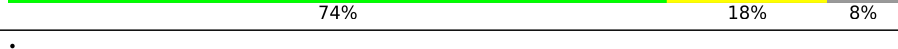
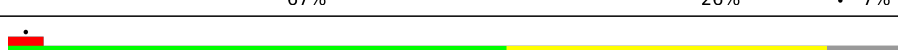
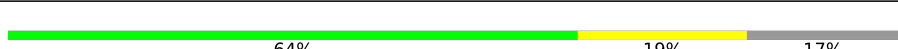
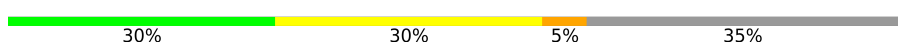
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	4520 (1.84 - 2.84)

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	Y	137	
2	X	142	
3	E	265	

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Mol	Chain	Length	Quality of chain
4	O	151	
5	W	130	
6	b	86	
7	e	62	
8	k	308	
9	B	263	
10	V	81	
11	a	139	
12	J	195	
13	C	275	
14	G	250	
15	H	192	
16	h	143	
17	L	159	
18	N	151	
19	n	25	
20	I	224	
21	A	1810	

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 49016 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 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Y	124	Total	C	N	O	S	0	0
			1014	648	196	168	2		

- Molecule 2 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	X	140	Total	C	N	O	S	0	0
			1088	690	212	183	3		

- Molecule 3 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	260	Total	C	N	O	S	0	0
			2077	1322	387	361	7		

- Molecule 4 is a protein called 30S ribosomal protein S11, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	O	130	Total	C	N	O	S	0	0
			984	603	195	182	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	138	IAS	ASP	conflict	UNP A0A3B6SS17

- Molecule 5 is a protein called Small ribosomal subunit protein uS8c.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	W	129	Total	C	N	O	S	0	0
			1032	659	188	180	5		

- Molecule 6 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	b	83	Total	C	N	O	S	0	0
			645	405	117	116	7		

- Molecule 7 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	e	48	Total	C	N	O	S	0	0
			383	232	87	64			

- Molecule 8 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	k	199	Total	C	N	O	S	0	0
			1586	1004	285	286	11		

- Molecule 9 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	210	Total	C	N	O	S	0	0
			1716	1094	310	303	9		

- Molecule 10 is a protein called Genome assembly, chromosome: II.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	V	81	Total	C	N	O	S	0	0
			630	389	116	122	3		

- Molecule 11 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	a	98	Total	C	N	O	S	0	0
			794	487	172	128	7		

- Molecule 12 is a protein called 30S ribosomal protein S4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	181	Total	C	N	O	S	0	0
			1494	947	298	245	4		

- Molecule 13 is a protein called S5 DRBM domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	C	214	Total	C	N	O	S	0	0
			1660	1070	294	287	9		

- Molecule 14 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	230	Total	C	N	O	S	0	0
			1856	1157	366	325	8		

- Molecule 15 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	184	Total	C	N	O	S	0	0
			1508	962	278	266	2		

- Molecule 16 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	h	27	Total	C	N	O	S	0	0
			208	129	34	42	3		

- Molecule 17 is a protein called Small ribosomal subunit protein uS17 N-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	146	Total	C	N	O	S	0	0
			1167	745	224	193	5		

- Molecule 18 is a protein called Small ribosomal subunit protein uS15 N-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	141	Total	C	N	O	S	0	0
			1138	731	215	190	2		

- Molecule 19 is a protein called Large ribosomal subunit protein eL41z/eL41y/eL41x/eL41w/eL41v.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	n	23	Total	C	N	O	S	0	0
			222	136	59	24	3		

- Molecule 20 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	I	186	Total	C	N	O	S	0	0
			1510	936	302	268	4		

- Molecule 21 is a RNA chain called RNA (1177-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
21	A	1177	Total	C	N	O	P	0	0
			25190	11273	4545	8196	1176		

- Molecule 22 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
22	a	1	Total	Zn	0
			1	1	

- Molecule 23 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
23	G	1	Total	Mg	0
			1	1	
23	A	31	Total	Mg	0
			31	31	

- Molecule 24 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
24	A	14	Total	K	0
			14	14	

- Molecule 25 is water.

Mol	Chain	Residues	Atoms		AltConf
25	Y	6	Total	O	0
			6	6	
25	X	14	Total	O	0
			14	14	
25	E	24	Total	O	0
			24	24	
25	O	3	Total	O	0
			3	3	

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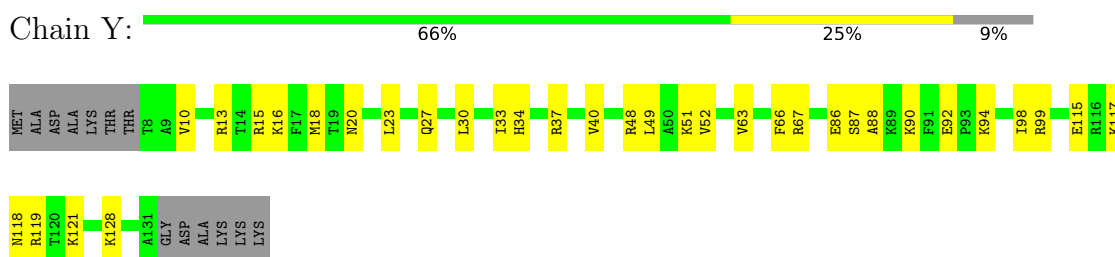
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Mol	Chain	Residues	Atoms		AltConf
25	W	6	Total 6	O 6	0
25	e	3	Total 3	O 3	0
25	B	2	Total 2	O 2	0
25	a	8	Total 8	O 8	0
25	J	14	Total 14	O 14	0
25	C	10	Total 10	O 10	0
25	G	7	Total 7	O 7	0
25	L	24	Total 24	O 24	0
25	N	3	Total 3	O 3	0
25	I	18	Total 18	O 18	0
25	A	925	Total 925	O 925	0

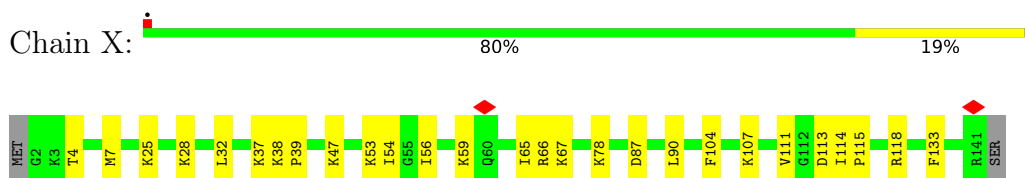
3 Residue-property plots

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

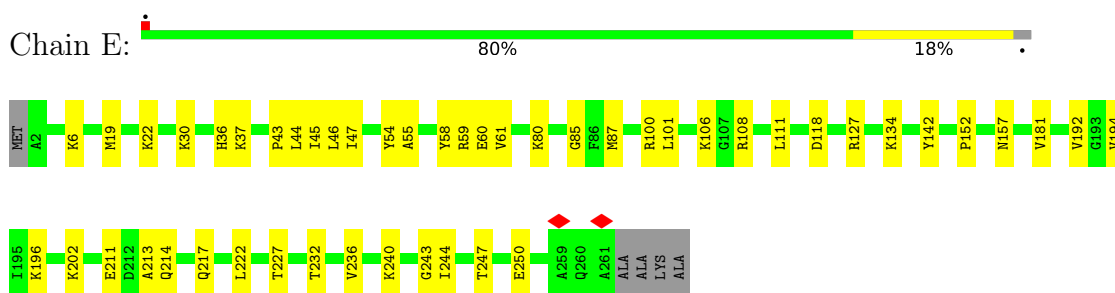
- Molecule 1: 40S ribosomal protein S24



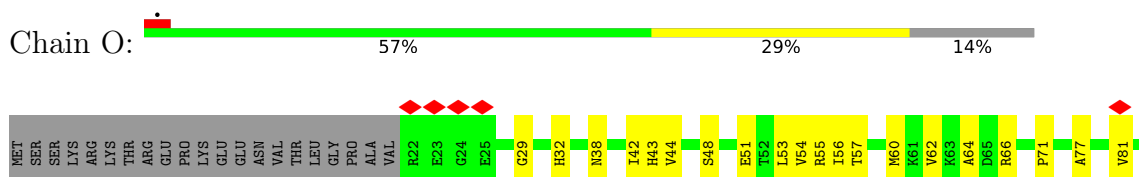
- Molecule 2: 40S ribosomal protein S23



- Molecule 3: 40S ribosomal protein S4



- Molecule 4: 30S ribosomal protein S11, chloroplastic





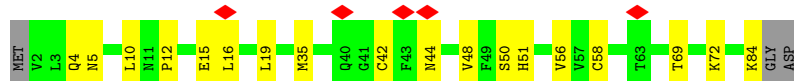
- Molecule 5: Small ribosomal subunit protein uS8c

Chain W: 72% 27%



- Molecule 6: 40S ribosomal protein S27

Chain b: 6% 76% 21%



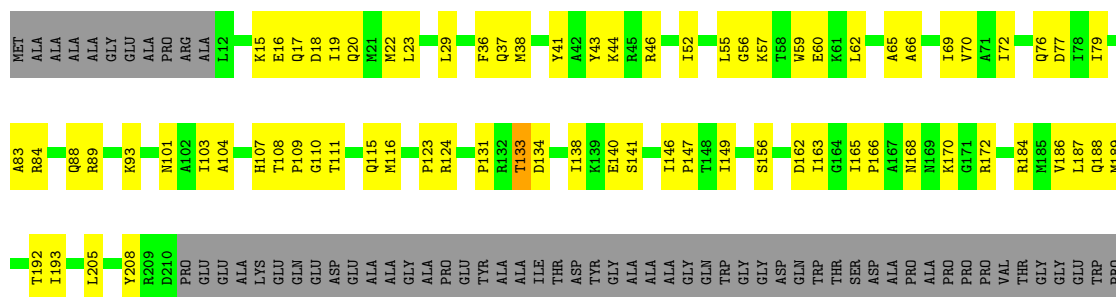
- Molecule 7: 40S ribosomal protein S30

Chain e: 60% 18% 23%



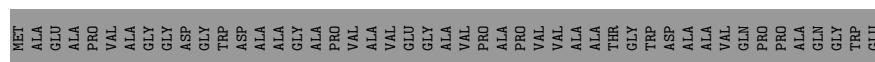
- Molecule 8: Small ribosomal subunit protein uS2

