



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 04:19 AM UTC

PDB ID : 6YSI / pdb_00006ysi
EMDB ID : EMD-10898
Title : Acinetobacter baumannii ribosome-tigecycline complex - 50S subunit
Authors : Nicholson, D.; Edwards, T.A.; O'Neill, A.J.; Ranson, N.A.
Deposited on : 2020-04-22
Resolution : 2.50 Å(reported)
Based on initial models : 5AFI, 5MDZ

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:

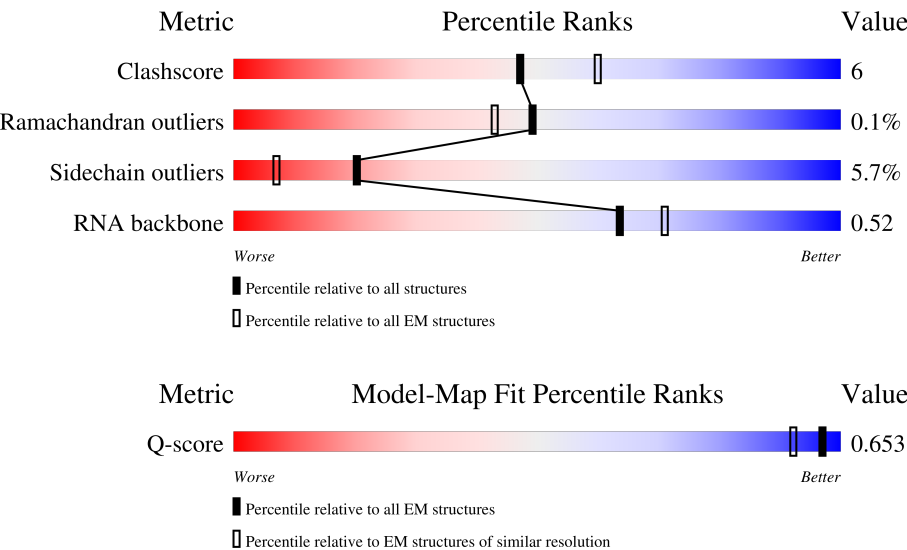
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

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

The reported resolution of this entry is 2.50 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.



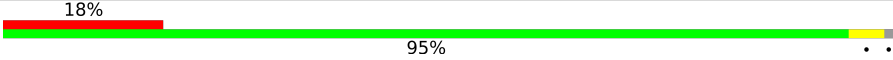
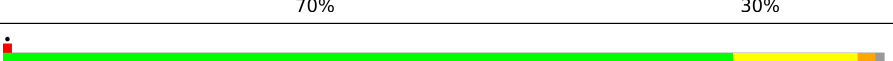
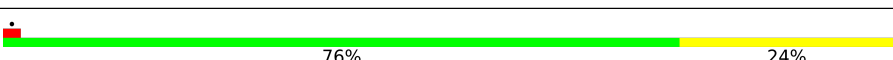
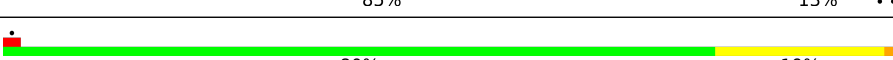
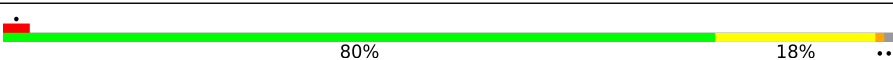
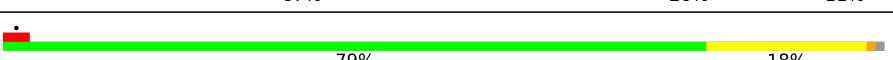
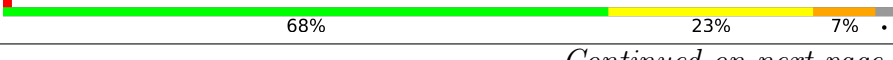
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7115 (2.00 - 3.00)

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	A	274	
2	B	212	
3	C	200	

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Mol	Chain	Length	Quality of chain
4	D	178	
5	E	177	
6	F	142	
7	G	122	
8	H	146	
9	I	137	
10	J	125	
11	K	116	
12	L	122	
13	M	119	
14	N	103	
15	O	110	
16	P	106	
17	Q	105	
18	R	98	
19	S	85	
20	T	78	
21	U	65	
22	V	58	
23	W	74	
24	X	61	
25	Y	51	
26	Z	44	
27	1	2903	
28	5	117	

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Mol	Chain	Length	Quality of chain
29	6	77	6%5%• 94%
29	8	77	6%5%•• 90%
30	a	64	• 86%11%••
31	b	38	• 79%21%

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 83855 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 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	272	Total	C	N	O	S	0	0
			2109	1301	435	365	8		

- Molecule 2 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	211	Total	C	N	O	S	0	0
			1571	972	297	299	3		

- Molecule 3 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	199	Total	C	N	O	S	0	0
			1485	933	278	270	4		

- Molecule 4 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	176	Total	C	N	O	0	0
			865	513	176	176		

- Molecule 5 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	175	Total	C	N	O	S	0	0
			1327	838	238	250	1		

- Molecule 6 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	142	Total	C	N	O	S	0	0
			1122	717	200	201	4		

- Molecule 7 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	122	Total	C	N	O	S	0	0
			945	592	180	168	5		

- Molecule 8 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	144	Total	C	N	O		0	0
			1071	663	213	195			

- Molecule 9 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	137	Total	C	N	O	S	0	0
			1086	687	210	184	5		

- Molecule 10 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	119	Total	C	N	O	S	1	0
			950	598	187	162	3		

- Molecule 11 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	115	Total	C	N	O	S	0	0
			864	532	175	156	1		

- Molecule 12 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	117	Total	C	N	O		0	0
			919	578	177	164			

- Molecule 13 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	117	Total	C	N	O	S	0	0
			934	589	197	146	2		

- Molecule 14 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	103	Total	C	N	O	S	0	0
			806	506	155	142	3		

- Molecule 15 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	109	Total	C	N	O	S	0	0
			825	514	158	149	4		

- Molecule 16 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	92	Total	C	N	O	S	0	0
			717	457	129	130	1		

- Molecule 17 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	102	Total	C	N	O	S	0	0
			761	473	141	147			

- Molecule 18 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	96	Total	C	N	O	S	0	0
			753	472	142	138	1		

- Molecule 19 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	76	Total	C	N	O	S	0	0
			577	358	111	106	2		

- Molecule 20 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	77	Total	C	N	O	S	0	0
			631	395	130	104	2		

- Molecule 21 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	61	Total	C	N	O	S	0	0
			490	304	94	91	1		

- Molecule 22 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	57	Total	C	N	O	S	0	0
			453	281	87	81	4		

- Molecule 23 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	W	43	Total	C	N	O	0	0
			213	127	43	43		

- Molecule 24 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	54	Total	C	N	O	S	0	0
			447	265	100	81	1		

- Molecule 25 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	51	Total	C	N	O	S	0	0
			426	274	77	72	3		

- Molecule 26 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	44	Total	C	N	O	S	0	0
			362	222	85	53	2		

- Molecule 27 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	1	2672	Total	C	N	O	P	0	0
			57324	25584	10504	18564	2672		

- Molecule 28 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	5	115	Total	C	N	O	P	0	0
			2450	1095	440	800	115		

- Molecule 29 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	6	5	Total	C	N	O	P	0	0
			112	49	23	35	5		
29	8	8	Total	C	N	O	P	0	0
			169	76	32	53	8		

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	a	63	Total	C	N	O	S	0	0
			508	319	110	75	4		

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	b	38	Total	C	N	O	S	0	0
			294	179	64	47	4		

- Molecule 32 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
32	1	159	Total	Mg	0
			159	159	
32	5	3	Total	Mg	0
			3	3	

- Molecule 33 is TIGECYCLINE (CCD ID: T1C) (formula: C₂₉H₄₁N₅O₈) (labeled as "Ligand of Interest" by depositor).



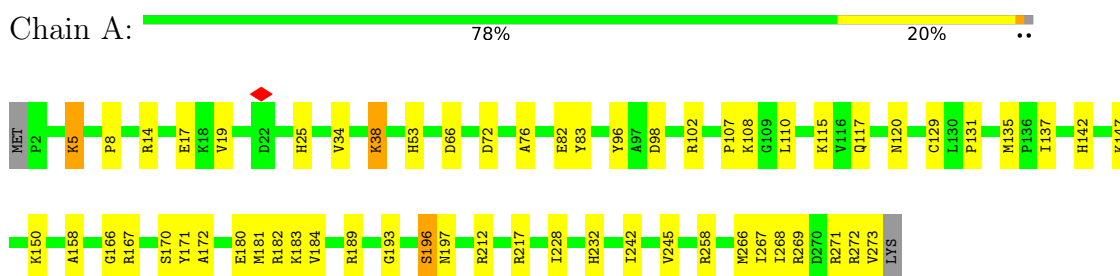
- Molecule 34 is ZINC ION (CCD ID: ZN) (formula: Zn).



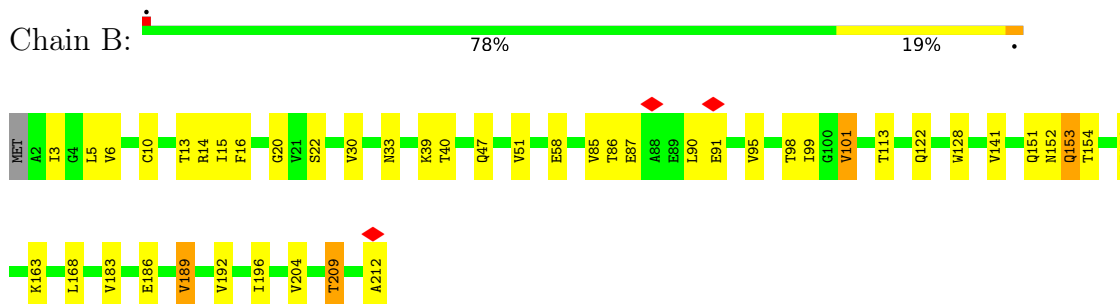
3 Residue-property plots [i](#)

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.

