



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 10:52 AM UTC

PDB ID : 8CF8 / pdb_00008cf8
EMDB ID : EMD-16620
Title : Eravacycline bound to the 30S head
Authors : Paternoga, H.; Koller, T.O.; Beckert, B.; Wilson, D.N.
Deposited on : 2023-02-03
Resolution : 2.20 Å(reported)

This is a Full wwPDB EM Validation 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

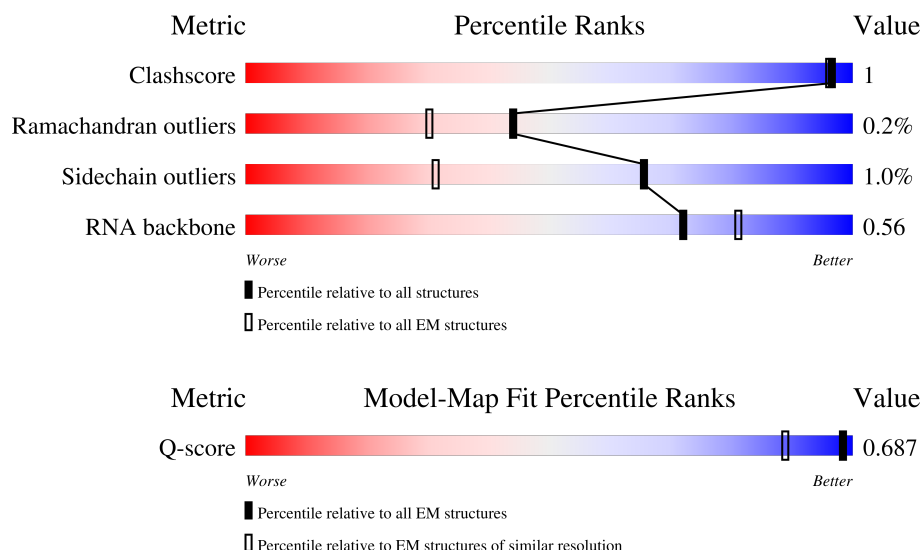
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.20 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	3184 (1.71 - 2.70)

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	1540	
2	B	241	
3	C	233	

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Mol	Chain	Length	Quality of chain
4	G	179	15% 80% 16%
5	I	130	96% ...
6	J	103	21% 83% 12% 5%
7	M	118	92% 5% ..
8	N	101	96% ..
9	S	92	89% 9%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 19324 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 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	460	Total	C	N	O	P	0	0
			9841	4394	1786	3201	460		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	222	Total	C	N	O	S	0	0
			1740	1101	313	318	8		

- Molecule 3 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 4 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	150	Total	C	N	O	S	0	0
			1182	737	227	214	4		

- Molecule 5 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 6 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 7 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

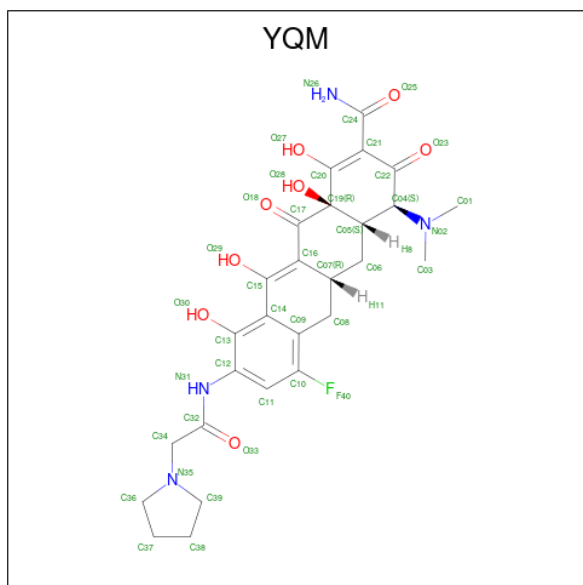
- Molecule 8 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 9 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	S	84	Total	C	N	O	S	0	0
			668	427	127	112	2		

- Molecule 10 is Eravacycline (CCD ID: YQM) (formula: C₂₇H₃₁FN₄O₈) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
10	A	1	Total	C	F	N	O	0
			40	27	1	4	8	

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
11	A	32	Total 32	Mg 32	0

- Molecule 12 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
12	A	11	Total 11	K 11	0
12	M	1	Total 1	K 1	0

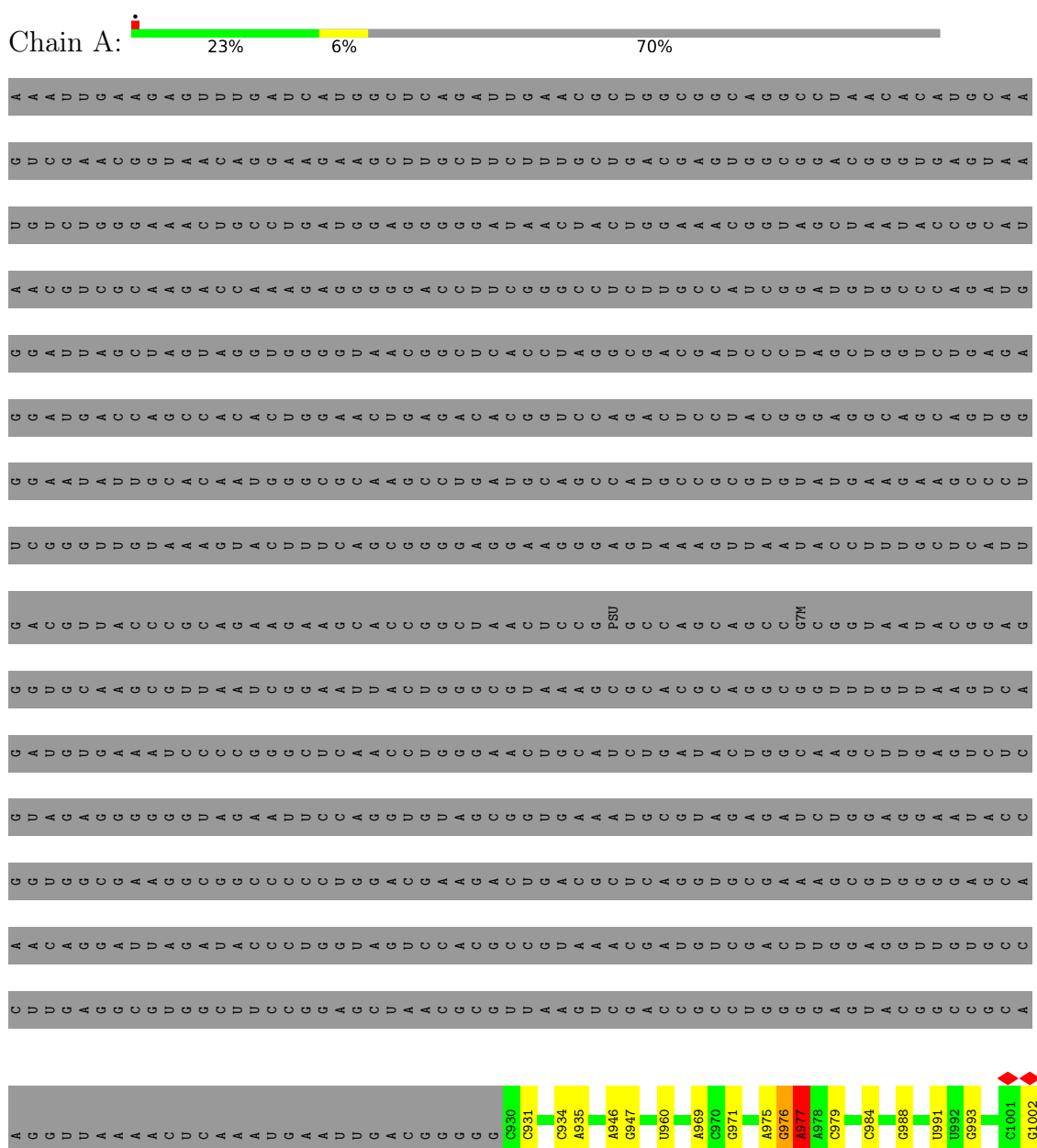
- Molecule 13 is water.

