WORLDWIDE PDB
PROTEIN DATA BANK

wwPDB EM Validation Summary Report (i)

Sep 13, 2023 – 01:12 pm BST

PDB ID	:	8CA7
EMDB ID	:	EMD-16520
Title	:	Omadacycline and spectinomycin bound to the 30S ribosomal subunit head
Authors	:	Paternoga, H.; Crowe-McAuliffe, C.; Wilson, D.N.
Deposited on	:	2023-01-24
Resolution	:	2.06 Å(reported)
Based on initial model	:	7k00

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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 2.06 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.
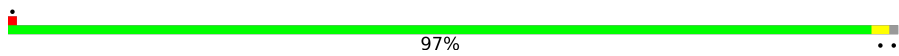
Metric	Percentile Ranks	Value
Clashscore		1
Ramachandran outliers		0.1%
Sidechain outliers		0.9%
RNA backbone		0.57

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures
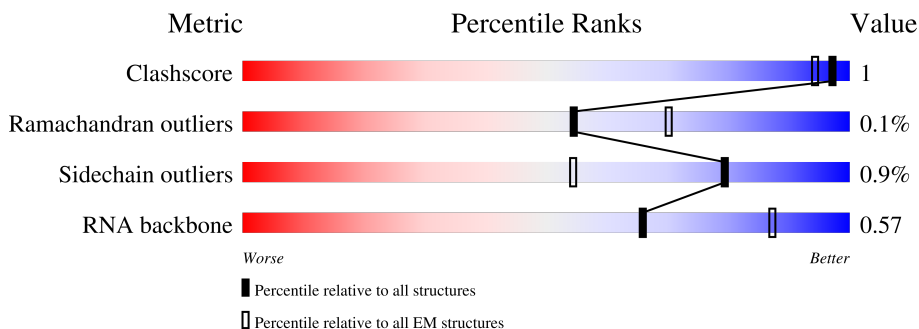
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	A	1540	· 27% 5% 67%
2	C	233	85% · 12%
3	E	167	7% 22% 78%
4	G	179	6% 55% · 44%
5	I	130	89% 5% · ·
6	J	103	6% 71% 10% 19%
7	M	118	· 92% · ·

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Mol	Chain	Length	Quality of chain
8	N	101	97%
9	S	92	88% 9%

2 Entry composition ⓘ

There are 14 unique types of molecules in this entry. The entry contains 18093 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	502	Total 10741	C 4797	N 1950	O 3492	P 502	0	0

- Molecule 2 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 3 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	36	Total 272	C 172	N 51	O 48	S 1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	101	Total 793	C 497	N 147	O 146	S 3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	125	Total 1001	C 622	N 200	O 176	S 3	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
6	J	83	Total 667	C 419	N 131	O 117	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	113	Total 876	C 541	N 177	O 155	S 3	0	0

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

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

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

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

- Molecule 10 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 11 is Omadacycline (three-letter code: U3B) (formula: $C_{29}H_{40}N_4O_7$) (labeled as "Ligand of Interest" by depositor).
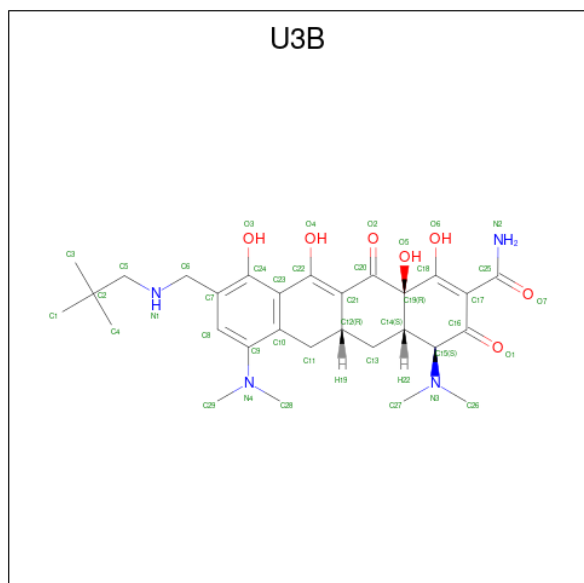
Mol	Chain	Residues	Atoms				AltConf
11	A	1	Total 40	C 29	N 4	O 7	0