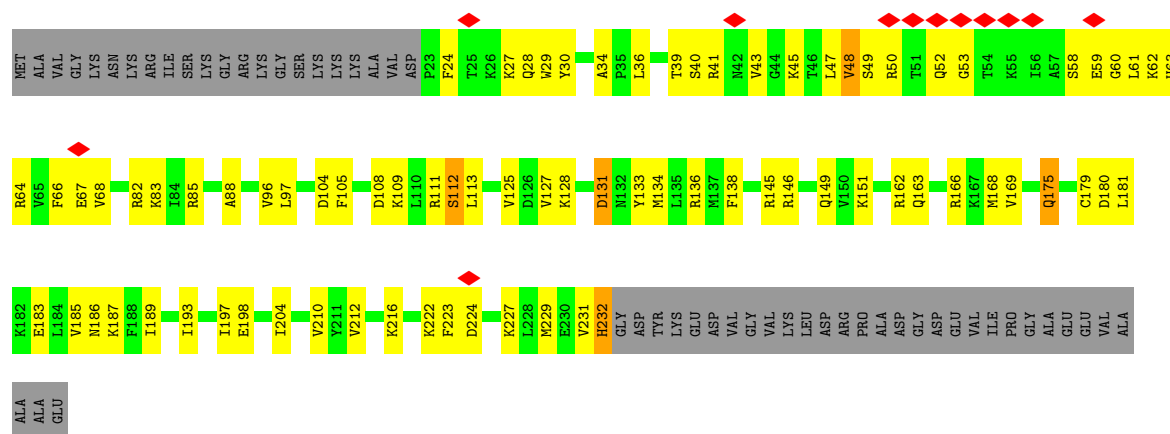
Chain k: 41% 24% 35%



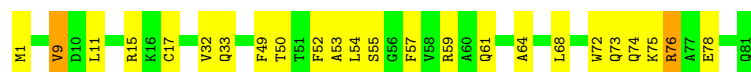
- Molecule 9: Small ribosomal subunit protein eS1

Chain B: 5% 49% 29% 20%

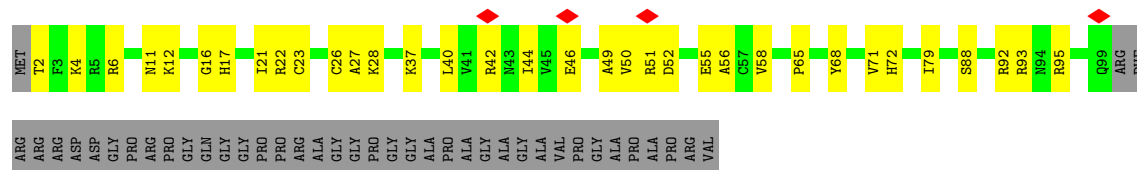




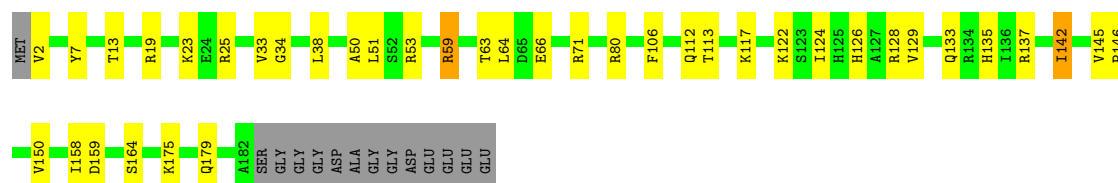
- Molecule 10: Genome assembly, chromosome: II



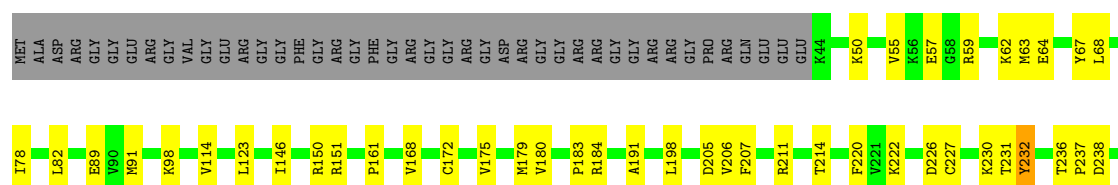
- Molecule 11: 40S ribosomal protein S26

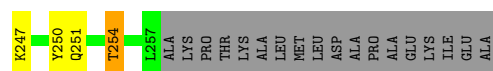


- Molecule 12: 30S ribosomal protein S4, chloroplastic



- Molecule 13: S5 DRBM domain-containing protein

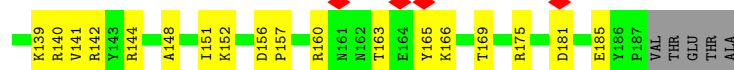
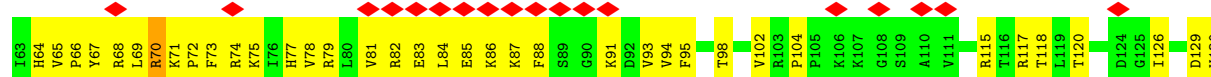
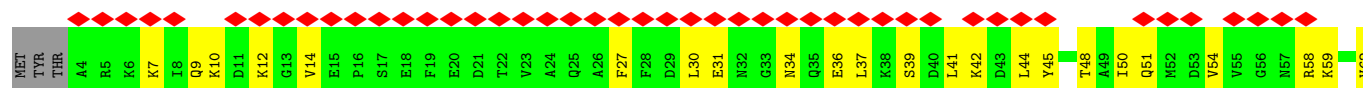




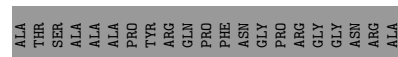
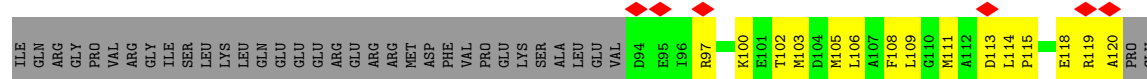
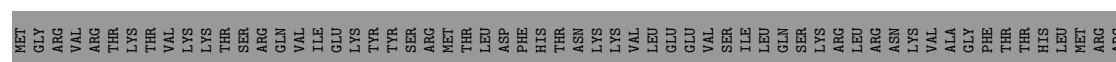
- Molecule 14: 40S ribosomal protein S6



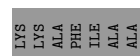
- Molecule 15: 40S ribosomal protein S7

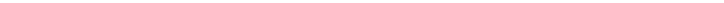


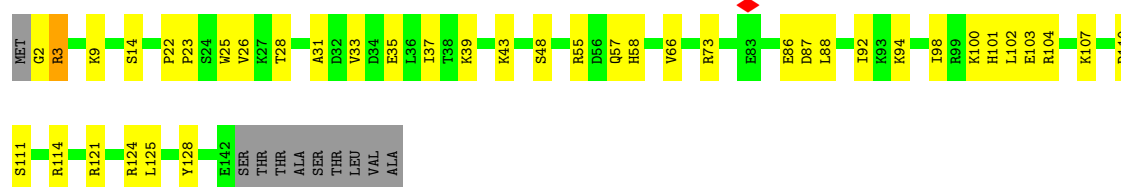
- Molecule 16: 40S ribosomal protein S17

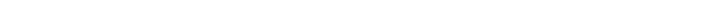


- Molecule 17: Small ribosomal subunit protein uS17 N-terminal domain-containing protein



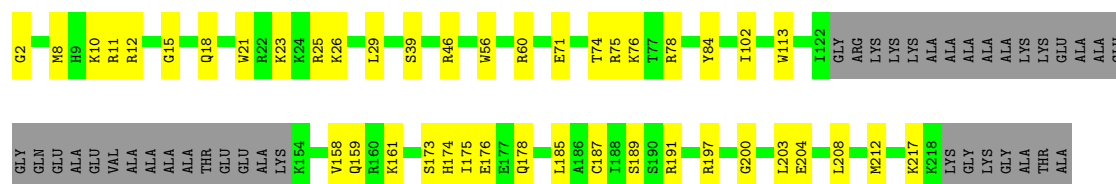
- Chain N:  67% 26% 7%



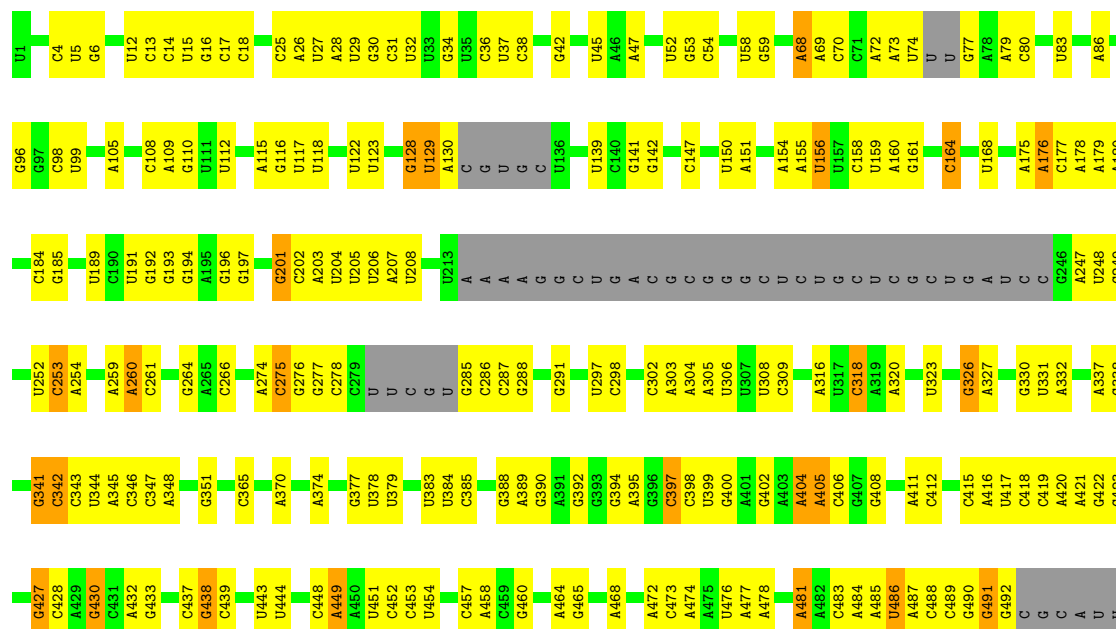
- Chain n: 