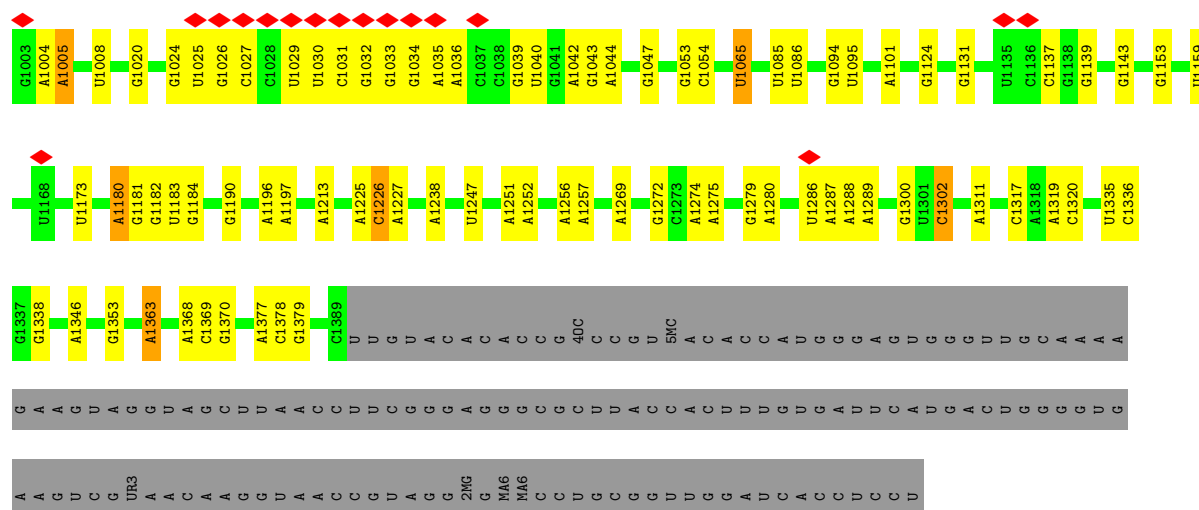
Mol	Chain	Residues	Atoms		AltConf
13	A	551	Total 551	O 551	0
13	C	29	Total 29	O 29	0
13	G	6	Total 6	O 6	0
13	I	23	Total 23	O 23	0
13	J	15	Total 15	O 15	0
13	M	13	Total 13	O 13	0
13	N	31	Total 31	O 31	0
13	S	13	Total 13	O 13	0

3 Residue-property plots

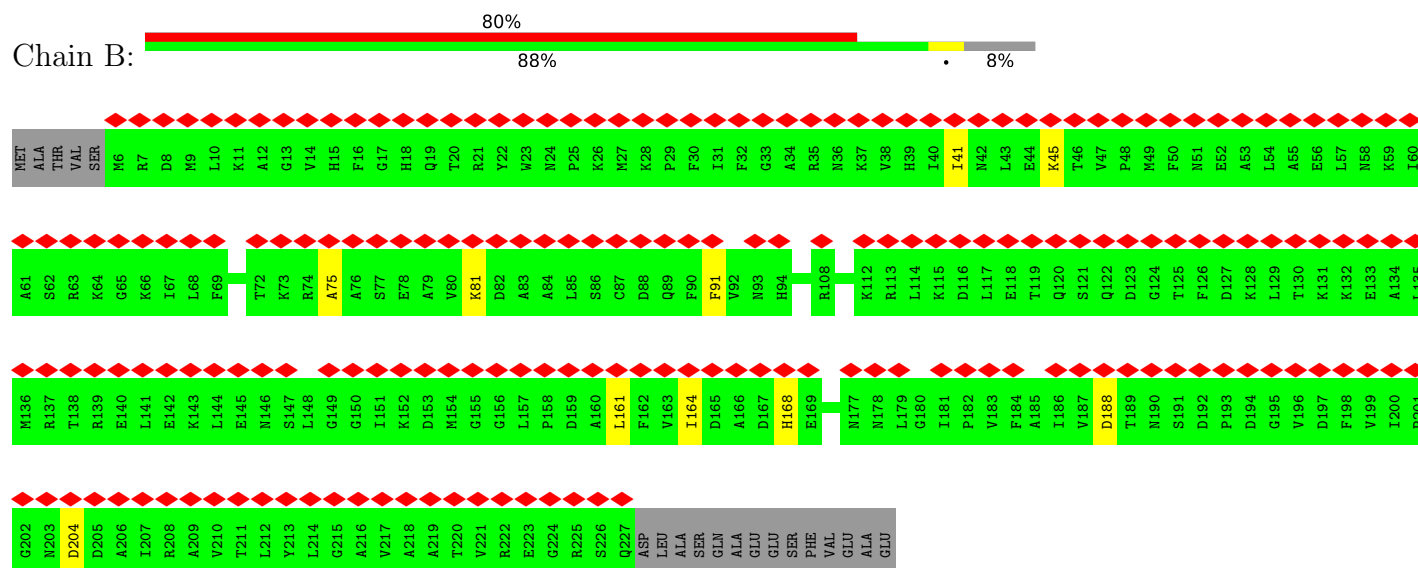
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 16S rRNA

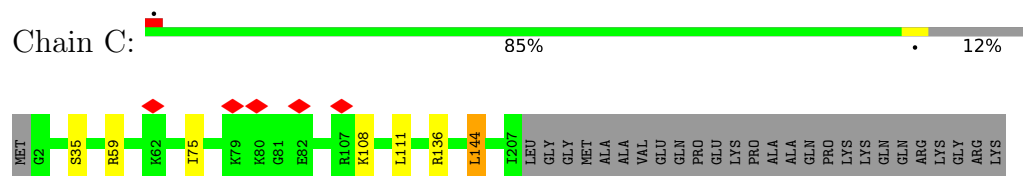




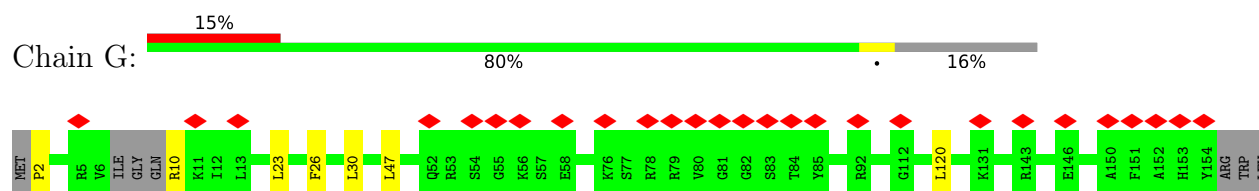
• Molecule 2: 30S ribosomal protein S2



• Molecule 3: Small ribosomal subunit protein uS3

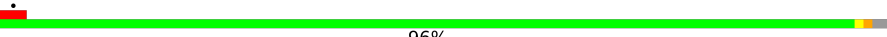


• Molecule 4: 30S ribosomal protein S7



SER
LEU
ARG
SER
PHE
SER
HIS
GLN
ALA
GLY
ALA
SER
SER
LYS
GLN
PRO
ALA
LEU
GLY
TYR
LEU
ASN

- Molecule 5: Small ribosomal subunit protein uS9

Chain I:  96% ...

MET
ALA
GLU
M4
D56
R85
R99
K129
R130

- Molecule 6: Small ribosomal subunit protein uS10

Chain J:  21% 83% 12% 5%

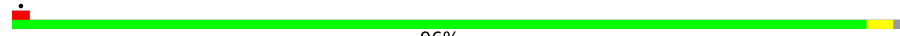
MET
GLN
ASN
GLN
R5
I6
R7
L10
T22
V26
E27
K30
R31
T32
G33
A34
Q35
V36
R37
V57
R62
E66
V77
E78
P79
T80
E81
K82
T83
V84
D85
A86
L87
M88
R89
L90
D91
L92
L102
GLY

- Molecule 7: Small ribosomal subunit protein uS13

Chain M:  92% 5% ..

MET
A2
I17
Y86
R87
R90
H91
R92
P96
R107
P115
I116
LYS
LYS

- Molecule 8: Small ribosomal subunit protein uS14

Chain N:  96% ..