- Molecule 12 is SPECTINOMYCIN (three-letter code: SCM) (formula: $C_{14}H_{24}N_2O_7$) (labeled as "Ligand of Interest" by depositor).
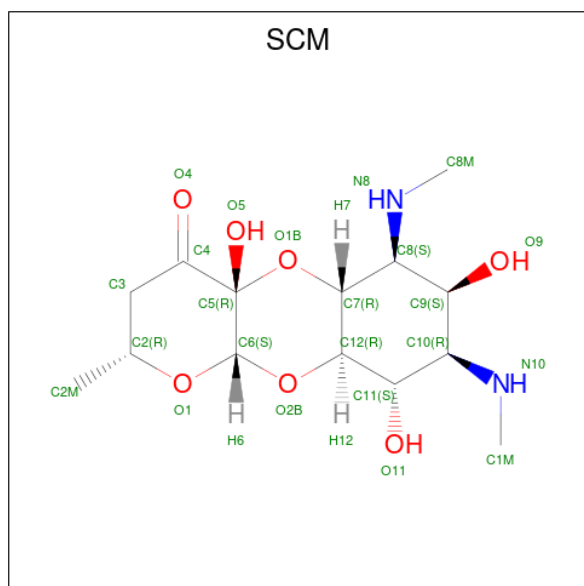
Mol	Chain	Residues	Atoms				AltConf
12	A	1	Total 23	C 14	N 2	O 7	0

- Molecule 13 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
13	A	25	Total 25	Mg 25	0
13	M	1	Total 1	Mg 1	0

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		AltConf
14	A	449	Total 449	O 449	0
14	C	21	Total 21	O 21	0
14	G	1	Total 1	O 1	0