- Chain I: 64% 19% 17%



- Chain A:





G1800	A1732	U1665	U1665
G1803	A1733	U1666	U1666
G1804	G1734	G1667	U1667
A1805	U1735	A1668	A1668
U1806	C1736	A1669	A1669
C1807	C1737	U1670	U1670
A1808	A1738	G1671	G1671
U1809	U1739	G1672	G1672
U1810	U1740	U1673	U1673
G1811	G1741	C1674	C1674
	A1742	C1675	C1675
	A1743	G1676	G1676
	C1744	G1677	G1677
	G1745	U1678	U1678
	U1746	G1679	G1679
	U1747	A1680	A1680
	A1748	A1681	A1681
	U1749	C1682	C1682
	C1750	U1683	U1683
	A1751	A1684	A1684
	U1752		
	U1753	G1689	G1689
	U1754	A1690	A1690
	A1755		
	G1756	G1695	G1695
		G1696	G1696
	A1761	C1697	C1697
	G1762	G1698	G1698
	G1763	A1699	A1699
	A1764	C1700	C1700
	G1765	G1701	G1701
	A1766	G1702	G1702
	A1767	G	G
	G1768	G	G
	U1769	C	C
	C1770	G	G
	G1771	G	G
	U1772	U	U
	A1773	U	U
	A1774	C	C
	G1775	C	C
	A1776	C	C
	A1777	C	C
		G	G
	U1780	C	C
	U1781	C	C
	U1782	C	C
		C	C
	A1787	G1719	G1719
	G1788		
		A1722	A1722
	G1791	C1723	C1723
	A1792	G1724	G1724
	A1793	U1725	U1725
	C1794	C1726	C1726
	C1795	G1727	G1727
	U1796	C1728	C1728
	G1797	G1729	G1729
	C1798	A1730	A1730
	G1799	G1731	G1731

U	C1634	C1643
C	U1635	A1644
A	U1636	A1645
PSU	U1637	C1646
C	G1638	C1647
A	U1639	G1648
A	A1640	C1649
G		C1650
C		G1651
PSU		U1652
C		C1653
G		G1654
C		C1655
G		U1656
U		C1657
PSU		C1658
G		U1659
A		A1660
C		C1661
A		C1662
U		G1663
C		A1664

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	256000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	84	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	9.900	Depositor
Minimum map value	-6.521	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.134	Depositor
Recommended contour level	0.4	Depositor
Map size ($\text{\AA}$)	412.80002, 412.80002, 412.80002	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.86, 0.86, 0.86	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PSU, MG, 4AC, ZN, IAS, OMC, AME, MA6, OMG, K, OMU, A2M, UY1, 6MZ

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	Y	0.30	0/1029	0.47	0/1366
2	X	0.32	0/1107	0.49	0/1474
3	E	0.22	0/2118	0.41	0/2846
4	O	0.37	0/988	0.58	1/1322 (0.1%)
5	W	0.47	0/1050	0.64	0/1405
6	b	0.20	0/656	0.41	0/883
7	e	0.33	0/387	0.56	0/510
8	k	0.34	0/1620	0.55	2/2193 (0.1%)
9	B	0.35	0/1745	0.59	0/2344
10	V	0.49	0/628	0.77	2/847 (0.2%)
11	a	0.38	0/809	0.55	0/1083
12	J	0.25	0/1522	0.46	1/2037 (0.0%)
13	C	0.34	0/1696	0.56	1/2292 (0.0%)
14	G	0.18	0/1876	0.41	0/2492
15	H	0.38	0/1535	0.64	1/2065 (0.0%)
16	h	0.59	0/209	0.91	0/279
17	L	0.28	0/1193	0.42	0/1599
18	N	0.21	0/1162	0.39	0/1560
19	n	0.57	0/223	0.93	0/283
20	I	0.23	0/1532	0.49	0/2046
21	A	0.20	2/26873 (0.0%)	0.30	1/41868 (0.0%)
All	All	0.26	2/49958 (0.0%)	0.41	9/72794 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	468	A2M	O3'-P	5.19	1.61	1.56
21	A	802	A2M	O3'-P	5.12	1.61	1.56

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	232	TYR	N-CA-C	-5.87	105.69	112.92
10	V	76	ARG	N-CA-C	-5.80	104.87	111.14
21	A	614	G	C4'-C3'-O3'	-5.60	104.60	113.00
8	k	133	THR	N-CA-C	-5.29	106.99	113.50
15	H	70	ARG	CA-C-O	-5.28	115.25	120.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Y	1014	0	1099	31	0
2	X	1088	0	1153	24	0
3	E	2077	0	2166	37	0
4	O	984	0	1011	43	0
5	W	1032	0	1068	27	0
6	b	645	0	664	15	0
7	e	383	0	406	9	0
8	k	1586	0	1590	61	0
9	B	1716	0	1790	71	0
10	V	630	0	614	18	0
11	a	794	0	812	33	0
12	J	1494	0	1563	32	0
13	C	1660	0	1743	37	0
14	G	1856	0	1995	46	0
15	H	1508	0	1573	74	0
16	h	208	0	205	15	0
17	L	1167	0	1228	22	0
18	N	1138	0	1228	32	0
19	n	222	0	271	8	0
20	I	1510	0	1555	32	0
21	A	25190	0	12722	490	0
22	a	1	0	0	1	0
23	A	31	0	0	0	0
23	G	1	0	0	0	0
24	A	14	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	A	925	0	0	22	0
25	B	2	0	0	0	0
25	C	10	0	0	0	0
25	E	24	0	0	0	0
25	G	7	0	0	0	0
25	I	18	0	0	1	0
25	J	14	0	0	0	0
25	L	24	0	0	2	0
25	N	3	0	0	0	0
25	O	3	0	0	0	0
25	W	6	0	0	0	0
25	X	14	0	0	0	0
25	Y	6	0	0	1	0
25	a	8	0	0	0	0
25	e	3	0	0	0	0
All	All	49016	0	36456	999	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 999 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:1672:G:H1	21:A:1749:U:H3	1.13	0.94
8:k:172:ARG:HD3	8:k:208:TYR:HD2	1.34	0.91
19:n:10:MET:HE1	21:A:1118:A:H5'	1.51	0.90
16:h:105:MET:HE3	16:h:109:LEU:HD12	1.56	0.87
20:I:2:GLY:N	21:A:1740:U:HO2'	1.72	0.87

There are no symmetry-related clashes.

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	
1	Y	122/137 (89%)	121 (99%)	1 (1%)	0	100	100
2	X	138/142 (97%)	132 (96%)	6 (4%)	0	100	100
3	E	258/265 (97%)	253 (98%)	5 (2%)	0	100	100
4	O	126/151 (83%)	123 (98%)	3 (2%)	0	100	100
5	W	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
6	b	81/86 (94%)	72 (89%)	9 (11%)	0	100	100
7	e	44/62 (71%)	42 (96%)	2 (4%)	0	100	100
8	k	197/308 (64%)	192 (98%)	5 (2%)	0	100	100
9	B	208/263 (79%)	203 (98%)	5 (2%)	0	100	100
10	V	79/81 (98%)	77 (98%)	2 (2%)	0	100	100
11	a	96/139 (69%)	94 (98%)	2 (2%)	0	100	100
12	J	179/195 (92%)	177 (99%)	2 (1%)	0	100	100
13	C	212/275 (77%)	206 (97%)	6 (3%)	0	100	100
14	G	228/250 (91%)	225 (99%)	3 (1%)	0	100	100
15	H	182/192 (95%)	170 (93%)	12 (7%)	0	100	100
16	h	25/143 (18%)	23 (92%)	2 (8%)	0	100	100
17	L	144/159 (91%)	143 (99%)	1 (1%)	0	100	100
18	N	139/151 (92%)	136 (98%)	3 (2%)	0	100	100
19	n	21/25 (84%)	21 (100%)	0	0	100	100
20	I	182/224 (81%)	176 (97%)	6 (3%)	0	100	100
All	All	2788/3378 (82%)	2712 (97%)	76 (3%)	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	Y	108/117 (92%)	108 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	X	111/113 (98%)	109 (98%)	2 (2%)	51	64
3	E	222/224 (99%)	222 (100%)	0	100	100
4	O	101/120 (84%)	100 (99%)	1 (1%)	68	79
5	W	111/112 (99%)	111 (100%)	0	100	100
6	b	76/78 (97%)	75 (99%)	1 (1%)	61	73
7	e	39/49 (80%)	39 (100%)	0	100	100
8	k	170/233 (73%)	169 (99%)	1 (1%)	78	86
9	B	189/228 (83%)	184 (97%)	5 (3%)	40	53
10	V	65/65 (100%)	64 (98%)	1 (2%)	57	69
11	a	85/108 (79%)	84 (99%)	1 (1%)	63	75
12	J	154/162 (95%)	152 (99%)	2 (1%)	61	73
13	C	181/219 (83%)	179 (99%)	2 (1%)	65	77
14	G	202/215 (94%)	201 (100%)	1 (0%)	81	88
15	H	164/171 (96%)	163 (99%)	1 (1%)	78	86
16	h	22/124 (18%)	21 (96%)	1 (4%)	24	32
17	L	125/132 (95%)	125 (100%)	0	100	100
18	N	123/131 (94%)	121 (98%)	2 (2%)	55	67
19	n	22/24 (92%)	22 (100%)	0	100	100
20	I	160/179 (89%)	158 (99%)	2 (1%)	61	73
All	All	2430/2804 (87%)	2407 (99%)	23 (1%)	68	80

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	C	232	TYR
15	H	126	ILE
14	G	200	LYS
16	h	108	PHE
9	B	112	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
13	C	97	GLN

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Mol	Chain	Res	Type
13	C	120	HIS
20	I	194	GLN
20	I	85	ASN
20	I	174	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	A	1164/1810 (64%)	207 (17%)	0

5 of 207 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	A	14	C
21	A	25	C
21	A	26	A
21	A	34	G
21	A	42	G

There are no RNA pucker outliers to report.