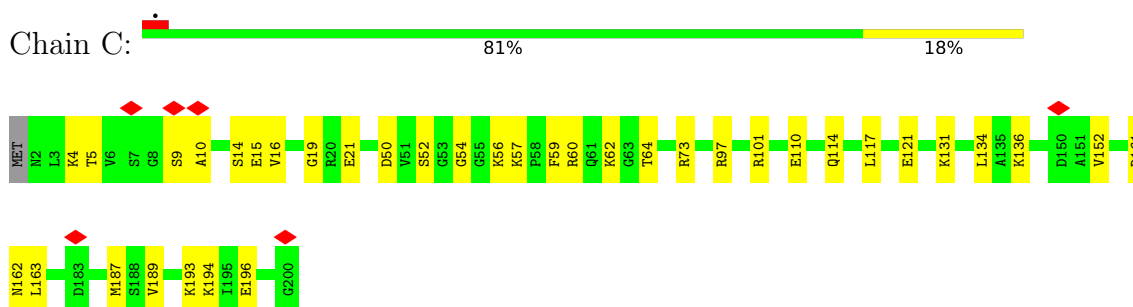
- Molecule 1: 50S ribosomal protein L2



- Molecule 2: 50S ribosomal protein L3

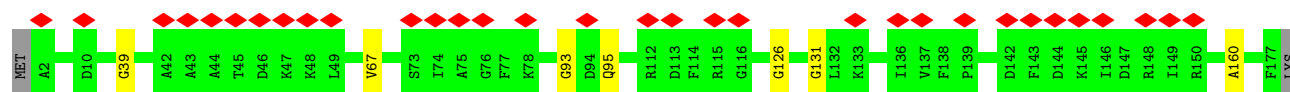


- Molecule 3: 50S ribosomal protein L4

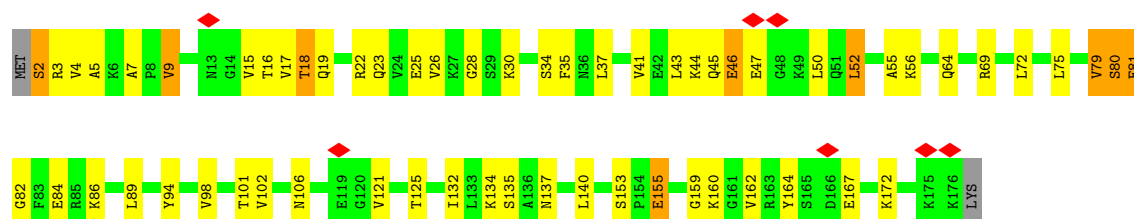


- Molecule 4: 50S ribosomal protein L5

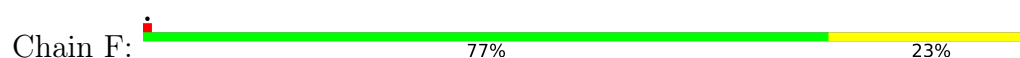




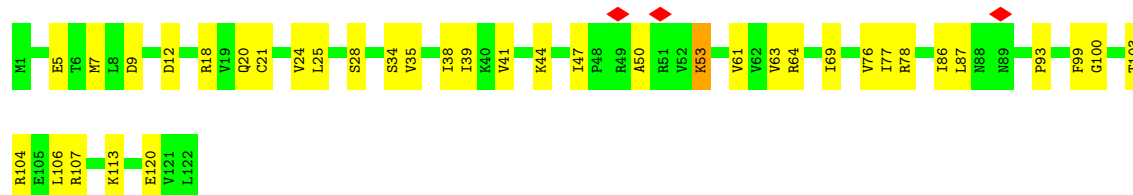
• Molecule 5: 50S ribosomal protein L6



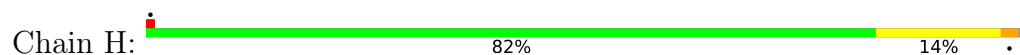
• Molecule 6: 50S ribosomal protein L13



• Molecule 7: 50S ribosomal protein L14



• Molecule 8: 50S ribosomal protein L15



• Molecule 9: 50S ribosomal protein L16





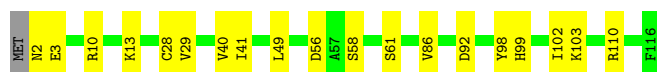
- Molecule 10: 50S ribosomal protein L17

Chain J: 86% 9% 5%



- Molecule 11: 50S ribosomal protein L18

Chain K: 83% 16%



- Molecule 12: 50S ribosomal protein L19

Chain L: 5% 77% 19%



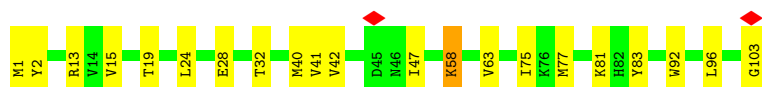
- Molecule 13: 50S ribosomal protein L20

Chain M: 85% 13%



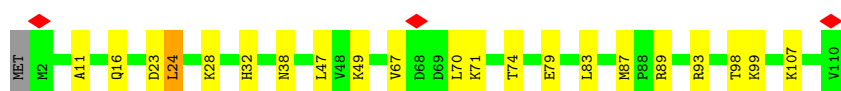
- Molecule 14: 50S ribosomal protein L21

Chain N: 80% 19%

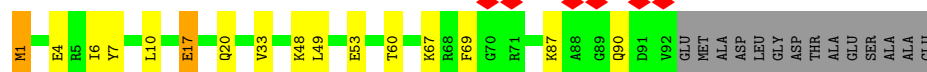
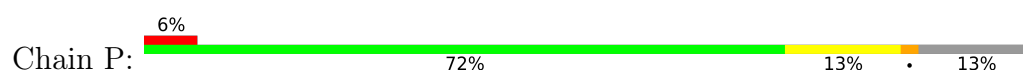


- Molecule 15: 50S ribosomal protein L22

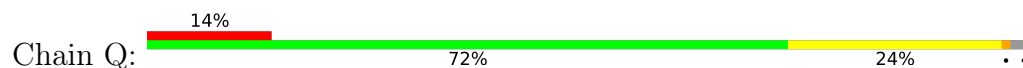
Chain O: 80% 18%



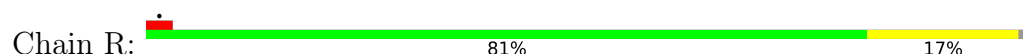
- Molecule 16: 50S ribosomal protein L23



- Molecule 17: 50S ribosomal protein L24



- Molecule 18: 50S ribosomal protein L25



- Molecule 19: 50S ribosomal protein L27



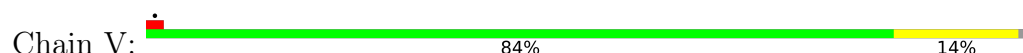
- Molecule 20: 50S ribosomal protein L28



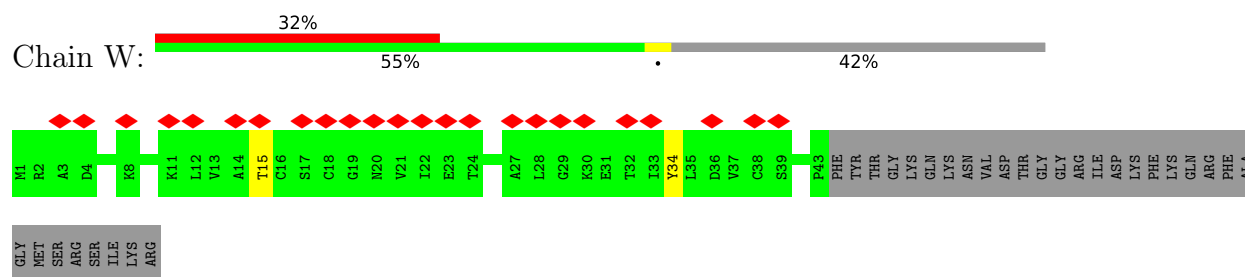
- Molecule 21: 50S ribosomal protein L29



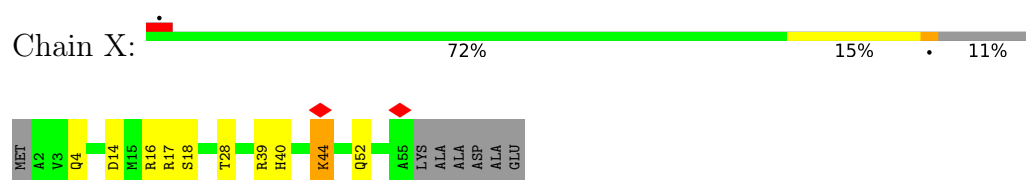
- Molecule 22: 50S ribosomal protein L30



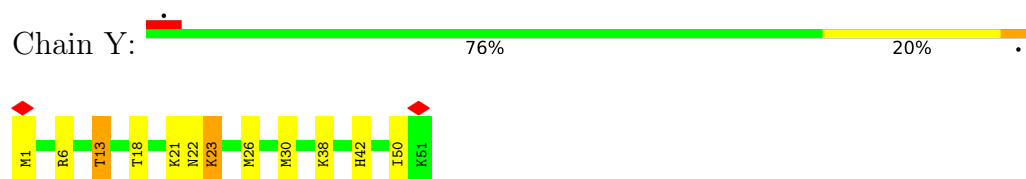
- Molecule 23: 50S ribosomal protein L31



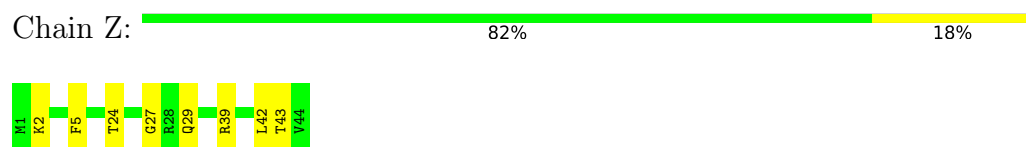
- Molecule 24: 50S ribosomal protein L32



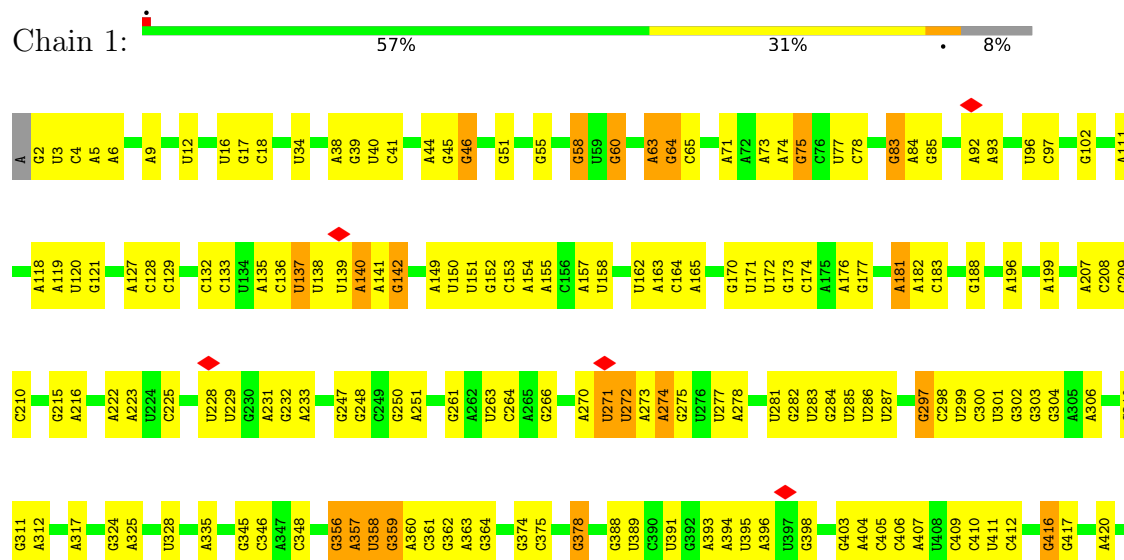
- Molecule 25: 50S ribosomal protein L33