MET
A2
E10
N35
D38
R63
A99
S100
W101

- Molecule 9: Small ribosomal subunit protein uS19

Chain S:  89% 9%

MET
P2
D27
K28
A50
H57
A84
A85
ASP
LYS
LYS
LYS
ALA
LYS
LYS
LYS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	275137	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.097	Depositor
Minimum map value	-0.033	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0114	Depositor
Map size (Å)	460.80002, 460.80002, 460.80002	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.768, 0.768, 0.768	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MC, 2MG, YQM, MG, K

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	0.50	0/10934	1.00	23/17047 (0.1%)
2	B	0.53	0/1771	1.10	0/2385
3	C	0.50	0/1651	0.95	0/2225
4	G	0.51	0/1197	1.02	1/1604 (0.1%)
5	I	0.48	0/1034	0.99	0/1375
6	J	0.50	0/796	0.95	0/1077
7	M	0.52	0/900	0.99	0/1204
8	N	0.52	0/817	0.96	0/1088
9	S	0.51	0/685	0.90	0/922
All	All	0.50	0/19785	1.00	24/28927 (0.1%)

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
3	C	0	1
4	G	0	1
5	I	0	2
6	J	0	3
7	M	0	4
All	All	0	11

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1377	A	O3'-P-O5'	-8.40	91.40	104.00
1	A	1131	G	O3'-P-O5'	-7.56	92.65	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1272	G	O3'-P-O5'	-7.54	92.69	104.00
1	A	976	G	O3'-P-O5'	-7.19	93.21	104.00
1	A	1182	G	O3'-P-O5'	-6.47	94.30	104.00
1	A	1153	G	O3'-P-O5'	-5.99	95.02	104.00
1	A	1247	U	O3'-P-O5'	-5.89	95.16	104.00
1	A	1190	G	O3'-P-O5'	-5.87	95.19	104.00
1	A	1005	A	O3'-P-O5'	-5.67	95.50	104.00
1	A	1279	G	O3'-P-O5'	-5.64	95.54	104.00
1	A	977	A	O3'-P-O5'	-5.62	95.57	104.00
1	A	1311	A	O3'-P-O5'	-5.56	95.66	104.00
1	A	1173	U	O3'-P-O5'	-5.50	95.75	104.00
1	A	1047	G	O3'-P-O5'	-5.50	95.76	104.00
1	A	1269	A	O3'-P-O5'	-5.40	95.91	104.00
1	A	1363	A	O3'-P-O5'	-5.35	95.97	104.00
1	A	988	G	O3'-P-O5'	-5.20	96.20	104.00
1	A	1274	A	O3'-P-O5'	-5.18	96.22	104.00
1	A	1065	U	O3'-P-O5'	-5.18	96.23	104.00
4	G	2	PRO	CA-N-CD	-5.10	104.86	112.00
1	A	991	U	O3'-P-O5'	-5.05	96.42	104.00
1	A	1180	A	O3'-P-O5'	-5.05	96.42	104.00
1	A	1181	G	O3'-P-O5'	-5.04	96.43	104.00
1	A	1369	C	O3'-P-O5'	-5.01	96.49	104.00

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	136	ARG	Sidechain
4	G	10	ARG	Sidechain
5	I	85	ARG	Sidechain
5	I	99	ARG	Sidechain
6	J	37	ARG	Sidechain
6	J	62	ARG	Sidechain
6	J	7	ARG	Sidechain
7	M	107	ARG	Sidechain
7	M	87	ARG	Sidechain
7	M	90	ARG	Sidechain
7	M	92	ARG	Sidechain

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	A	9841	0	4966	9	0
2	B	1740	0	1766	2	0
3	C	1624	0	1696	3	0
4	G	1182	0	1231	2	0
5	I	1022	0	1070	1	0
6	J	786	0	828	5	0
7	M	891	0	952	5	0
8	N	805	0	844	2	0
9	S	668	0	693	1	0
10	A	40	0	0	0	0
11	A	32	0	0	0	0
12	A	11	0	0	0	0
12	M	1	0	0	0	0
13	A	551	0	0	0	0
13	C	29	0	0	0	0
13	G	6	0	0	0	0
13	I	23	0	0	0	0
13	J	15	0	0	0	0
13	M	13	0	0	0	0
13	N	31	0	0	0	0
13	S	13	0	0	0	0
All	All	19324	0	14046	25	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 1.

All (25) 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:A:1180:A:P	5:I:99:ARG:HH22	2.25	0.59
7:M:90:ARG:HD3	7:M:96:PRO:O	2.06	0.56
6:J:10:LEU:HD12	6:J:22:THR:HG23	1.93	0.50
3:C:108:LYS:HB3	3:C:111:LEU:HD23	1.95	0.48
3:C:35:SER:OG	3:C:59:ARG:NH2	2.48	0.46
8:N:10:GLU:HG3	8:N:63:ARG:HD2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:81:LYS:HG3	2:B:91:PHE:CZ	2.49	0.46
1:A:946:A:H2'	1:A:947:G:C8	2.51	0.46
2:B:188:ASP:HB2	2:B:204:ASP:OD2	2.16	0.46
7:M:86:TYR:CZ	7:M:90:ARG:HD2	2.51	0.46
1:A:1226:C:OP1	7:M:90:ARG:NH2	2.47	0.45
4:G:23:LEU:HD11	4:G:47:LEU:HD11	1.98	0.44
6:J:26:VAL:HG12	6:J:36:VAL:HG11	1.99	0.44
6:J:66:GLU:HB2	8:N:99:ALA:HB2	1.99	0.44
1:A:1302:C:C5	7:M:17:ILE:HG13	2.52	0.43
1:A:977:A:O2'	1:A:979:C:OP2	2.32	0.43
4:G:26:PHE:HZ	4:G:120:LEU:HD11	1.83	0.43
3:C:111:LEU:HD21	3:C:144:LEU:HB3	2.01	0.42
1:A:1251:A:H2'	1:A:1252:A:O4'	2.21	0.41
6:J:6:ILE:HD11	6:J:84:VAL:HG22	2.03	0.41
9:S:50:ALA:HB1	9:S:57:HIS:HB3	2.02	0.41
1:A:1053:G:H4'	1:A:1054:C:H3'	2.03	0.41
1:A:1226:C:P	7:M:90:ARG:HH22	2.43	0.41
1:A:1288:A:H2'	1:A:1289:A:O4'	2.21	0.40
6:J:35:GLN:HG3	6:J:77:VAL:HB	2.03	0.40

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	B	220/241 (91%)	201 (91%)	18 (8%)	1 (0%)	24	27
3	C	204/233 (88%)	200 (98%)	4 (2%)	0	100	100
4	G	146/179 (82%)	138 (94%)	8 (6%)	0	100	100
5	I	125/130 (96%)	119 (95%)	6 (5%)	0	100	100
6	J	96/103 (93%)	91 (95%)	4 (4%)	1 (1%)	12	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	M	113/118 (96%)	110 (97%)	3 (3%)	0	100	100
8	N	98/101 (97%)	98 (100%)	0	0	100	100
9	S	82/92 (89%)	81 (99%)	1 (1%)	0	100	100
All	All	1084/1197 (91%)	1038 (96%)	44 (4%)	2 (0%)	44	51

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	75	ALA
6	J	57	VAL

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	
2	B	184/199 (92%)	179 (97%)	5 (3%)	39	53
3	C	170/190 (90%)	168 (99%)	2 (1%)	63	78
4	G	124/147 (84%)	123 (99%)	1 (1%)	73	85
5	I	105/107 (98%)	105 (100%)	0	100	100
6	J	86/90 (96%)	85 (99%)	1 (1%)	63	78
7	M	93/96 (97%)	93 (100%)	0	100	100
8	N	83/84 (99%)	83 (100%)	0	100	100
9	S	72/79 (91%)	72 (100%)	0	100	100
All	All	917/992 (92%)	908 (99%)	9 (1%)	65	81

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	41	ILE
2	B	45	LYS
2	B	161	LEU
2	B	164	ILE

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Mol	Chain	Res	Type
2	B	168	HIS
3	C	75	ILE
3	C	144	LEU
4	G	30	LEU
6	J	35	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	19	GLN
2	B	51	ASN
2	B	58	ASN
2	B	190	ASN
2	B	203	ASN
3	C	6	HIS
4	G	97	ASN
7	M	14	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	459/1540 (29%)	74 (16%)	8 (1%)

All (74) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	931	C
1	A	934	C
1	A	935	A
1	A	960	U
1	A	969	A
1	A	971	G
1	A	975	A
1	A	976	G
1	A	977	A
1	A	984	C
1	A	993	G
1	A	1002	G
1	A	1004	A
1	A	1005	A

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Mol	Chain	Res	Type
1	A	1008	U
1	A	1020	G
1	A	1024	G
1	A	1025	U
1	A	1026	G
1	A	1027	C
1	A	1029	U
1	A	1030	U
1	A	1031	C
1	A	1032	G
1	A	1033	G
1	A	1034	G
1	A	1035	A
1	A	1036	A
1	A	1039	G
1	A	1040	U
1	A	1042	A
1	A	1043	G
1	A	1044	A
1	A	1065	U
1	A	1085	U
1	A	1086	U
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1124	G
1	A	1137	C
1	A	1139	G
1	A	1143	G
1	A	1159	U
1	A	1183	U
1	A	1184	G
1	A	1196	A
1	A	1197	A
1	A	1213	A
1	A	1225	A
1	A	1226	C
1	A	1227	A
1	A	1238	A
1	A	1256	A
1	A	1257	A
1	A	1275	A

Continued on next page...