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

57 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	$\# Z > 2$
21	A2M	A	623	21,23	22,25,26	0.31	0	31,36,39	0.57	0
21	PSU	A	811	21	18,21,22	0.51	0	22,30,33	0.59	0
21	PSU	A	607	21	18,21,22	0.53	0	22,30,33	0.56	0
21	6MZ	A	1774	21,24,23	22,25,26	0.38	0	30,36,39	0.81	1 (3%)
21	A2M	A	440	21	22,25,26	0.17	0	31,36,39	0.37	0
21	OMU	A	168	21	19,22,23	0.41	0	26,31,34	0.88	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	OMU	A	1014	21	19,22,23	0.34	0	26,31,34	0.50	0
21	PSU	A	258	21	18,21,22	0.50	0	22,30,33	0.59	0
21	PSU	A	300	21	18,21,22	0.50	0	22,30,33	0.56	0
21	PSU	A	111	21,24	18,21,22	0.52	0	22,30,33	0.59	0
21	PSU	A	1637	21	18,21,22	0.52	0	22,30,33	0.57	0
21	A2M	A	545	21	22,25,26	0.20	0	31,36,39	0.56	0
21	OMU	A	123	21	19,22,23	0.36	0	26,31,34	0.46	0
21	PSU	A	208	21	18,21,22	0.50	0	22,30,33	0.59	0
21	OMC	A	38	21	19,22,23	0.33	0	26,31,34	0.51	0
21	A2M	A	468	21	22,25,26	0.24	0	31,36,39	0.65	0
21	OMG	A	599	21	23,26,27	0.36	0	33,38,41	0.42	0
21	OMC	A	418	21	19,22,23	0.30	0	26,31,34	0.47	0
21	A2M	A	1761	21	22,25,26	0.16	0	31,36,39	0.39	0
21	OMU	A	615	21	19,22,23	1.70	4 (21%)	26,31,34	1.83	6 (23%)
21	4AC	A	1784	21	21,24,25	0.43	0	29,34,37	0.60	0
21	A2M	A	28	21	22,25,26	0.24	0	31,36,39	0.38	0
21	MA6	A	1792	21	23,26,27	0.36	0	34,38,41	0.71	2 (5%)
21	PSU	A	1108	21	18,21,22	0.53	0	22,30,33	0.57	0
21	PSU	A	1310	21	18,21,22	0.53	0	22,30,33	0.40	0
21	UY1	A	604	21	19,22,23	0.50	0	22,31,34	0.61	0
21	PSU	A	121	21	18,21,22	0.50	0	22,30,33	0.76	0
21	PSU	A	1306	21	18,21,22	0.57	0	22,30,33	0.55	0
21	PSU	A	362	21	18,21,22	0.50	0	22,30,33	0.63	0
10	AME	V	1	10	9,10,11	1.37	1 (11%)	9,11,13	1.62	2 (22%)
21	PSU	A	1084	21	18,21,22	0.48	0	22,30,33	0.63	0
21	PSU	A	806	21	18,21,22	0.48	0	22,30,33	0.61	0
21	PSU	A	1004	21	18,21,22	0.49	0	22,30,33	0.59	0
21	PSU	A	636	21	18,21,22	0.55	0	22,30,33	0.58	0
21	PSU	A	1122	21	18,21,22	0.50	0	22,30,33	0.61	0
21	OMG	A	1131	21	23,26,27	0.36	0	33,38,41	0.46	0
21	PSU	A	308	21	18,21,22	0.56	0	22,30,33	0.57	0
21	MA6	A	1793	21	23,26,27	0.35	0	34,38,41	0.89	2 (5%)
21	A2M	A	802	21	22,25,26	0.22	0	31,36,39	0.70	1 (3%)
21	A2M	A	424	21	22,25,26	0.22	0	31,36,39	0.55	0
21	OMC	A	1648	21	19,22,23	0.33	0	26,31,34	0.50	0
21	OMG	A	434	21	23,26,27	0.34	0	33,38,41	0.39	0
21	PSU	A	103	21	18,21,22	0.52	0	22,30,33	0.56	0
21	PSU	A	35	21	18,21,22	0.52	0	22,30,33	0.58	0
21	A2M	A	162	21	22,25,26	0.18	0	31,36,39	0.55	0
21	PSU	A	606	21	18,21,22	0.53	0	22,30,33	0.59	0
21	PSU	A	764	21	18,21,22	0.50	0	22,30,33	0.66	0
21	PSU	A	306	21	18,21,22	0.54	0	22,30,33	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	PSU	A	765	21	18,21,22	0.48	0	22,30,33	0.59	0
21	OMG	A	392	21	23,26,27	0.35	0	33,38,41	0.44	0
21	A2M	A	979	21	22,25,26	0.25	0	31,36,39	0.55	0
4	IAS	O	138	4	6,7,8	0.82	0	6,8,10	1.06	0
21	OMG	A	246	21	23,26,27	0.33	0	33,38,41	0.44	0
21	PSU	A	255	21,23	18,21,22	0.50	0	22,30,33	0.60	0
21	PSU	A	1295	21	18,21,22	0.46	0	22,30,33	0.60	0
21	OMG	A	1300	21	23,26,27	0.35	0	33,38,41	0.49	0
21	PSU	A	1100	21	18,21,22	0.54	0	22,30,33	0.55	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	A2M	A	623	21,23	-	3/9/27/28	0/3/3/3
21	PSU	A	811	21	-	0/7/25/26	0/2/2/2
21	PSU	A	607	21	-	0/7/25/26	0/2/2/2
21	6MZ	A	1774	21,24,23	-	0/9/27/28	0/3/3/3
21	A2M	A	440	21	-	0/9/27/28	0/3/3/3
21	OMU	A	168	21	-	0/9/27/28	0/2/2/2
21	OMU	A	1014	21	-	0/9/27/28	0/2/2/2
21	PSU	A	258	21	-	0/7/25/26	0/2/2/2
21	PSU	A	300	21	-	0/7/25/26	0/2/2/2
21	PSU	A	111	21,24	-	0/7/25/26	0/2/2/2
21	PSU	A	1637	21	-	0/7/25/26	0/2/2/2
21	A2M	A	545	21	-	1/9/27/28	0/3/3/3
21	OMU	A	123	21	-	1/9/27/28	0/2/2/2
21	PSU	A	208	21	-	0/7/25/26	0/2/2/2
21	OMC	A	38	21	-	0/9/27/28	0/2/2/2
21	A2M	A	468	21	-	2/9/27/28	0/3/3/3
21	OMG	A	599	21	-	1/9/27/28	0/3/3/3
21	OMC	A	418	21	-	0/9/27/28	0/2/2/2
21	A2M	A	1761	21	-	2/9/27/28	0/3/3/3
21	OMU	A	615	21	-	1/9/27/28	0/2/2/2
21	4AC	A	1784	21	-	0/11/29/30	0/2/2/2
21	A2M	A	28	21	-	0/9/27/28	0/3/3/3
21	MA6	A	1792	21	-	0/11/29/30	0/3/3/3
21	PSU	A	1108	21	-	0/7/25/26	0/2/2/2
21	PSU	A	1310	21	-	2/7/25/26	0/2/2/2
21	UY1	A	604	21	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	PSU	A	121	21	-	0/7/25/26	0/2/2/2
21	PSU	A	1306	21	-	0/7/25/26	0/2/2/2
21	PSU	A	362	21	-	0/7/25/26	0/2/2/2
10	AME	V	1	10	-	2/9/10/12	-
21	PSU	A	1084	21	-	0/7/25/26	0/2/2/2
21	PSU	A	806	21	-	0/7/25/26	0/2/2/2
21	PSU	A	1004	21	-	0/7/25/26	0/2/2/2
21	PSU	A	636	21	-	0/7/25/26	0/2/2/2
21	PSU	A	1122	21	-	0/7/25/26	0/2/2/2
21	OMG	A	1131	21	-	1/9/27/28	0/3/3/3
21	PSU	A	308	21	-	0/7/25/26	0/2/2/2
21	MA6	A	1793	21	-	2/11/29/30	0/3/3/3
21	A2M	A	802	21	-	0/9/27/28	0/3/3/3
21	A2M	A	424	21	-	0/9/27/28	0/3/3/3
21	OMC	A	1648	21	-	2/9/27/28	0/2/2/2
21	OMG	A	434	21	-	0/9/27/28	0/3/3/3
21	PSU	A	103	21	-	0/7/25/26	0/2/2/2
21	PSU	A	35	21	-	0/7/25/26	0/2/2/2
21	A2M	A	162	21	-	0/9/27/28	0/3/3/3
21	PSU	A	606	21	-	0/7/25/26	0/2/2/2
21	PSU	A	764	21	-	0/7/25/26	0/2/2/2
21	PSU	A	306	21	-	0/7/25/26	0/2/2/2
21	PSU	A	765	21	-	0/7/25/26	0/2/2/2
21	OMG	A	392	21	-	2/9/27/28	0/3/3/3
21	A2M	A	979	21	-	0/9/27/28	0/3/3/3
4	IAS	O	138	4	-	1/7/7/8	-
21	OMG	A	246	21	-	2/9/27/28	0/3/3/3
21	PSU	A	255	21,23	-	0/7/25/26	0/2/2/2
21	PSU	A	1295	21	-	0/7/25/26	0/2/2/2
21	OMG	A	1300	21	-	0/9/27/28	0/3/3/3
21	PSU	A	1100	21	-	0/7/25/26	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	615	OMU	C4-N3	-4.31	1.30	1.38
21	A	615	OMU	C2-N3	-4.04	1.30	1.38
10	V	1	AME	CT1-N	3.31	1.45	1.34
21	A	615	OMU	C5-C4	-2.53	1.38	1.43
21	A	615	OMU	C6-N1	-2.07	1.33	1.38

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	615	OMU	N3-C2-N1	4.45	120.80	114.89
21	A	615	OMU	C4-N3-C2	-4.42	120.75	126.58
21	A	615	OMU	C5-C4-N3	4.33	121.32	114.84
21	A	1774	6MZ	C9-N6-C6	3.27	125.69	122.87
21	A	1793	MA6	N1-C6-N6	-3.22	113.56	117.08

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	A	246	OMG	O4'-C4'-C5'-O5'
21	A	615	OMU	C1'-C2'-O2'-CM2
21	A	623	A2M	O4'-C4'-C5'-O5'
21	A	1310	PSU	C2'-C1'-C5-C4
21	A	1648	OMC	O4'-C1'-N1-C2

There are no ring outliers.

