wwPDB EM Validation Summary Report ⓘ

Nov 12, 2026 – 12:32 pm GMT

PDB ID	:	29GX / pdb_000029gx
EMDB ID	:	EMD-57157
Title	:	Interaction of G4C2 repeat expansion in C9orf72 with ES9S of the 16S rRNA
Authors	:	von Loeffelholz, O.; Klaholz, B.; Barchet, C.
Deposited on	:	2026-03-11
Resolution	:	2.80 Å(reported)
Based on initial models	:	., 8qoi

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:

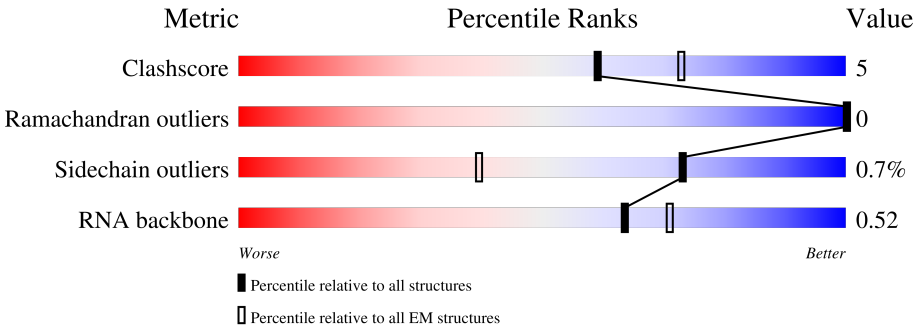
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

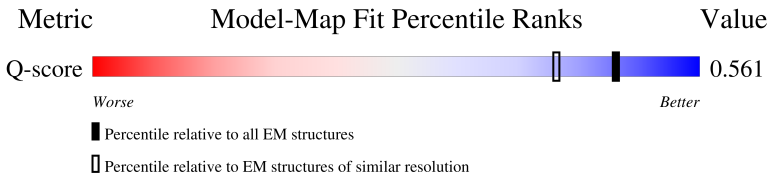
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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.





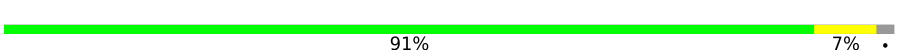
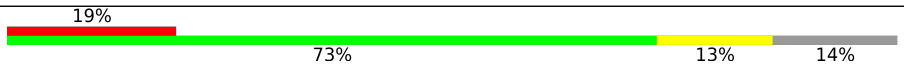
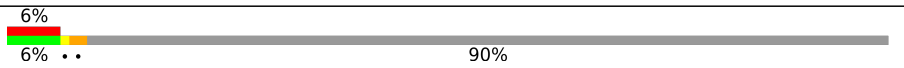
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11806 (2.30 - 3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	S2	1869	16% 6% • 77%
2	Sf	156	6% 32% 7% 61%
3	SD	243	• 84% 8% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	SF	204	
5	SK	165	
6	SP	145	
7	SQ	146	
8	SS	152	
9	ST	145	
10	SU	119	
11	Sc	69	
12	Sd	56	
13	Sg	317	
14	SM	132	
15	SZ	125	
16	SR	135	
17	C	360	

2 Entry composition (i)

There are 21 unique types of molecules in this entry. The entry contains 25368 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	S2	438	9347	4178	1658	3073	438	0	0

- Molecule 2 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	Sf	61	497	312	94	84	7	0	0

- Molecule 3 is a protein called 40S ribosomal protein S3.

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

- Molecule 4 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	SF	183	1452	909	272	264	7	0	0

- Molecule 5 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	SK	94	788	518	135	129	6	0	0

- Molecule 6 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	SP	123	1005	638	188	172	7	0	0

- Molecule 7 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SQ	140	Total	C	N	O	S	0	0
			1112	709	208	192	3		

- Molecule 8 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	SS	144	Total	C	N	O	S	0	0
			1190	746	241	202	1		

- Molecule 9 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	ST	142	Total	C	N	O	S	0	0
			1104	692	212	197	3		

- Molecule 10 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	SU	101	Total	C	N	O	S	0	0
			803	504	153	142	4		

- Molecule 11 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Sc	64	Total	C	N	O	S	0	0
			506	308	102	94	2		

- Molecule 12 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Sd	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 13 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Sg	302	Total	C	N	O	S	0	0
			2354	1486	412	444	12		

- Molecule 14 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	SM	114	Total	C	N	O	S	0	0
			868	541	153	167	7		

- Molecule 15 is a protein called Small ribosomal subunit protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	SZ	72	Total	C	N	O	S	0	0
			574	368	104	101	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	SR	77	Total	C	N	O	S	0	0
			632	398	126	106	2		

- Molecule 17 is a RNA chain called G4C2 repeat expansion in C9orf72 transcript.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	C	36	Total	C	N	O	P	0	0
			793	348	156	253	36		

- Molecule 18 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
18	S2	6	Total	K	0
			6	6	
18	SS	1	Total	K	0
			1	1	
18	Sd	1	Total	K	0
			1	1	

- Molecule 19 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
19	S2	23	Total	Mg	0
			23	23	
19	ST	1	Total	Mg	0
			1	1	

- Molecule 20 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
20	Sf	1	Total Zn 1 1	0
20	Sd	1	Total Zn 1 1	0

- Molecule 21 is water.

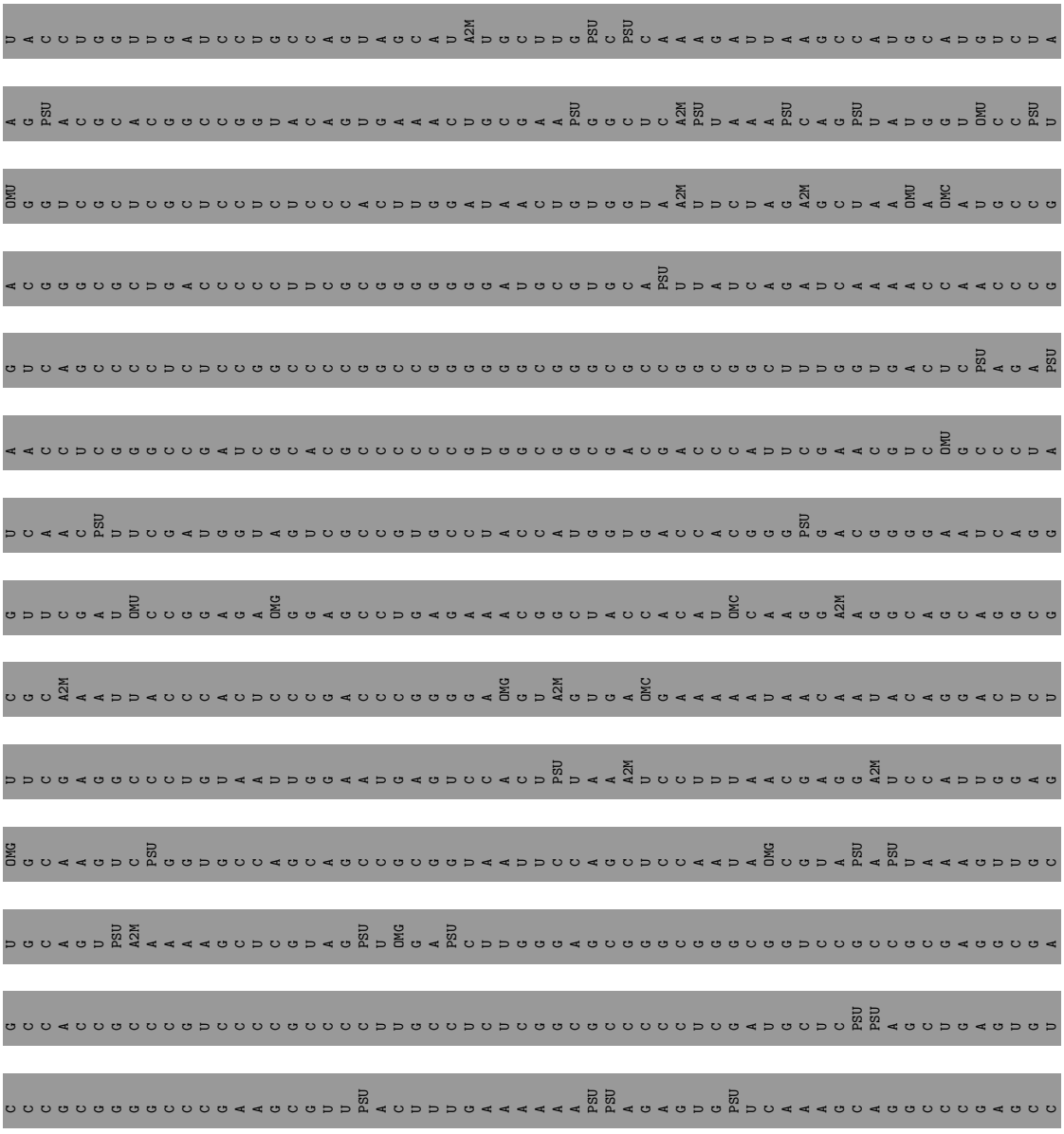
Mol	Chain	Residues	Atoms	AltConf
21	S2	100	Total O 100 100	0
21	SQ	1	Total O 1 1	0
21	SS	2	Total O 2 2	0
21	ST	2	Total O 2 2	0