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Mol	Chain	Res	Type
1	A	1280	A
1	A	1286	U
1	A	1287	A
1	A	1300	G
1	A	1302	C
1	A	1317	C
1	A	1319	A
1	A	1320	C
1	A	1335	U
1	A	1336	C
1	A	1338	G
1	A	1346	A
1	A	1353	G
1	A	1363	A
1	A	1368	A
1	A	1370	G
1	A	1378	C
1	A	1379	G

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1024	G
1	A	1025	U
1	A	1035	A
1	A	1042	A
1	A	1124	G
1	A	1225	A
1	A	1319	A
1	A	1335	U

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

3 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	5MC	A	967	1	19,22,23	0.38	0	26,32,35	0.79	0
1	2MG	A	966	1	23,26,27	0.43	0	33,38,41	0.54	0
1	2MG	A	1207	12,1	23,26,27	0.41	0	33,38,41	0.59	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	5MC	A	967	1	-	0/7/25/26	0/2/2/2
1	2MG	A	966	1	-	0/9/27/28	0/3/3/3
1	2MG	A	1207	12,1	-	0/9/27/28	0/3/3/3

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.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 45 ligands modelled in this entry, 44 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	YQM	A	1601	11	43,44,44	2.17	8 (18%)	53,69,69	2.46	13 (24%)

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
10	YQM	A	1601	11	-	3/16/81/81	0/5/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1601	YQM	O23-C22	6.37	1.33	1.22
10	A	1601	YQM	O18-C17	6.29	1.33	1.22
10	A	1601	YQM	C15-C16	5.56	1.45	1.36
10	A	1601	YQM	C24-N26	4.93	1.47	1.33
10	A	1601	YQM	C17-C16	-4.70	1.36	1.46
10	A	1601	YQM	C19-C20	3.66	1.55	1.52
10	A	1601	YQM	C19-C17	-2.70	1.51	1.55
10	A	1601	YQM	O27-C20	-2.44	1.24	1.32

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1601	YQM	C34-N35-C39	8.27	124.05	113.34
10	A	1601	YQM	C39-N35-C36	7.64	113.07	104.04
10	A	1601	YQM	C34-N35-C36	7.36	122.88	113.34
10	A	1601	YQM	C11-C10-C09	-4.63	121.01	124.45
10	A	1601	YQM	C03-N02-C04	4.37	124.07	114.10
10	A	1601	YQM	O27-C20-C19	3.97	119.11	113.37
10	A	1601	YQM	C19-C20-C21	-3.86	117.35	122.89
10	A	1601	YQM	C07-C16-C15	-2.73	117.47	121.44
10	A	1601	YQM	O18-C17-C19	-2.46	114.42	119.11
10	A	1601	YQM	C01-N02-C04	2.30	119.35	114.10
10	A	1601	YQM	C06-C07-C16	2.29	115.25	110.28
10	A	1601	YQM	C11-C12-C13	-2.19	118.41	120.53
10	A	1601	YQM	C03-N02-C01	2.07	116.57	110.49

There are no chirality outliers.

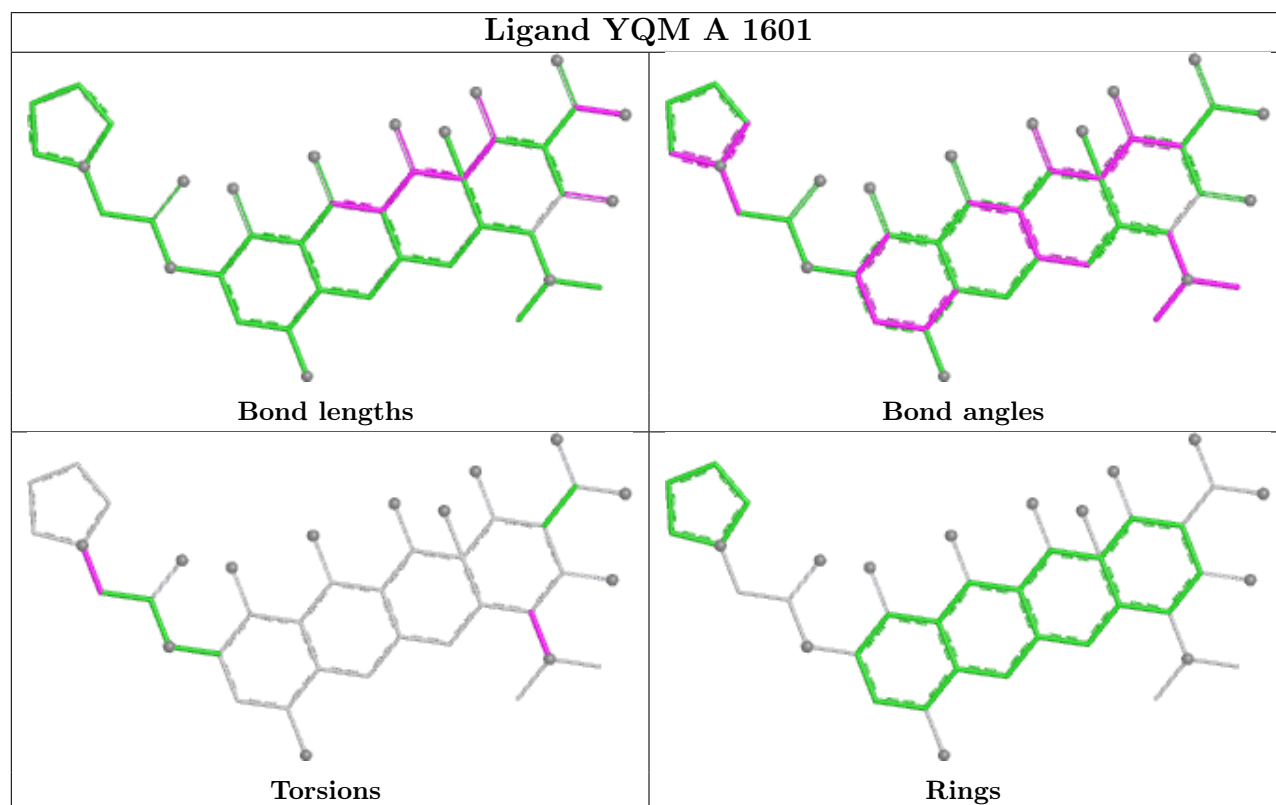
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	1601	YQM	C32-C34-N35-C39
10	A	1601	YQM	C05-C04-N02-C03
10	A	1601	YQM	C22-C04-N02-C03

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

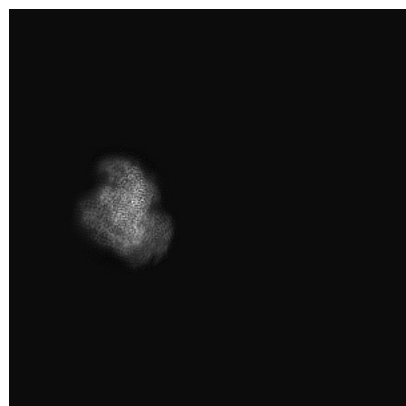
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16620. These allow visual inspection of the internal detail of the map and identification of artifacts.

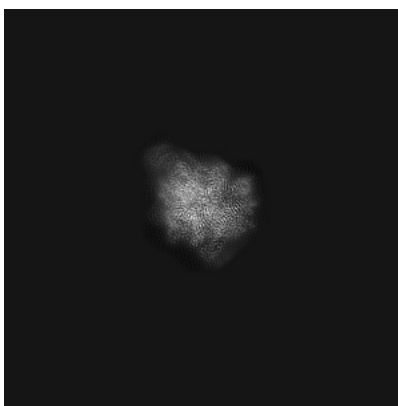
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