22 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	607	PSU	2	0
21	A	1774	6MZ	2	0
21	A	1014	OMU	2	0
21	A	1637	PSU	1	0
21	A	123	OMU	1	0
21	A	208	PSU	2	0
21	A	38	OMC	1	0
21	A	418	OMC	3	0
21	A	1761	A2M	1	0
21	A	615	OMU	1	0
21	A	28	A2M	1	0
21	A	1792	MA6	2	0
21	A	1108	PSU	1	0
21	A	1306	PSU	1	0
21	A	636	PSU	2	0
21	A	1122	PSU	2	0
21	A	308	PSU	2	0
21	A	1793	MA6	1	0
21	A	1648	OMC	4	0
21	A	606	PSU	2	0
21	A	306	PSU	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	392	OMG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 47 ligands modelled in this entry, 47 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

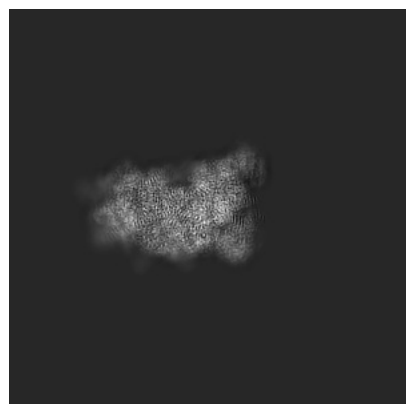
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18951. These allow visual inspection of the internal detail of the map and identification of artifacts.

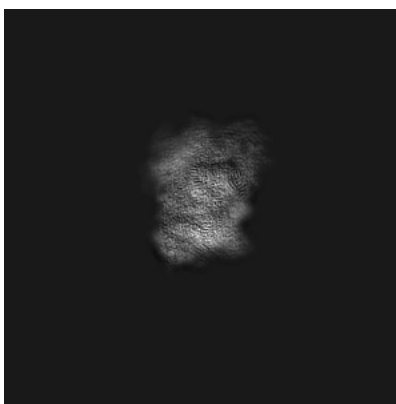
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

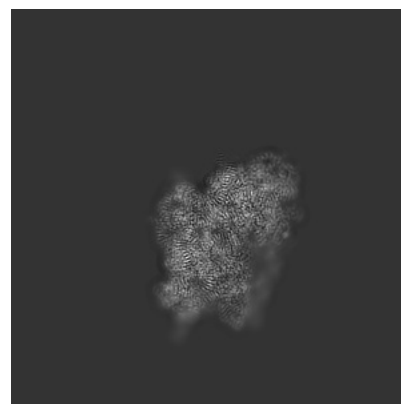
6.1.1 Primary map



X

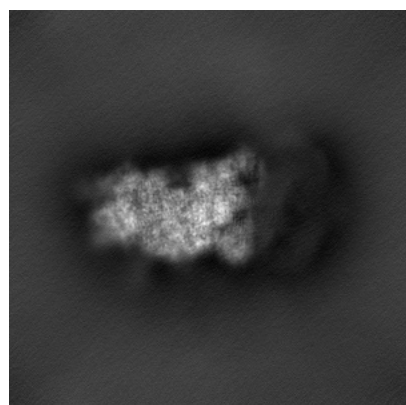


Y

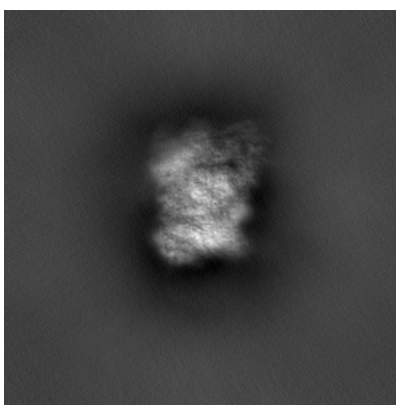


Z

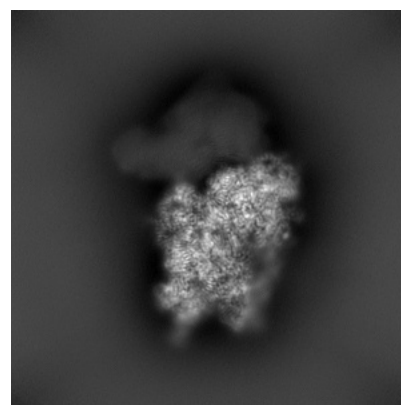
6.1.2 Raw map



X



Y

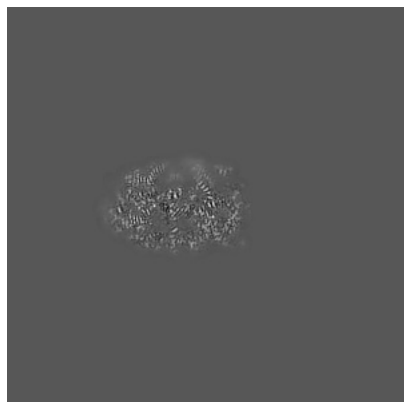


Z

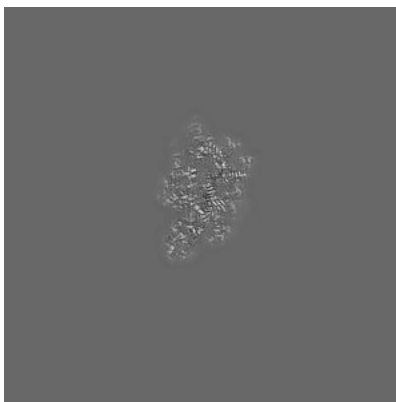
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

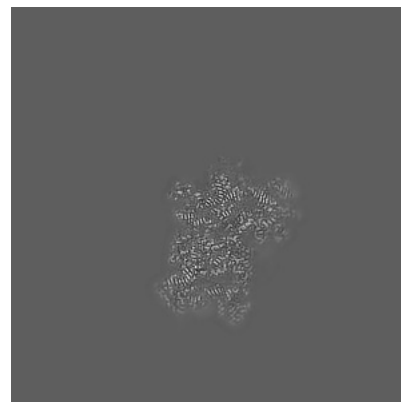
6.2.1 Primary map



X Index: 240

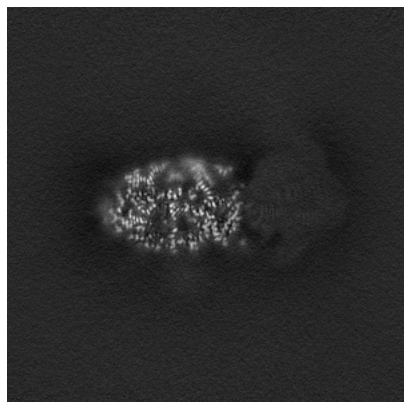


Y Index: 240

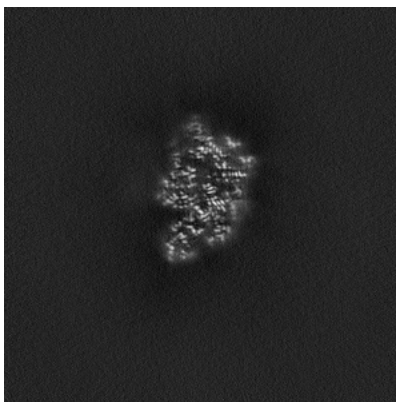


Z Index: 240

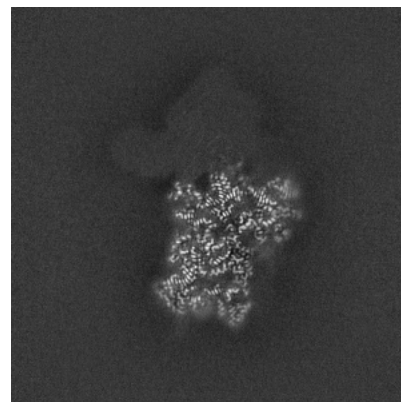
6.2.2 Raw map



X Index: 240



Y Index: 240

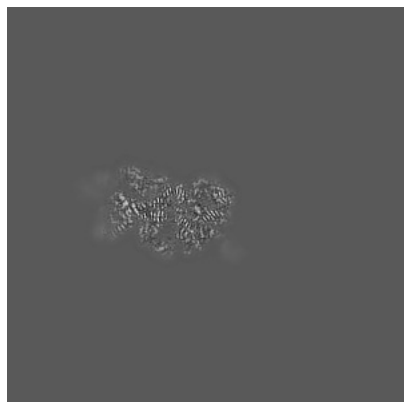


Z Index: 240

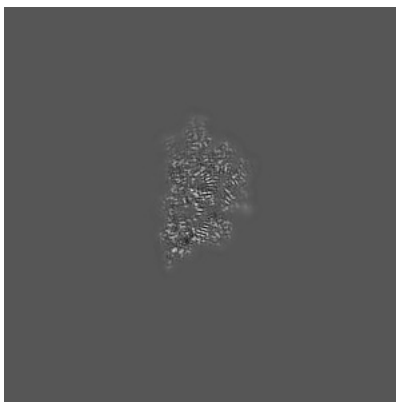
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