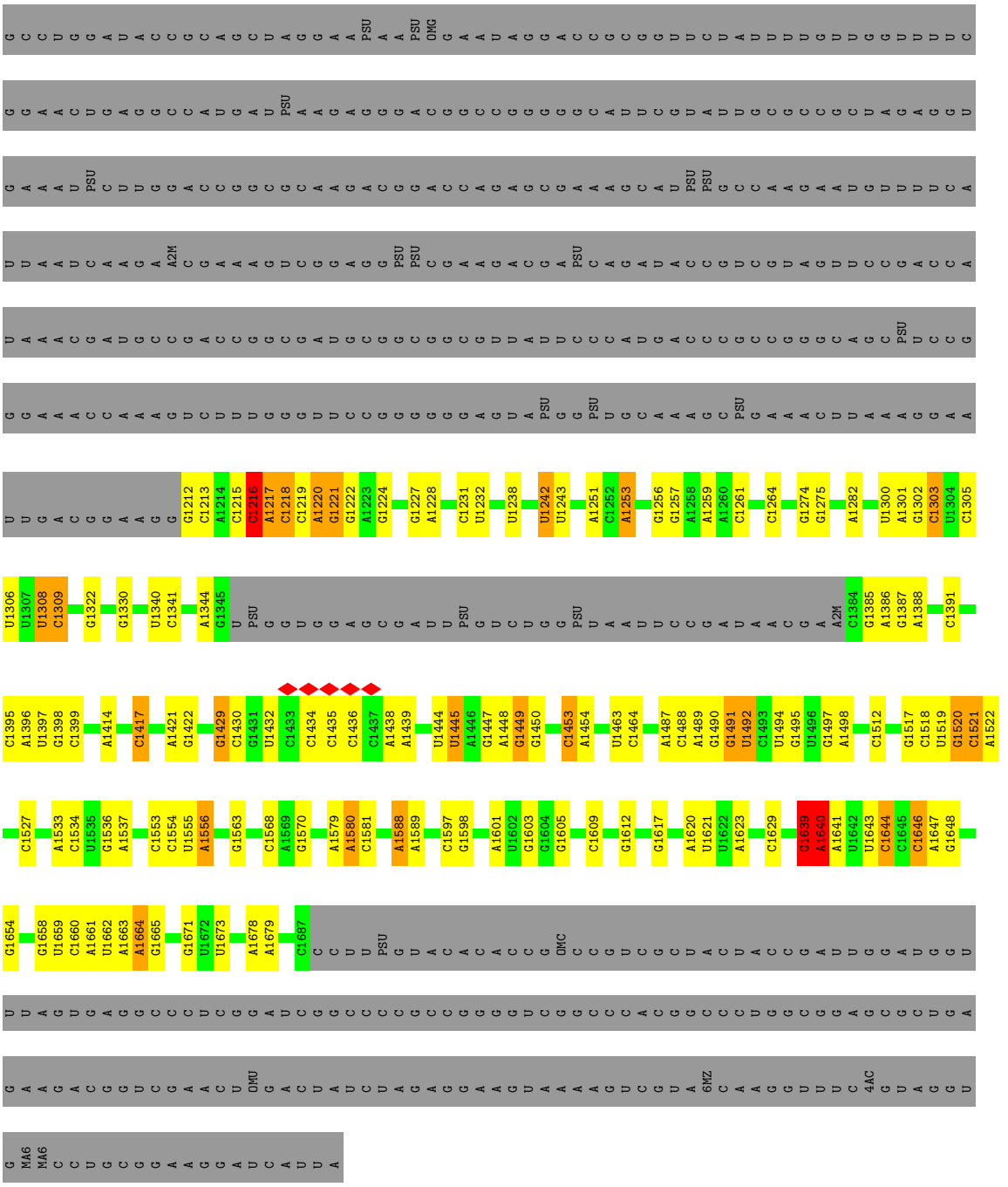
3 Residue-property plots (i)

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: 18S ribosomal RNA

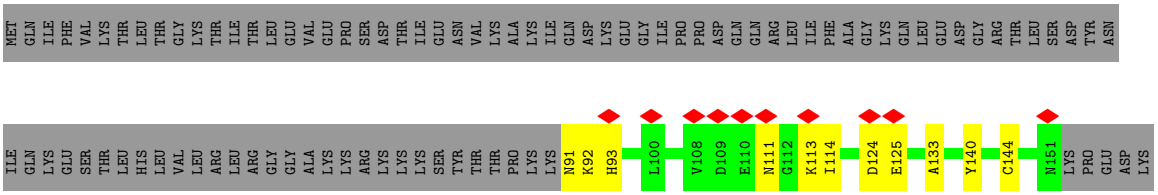
Chain S2: 16% 6% 77%





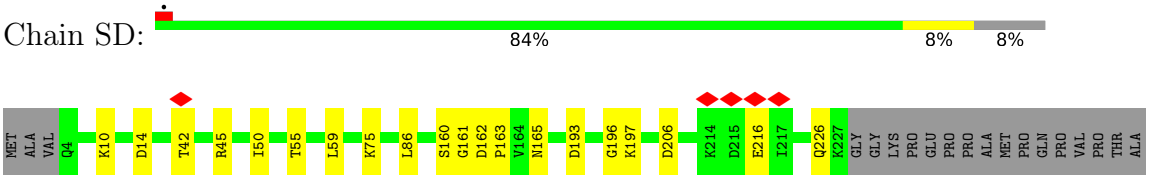
• Molecule 2: Ubiquitin





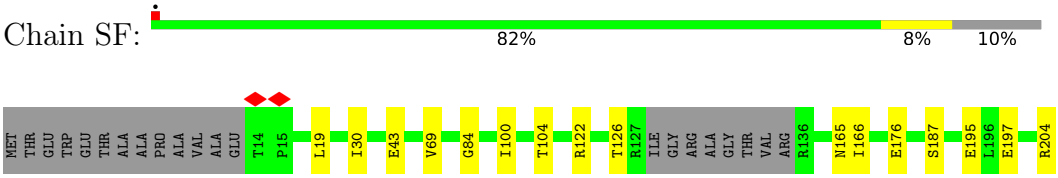
• Molecule 3: 40S ribosomal protein S3

Chain SD:



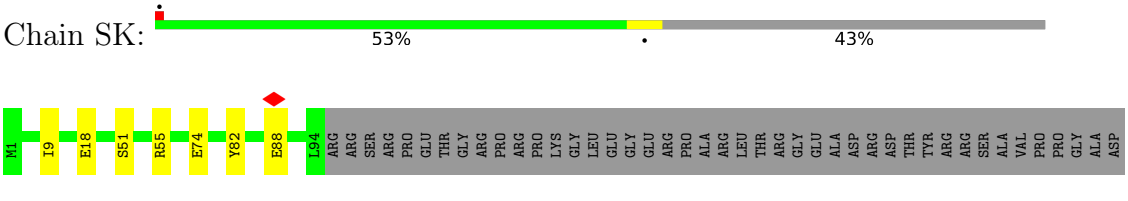
• Molecule 4: 40S ribosomal protein S5

Chain SF:



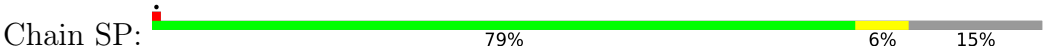
• Molecule 5: 40S ribosomal protein S10

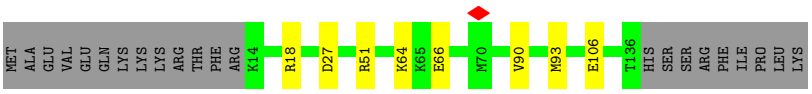
Chain SK:



• Molecule 6: 40S ribosomal protein S15

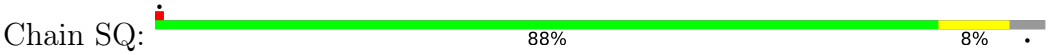
Chain SP:





• Molecule 7: 40S ribosomal protein S16

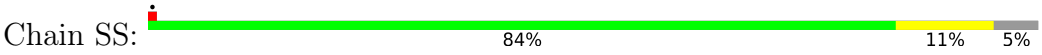
Chain SQ:

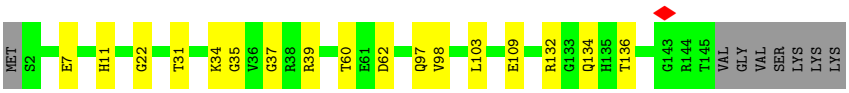




• Molecule 8: 40S ribosomal protein S18

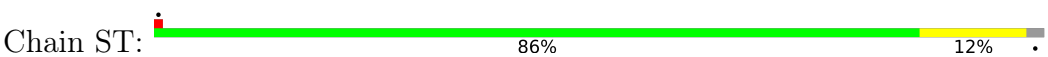
Chain SS:





• Molecule 9: Small ribosomal subunit protein eS19

Chain ST:

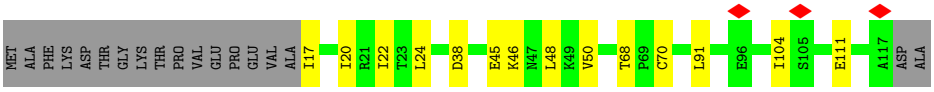




• Molecule 10: 40S ribosomal protein S20

Chain SU:





• Molecule 11: 40S ribosomal protein S28

Chain Sc:

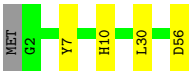




• Molecule 12: 40S ribosomal protein S29

Chain Sd:

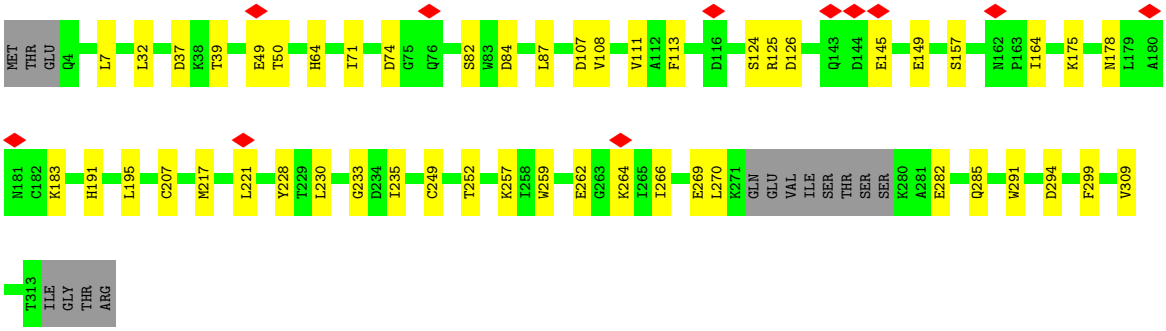




• Molecule 13: Receptor of activated protein C kinase 1

Chain Sg:

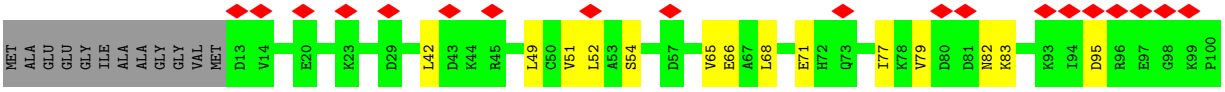


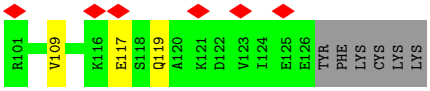


• Molecule 14: 40S ribosomal protein S12

Chain SM:



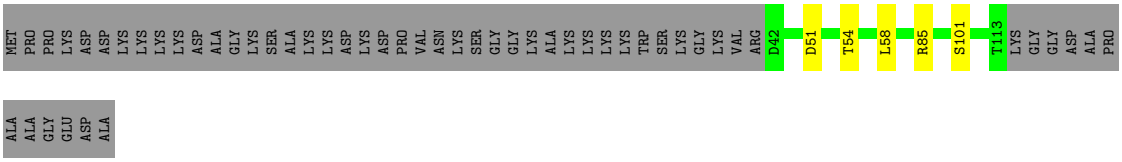




• Molecule 15: Small ribosomal subunit protein eS25

Chain SZ:

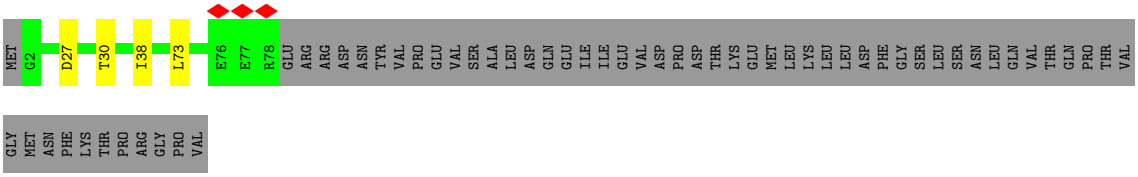




• Molecule 16: 40S ribosomal protein S17

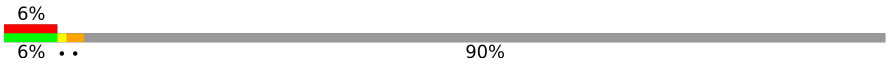
Chain SR:

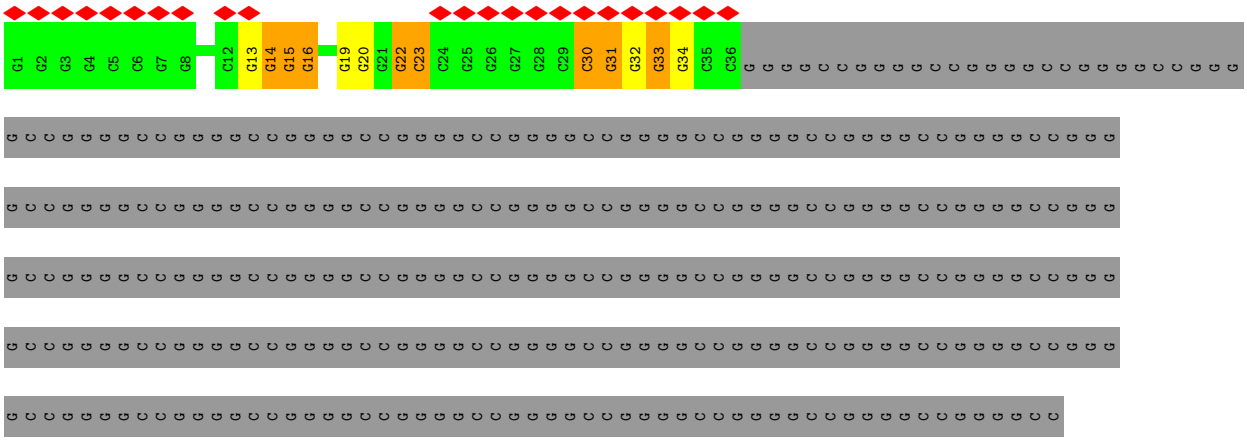




• Molecule 17: G4C2 repeat expansion in C9orf72 transcript

Chain C:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	34317	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	5000	Depositor
Maximum defocus (nm)	30000	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	52.530	Depositor
Minimum map value	-16.818	Depositor
Average map value	-0.470	Depositor
Map value standard deviation	1.703	Depositor
Recommended contour level	7.72	Depositor
Map size (Å)	306.18, 306.18, 306.18	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.729, 0.729, 0.729	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NMM, OMU, OMG, ZN, UY1, K, OMC, B8N, G7M, A2M, 4AC, MG, PSU

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	S2	0.34	1/9979 (0.0%)	0.78	29/15544 (0.2%)
2	Sf	0.14	0/507	0.36	0/673
3	SD	0.10	0/1773	0.22	0/2387
4	SF	0.10	0/1473	0.26	0/1980
5	SK	0.12	0/812	0.24	0/1097
6	SP	0.10	0/1024	0.25	0/1369
7	SQ	0.11	0/1130	0.27	0/1514
8	SS	0.10	0/1208	0.25	0/1618
9	ST	0.11	0/1110	0.25	0/1487
10	SU	0.15	0/813	0.31	0/1092
11	Sc	0.11	0/508	0.30	0/680
12	Sd	0.10	0/470	0.27	0/623
13	Sg	0.10	0/2410	0.25	0/3279
14	SM	0.11	0/876	0.26	0/1180
15	SZ	0.09	0/580	0.26	0/780
16	SR	0.09	0/639	0.23	0/851
17	C	0.27	0/888	0.88	4/1388 (0.3%)
All	All	0.23	1/26200 (0.0%)	0.57	33/37542 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1639	G7M	O3'-P	10.40	1.66	1.56

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	C	19	G	O3'-P-O5'	-16.41	72.83	104.00
1	S2	1639	G7M	O3'-P-O5'	16.22	134.82	104.00
1	S2	1639	G7M	P-O3'-C3'	-14.30	102.54	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S2	1639	G7M	OP2-P-O3'	-14.11	74.17	105.20
1	S2	1212	G	P-O3'-C3'	-10.16	107.50	119.70

There are no chirality outliers.

There are no planarity outliers.

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	S2	9347	0	4726	72	0
2	Sf	497	0	495	8	0
3	SD	1745	0	1839	17	0
4	SF	1452	0	1498	11	0
5	SK	788	0	810	7	0
6	SP	1005	0	1053	6	0
7	SQ	1112	0	1180	9	0
8	SS	1190	0	1249	13	0
9	ST	1104	0	1132	12	0
10	SU	803	0	873	12	0
11	Sc	506	0	536	7	0
12	Sd	459	0	448	3	0
13	Sg	2354	0	2310	30	0
14	SM	868	0	885	11	0
15	SZ	574	0	627	4	0
16	SR	632	0	688	3	0
17	C	793	0	397	13	0
18	S2	6	0	0	0	0
18	SS	1	0	0	0	0
18	Sd	1	0	0	0	0
19	S2	23	0	0	0	0
19	ST	1	0	0	0	0
20	Sd	1	0	0	0	0
20	Sf	1	0	0	0	0
21	S2	100	0	0	10	0
21	SQ	1	0	0	0	0
21	SS	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	ST	2	0	0	0	0
All	All	25368	0	20746	209	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 5.