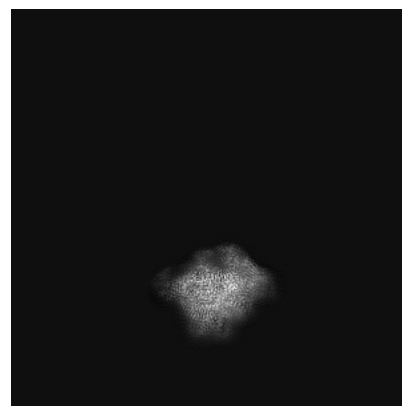
6.1.1 Primary map



X

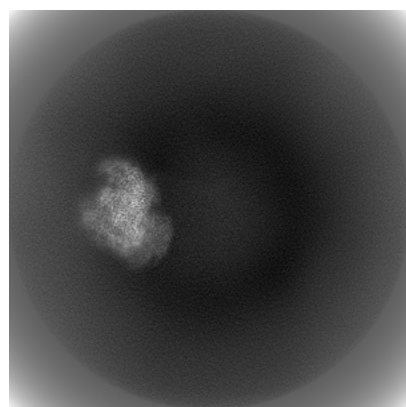


Y

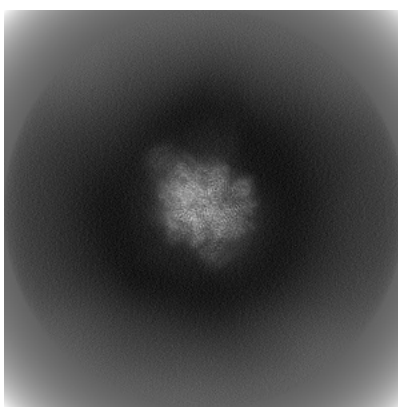


Z

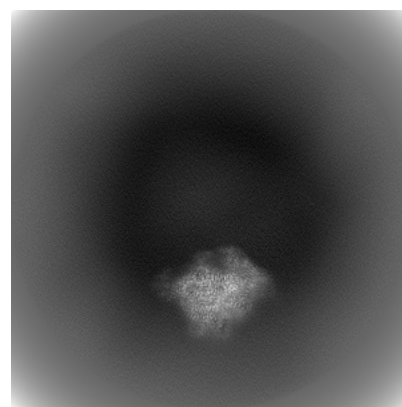
6.1.2 Raw map



X



Y

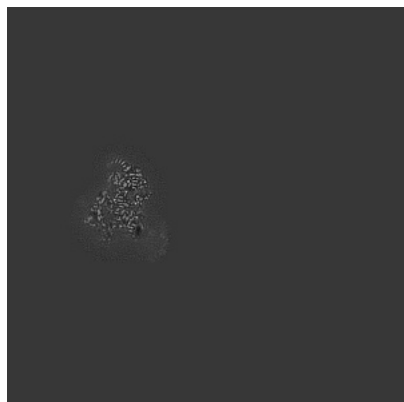


Z

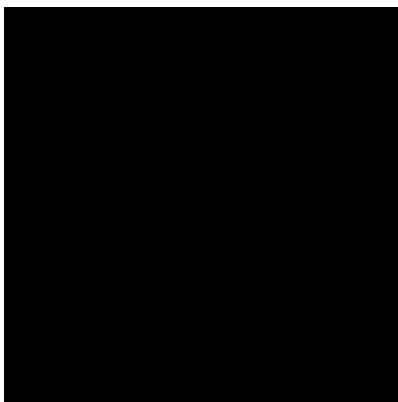
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 300

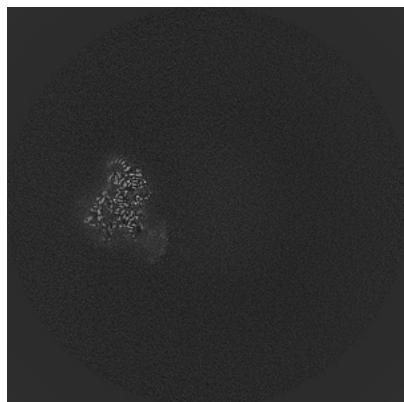


Y Index: 300

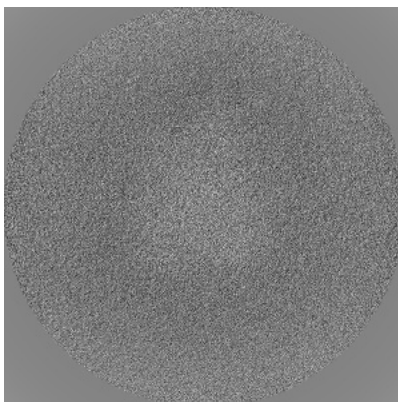


Z Index: 300

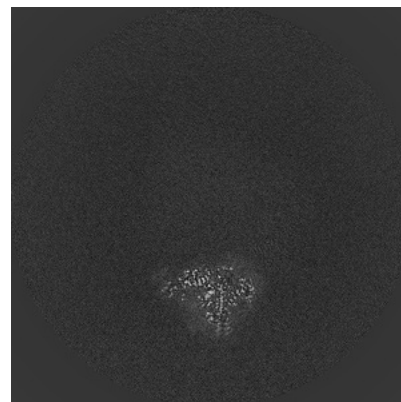
6.2.2 Raw map



X Index: 300



Y Index: 300



Z Index: 300

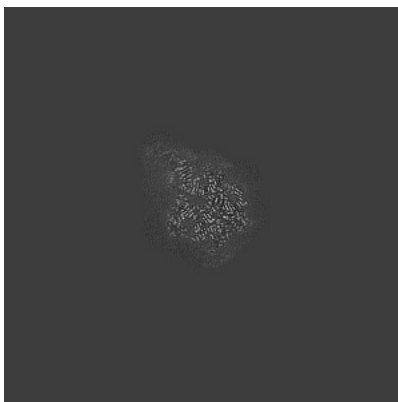
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