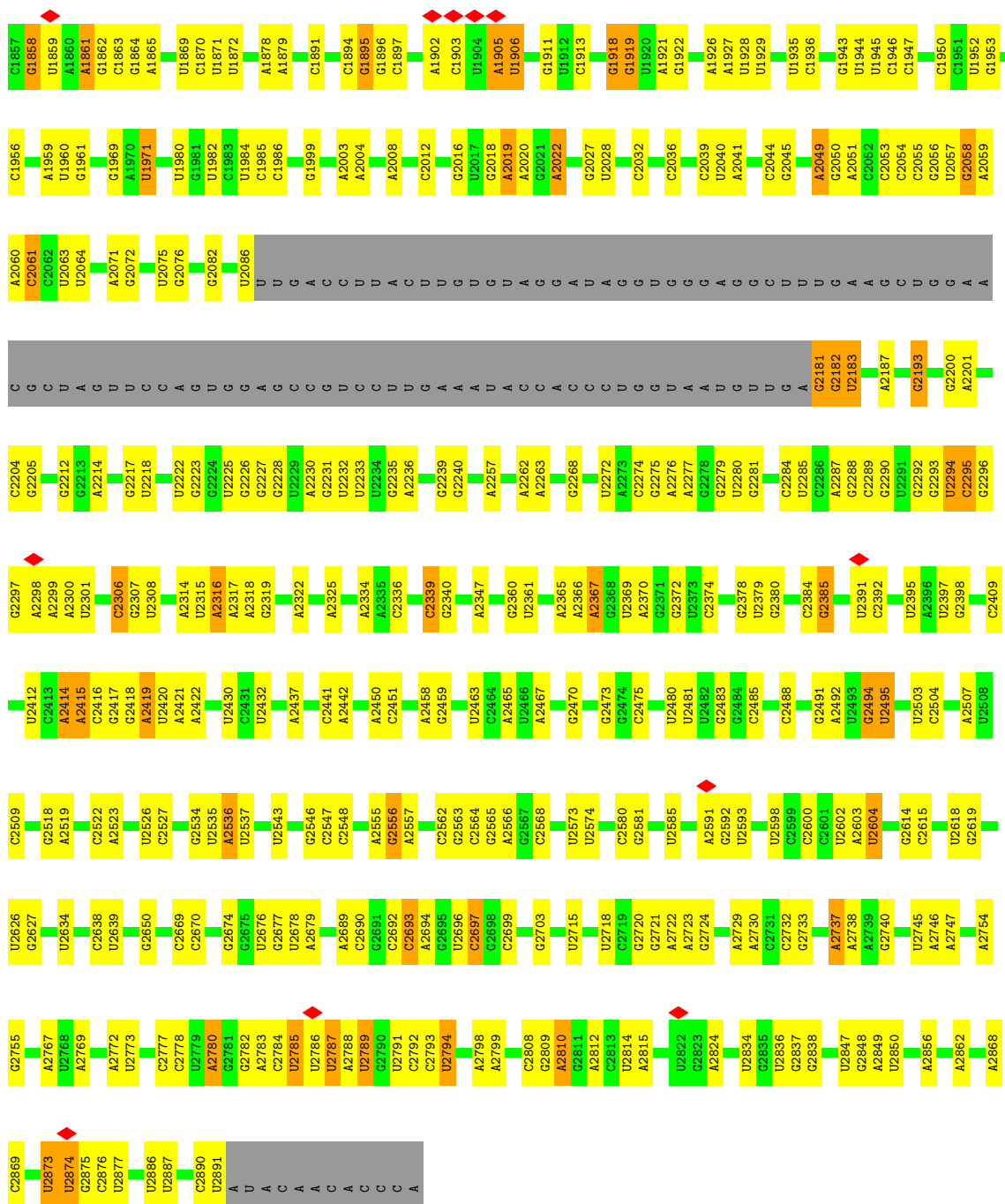
- Molecule 26: 50S ribosomal protein L34



- Molecule 27: 23S ribosomal RNA



A1746	G1640	G	G1463	U1367	G1113	U	G983	G	G766	G647	U557	C428
A1747	A1643	A1535	U1464	G1368	G1114	G	C984	G	G767	U648	U564	U429
A1748	G1644	A1645	G1465	G1258	G1115	G	A986	U	A773	U649	U565	A439
C1749		U1541	G1466	G1259		C			A774	A657	A566	
			G1467	A1374	G1119	U	G987	C	G775	U658	U567	C448
	U1648	G1551	C1468	U1375	U1120	U	U989	A	G776	A659	A568	A449
C1649	C1649	U1554	A1469	A1380	G1121	A	A990	U	A779	G660	G569	
U1650		C1555	U1470	A1381	U1122	G	A991	C	C782	A661	G570	G457
	A1660	G1556	U1472	U1382	A1123	A	G992	C	A783	A666	U571	A458
G1765		U1557	A1473	A1383	A1124	G	G993	C	C784	A667	C572	G459
U1766		G1558	U1474	U1384	C1125	C		A	U784		A573	G460
U1767	G1665	G1559	C1475		G1126	A	C996	C	G785	U677	G576	G468
U1768	A1688	A1560	U1476	A1388		G	A1000	U	C786	C678		
		A1561	U1477	U1389	G1129	C	A1001	C	G787	U579		A471
U1771	U1671	A1562	A1478		C1130	C	U1002	A	G796	U580		A472
A1772	G1672			U1393	U1131	A	C1003	C	C797	G691		G473
A1773	G1673	U1569	U1482	U1394	A1132	C	U1004	C	U798	U694		A474
	U1674	A1570	A1483	G1395	A1133	C	A1005	A		G695		A475
U1779		A1571	U1484	U1396	A1134	C	U1006		C803	U697		
A1780		G1572	U1485	G1397		U	U1009		U804	A697		U480
	U1679		G1490	G1404	G1140	U	A1010		C805	U698		G483
A1783	A1680	U1575		C1405	U1141	U	A1011		C806	U699		A484
C1784	A1681	C1576	G1494	G1406		A	G1012		A810	G702		G485
C1682	C1682	A1577	U1495	A1407	U1163	A	U1013		U818	G703		G486
		G1578	U1496	U1408	U1164	G	G1014		U819	A902		G487
A1691		U1579	U1497		U1165	A	G1015		C903	A902		G488
G1701	U1580	G1578	A1498	G1414	U1166	A	G1016		A915	C708		A489
U1702	A1581	U1579		A1415	U1167	A	A1017		U916	A709		G490
A1791	U1703	C1582		G1416	U1168	G	A1018		G917	C710		
A1792	G1704	A1583		G1417	U1169	C	C1020		A824	U711		A495
	U1705	U1705	G1503	G1418	U1170	G	U1021		G825	A712		U496
A1798	U1706	A1588	A1504	G1419	C1171	U	A1022		U830	C714		A497
A1799	G1707	A1589	U1505	G1420	G1172	A	U1023		C831	U715		U500
G1800	G1708	U1590	U1506	A1421		U	G1024		G836	A720		C501
	U1709	C1591	C1508	A1422	G1175	A	U1025		A837	A721		A520
	G1710			G1423	U1176	G			U838	A722		A521
	A1711		A1511	C1425	U1186	C	G1028		U839	A730		G522
G1815	U1712	U1599	U	U1430	U1187	U	A1030		A840	C731		C523
A1818		A1600	G	C1431	U1188	C			C941	U732		A524
		A1601	A	U1436	U1191	C	A1034		C842	G733		G525
C1832		G1619	C	C1435	U1200	U	U		A843	U734		U526
U1833		U1620	A	U1436	G1226	A	A		G847	A628		A530
			G	U1439	G1238	C	A		G848	G829		G531
A1836		A1623	U	U1440	G1239	G	A		G849	U633		U536
A1837		G1624	C	U1441	G1240	C	A		G850	U634		U537
		U1625	U		A1241	A	A		G855	A635		U538
A1842		A1626	C	U1446	A1242	U	A		C956	U636		G539
A1843		G1627	C	U1447	U1243	G	G		A857	G751		U540
U1844		A1628	U	U1448	G1244	G	A		U668	A752		G541
U1845		C1629	U	A1456		A	A		A			
U1846	U1726	G1630	U	A1457	U1251	G	A		G			A554
A1847	G1727	A1631	G	A1458	A1252	G	A		G			C555
U1848	A1728	A1632	U	A1459	A1253	G	A		G			C556
	G1729	G1633	C		G1254	G	U					
U1853		U1637	A									
U1854		U1638	A									
A1855		G1639	G									
G1856	G1745		C									



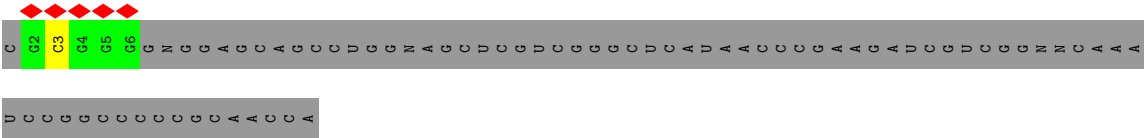
• Molecule 28: 5S ribosomal RNA

Chain 5: 68% 23% 7% .

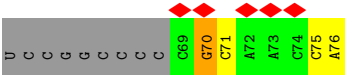
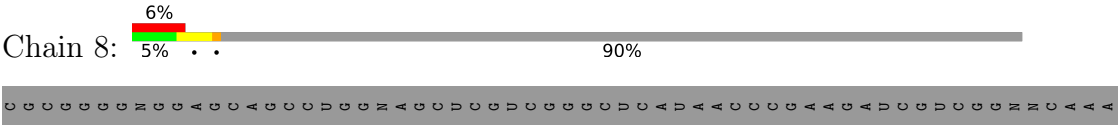


• Molecule 29: E-site tRNA

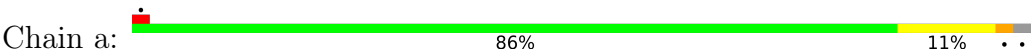
Chain 6: 6% 5% . 94%



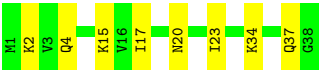
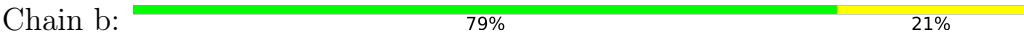
● Molecule 29: E-site tRNA



● Molecule 30: 50S ribosomal protein L35



● Molecule 31: 50S ribosomal protein L36



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	231159	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	62	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.576	Depositor
Minimum map value	-0.272	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	426.00003, 426.00003, 426.00003	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.065, 1.065, 1.065	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: T1C, 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	A	0.35	0/2150	0.48	0/2888
2	B	0.36	0/1589	0.46	0/2142
3	C	0.30	0/1506	0.41	0/2035
4	D	0.16	0/864	0.36	0/1199
5	E	0.24	0/1346	0.42	0/1818
6	F	0.33	0/1148	0.41	0/1548
7	G	0.33	0/955	0.44	0/1286
8	H	0.33	0/1079	0.46	0/1439
9	I	0.33	0/1103	0.45	0/1475
10	J	0.36	0/968	0.49	0/1298
11	K	0.28	0/872	0.45	0/1167
12	L	0.31	0/931	0.44	0/1249
13	M	0.36	0/947	0.42	0/1262
14	N	0.32	0/817	0.42	0/1094
15	O	0.31	0/830	0.38	0/1113
16	P	0.27	0/723	0.38	0/967
17	Q	0.28	0/765	0.46	0/1027
18	R	0.29	0/763	0.42	0/1026
19	S	0.38	0/585	0.48	0/783
20	T	0.33	0/641	0.42	0/856
21	U	0.22	0/491	0.40	0/651
22	V	0.29	0/458	0.38	0/612
23	W	0.14	0/212	0.39	0/294
24	X	0.32	0/453	0.46	0/604
25	Y	0.31	0/433	0.44	0/573
26	Z	0.36	0/366	0.48	0/481
27	1	0.44	0/64198	0.38	0/100128
28	5	0.33	0/2739	0.39	0/4266
29	6	0.17	0/125	0.24	0/194
29	8	0.18	0/188	0.32	0/290
30	a	0.35	0/514	0.48	0/678
31	b	0.36	0/295	0.46	0/389

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.41	0/91054	0.40	0/136832

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
8	H	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	H	37	ILE	Peptide

5.2 Too-close contacts [i](#)

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	A	2109	0	2175	38	0
2	B	1571	0	1610	26	0
3	C	1485	0	1504	20	0
4	D	865	0	408	5	0
5	E	1327	0	1386	39	0
6	F	1122	0	1146	20	0
7	G	945	0	1007	22	0
8	H	1071	0	1141	15	0
9	I	1086	0	1162	19	0
10	J	950	0	998	5	0
11	K	864	0	905	9	0
12	L	919	0	973	18	0
13	M	934	0	997	14	0
14	N	806	0	842	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	O	825	0	891	13	0
16	P	717	0	777	11	0
17	Q	761	0	811	15	0
18	R	753	0	774	9	0
19	S	577	0	580	9	0
20	T	631	0	667	8	0
21	U	490	0	531	10	0
22	V	453	0	482	5	0
23	W	213	0	100	1	0
24	X	447	0	435	8	0
25	Y	426	0	462	8	0
26	Z	362	0	401	5	0
27	1	57324	0	28814	509	0
28	5	2450	0	1241	16	0
29	6	112	0	56	0	0
29	8	169	0	89	1	0
30	a	508	0	566	4	0
31	b	294	0	326	7	0
32	1	159	0	0	0	0
32	5	3	0	0	0	0
33	1	42	0	38	3	0
33	5	84	0	76	7	0
34	b	1	0	0	0	0
All	All	83855	0	54371	811	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 6.