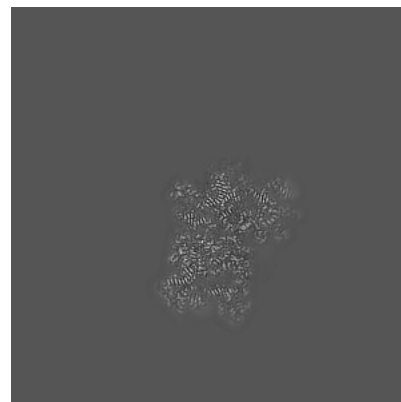
6.3.1 Primary map



X Index: 210

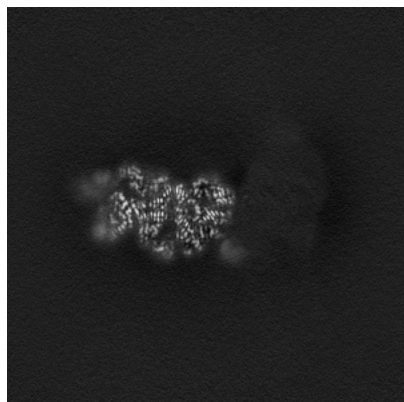


Y Index: 229

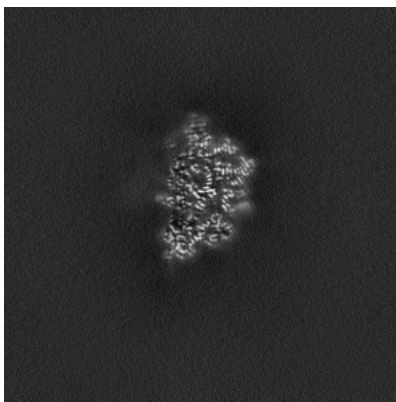


Z Index: 241

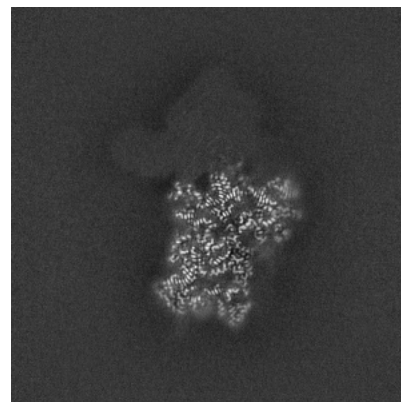
6.3.2 Raw map



X Index: 210



Y Index: 234

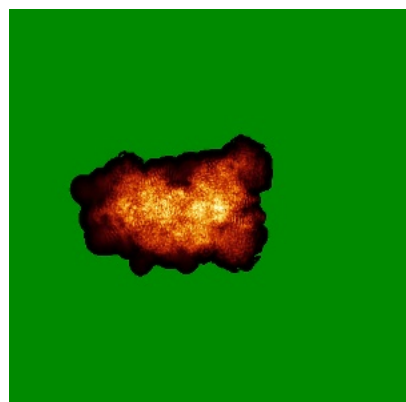


Z Index: 240

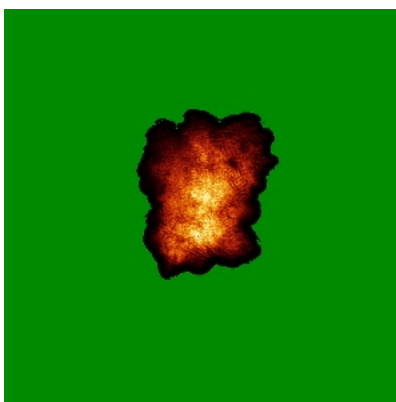
The images above show the largest variance slices of the map in three orthogonal directions.

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

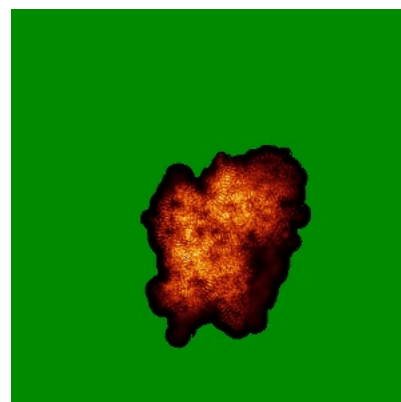
6.4.1 Primary map



X

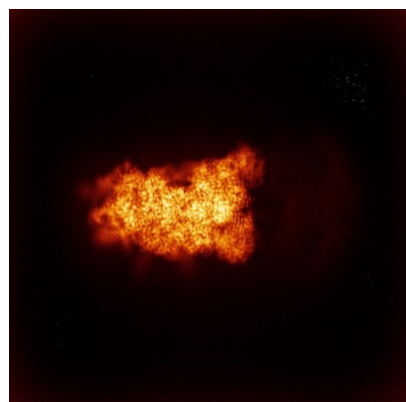


Y

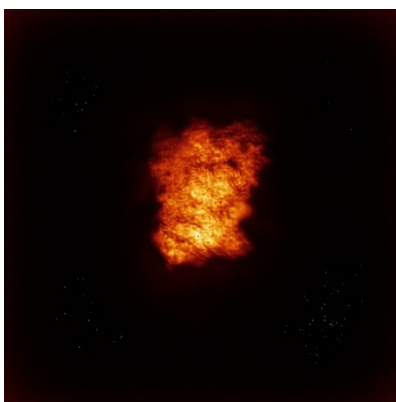


Z

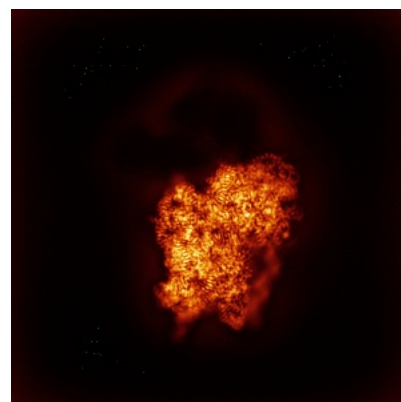
6.4.2 Raw map



X



Y



Z

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

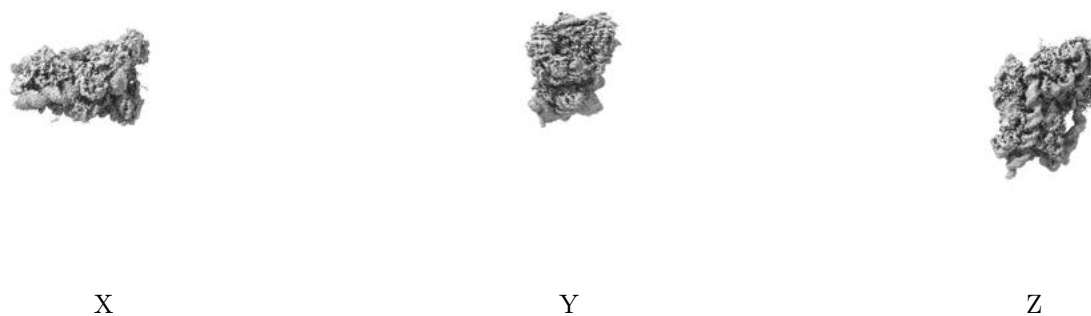
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. 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.

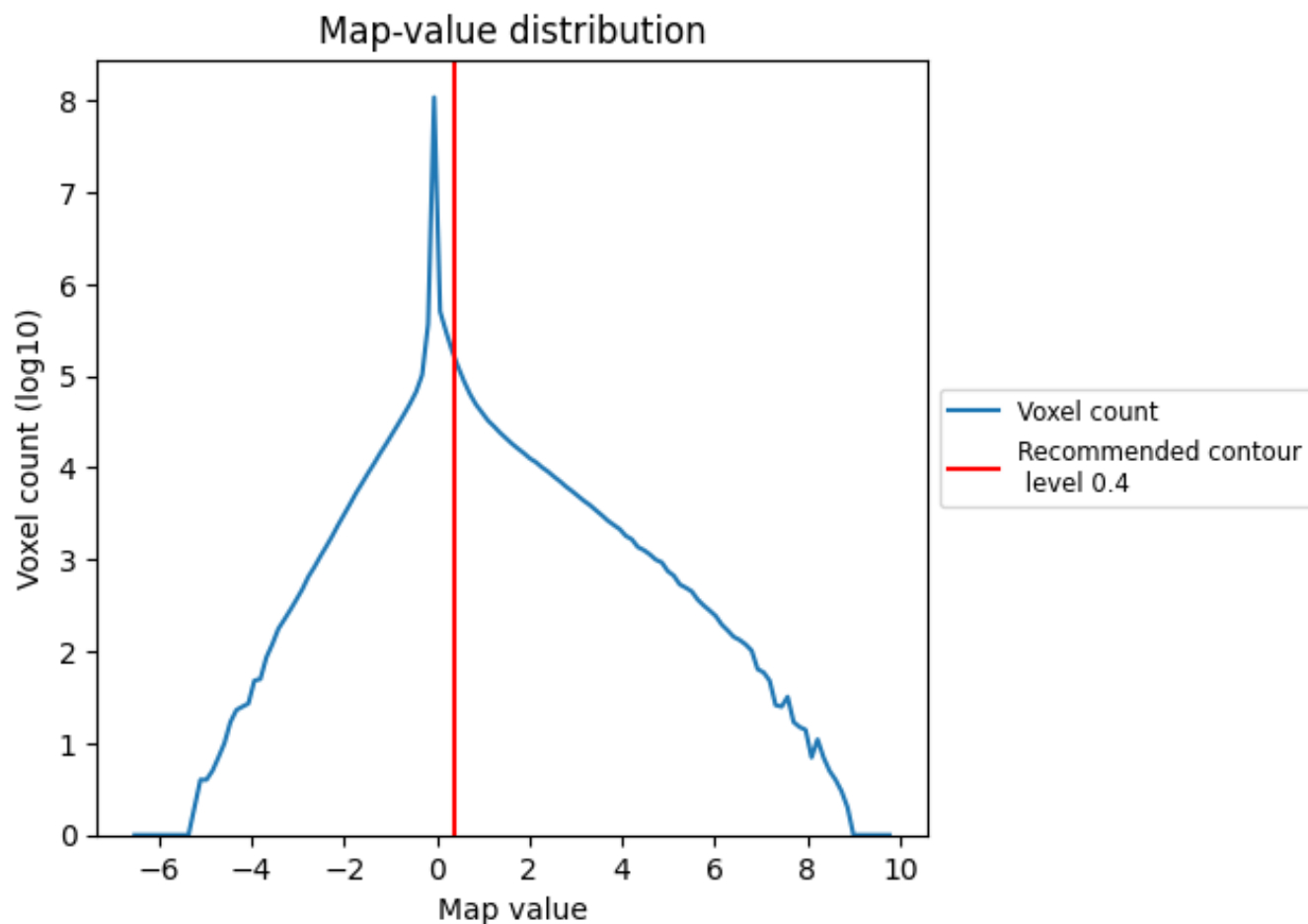
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