The worst 5 of 209 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)
1:S2:1396:A:O2'	1:S2:1398:G:N7	2.08	0.86
1:S2:1517:G:O6	21:S2:2002:HOH:O	1.95	0.84
9:ST:32:GLU:OE1	9:ST:32:GLU:N	2.10	0.84
1:S2:1388:A:N7	21:S2:2008:HOH:O	2.10	0.83
17:C:33:G:OP2	17:C:33:G:N2	2.10	0.83

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	
2	Sf	59/156 (38%)	55 (93%)	4 (7%)	0	100	100
3	SD	222/243 (91%)	218 (98%)	4 (2%)	0	100	100
4	SF	179/204 (88%)	174 (97%)	5 (3%)	0	100	100
5	SK	92/165 (56%)	89 (97%)	3 (3%)	0	100	100
6	SP	121/145 (83%)	120 (99%)	1 (1%)	0	100	100
7	SQ	138/146 (94%)	132 (96%)	6 (4%)	0	100	100
8	SS	142/152 (93%)	142 (100%)	0	0	100	100
9	ST	139/145 (96%)	138 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	SU	99/119 (83%)	95 (96%)	4 (4%)	0	100	100
11	Sc	62/69 (90%)	60 (97%)	2 (3%)	0	100	100
12	Sd	53/56 (95%)	51 (96%)	2 (4%)	0	100	100
13	Sg	298/317 (94%)	283 (95%)	15 (5%)	0	100	100
14	SM	112/132 (85%)	109 (97%)	3 (3%)	0	100	100
15	SZ	70/125 (56%)	69 (99%)	1 (1%)	0	100	100
16	SR	75/135 (56%)	75 (100%)	0	0	100	100
All	All	1861/2309 (81%)	1810 (97%)	51 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Sf	54/140 (39%)	53 (98%)	1 (2%)	50	81
3	SD	188/202 (93%)	188 (100%)	0	100	100
4	SF	156/170 (92%)	156 (100%)	0	100	100
5	SK	85/136 (62%)	85 (100%)	0	100	100
6	SP	109/130 (84%)	108 (99%)	1 (1%)	70	89
7	SQ	116/121 (96%)	116 (100%)	0	100	100
8	SS	125/132 (95%)	125 (100%)	0	100	100
9	ST	111/114 (97%)	111 (100%)	0	100	100
10	SU	93/107 (87%)	93 (100%)	0	100	100
11	Sc	57/62 (92%)	56 (98%)	1 (2%)	51	82
12	Sd	48/49 (98%)	47 (98%)	1 (2%)	47	79
13	Sg	261/275 (95%)	256 (98%)	5 (2%)	50	81
14	SM	94/108 (87%)	93 (99%)	1 (1%)	65	87
15	SZ	64/103 (62%)	63 (98%)	1 (2%)	55	83

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
16	SR	68/122 (56%)	68 (100%)	0	100 100
All	All	1629/1971 (83%)	1618 (99%)	11 (1%)	73 91

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	Sg	282	GLU
13	Sg	294	ASP
15	SZ	101	SER
14	SM	66	GLU
13	Sg	64	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
8	SS	101	ASN
14	SM	19	GLN
9	ST	63	HIS
16	SR	26	ASN
12	Sd	45	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	S2	436/1869 (23%)	65 (14%)	2 (0%)
17	C	35/360 (9%)	7 (20%)	1 (2%)
All	All	471/2229 (21%)	72 (15%)	3 (0%)

5 of 72 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	S2	1215	C
1	S2	1216	C
1	S2	1217	A
1	S2	1221	G
1	S2	1224	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	S2	1463	U
1	S2	1646	C
17	C	30	C

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

20 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	OMG	S2	1447	1	23,26,27	0.34	0	33,38,41	0.31	0
1	UY1	S2	1326	1,19	19,22,23	0.41	0	22,31,34	0.47	0
1	OMG	S2	1328	1,18	23,26,27	0.29	0	33,38,41	0.35	0
1	PSU	S2	1445	1	18,21,22	0.44	0	22,30,33	0.47	0
1	A2M	S2	1678	1	22,25,26	0.10	0	31,36,39	0.23	0
1	PSU	S2	1643	1,19	18,21,22	0.37	0	22,30,33	0.49	0
1	PSU	S2	1625	1	18,21,22	0.51	0	22,30,33	0.55	0
1	OMC	S2	1391	1	19,22,23	0.29	0	26,31,34	0.43	0
9	NMM	ST	67	9	9,11,12	0.61	0	6,12,14	1.69	2 (33%)
1	OMC	S2	1272	1	19,22,23	0.28	0	26,31,34	0.34	0
1	4AC	S2	1337	1	21,24,25	0.31	0	29,34,37	0.36	0
1	PSU	S2	1238	1	18,21,22	0.51	0	22,30,33	0.56	0
1	PSU	S2	1244	1	18,21,22	0.46	0	22,30,33	0.56	0
1	B8N	S2	1248	1	24,29,30	0.58	0	29,42,45	0.63	0
1	G7M	S2	1639	1	23,26,27	1.43	3 (13%)	35,39,42	1.33	4 (11%)
1	OMU	S2	1442	1,19	19,22,23	0.29	0	26,31,34	0.41	0
1	OMG	S2	1490	1,19	23,26,27	0.50	0	33,38,41	0.38	0
1	OMU	S2	1288	1	19,22,23	0.29	0	26,31,34	0.44	0
1	PSU	S2	1596	1	18,21,22	0.54	0	22,30,33	0.53	0
1	PSU	S2	1232	1	18,21,22	0.45	0	22,30,33	0.61	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
1	OMG	S2	1447	1	-	1/9/27/28	0/3/3/3
1	UY1	S2	1326	1,19	-	2/9/27/28	0/2/2/2
1	OMG	S2	1328	1,18	-	0/9/27/28	0/3/3/3
1	PSU	S2	1445	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	1678	1	-	1/9/27/28	0/3/3/3
1	PSU	S2	1643	1,19	-	0/7/25/26	0/2/2/2
1	PSU	S2	1625	1	-	0/7/25/26	0/2/2/2
1	OMC	S2	1391	1	-	0/9/27/28	0/2/2/2
9	NMM	ST	67	9	-	1/9/11/13	-
1	OMC	S2	1272	1	-	0/9/27/28	0/2/2/2
1	4AC	S2	1337	1	-	0/11/29/30	0/2/2/2
1	PSU	S2	1238	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1244	1	-	0/7/25/26	0/2/2/2
1	B8N	S2	1248	1	-	4/16/34/35	0/2/2/2
1	G7M	S2	1639	1	-	0/7/25/26	0/3/3/3
1	OMU	S2	1442	1,19	-	1/9/27/28	0/2/2/2
1	OMG	S2	1490	1,19	-	2/9/27/28	0/3/3/3
1	OMU	S2	1288	1	-	0/9/27/28	0/2/2/2
1	PSU	S2	1596	1	-	2/7/25/26	0/2/2/2
1	PSU	S2	1232	1	-	2/7/25/26	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1639	G7M	C8-N7	5.19	1.42	1.33
1	S2	1639	G7M	C8-N9	3.54	1.45	1.35
1	S2	1639	G7M	C5-N7	-2.36	1.36	1.39

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S2	1639	G7M	N9-C8-N7	-4.48	101.12	112.21
1	S2	1639	G7M	C8-N7-C5	4.33	113.19	107.78
9	ST	67	NMM	NE-CZ-NH2	-3.26	116.49	119.48
1	S2	1639	G7M	CN7-N7-C8	-2.94	120.30	124.84
9	ST	67	NMM	NE-CZ-NH1	2.23	124.45	120.26

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	ST	67	NMM	O-C-CA-CB
1	S2	1232	PSU	O4'-C1'-C5-C4
1	S2	1232	PSU	O4'-C1'-C5-C6
1	S2	1248	B8N	N3-C31-C32-C33
1	S2	1326	UY1	C1'-C2'-O2'-CM2

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	S2	1445	PSU	2	0
1	S2	1678	A2M	2	0
1	S2	1391	OMC	1	0
1	S2	1238	PSU	1	0
1	S2	1639	G7M	1	0
1	S2	1232	PSU	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 34 ligands modelled in this entry, 34 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	S2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S2	1638:G	O3'	1639:G7M	P	2.84

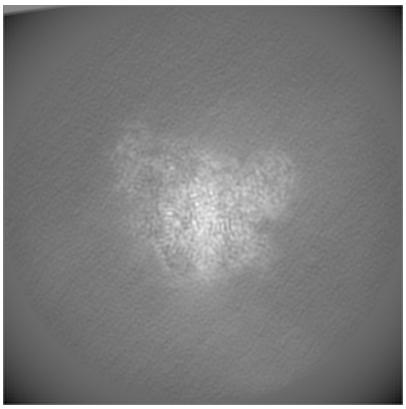
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-57157. These allow visual inspection of the internal detail of the map and identification of artifacts.

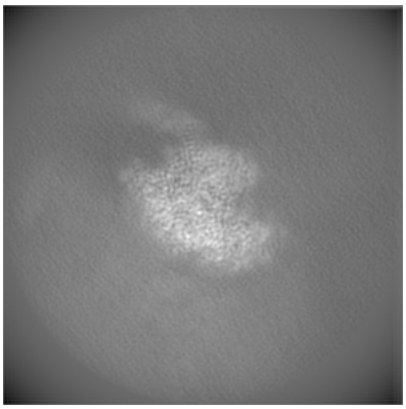
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