The worst 5 of 811 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)
27:1:1014:G:H1	27:1:1130:C:H5	1.15	0.88
27:1:703:G:N2	27:1:710:C:O2	2.06	0.87
27:1:2086:U:H3	27:1:2181:G:H1	0.88	0.87
13:M:6:ARG:NH2	27:1:576:G:N7	2.24	0.86
13:M:37:GLN:HE21	27:1:1240:G:H1	1.24	0.86

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	270/274 (98%)	263 (97%)	7 (3%)	0	100	100
2	B	209/212 (99%)	202 (97%)	6 (3%)	1 (0%)	24	43
3	C	197/200 (98%)	188 (95%)	8 (4%)	1 (0%)	24	43
4	D	174/178 (98%)	155 (89%)	19 (11%)	0	100	100
5	E	173/177 (98%)	160 (92%)	13 (8%)	0	100	100
6	F	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
7	G	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
8	H	142/146 (97%)	136 (96%)	6 (4%)	0	100	100
9	I	135/137 (98%)	131 (97%)	4 (3%)	0	100	100
10	J	118/125 (94%)	113 (96%)	5 (4%)	0	100	100
11	K	113/116 (97%)	110 (97%)	3 (3%)	0	100	100
12	L	115/122 (94%)	114 (99%)	1 (1%)	0	100	100
13	M	115/119 (97%)	114 (99%)	1 (1%)	0	100	100
14	N	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
15	O	107/110 (97%)	105 (98%)	2 (2%)	0	100	100
16	P	90/106 (85%)	87 (97%)	3 (3%)	0	100	100
17	Q	100/105 (95%)	90 (90%)	10 (10%)	0	100	100
18	R	94/98 (96%)	87 (93%)	7 (7%)	0	100	100
19	S	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
20	T	75/78 (96%)	75 (100%)	0	0	100	100
21	U	59/65 (91%)	52 (88%)	7 (12%)	0	100	100
22	V	55/58 (95%)	53 (96%)	2 (4%)	0	100	100
23	W	41/74 (55%)	32 (78%)	9 (22%)	0	100	100
24	X	52/61 (85%)	49 (94%)	3 (6%)	0	100	100
25	Y	49/51 (96%)	47 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	Z	42/44 (96%)	40 (95%)	2 (5%)	0	100	100
30	a	61/64 (95%)	58 (95%)	3 (5%)	0	100	100
31	b	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
All	All	3057/3210 (95%)	2917 (95%)	138 (4%)	2 (0%)	49	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	141	VAL
3	C	5	THR

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	A	218/220 (99%)	209 (96%)	9 (4%)	27	53
2	B	166/167 (99%)	152 (92%)	14 (8%)	10	22
3	C	145/155 (94%)	137 (94%)	8 (6%)	19	40
5	E	140/142 (99%)	124 (89%)	16 (11%)	5	12
6	F	117/117 (100%)	111 (95%)	6 (5%)	21	43
7	G	103/103 (100%)	96 (93%)	7 (7%)	14	31
8	H	106/108 (98%)	100 (94%)	6 (6%)	18	39
9	I	113/113 (100%)	107 (95%)	6 (5%)	20	42
10	J	97/101 (96%)	96 (99%)	1 (1%)	68	86
11	K	84/85 (99%)	80 (95%)	4 (5%)	23	46
12	L	99/102 (97%)	96 (97%)	3 (3%)	36	64
13	M	85/86 (99%)	84 (99%)	1 (1%)	63	83
14	N	84/84 (100%)	81 (96%)	3 (4%)	31	58
15	O	88/89 (99%)	84 (96%)	4 (4%)	24	49
16	P	78/87 (90%)	73 (94%)	5 (6%)	16	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	Q	83/85 (98%)	77 (93%)	6 (7%)	13	28
18	R	78/79 (99%)	76 (97%)	2 (3%)	40	68
19	S	59/64 (92%)	53 (90%)	6 (10%)	7	15
20	T	69/70 (99%)	64 (93%)	5 (7%)	13	28
21	U	53/56 (95%)	47 (89%)	6 (11%)	5	12
22	V	53/54 (98%)	50 (94%)	3 (6%)	18	39
24	X	46/50 (92%)	43 (94%)	3 (6%)	15	32
25	Y	47/47 (100%)	43 (92%)	4 (8%)	10	22
26	Z	36/36 (100%)	34 (94%)	2 (6%)	19	39
30	a	52/53 (98%)	49 (94%)	3 (6%)	18	38
31	b	33/33 (100%)	32 (97%)	1 (3%)	36	64
All	All	2332/2386 (98%)	2198 (94%)	134 (6%)	20	39

5 of 134 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	U	40	SER
22	V	3	THR
30	a	23	ARG
6	F	5	SER
6	F	4	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
6	F	138	GLN
22	V	14	HIS
12	L	44	GLN
21	U	44	GLN
20	T	35	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
27	1	2667/2903 (91%)	421 (15%)	17 (0%)
28	5	114/117 (97%)	21 (18%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	6	4/77 (5%)	1 (25%)	0
29	8	7/77 (9%)	3 (42%)	0
All	All	2792/3174 (87%)	446 (15%)	17 (0%)

5 of 446 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
27	1	34	U
27	1	46	G
27	1	51	G
27	1	55	G
27	1	58	G

5 of 17 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
27	1	2414	A
27	1	2745	U
27	1	1367	U
27	1	1404	G
27	1	1575	U

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 166 ligands modelled in this entry, 163 are monoatomic - leaving 3 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
33	T1C	1	3160	32	45,45,45	1.13	4 (8%)	56,72,72	0.83	0
33	T1C	5	201	32	45,45,45	1.13	4 (8%)	56,72,72	0.74	1 (1%)
33	T1C	5	205	32	45,45,45	1.15	4 (8%)	56,72,72	0.73	1 (1%)

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
33	T1C	1	3160	32	-	6/22/80/80	0/4/4/4
33	T1C	5	201	32	-	8/22/80/80	0/4/4/4
33	T1C	5	205	32	-	5/22/80/80	0/4/4/4

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	5	205	T1C	C21-N21	4.90	1.47	1.33
33	5	201	T1C	C21-N21	4.87	1.47	1.33
33	1	3160	T1C	C21-N21	4.86	1.47	1.33
33	1	3160	T1C	C4-N4	2.22	1.52	1.47
33	5	205	T1C	O11-C11	2.21	1.27	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	5	201	T1C	C1C-C1-C2	2.03	118.97	115.75
33	5	205	T1C	O1C-C1C-C12	-2.02	106.90	110.14

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

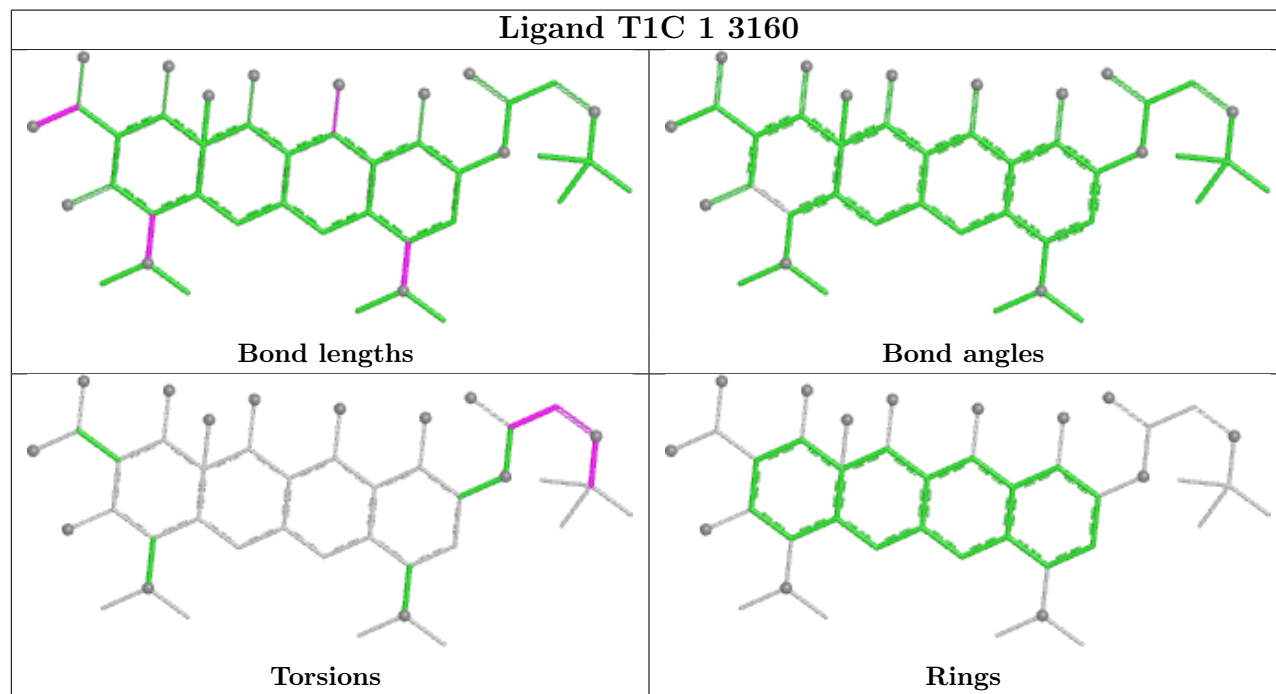
Mol	Chain	Res	Type	Atoms
33	1	3160	T1C	C94-C93-N92-C92
33	1	3160	T1C	C95-C93-N92-C92
33	1	3160	T1C	C96-C93-N92-C92
33	5	201	T1C	C94-C93-N92-C92
33	5	201	T1C	C95-C93-N92-C92