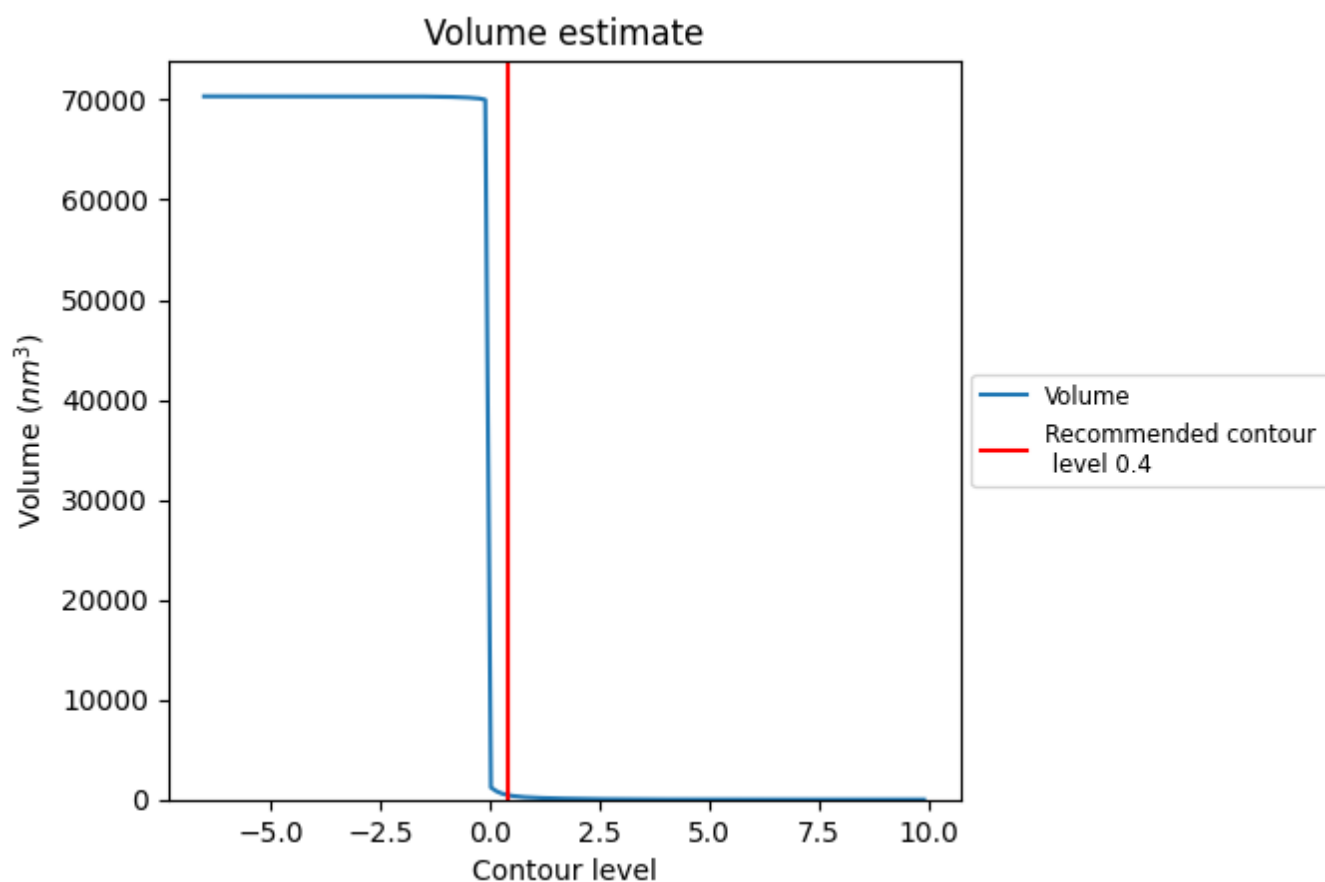
This section contains the results of statistical analysis of the map.

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.

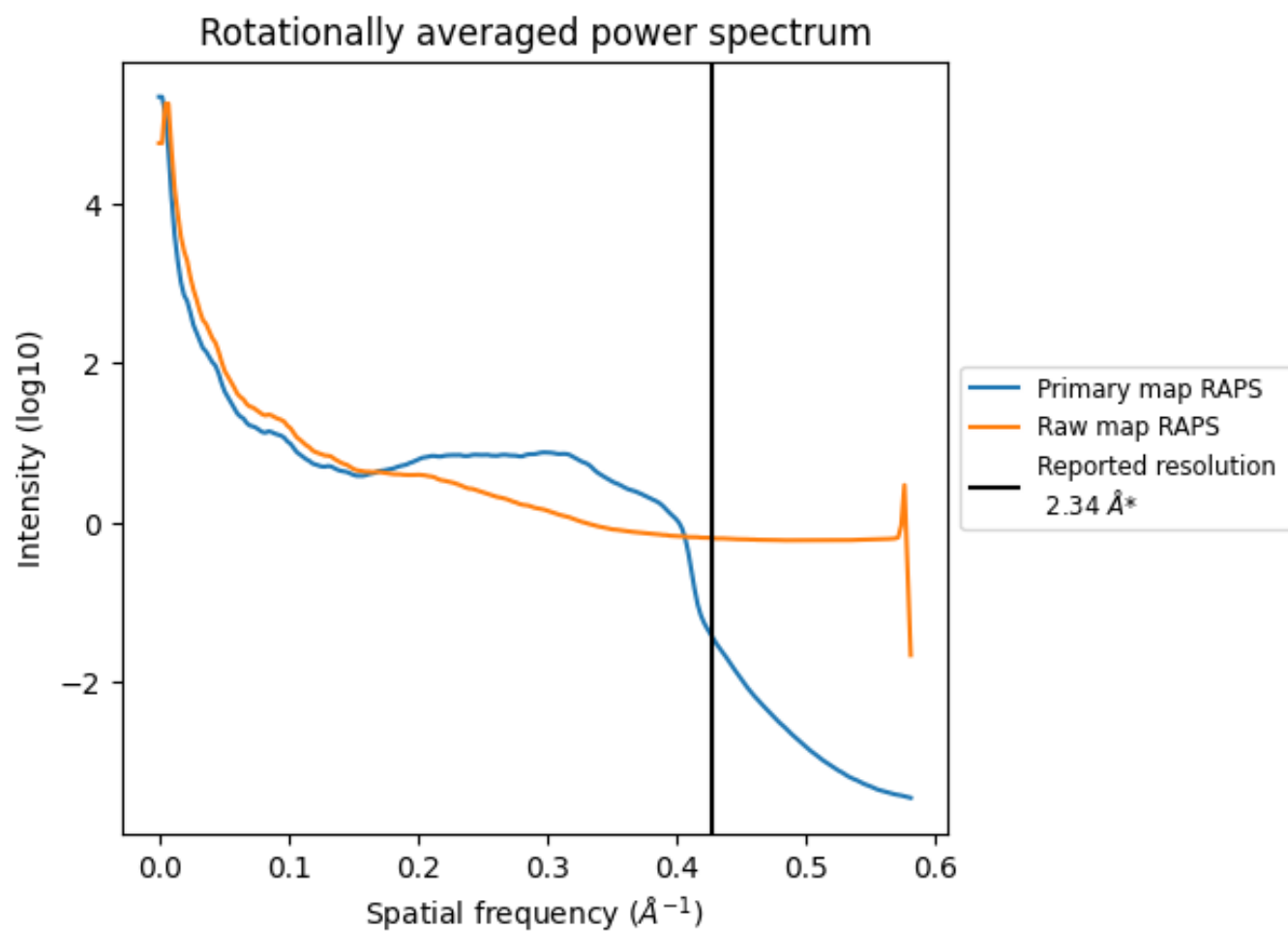
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 453 nm^3 ; this corresponds to an approximate mass of 409 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

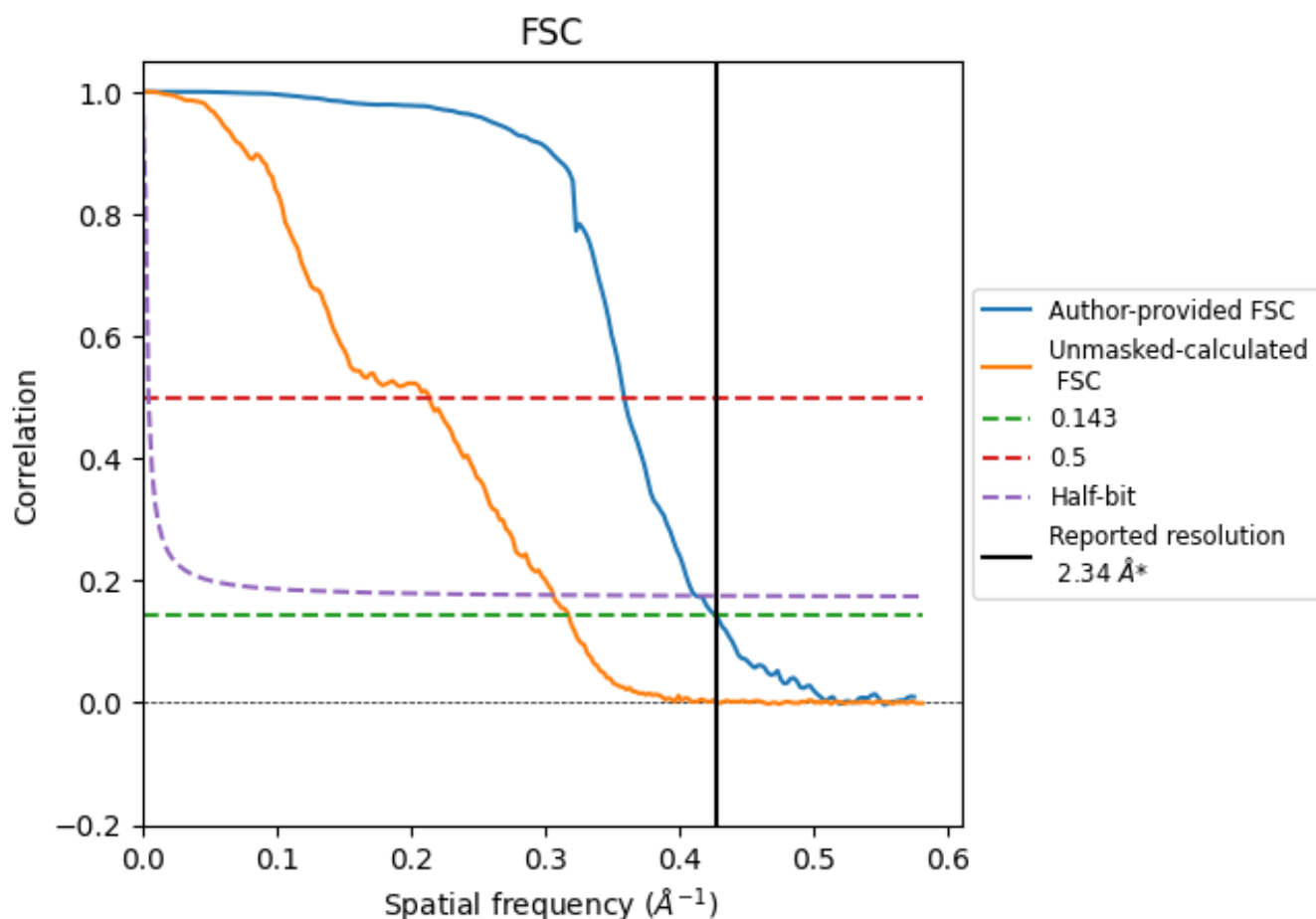


*Reported resolution corresponds to spatial frequency of 0.427 Å⁻¹

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 0.427 $\text{\AA}^{-1}$

8.2 Resolution estimates

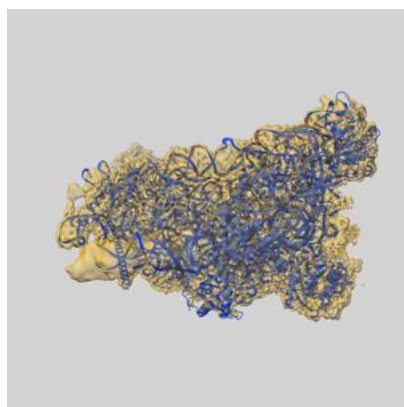
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.34	-	-
Author-provided FSC curve	2.34	2.78	2.42
Unmasked-calculated*	3.15	4.68	3.26