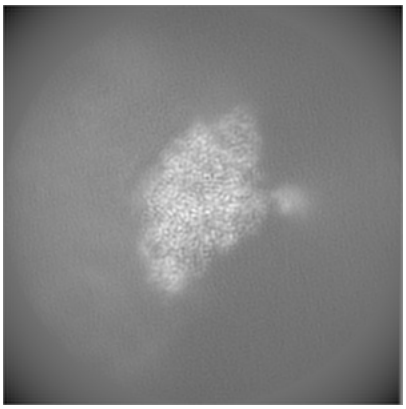
6.1.1 Primary map



X

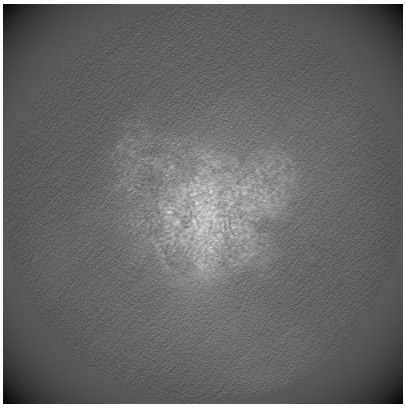


Y

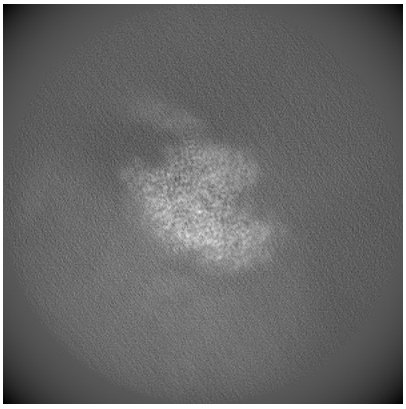


Z

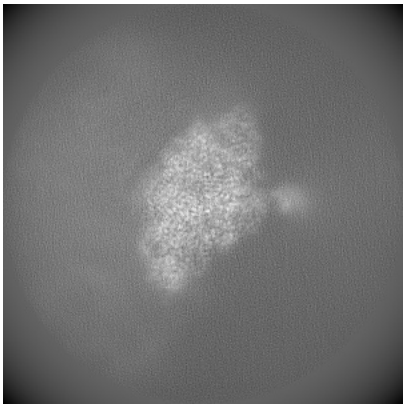
6.1.2 Raw map



X



Y

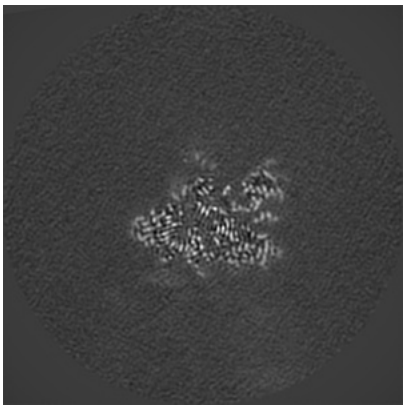


Z

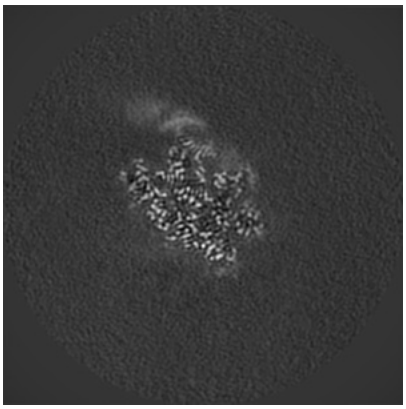
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

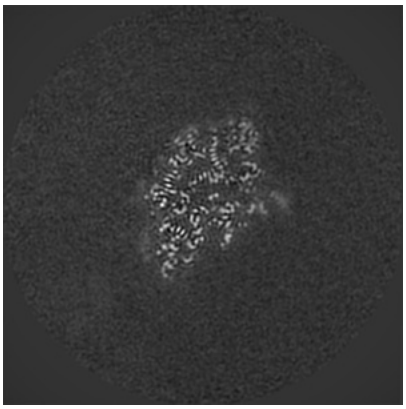
6.2.1 Primary map



X Index: 210

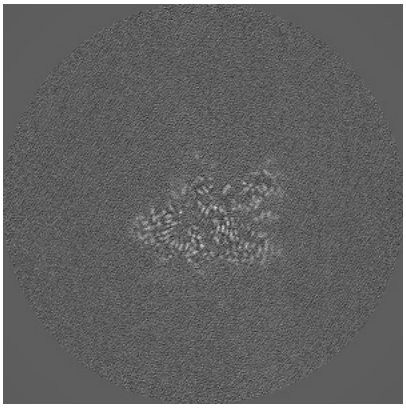


Y Index: 210

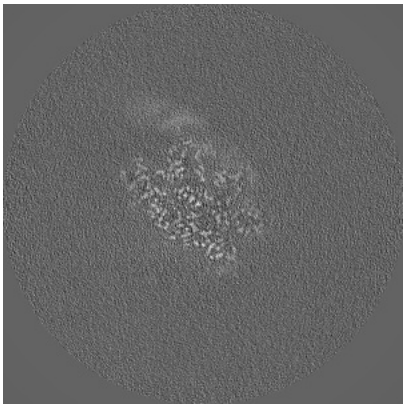


Z Index: 210

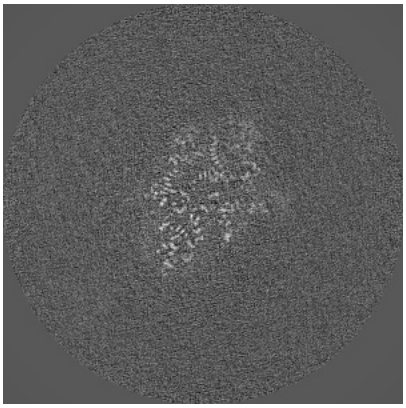
6.2.2 Raw map



X Index: 210



Y Index: 210

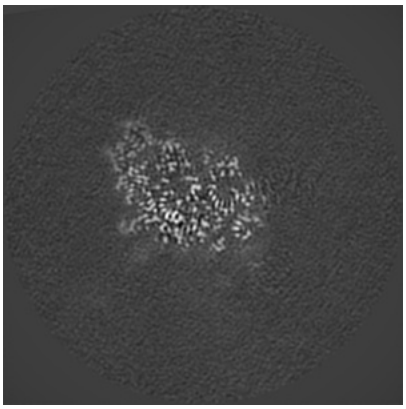


Z Index: 210

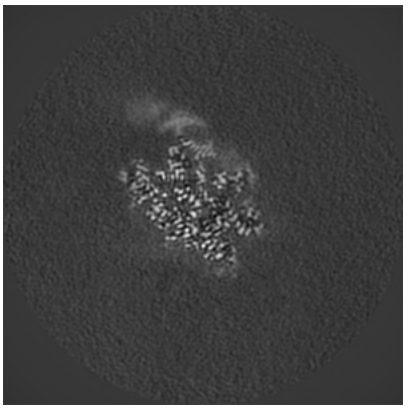
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

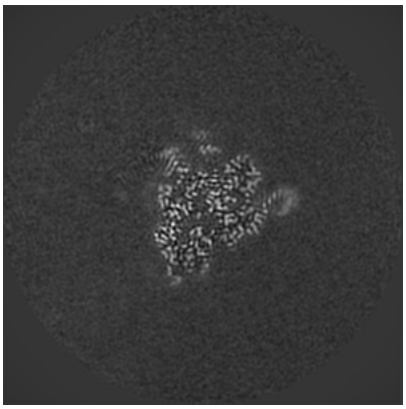
6.3.1 Primary map



X Index: 176

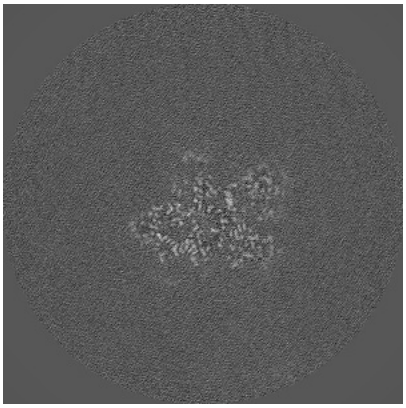


Y Index: 209

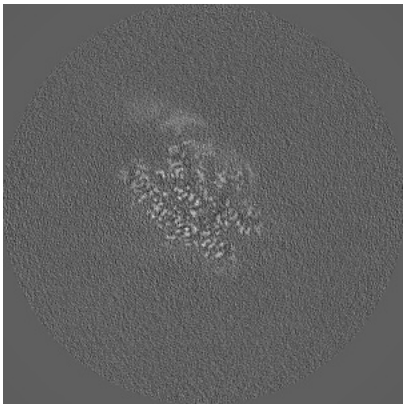


Z Index: 193

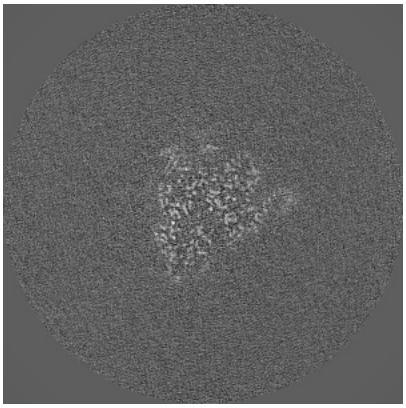
6.3.2 Raw map



X Index: 207



Y Index: 209

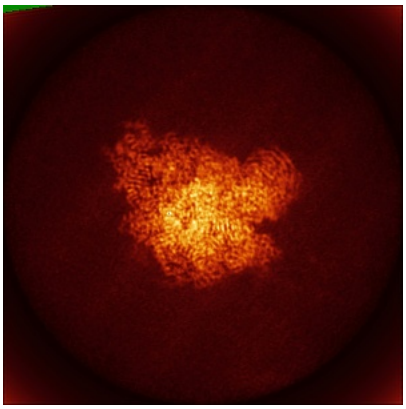


Z Index: 193

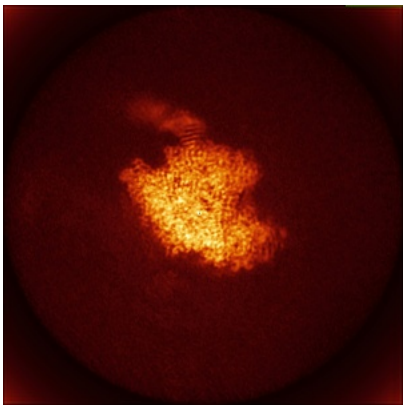
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