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| Mol	Chain	Residues	Atoms		AltConf
14	I	13	Total 13	O 13	0
14	J	9	Total 9	O 9	0
14	M	14	Total 14	O 14	0
14	N	26	Total 26	O 26	0
14	S	10	Total 10	O 10	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.
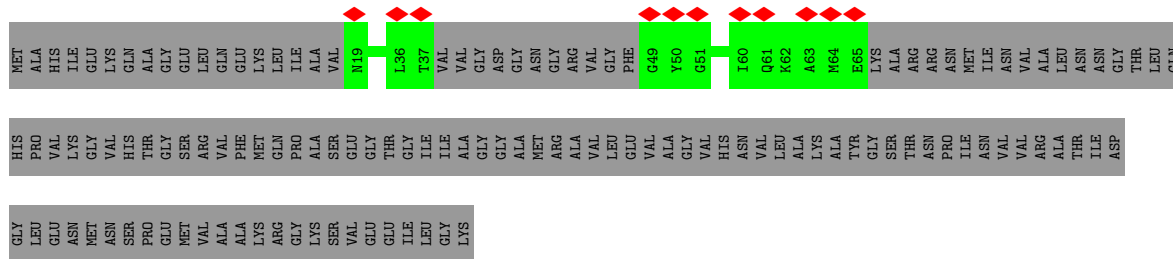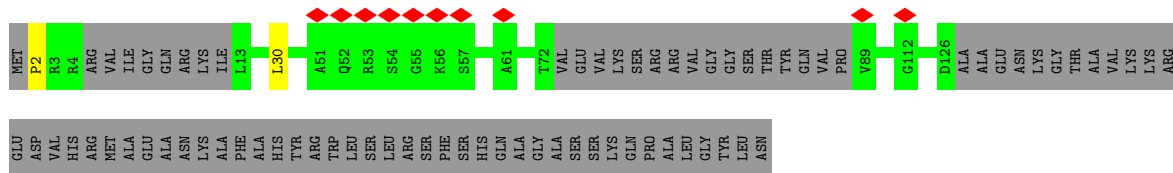
• Molecule 1: 16S rRNA
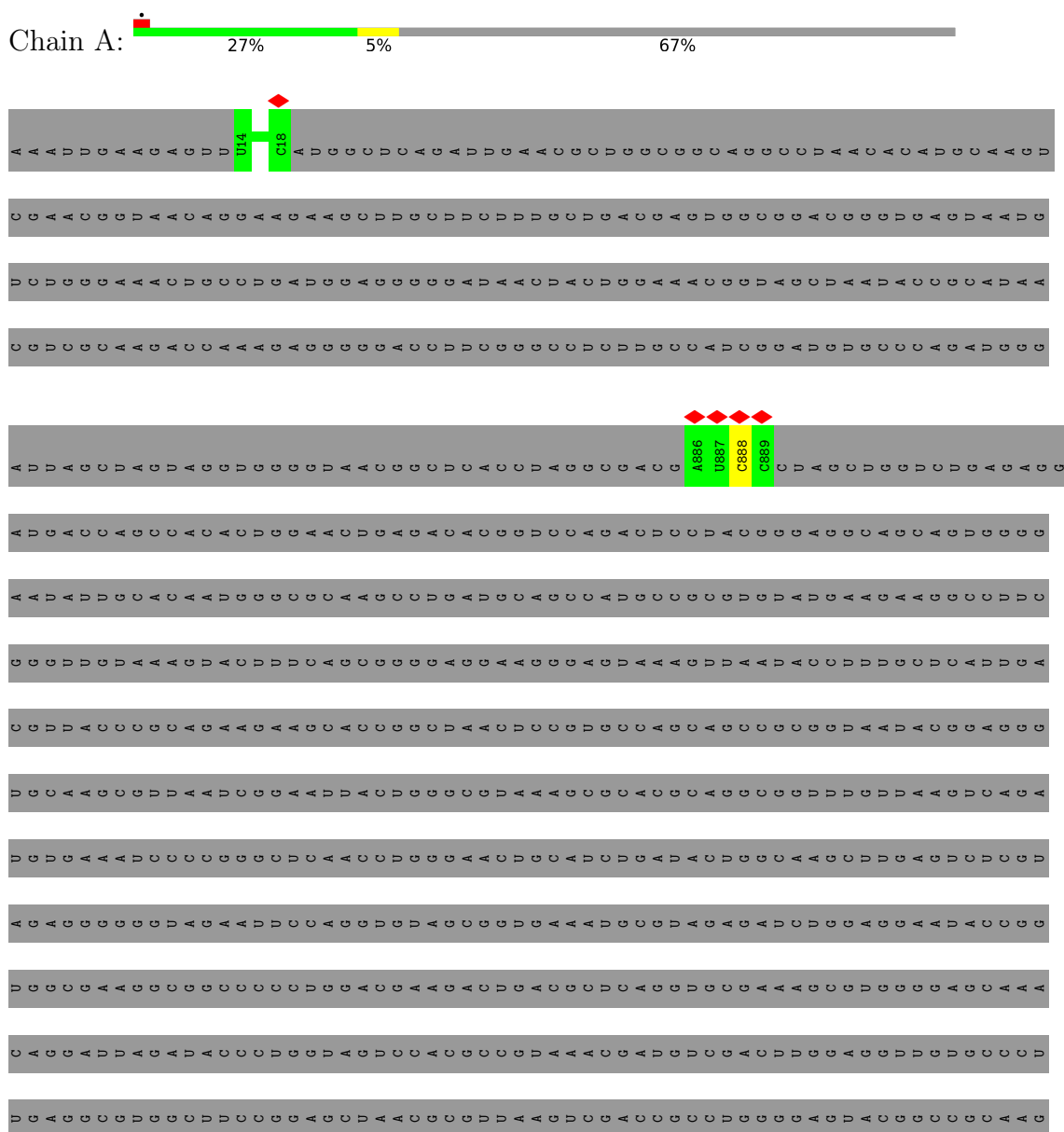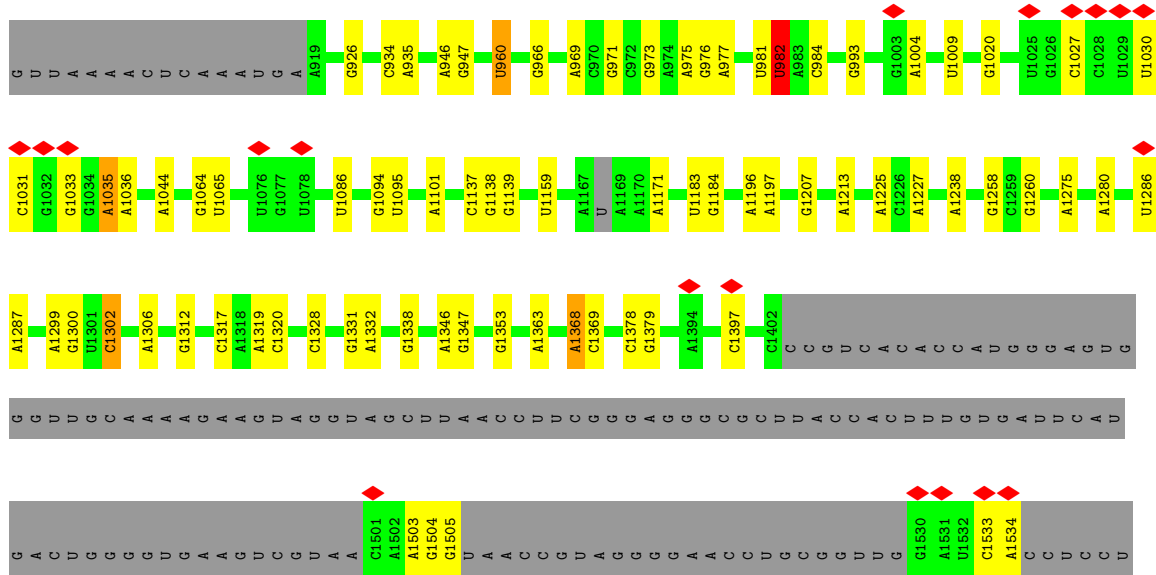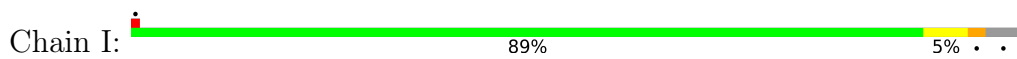
• Molecule 2: Small ribosomal subunit protein uS3