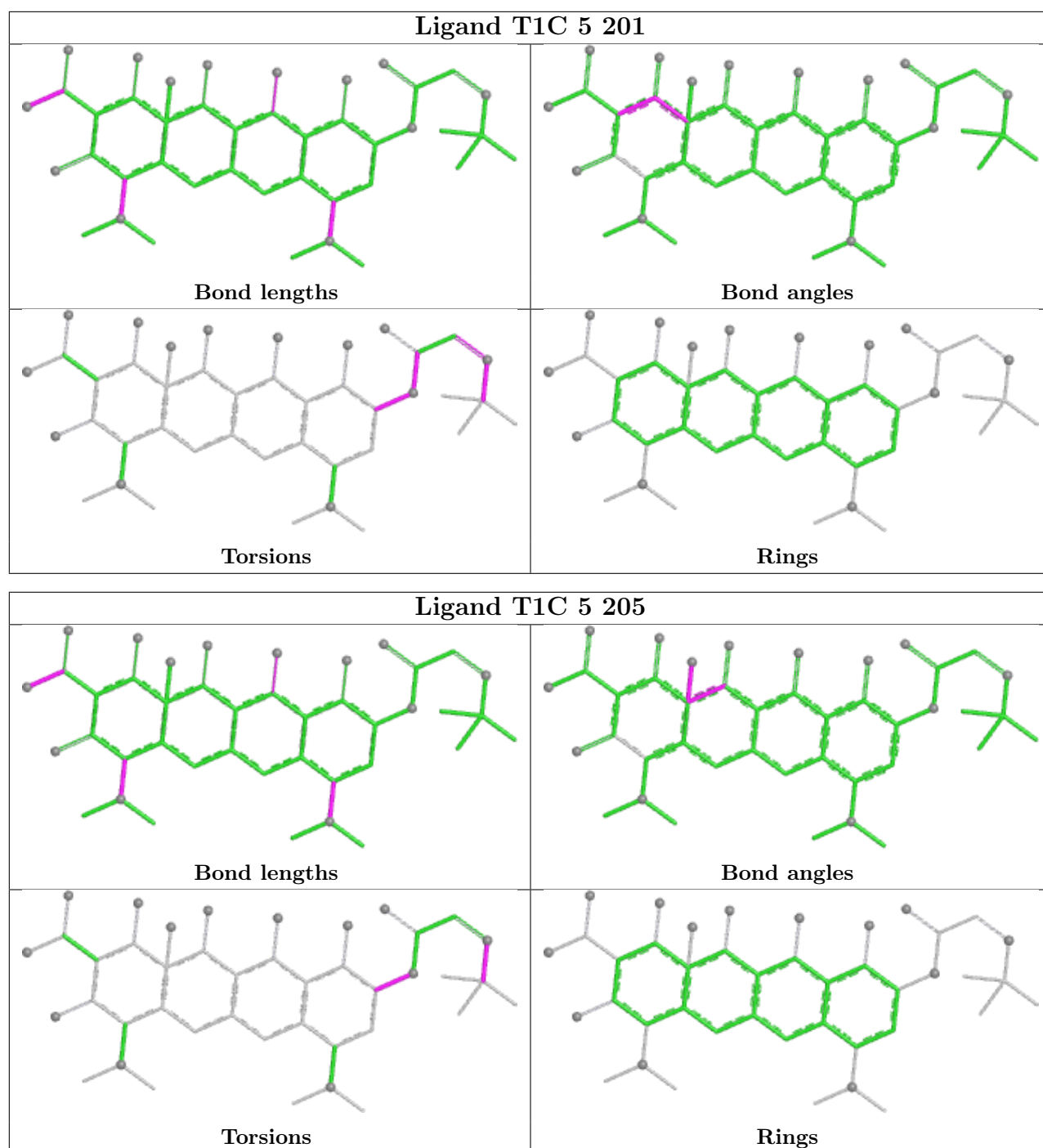
There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	1	3160	T1C	3	0
33	5	201	T1C	5	0
33	5	205	T1C	3	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

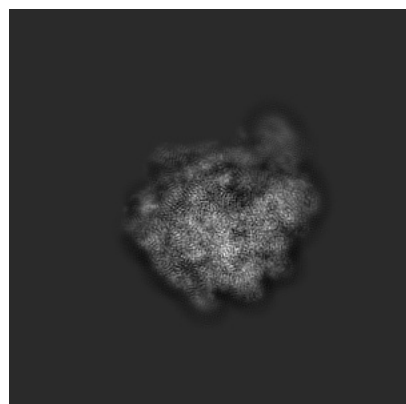
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10898. These allow visual inspection of the internal detail of the map and identification of artifacts.

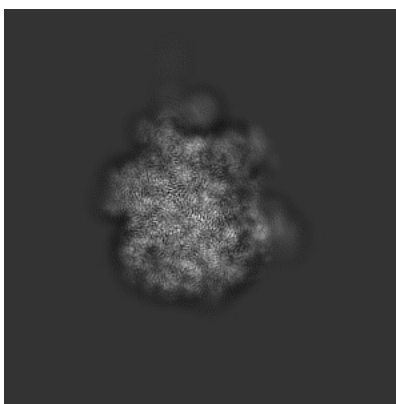
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

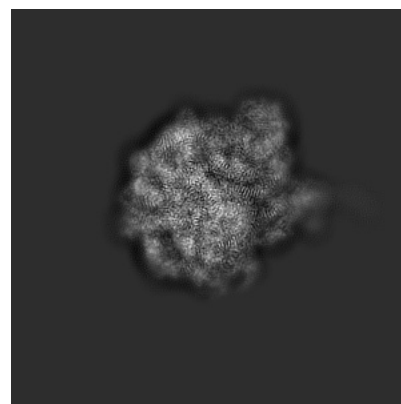
6.1.1 Primary map



X

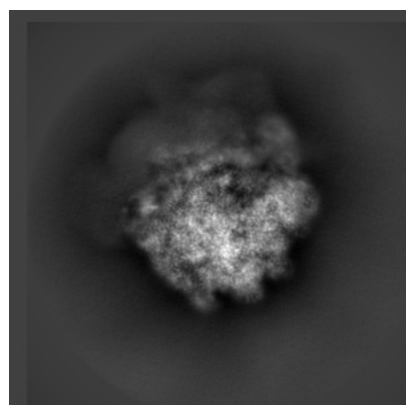


Y

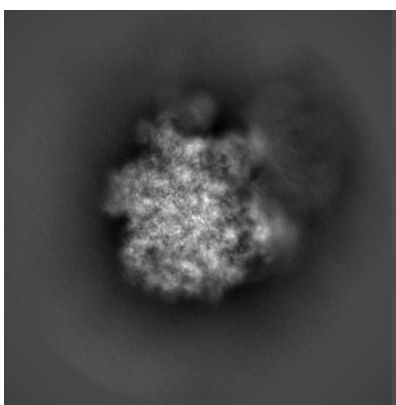


Z

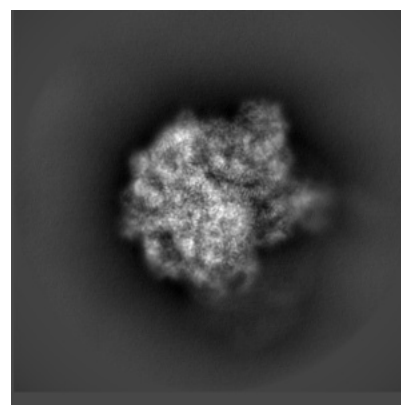
6.1.2 Raw map



X



Y

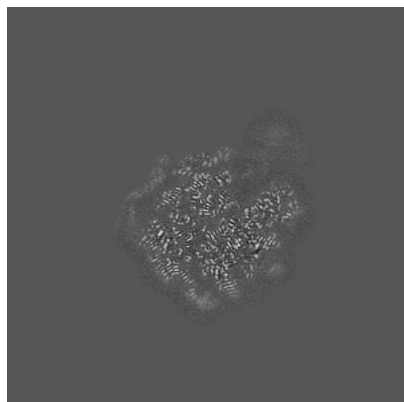


Z

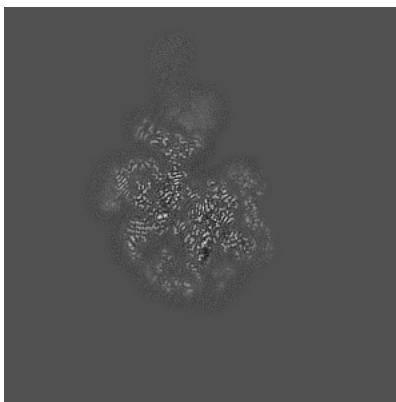
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

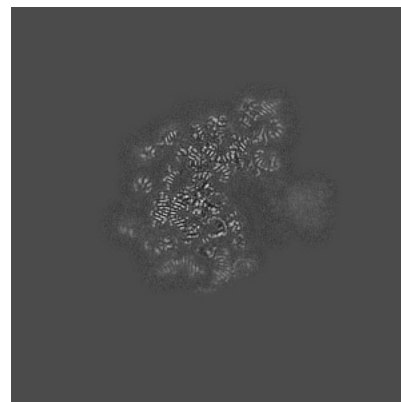
6.2.1 Primary map



X Index: 200

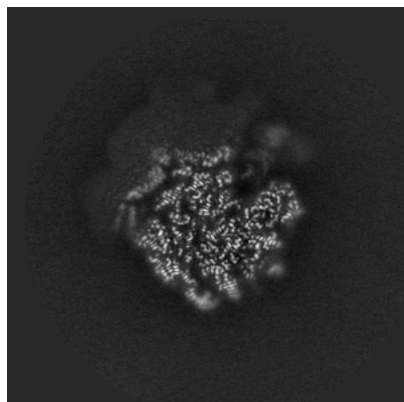


Y Index: 200

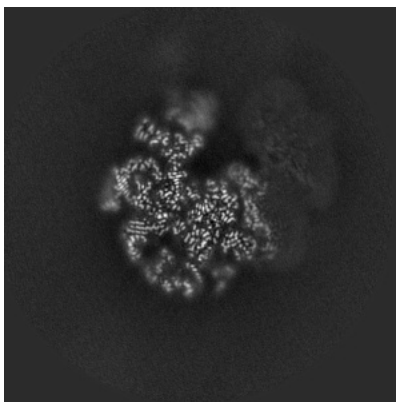


Z Index: 200

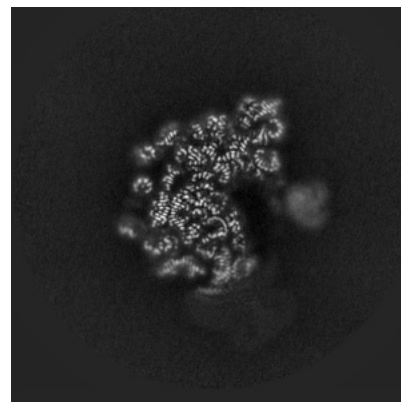
6.2.2 Raw map



X Index: 200



Y Index: 200

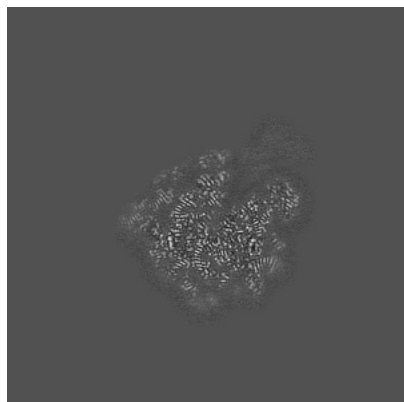


Z Index: 200

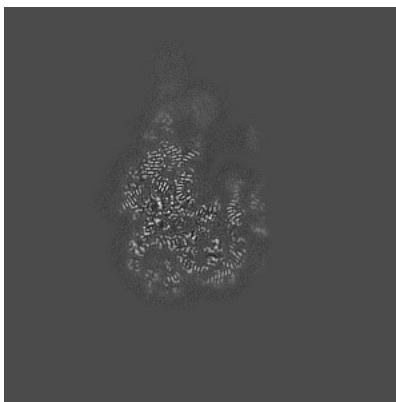
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