*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 3.15 differs from the reported value 2.34 by more than 10 %

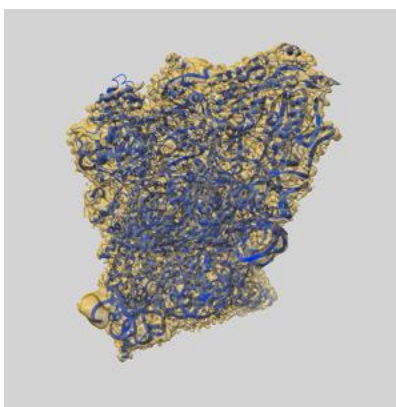
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-18951 and PDB model 8R6F. Per-residue inclusion information can be found in section [3](#) on page [9](#).

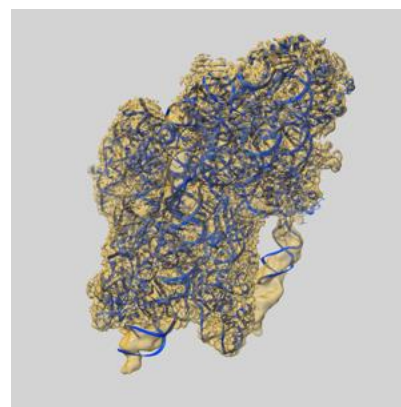
9.1 Map-model overlay [i](#)



X



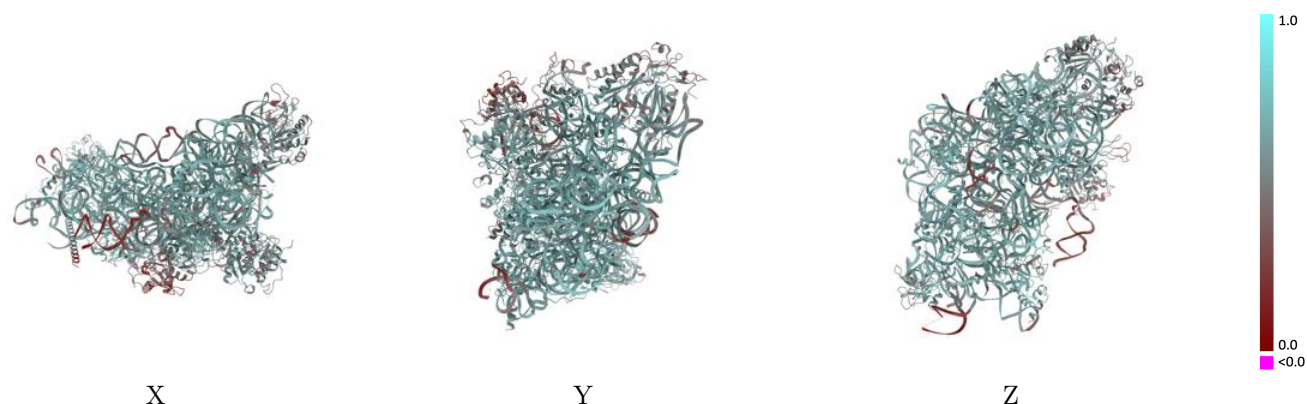
Y



Z

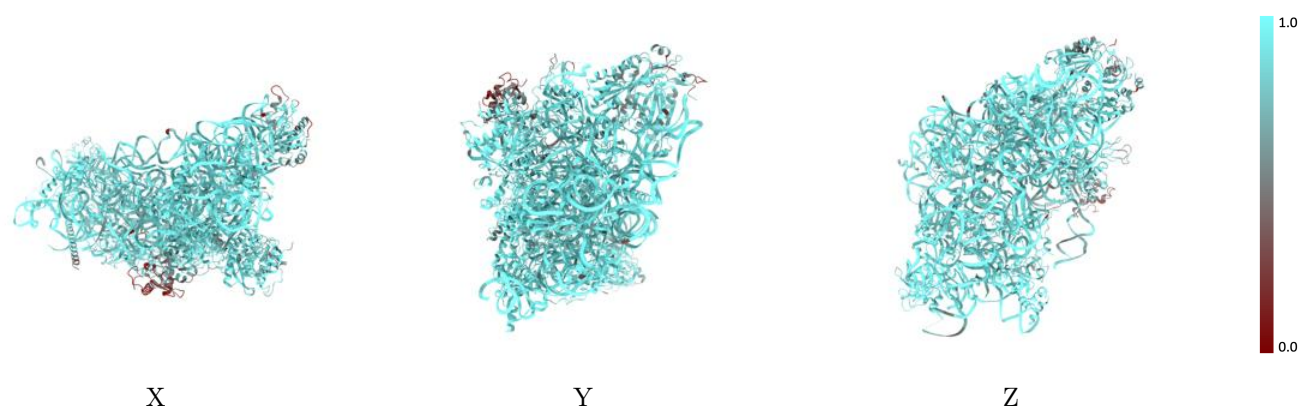
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



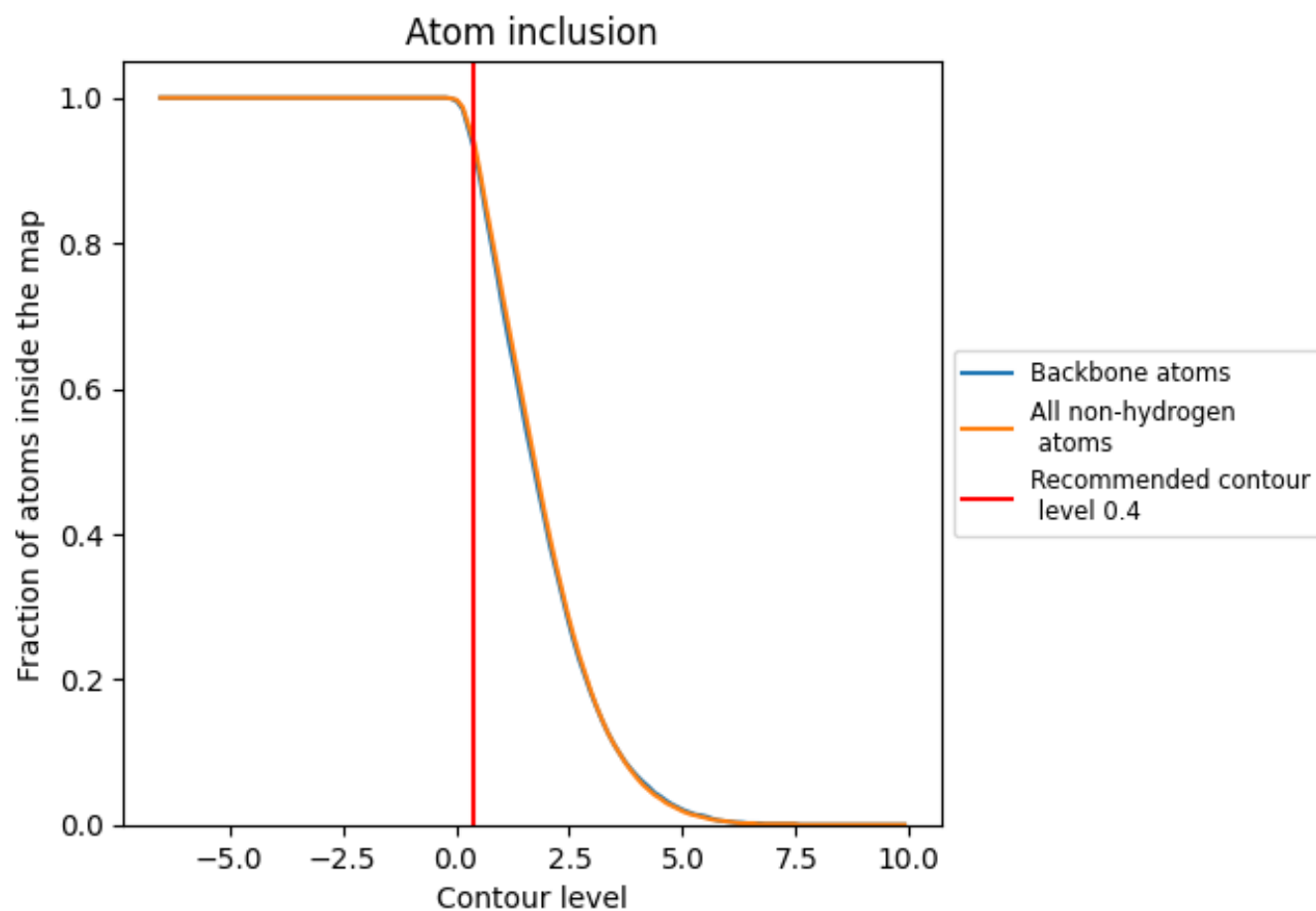
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9390	 0.6000
A	 0.9700	 0.6060
B	 0.8370	 0.5260
C	 0.9620	 0.6410
E	 0.9620	 0.6430
G	 0.9280	 0.5700
H	 0.5400	 0.4000
I	 0.9670	 0.6380
J	 0.9670	 0.6490
L	 0.9750	 0.6630
N	 0.9430	 0.5980
O	 0.8410	 0.5460
V	 0.9450	 0.6060
W	 0.9820	 0.6700
X	 0.9710	 0.6460
Y	 0.9610	 0.6320
a	 0.8850	 0.6060
b	 0.8410	 0.5120
e	 0.9180	 0.6070
h	 0.6030	 0.3810
k	 0.9410	 0.5810
n	 0.9310	 0.5990