Chain C:

85%   •   12%
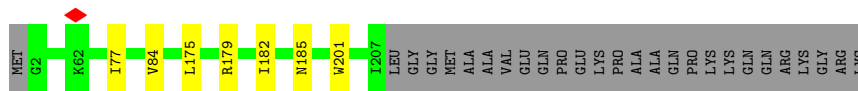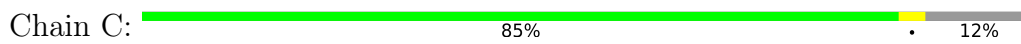
• Molecule 3: Small ribosomal subunit protein uS5

Chain E:

7%

22%   78%

• Molecule 4: 30S ribosomal protein S7

Chain G:

6%

55%   •   44%

• Molecule 5: Small ribosomal subunit protein uS9

Chain I:

89% | 5%

MET ALA GLU N4 R85 M88 E97 L98 R99 R109 R113 K114 R123 R124 S128 LYS ARG

• Molecule 6: Small ribosomal subunit protein uS10

6%

Chain J:

71% | 10% | 19%

MET GLN ASN GLN R5 E24 I25 V26 E27 T28 A29 K30 R31 A34 P39 L52 V57 N58 K59 R62 D63 Q64 V74 V77 GLU PRO THR GLU LYS THR VAL ASP ALA LEU MET ARG LEU ASP L92 V98 S101 LEU GLY

• Molecule 7: Small ribosomal subunit protein uS13

Chain M:

92%

MET A2 H12 I17 T28 I39 L56 K114 PRO ILE LYS LYS

• Molecule 8: Small ribosomal subunit protein uS14

Chain N:

97%

MET A2 R13 D38 R63 W101
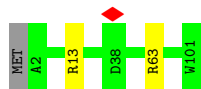
• Molecule 9: Small ribosomal subunit protein uS19

Chain S:

88% | 9%

MET P2 L13 S25 G26 D27 A50 H57 A85 ASP LYS LYS ALA LYS LYS LYS
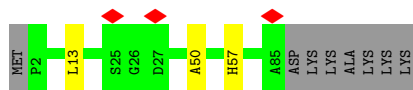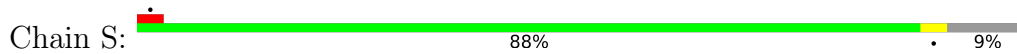
4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	514855	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 $(e^-/\text{Å}^2)$	44	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.253	Depositor
Minimum map value	-0.124	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	390.144, 390.144, 390.144	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.762, 0.762, 0.762	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SCM, K, MG, U3B, 2MG, 4OC, 5MC