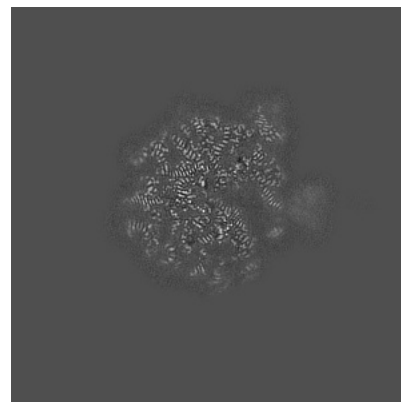
6.3.1 Primary map



X Index: 208

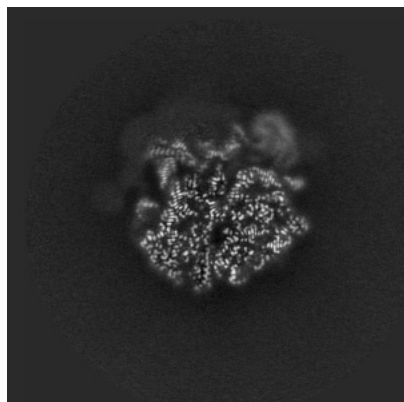


Y Index: 218

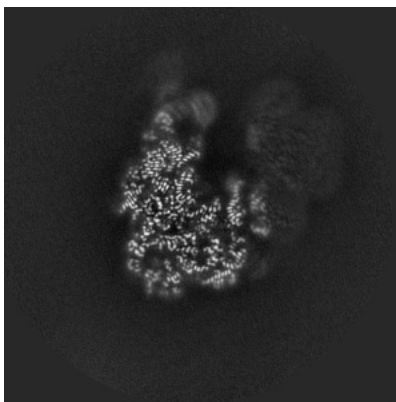


Z Index: 191

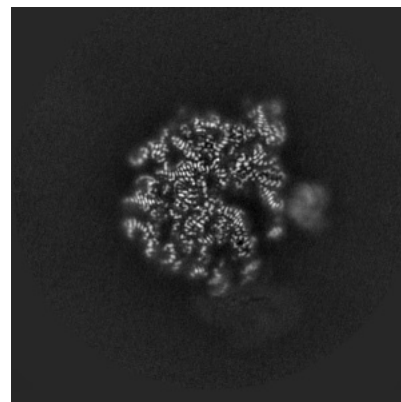
6.3.2 Raw map



X Index: 179



Y Index: 218

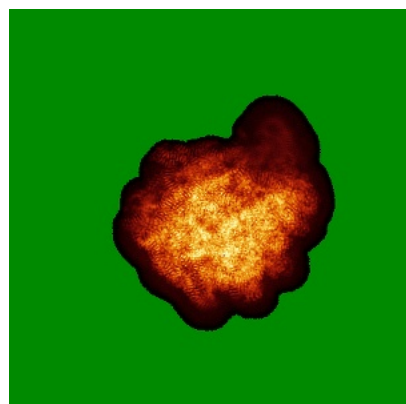


Z Index: 192

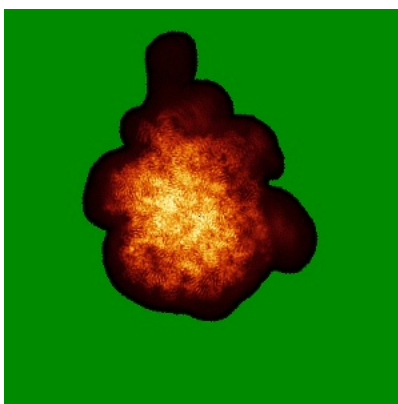
The images above show the largest variance slices of the map in three orthogonal directions.

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

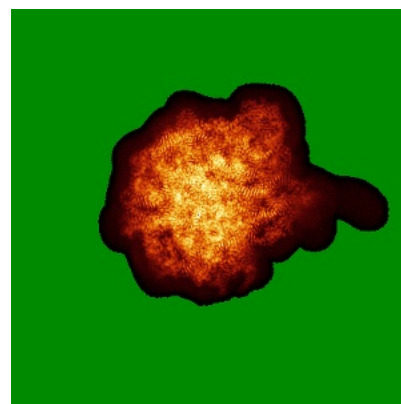
6.4.1 Primary map



X

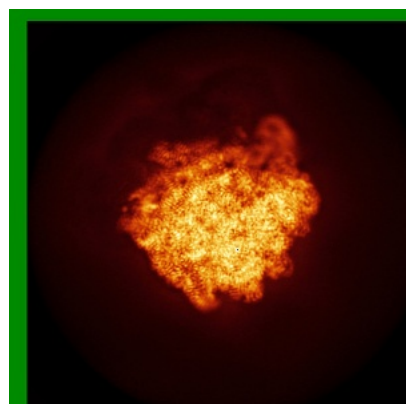


Y

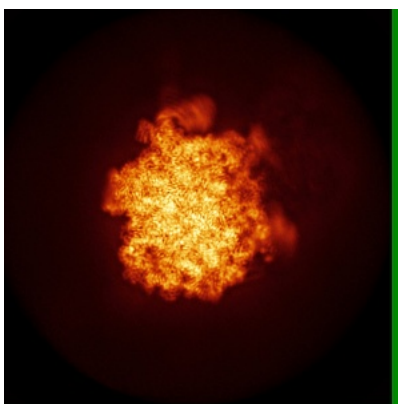


Z

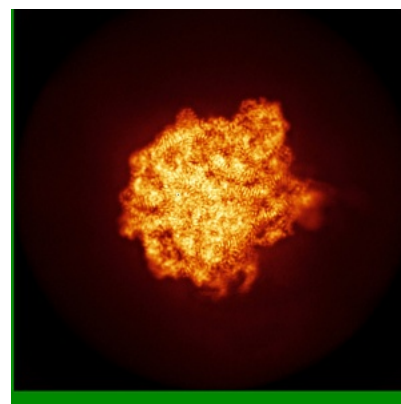
6.4.2 Raw map



X



Y

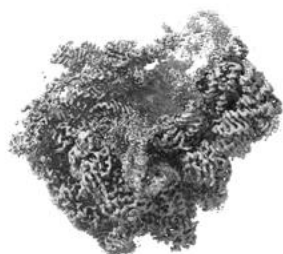


Z

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](#)

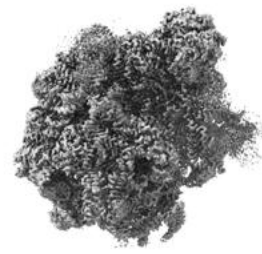
6.5.1 Primary map



X



Y



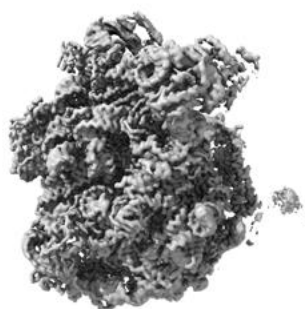
Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

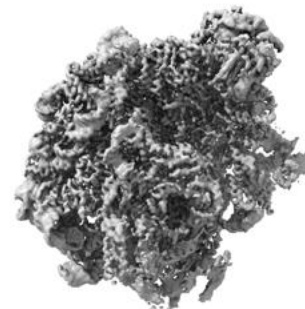
6.5.2 Raw map



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.

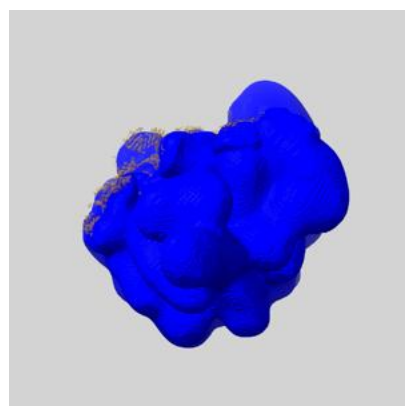
6.6 Mask visualisation [i](#)

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

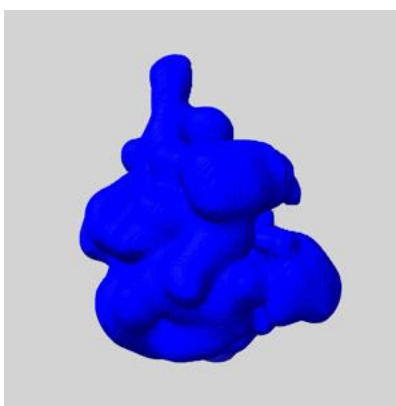
A mask typically either:

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

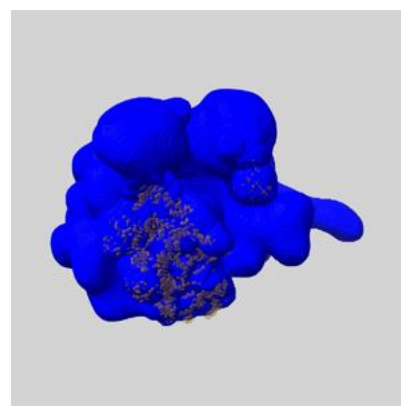
6.6.1 emd_10898_msk_1.map [i](#)