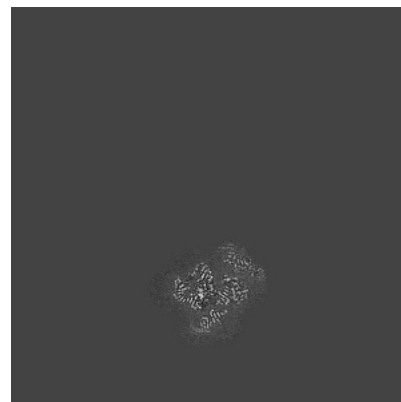
6.3.1 Primary map



X Index: 294

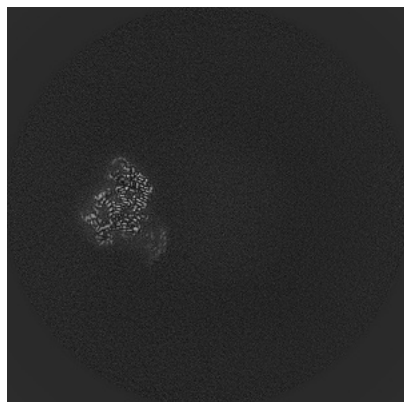


Y Index: 191

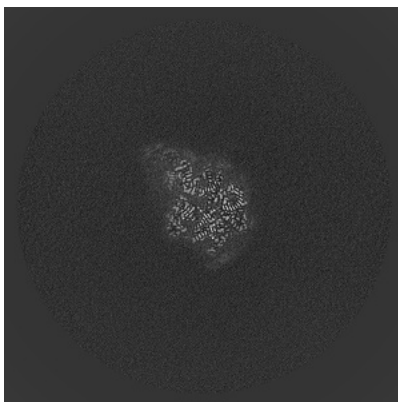


Z Index: 284

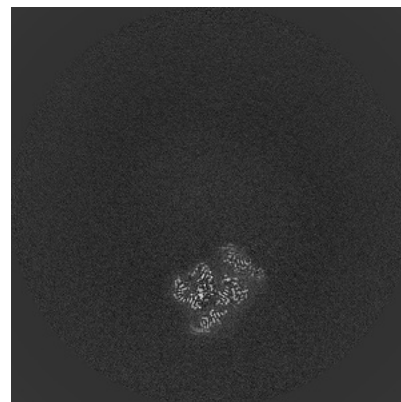
6.3.2 Raw map



X Index: 294



Y Index: 190

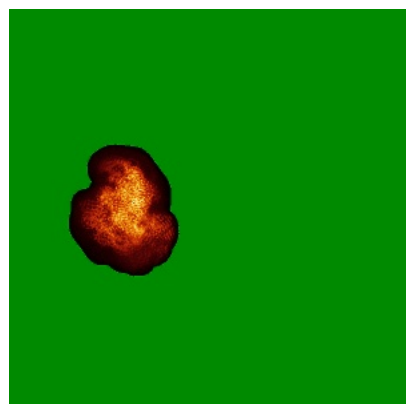


Z Index: 284

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

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

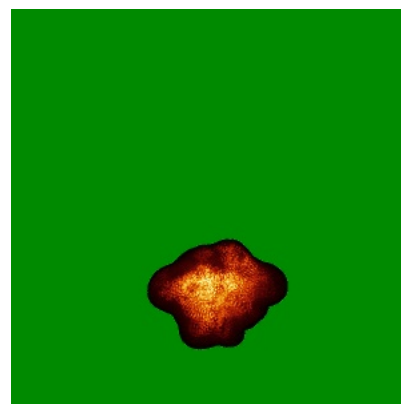
6.4.1 Primary map



X

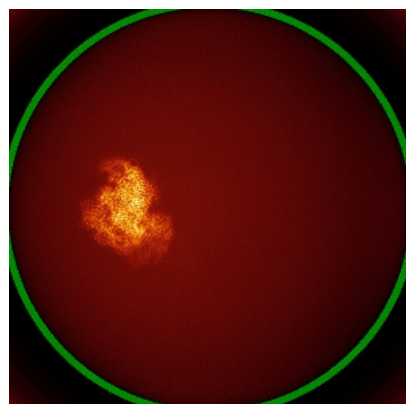


Y

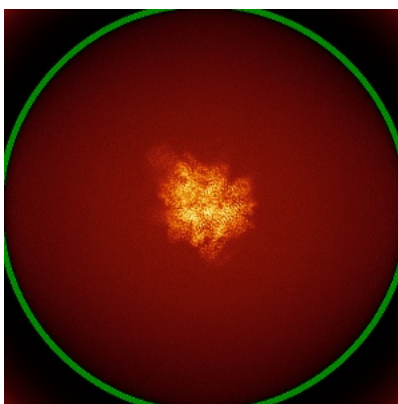


Z

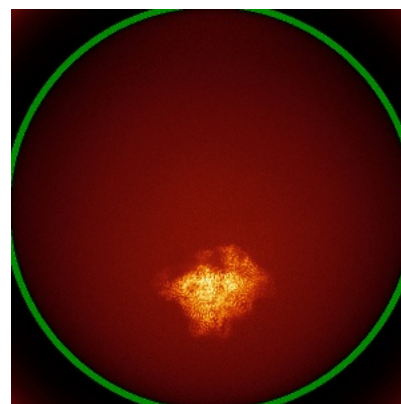
6.4.2 Raw map



X



Y

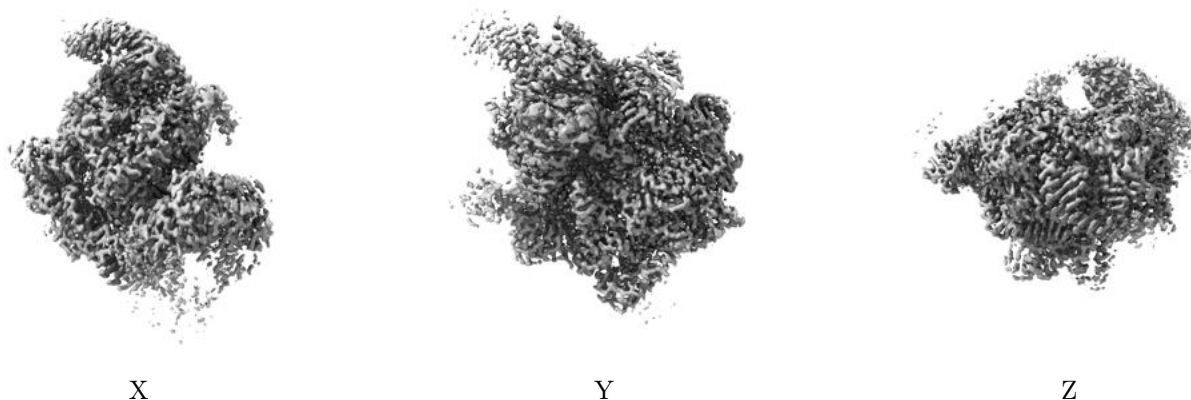


Z

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 0.0114. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

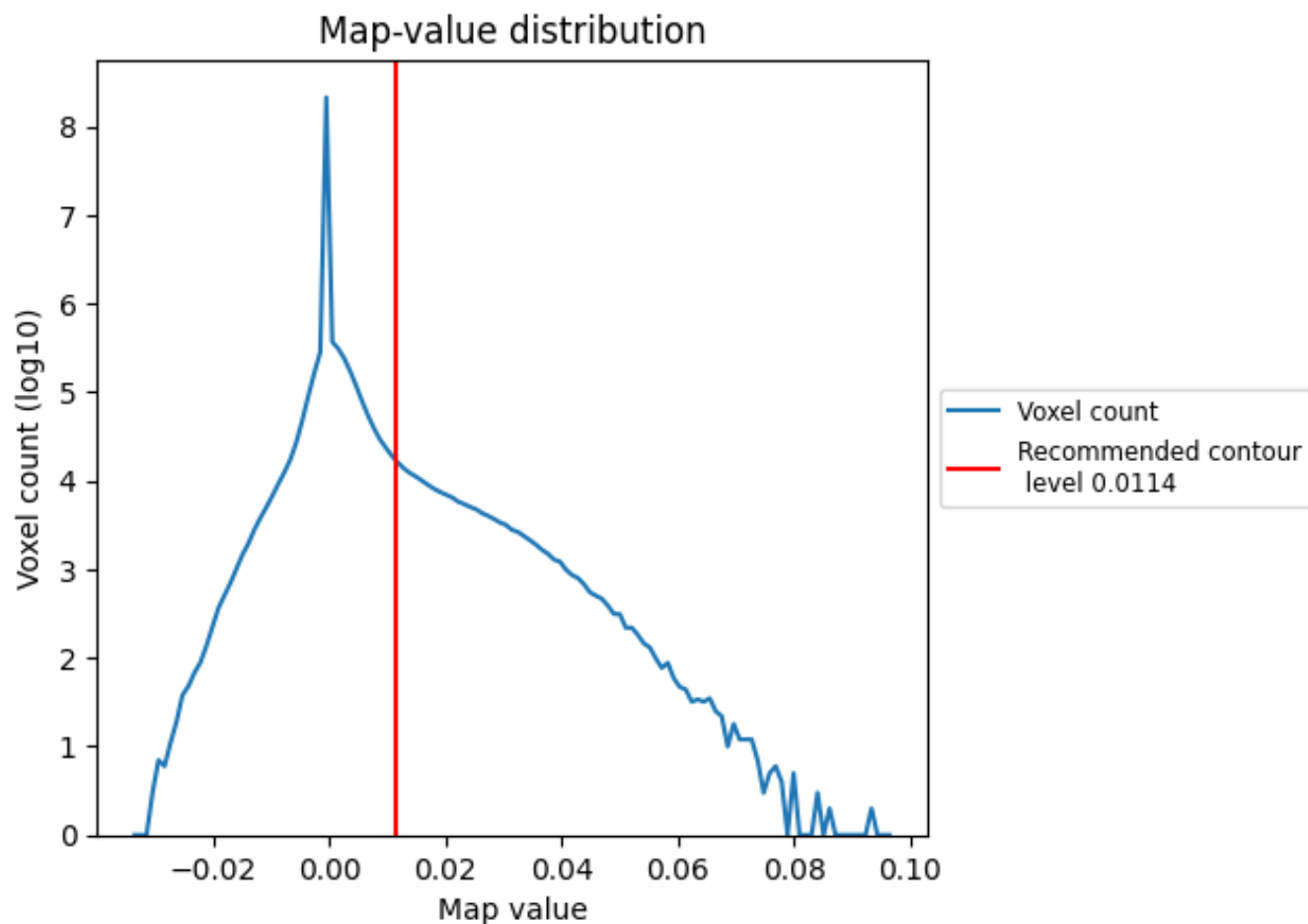
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

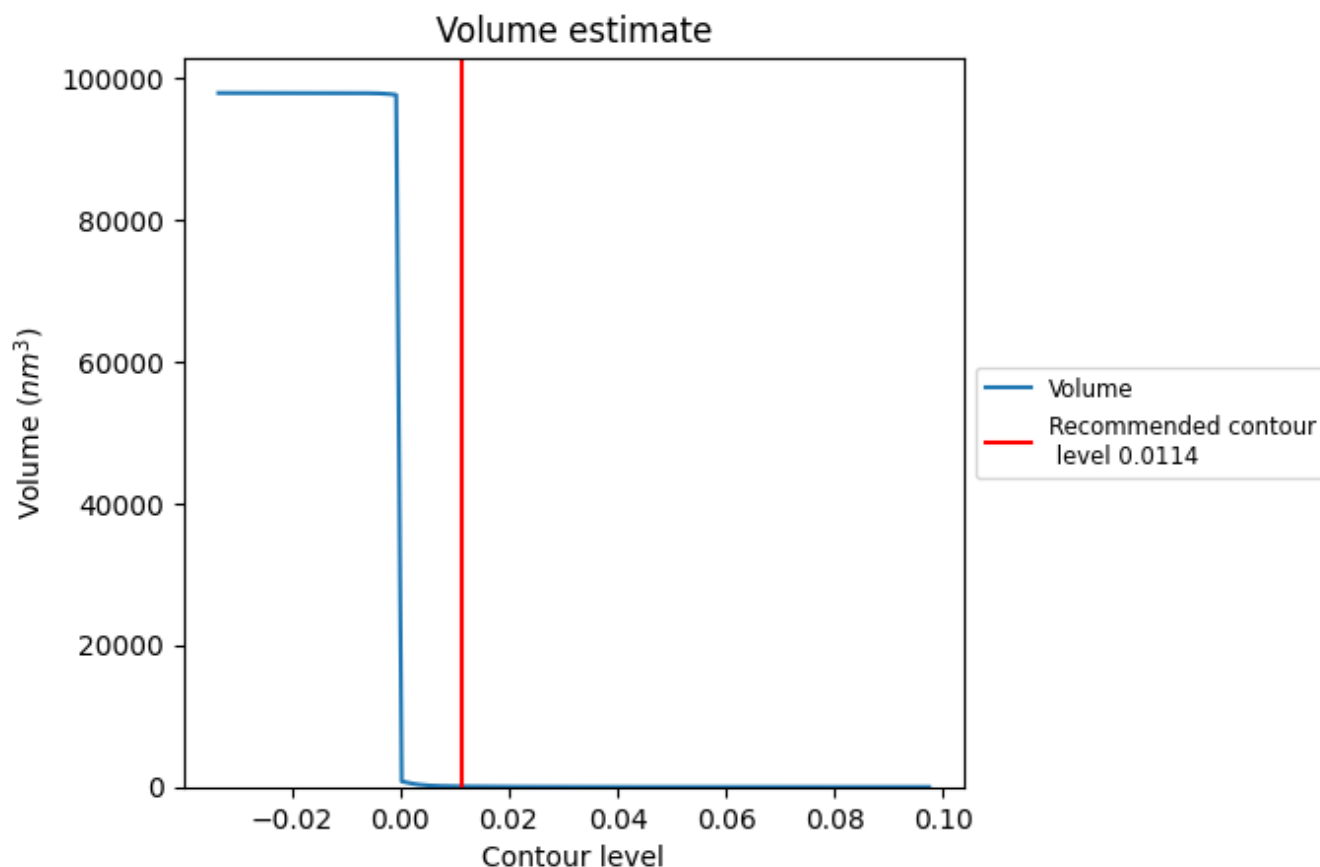
This section contains the results of statistical analysis of the map.