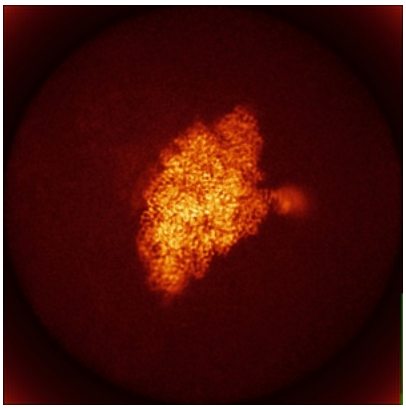
6.4.1 Primary map



X

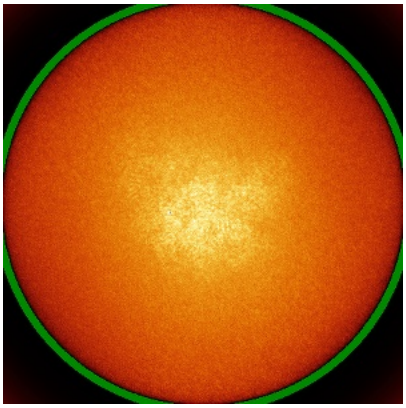


Y

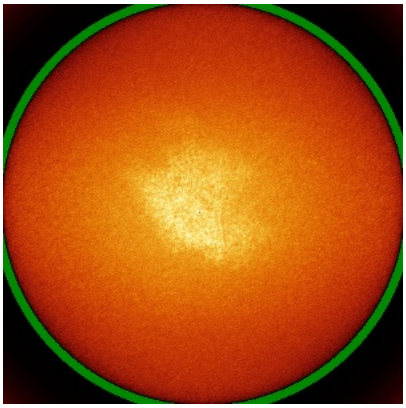


Z

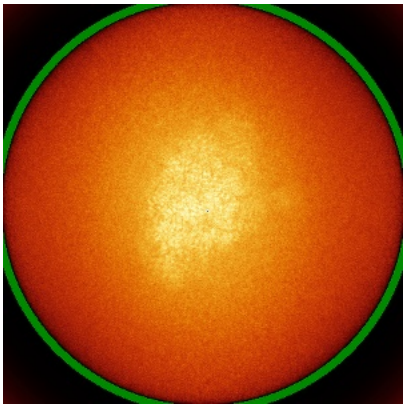
6.4.2 Raw map



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)

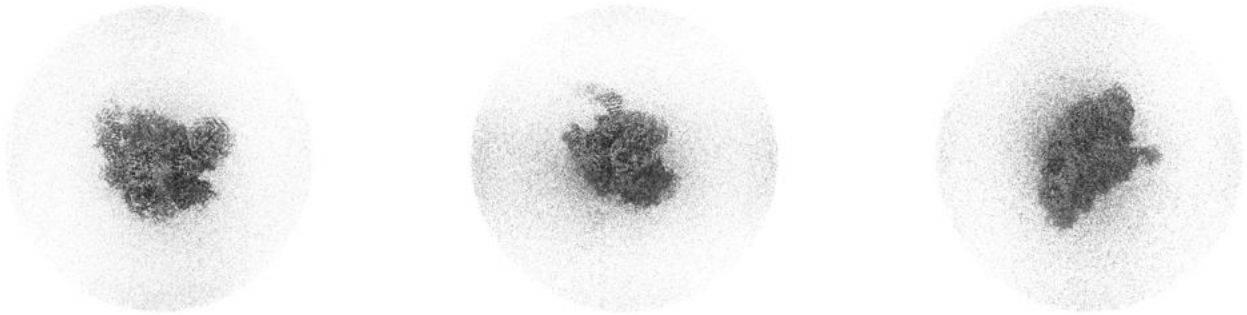
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 7.72. 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.

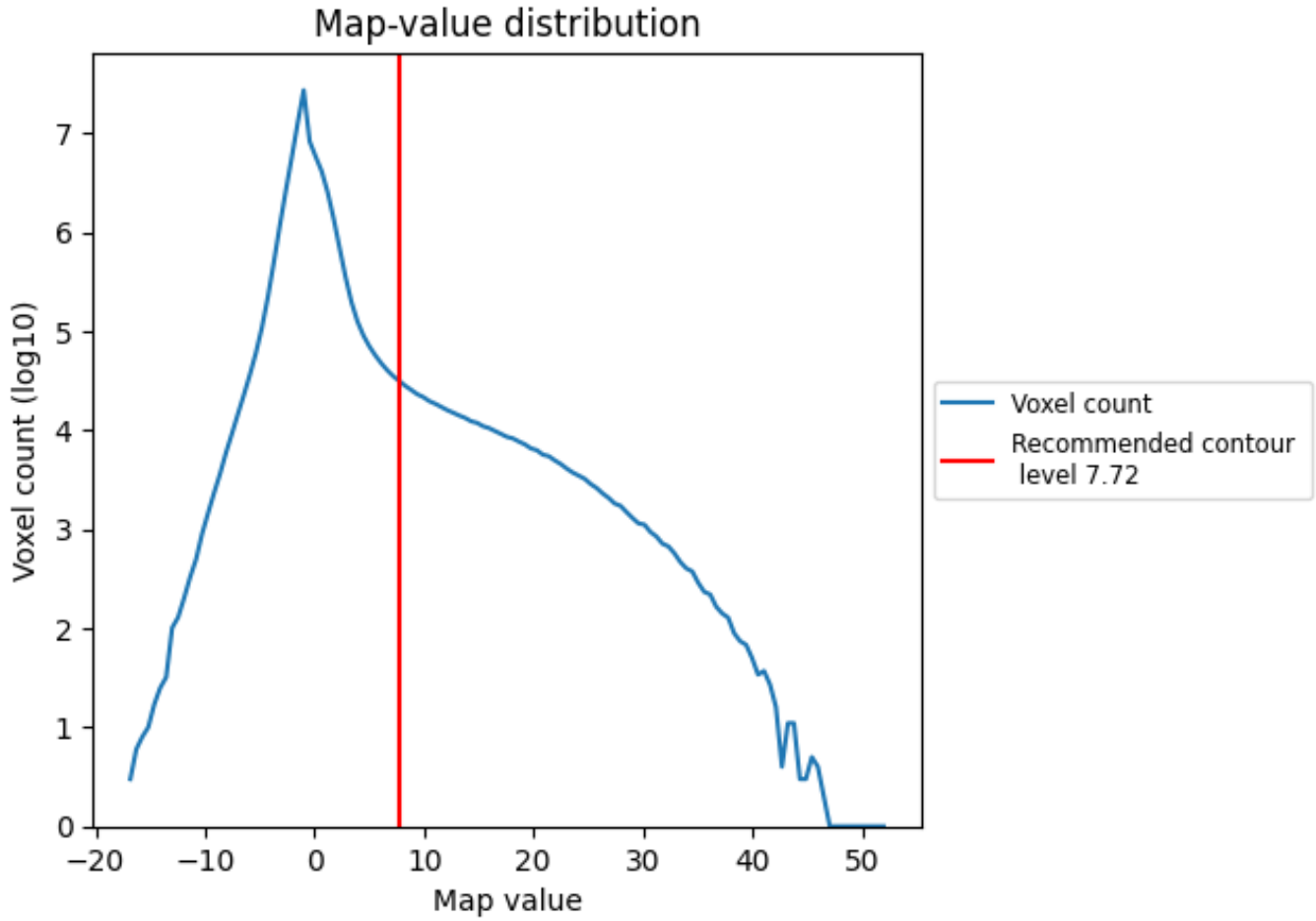
6.6 Mask visualisation (i)

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

7 Map analysis

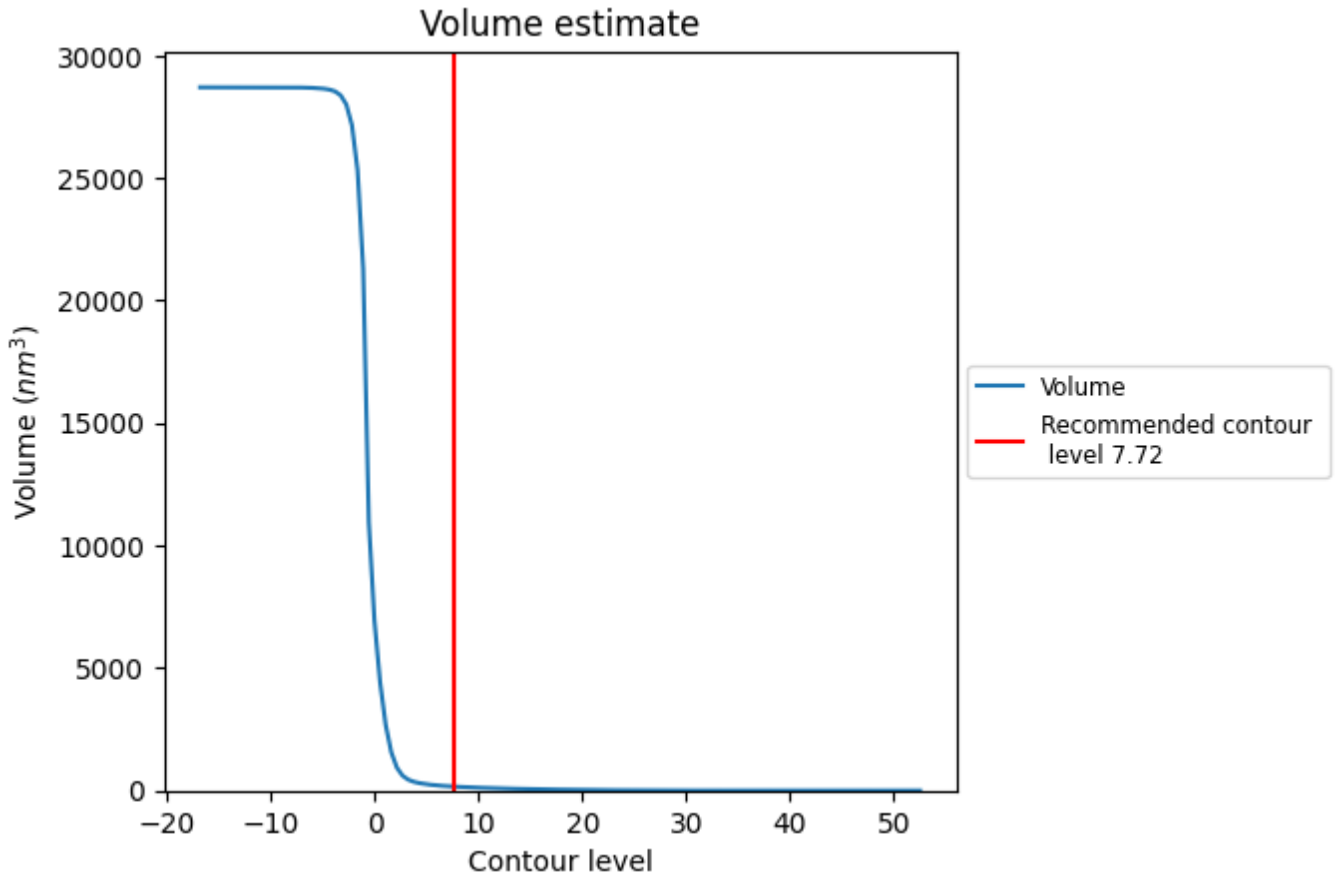
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