X



Y

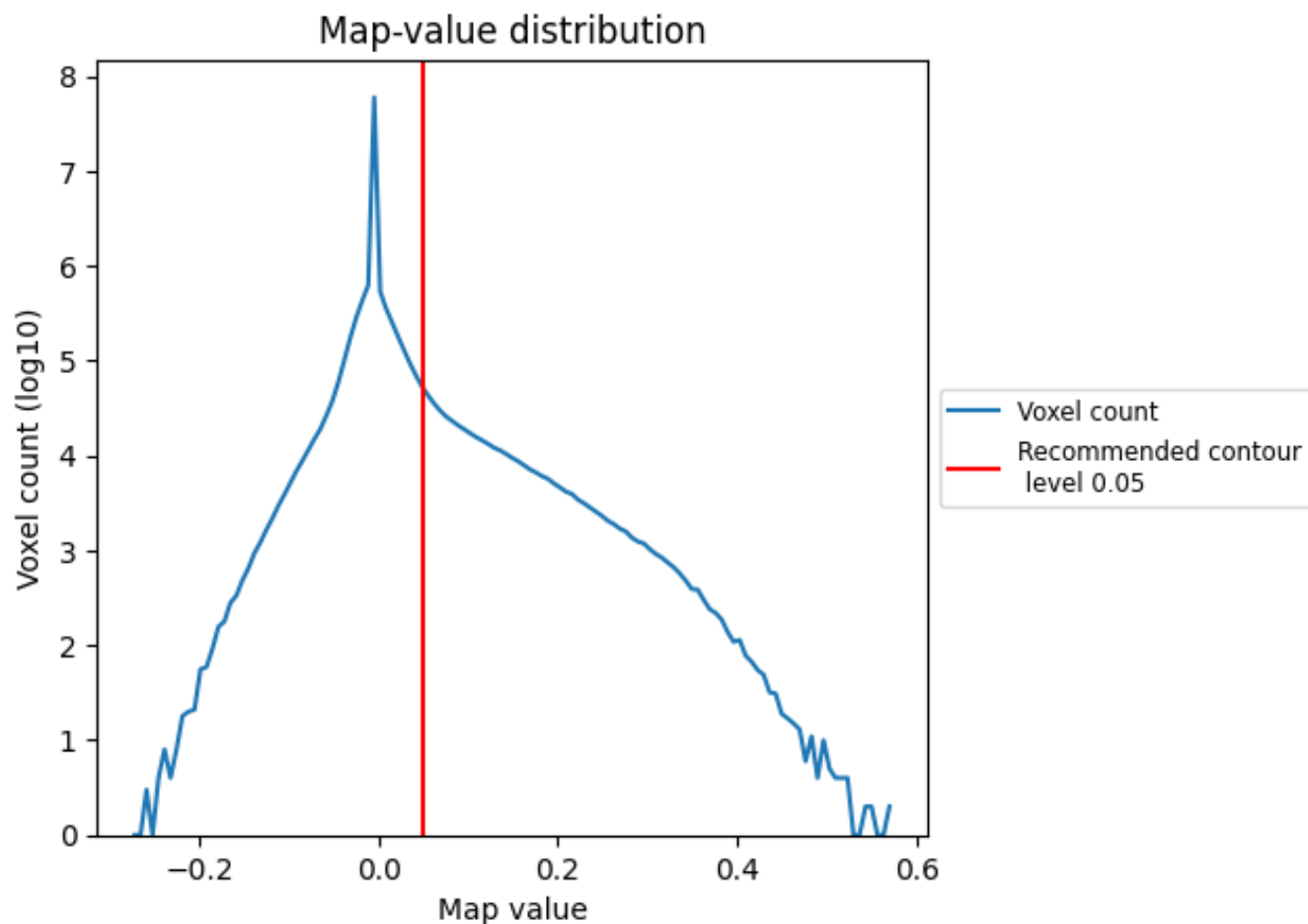


Z

7 Map analysis [i](#)

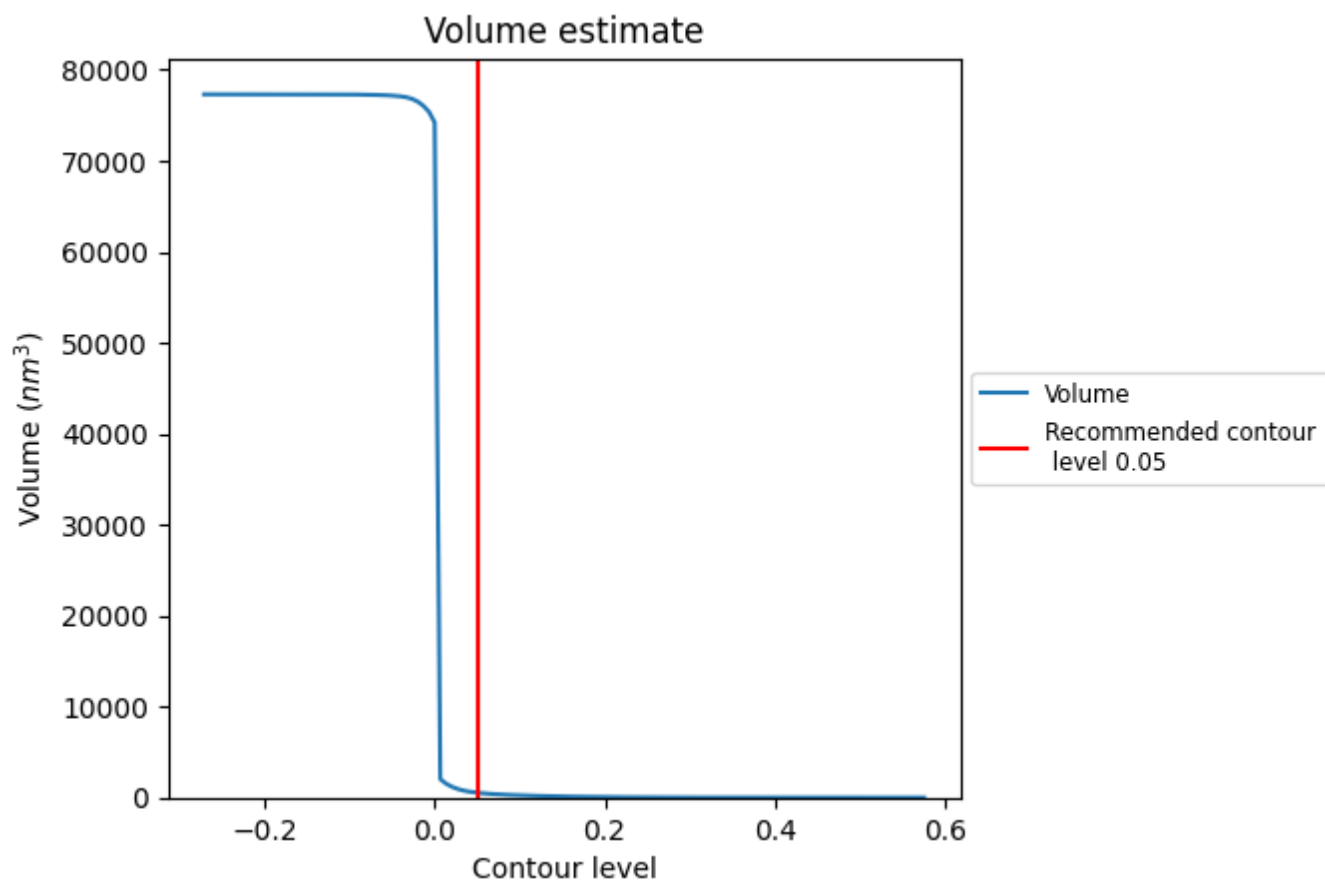
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

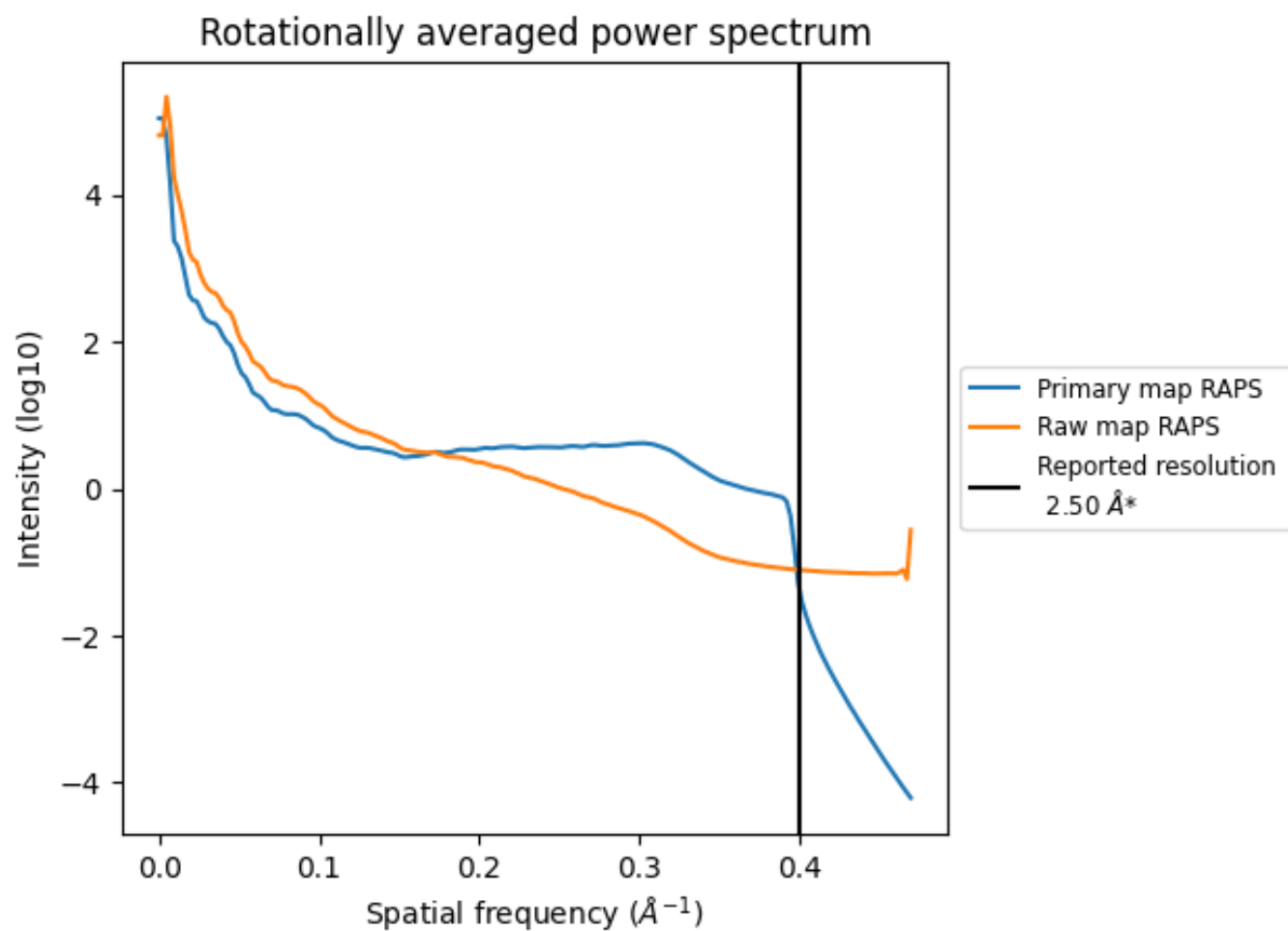
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 530 nm³; this corresponds to an approximate mass of 479 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 ⓘ

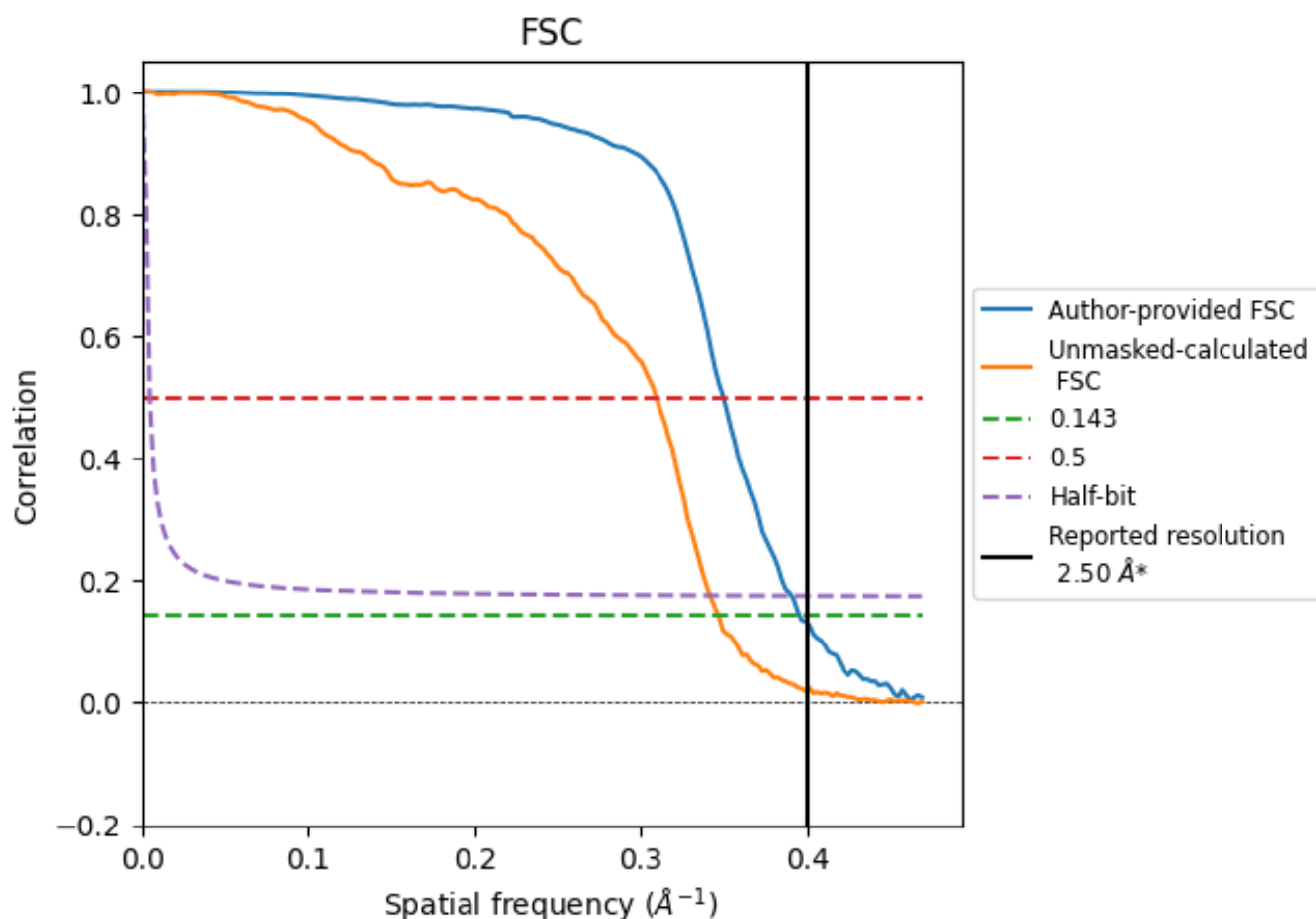


*Reported resolution corresponds to spatial frequency of 0.400 $\text{\AA}^{-1}$

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 0.400 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