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.

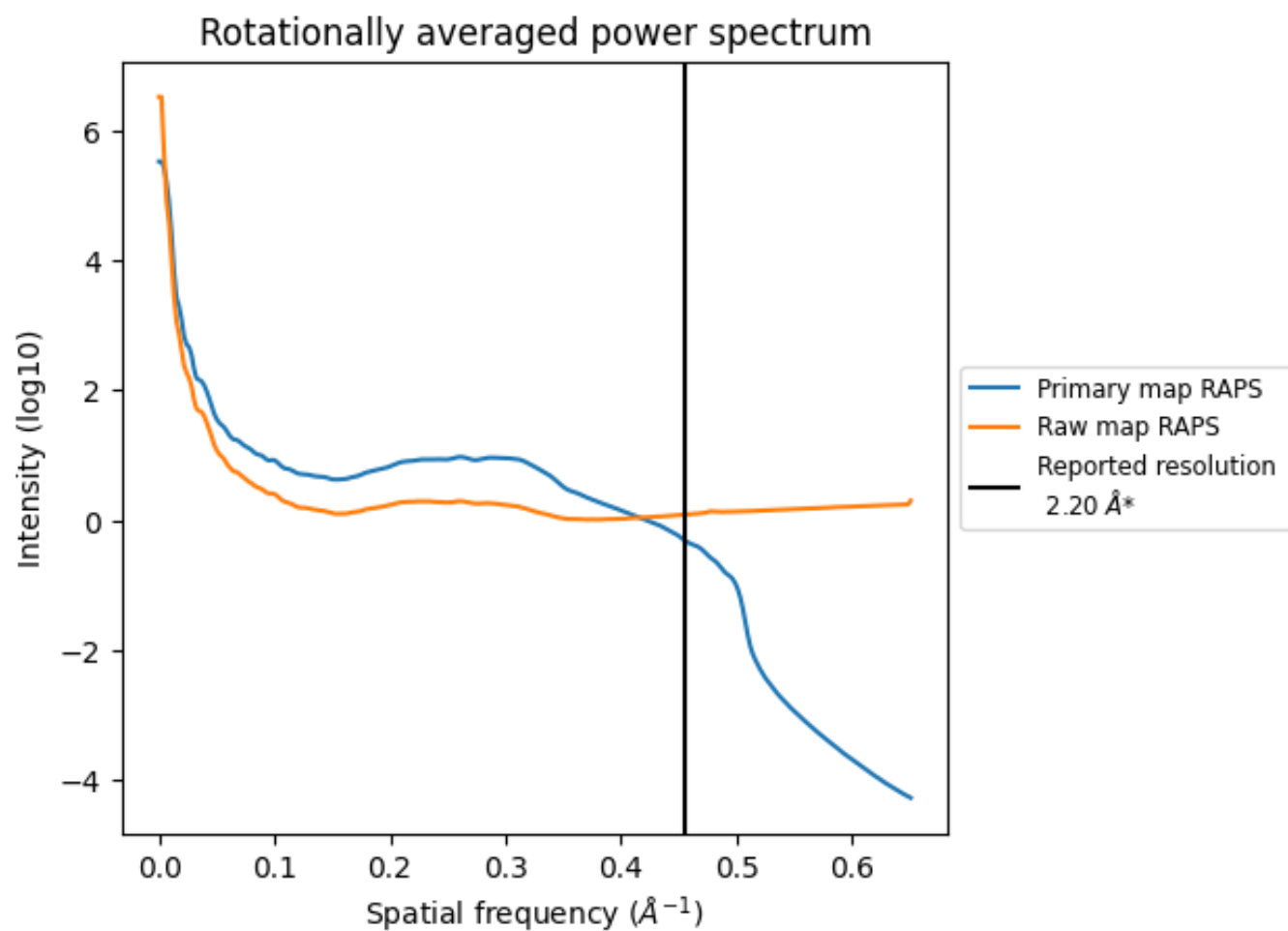
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 79 nm^3 ; this corresponds to an approximate mass of 71 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 ⓘ

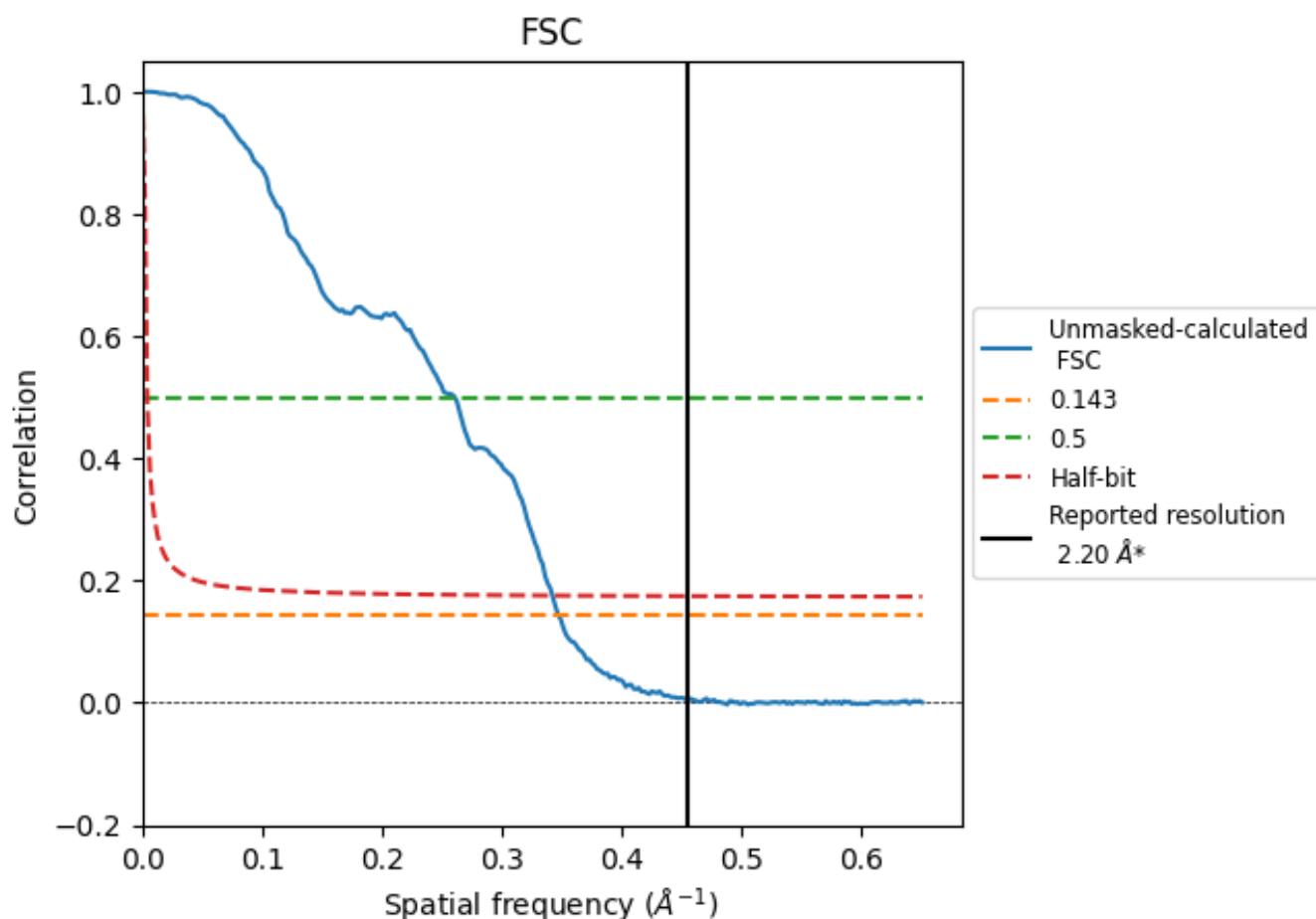


*Reported resolution corresponds to spatial frequency of 0.455 $\text{\AA}^{-1}$

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 0.455 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