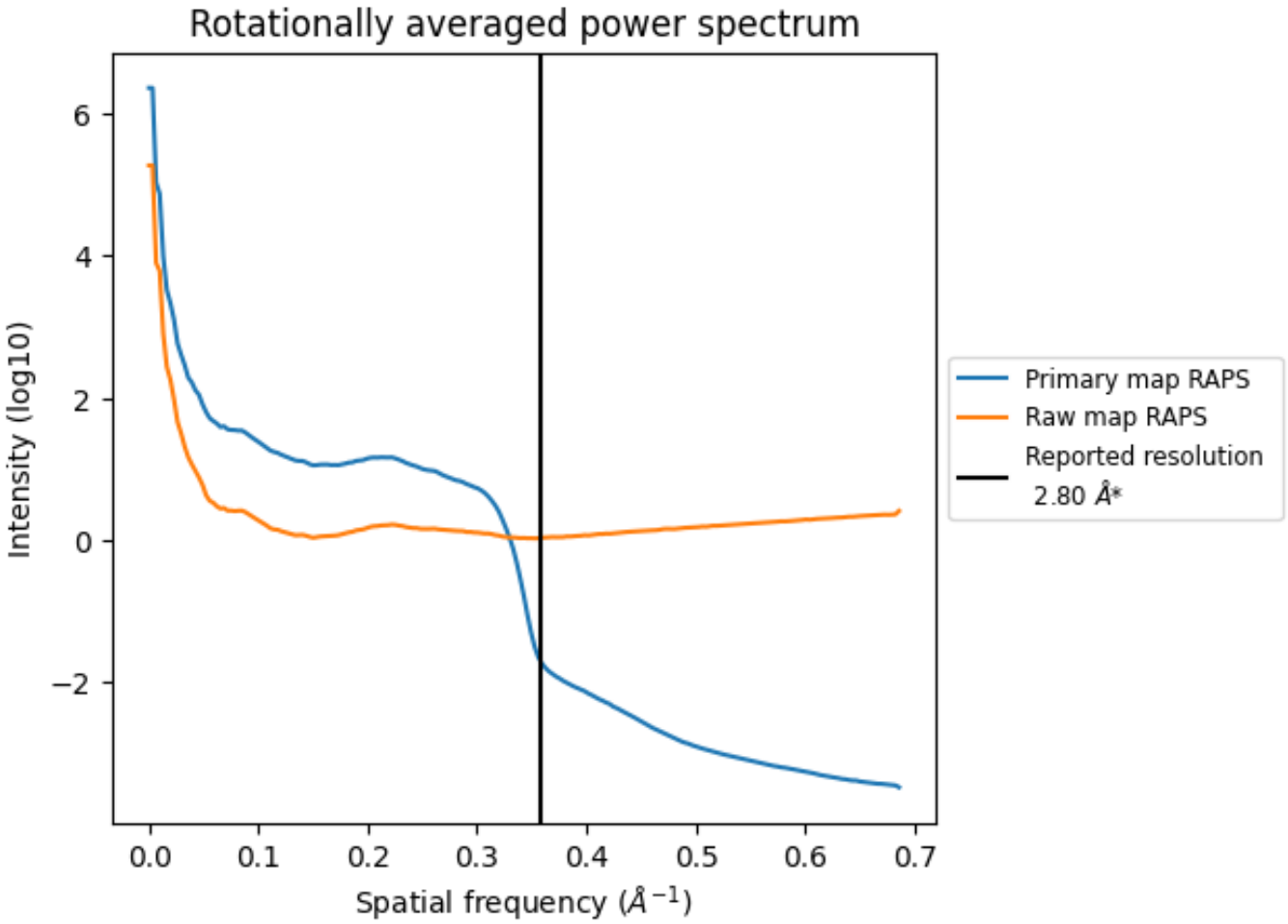
7.2 Volume estimate (i)



The volume at the recommended contour level is 160 nm^3; this corresponds to an approximate mass of 145 kDa.

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

7.3 Rotationally averaged power spectrum (i)

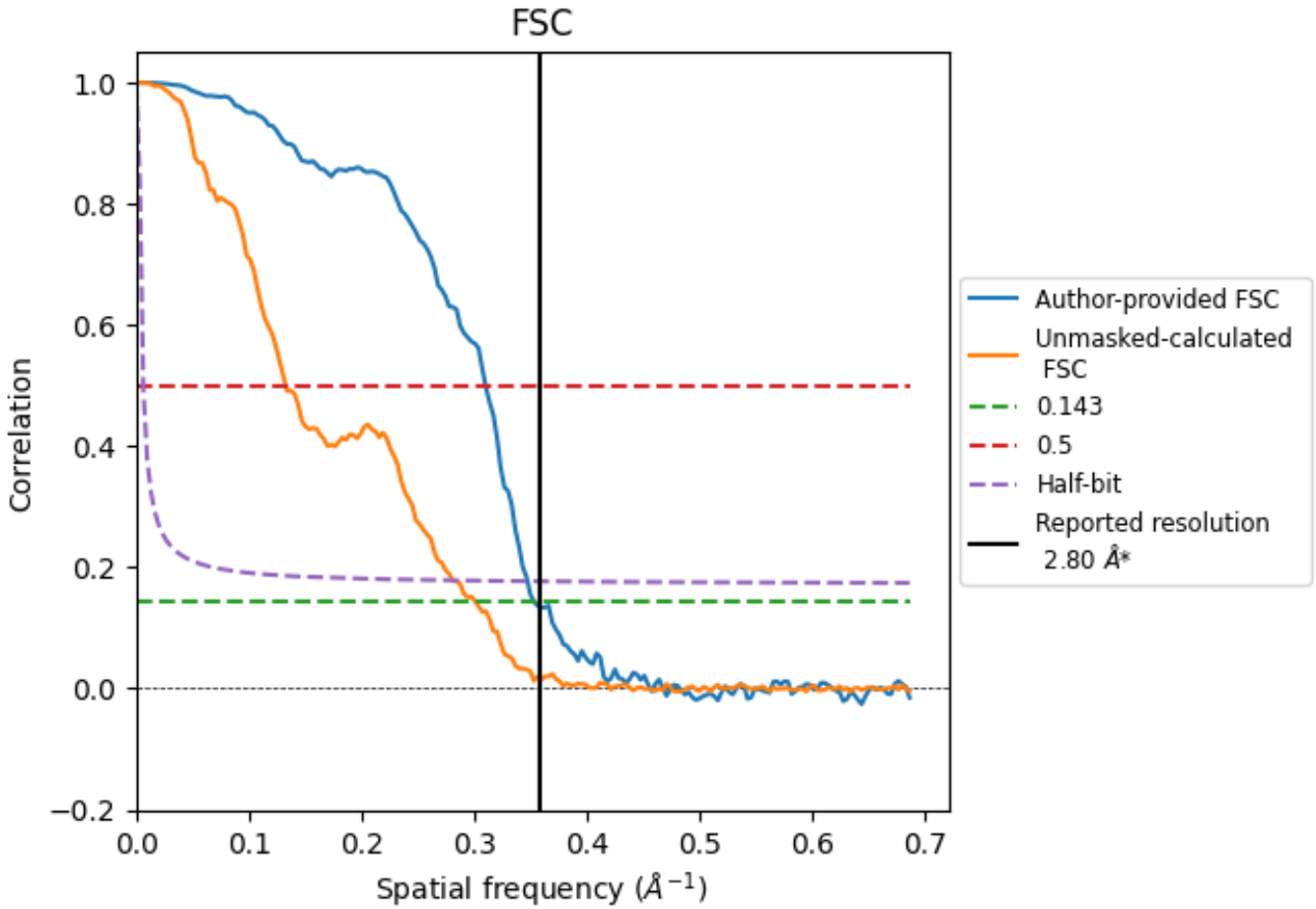


*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

8.2 Resolution estimates (i)

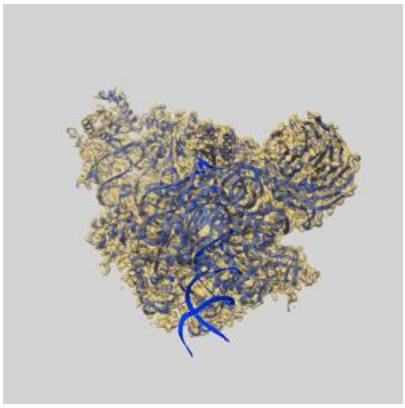
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.83	3.23	2.88
Unmasked-calculated*	3.32	7.54	3.56

*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 3.32 differs from the reported value 2.8 by more than 10 %

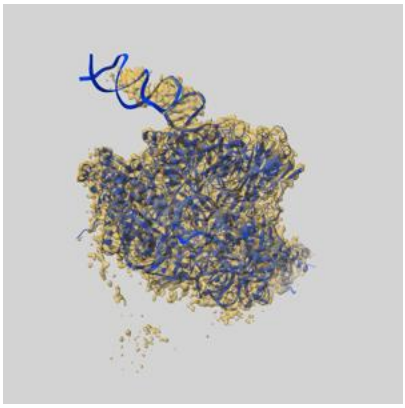
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-57157 and PDB model 29GX. Per-residue inclusion information can be found in section 3 on page 8.