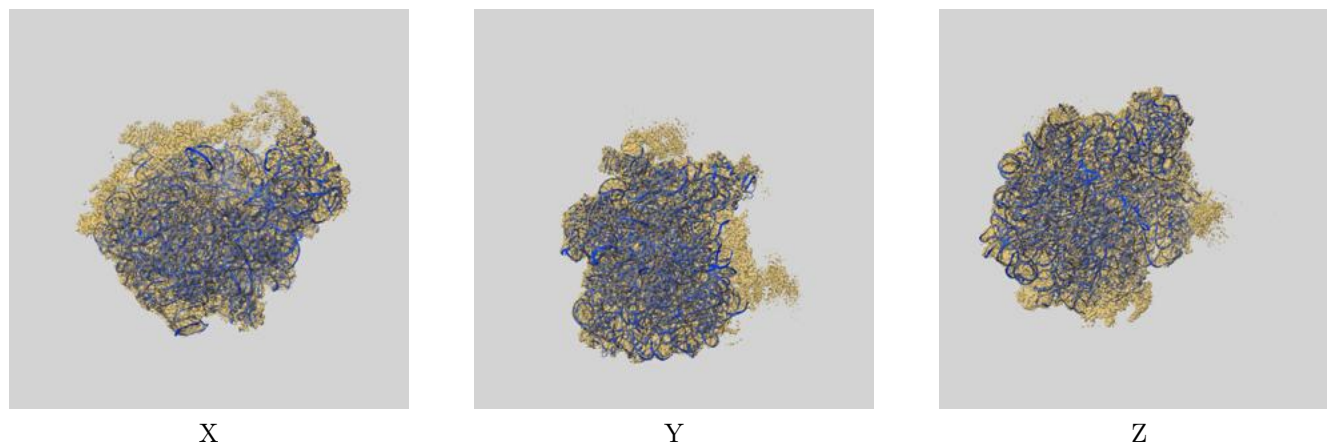
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.53	2.86	2.56
Unmasked-calculated*	2.88	3.23	2.92

*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 2.88 differs from the reported value 2.5 by more than 10 %

9 Map-model fit [i](#)

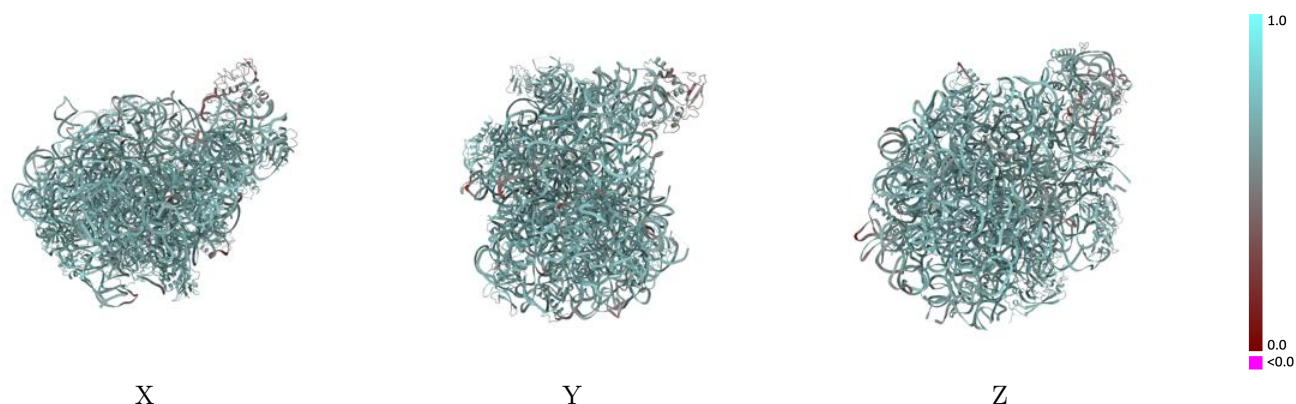
This section contains information regarding the fit between EMDB map EMD-10898 and PDB model 6YSI. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



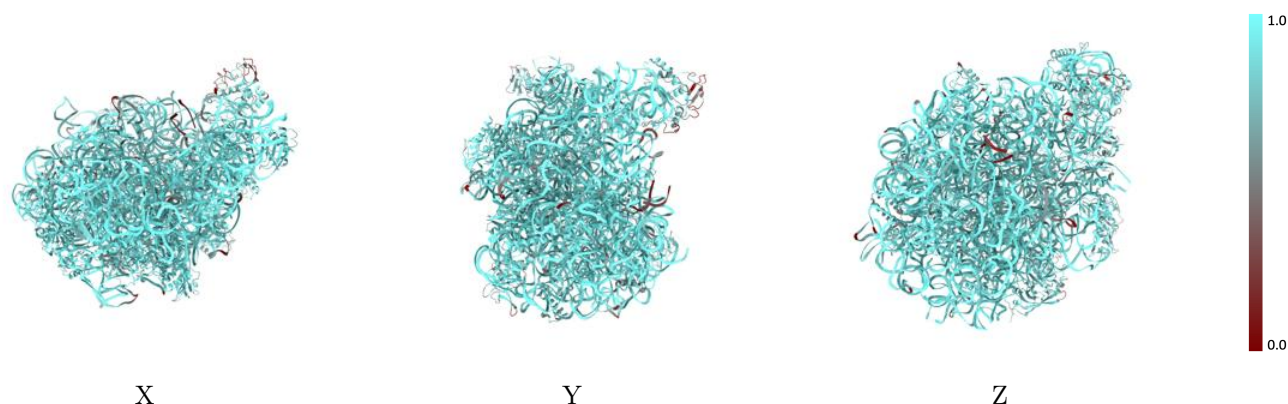
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



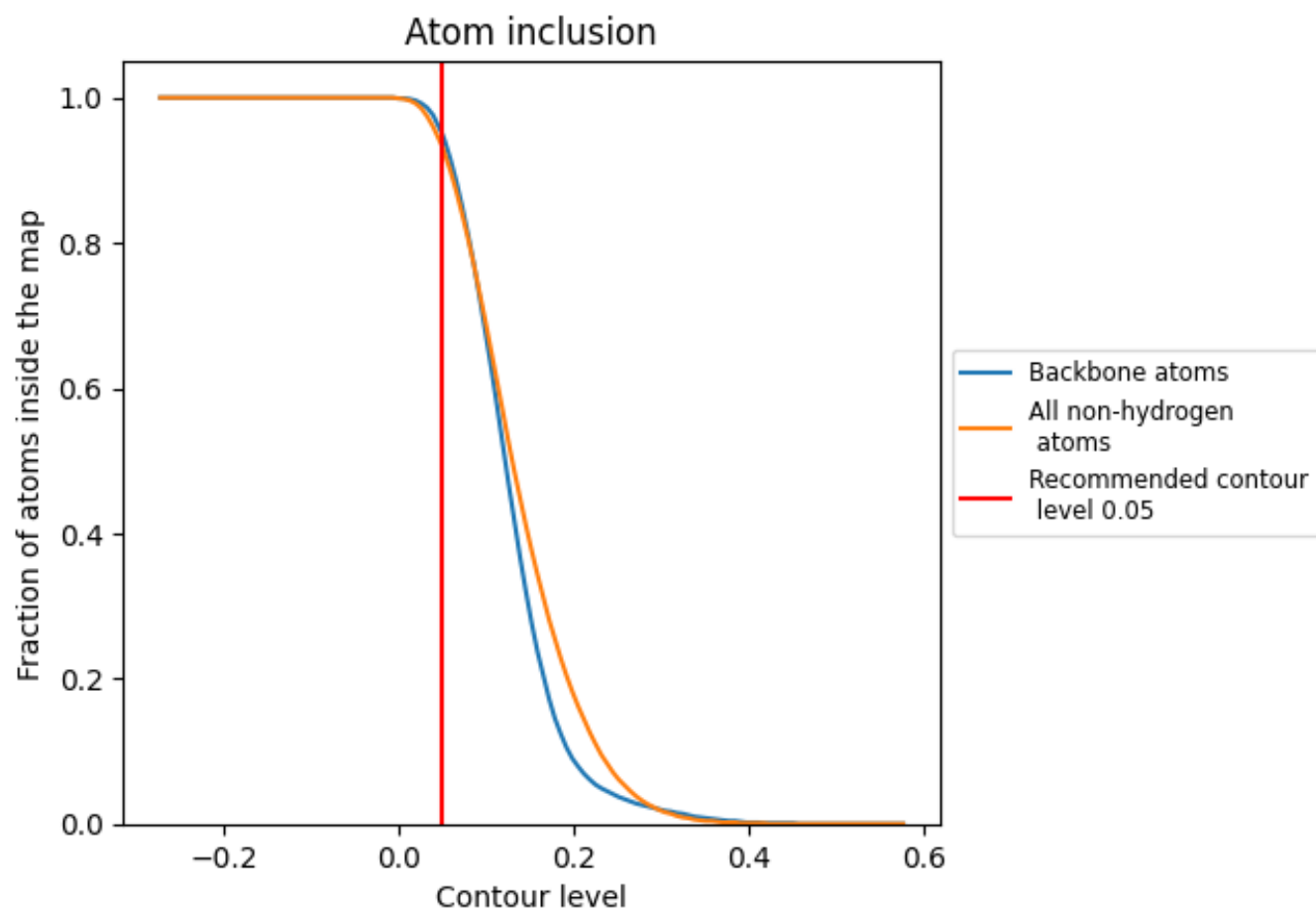
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 93% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9330	 0.6530
1	 0.9610	 0.6570
5	 0.9400	 0.6210
6	 0.2050	 0.5220
8	 0.2600	 0.5620
A	 0.9100	 0.6730
B	 0.9110	 0.6660
C	 0.8870	 0.6490
D	 0.7120	 0.5180
E	 0.7590	 0.5990
F	 0.9090	 0.6690
G	 0.8500	 0.6590
H	 0.9070	 0.6670
I	 0.8640	 0.6580
J	 0.9510	 0.6790
K	 0.8760	 0.6310
L	 0.8560	 0.6550
M	 0.9590	 0.6860
N	 0.8980	 0.6580
O	 0.8770	 0.6670
P	 0.7990	 0.6400
Q	 0.7220	 0.5950
R	 0.8410	 0.6410
S	 0.9340	 0.6830
T	 0.8730	 0.6660
U	 0.7770	 0.6070
V	 0.9120	 0.6650
W	 0.4790	 0.4480
X	 0.8780	 0.6640
Y	 0.8370	 0.6520
Z	 0.9440	 0.6920
a	 0.9690	 0.6920
b	 0.9370	 0.6730