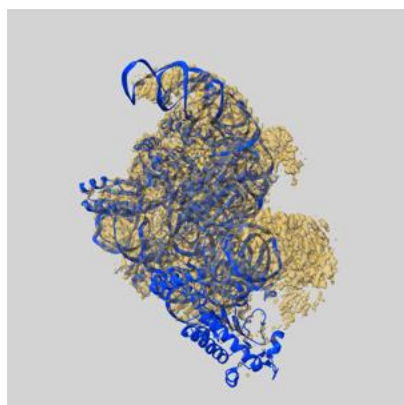
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.88	3.83	2.92

*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 2.2 by more than 10 %

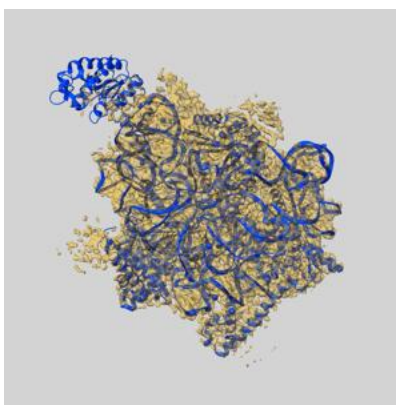
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16620 and PDB model 8CF8. Per-residue inclusion information can be found in section [3](#) on page [7](#).

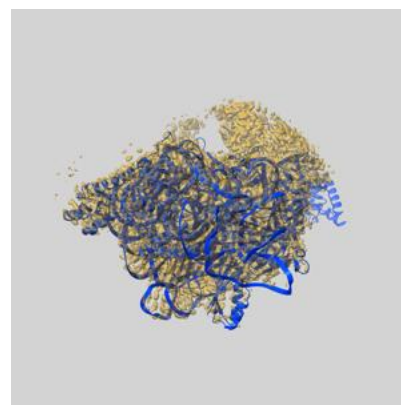
9.1 Map-model overlay [i](#)



X



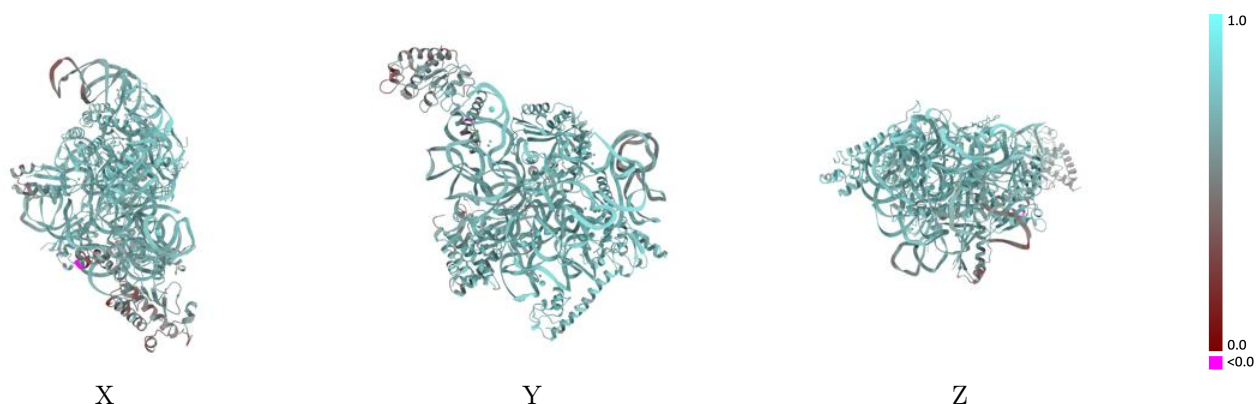
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0114 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](#)

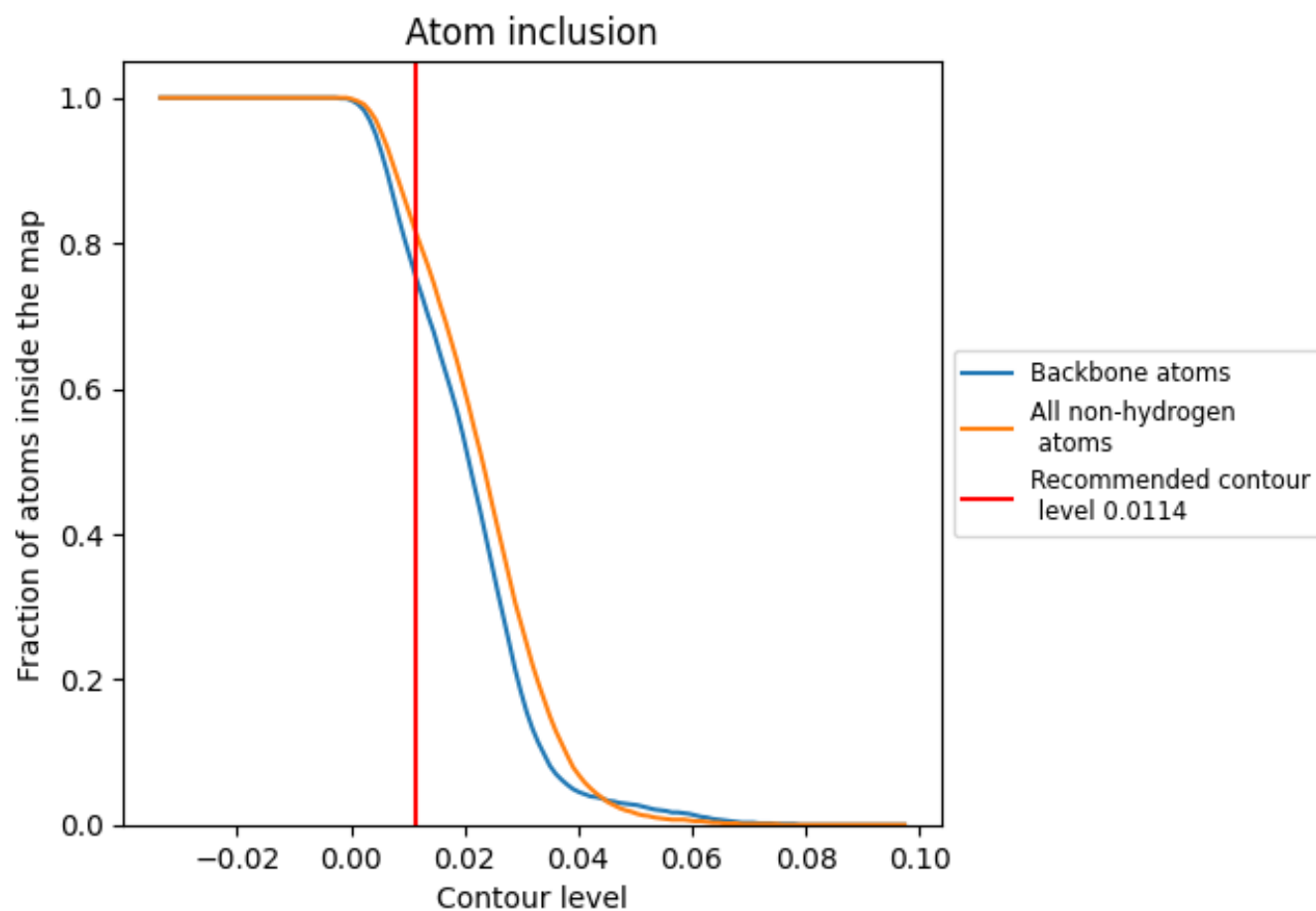


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 82% 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 (0.0114) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8160	0.6870
A	0.9220	0.7050
B	0.1500	0.5170
C	0.8850	0.7200
G	0.6970	0.6570
I	0.8720	0.7030
J	0.7210	0.6640
M	0.8720	0.7240
N	0.9250	0.7380
S	0.9000	0.7400

1.0

0.0

<0.0