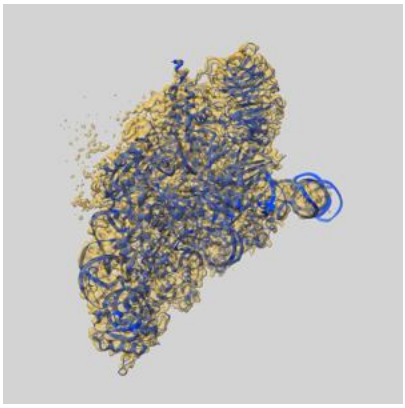
9.1 Map-model overlay



X



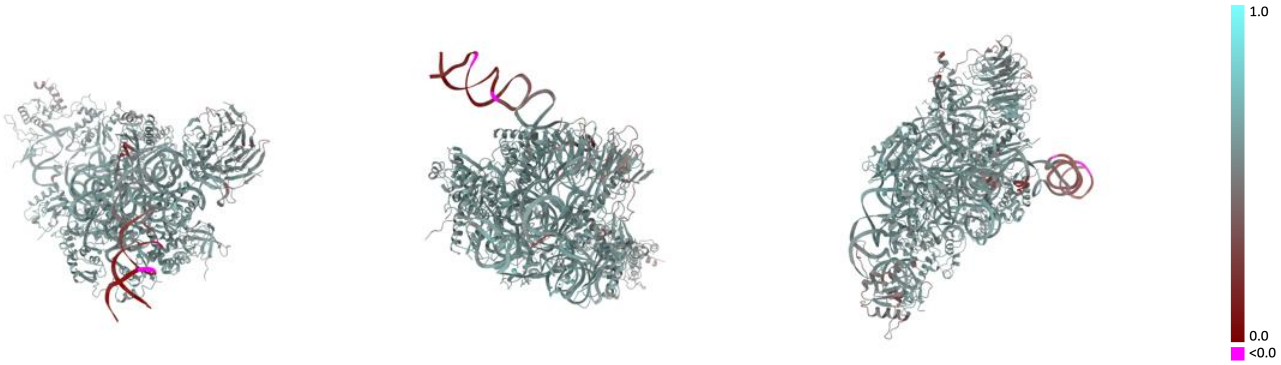
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 7.72 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.

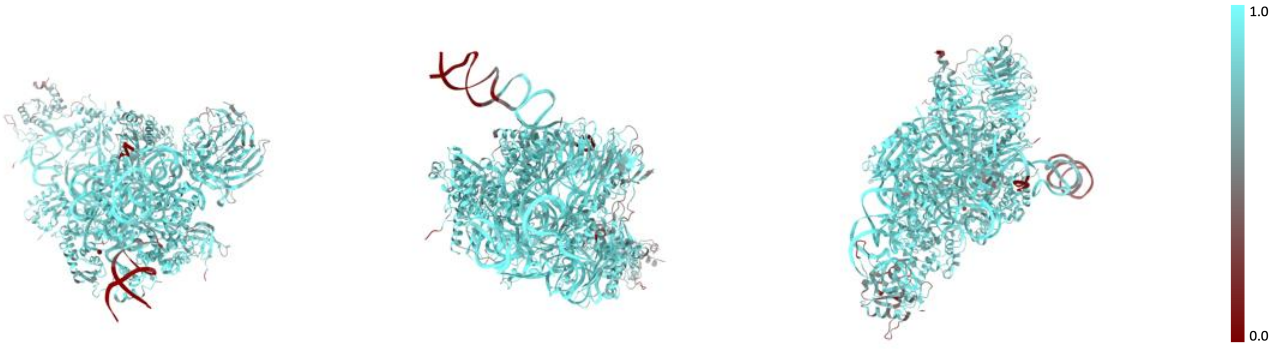
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

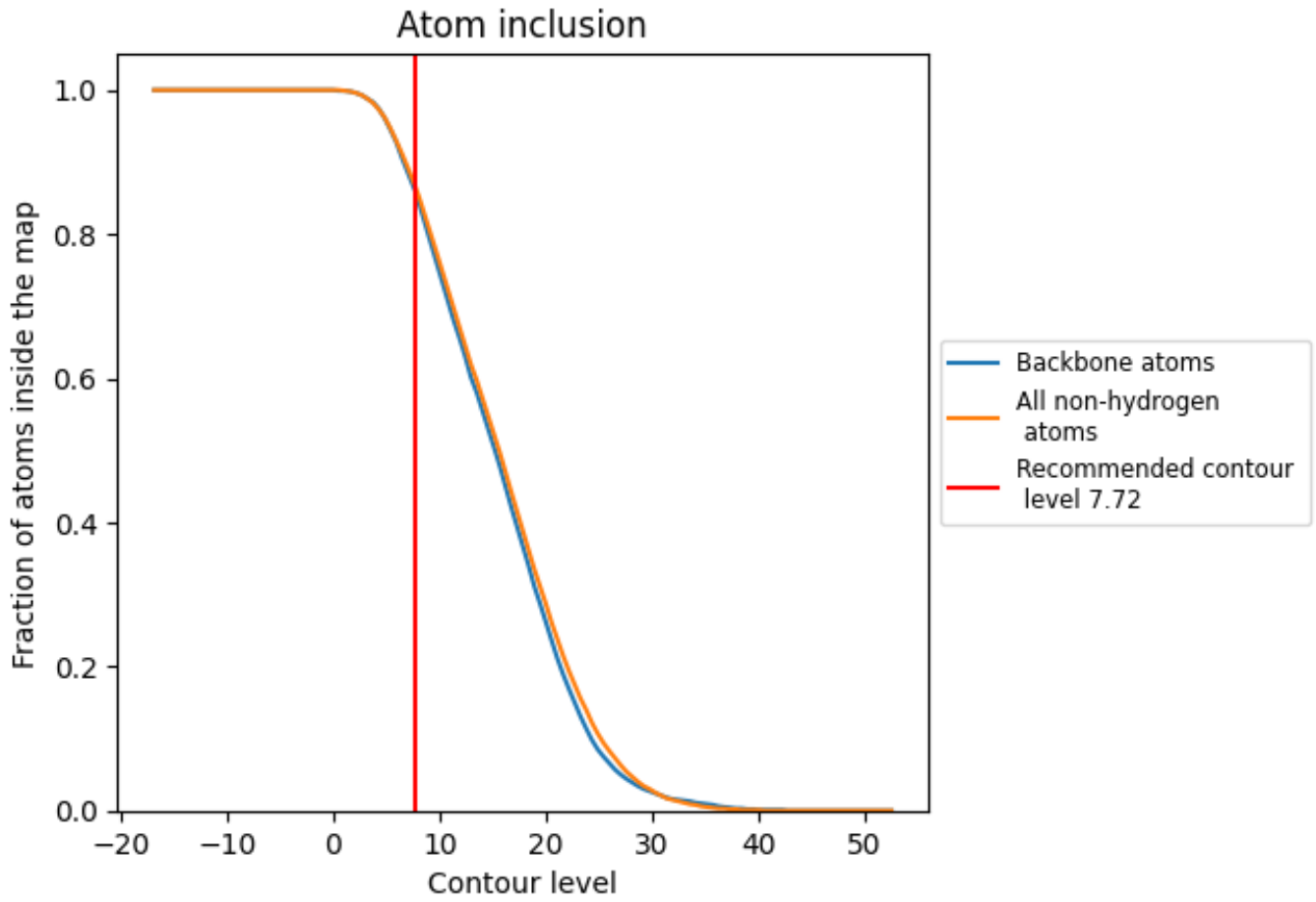
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (7.72).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 87% 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 (7.72) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8670	0.5610
C	0.2810	0.1590
S2	0.9600	0.5840
SD	0.8450	0.5660
SF	0.9070	0.5840
SK	0.8950	0.5840
SM	0.5640	0.4790
SP	0.8940	0.5870
SQ	0.9200	0.6040
SR	0.8210	0.5550
SS	0.8640	0.5800
ST	0.8990	0.5990
SU	0.8120	0.5560
SZ	0.8630	0.5730
Sc	0.7980	0.5500
Sd	0.9300	0.6160
Sf	0.7070	0.5270
Sg	0.8230	0.5440