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	0.54	0/11912	1.16	11/18560 (0.1%)
2	C	0.29	0/1651	0.62	0/2225
3	E	0.36	0/274	0.65	0/363
4	G	0.32	0/801	0.67	0/1073
5	I	0.32	0/1013	0.72	0/1350
6	J	0.29	0/675	0.67	0/911
7	M	0.30	0/884	0.64	0/1181
8	N	0.31	0/817	0.62	0/1088
9	S	0.32	0/685	0.63	0/922
All	All	0.47	0/18712	1.02	11/27673 (0.0%)

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
2	C	0	1
5	I	0	5
6	J	0	1
8	N	0	1
All	All	0	8

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	981	U	OP1-P-O3'	11.24	129.92	105.20
1	A	982	U	O5'-P-OP2	-10.63	96.13	105.70
1	A	981	U	OP2-P-O3'	-10.61	81.86	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	973	G	O5'-P-OP2	-6.57	99.79	105.70
1	A	1331	G	O4'-C1'-N9	6.24	113.19	108.20

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	179	ARG	Sidechain
5	I	109	ARG	Sidechain
5	I	123	ARG	Sidechain
5	I	85	ARG	Sidechain
5	I	99	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	10741	0	5429	6	0
2	C	1624	0	1696	2	0
3	E	272	0	286	0	0
4	G	793	0	827	0	0
5	I	1001	0	1044	4	0
6	J	667	0	704	5	0
7	M	876	0	934	3	0
8	N	805	0	844	1	0
9	S	668	0	693	1	0
10	A	14	0	0	0	0
11	A	40	0	0	0	0
12	A	23	0	24	0	0
13	A	25	0	0	0	0
13	M	1	0	0	0	0
14	A	449	0	0	0	0
14	C	21	0	0	0	0
14	G	1	0	0	0	0
14	I	13	0	0	0	0
14	J	9	0	0	0	0
14	M	14	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	N	26	0	0	0	0
14	S	10	0	0	0	0
All	All	18093	0	12481	17	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.

The worst 5 of 17 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)
5:I:99:ARG:HH21	5:I:99:ARG:HG3	1.71	0.56
1:A:1302:C:C5	7:M:17:ILE:HG13	2.44	0.53
2:C:175:LEU:HD23	2:C:182:ILE:HD13	1.91	0.52
5:I:85:ARG:HA	5:I:88:MET:HE2	1.94	0.49
9:S:50:ALA:HB1	9:S:57:HIS:HB3	1.94	0.49

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	
2	C	204/233 (88%)	197 (97%)	7 (3%)	0	100	100
3	E	32/167 (19%)	32 (100%)	0	0	100	100
4	G	95/179 (53%)	92 (97%)	3 (3%)	0	100	100
5	I	123/130 (95%)	114 (93%)	9 (7%)	0	100	100
6	J	79/103 (77%)	77 (98%)	1 (1%)	1 (1%)	12	4
7	M	111/118 (94%)	108 (97%)	3 (3%)	0	100	100
8	N	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
9	S	82/92 (89%)	81 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	824/1123 (73%)	798 (97%)	25 (3%)	1 (0%)	54	45

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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	C	170/190 (90%)	168 (99%)	2 (1%)	71	69
3	E	27/126 (21%)	27 (100%)	0	100	100
4	G	85/147 (58%)	83 (98%)	2 (2%)	49	43
5	I	103/107 (96%)	102 (99%)	1 (1%)	76	75
6	J	72/90 (80%)	72 (100%)	0	100	100
7	M	91/96 (95%)	91 (100%)	0	100	100
8	N	83/84 (99%)	83 (100%)	0	100	100
9	S	72/79 (91%)	71 (99%)	1 (1%)	67	64
All	All	703/919 (76%)	697 (99%)	6 (1%)	79	78

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	G	30	LEU
5	I	97	GLU
9	S	13	LEU
2	C	201	TRP
2	C	185	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
6	J	64	GLN
8	N	4	GLN
9	S	83	HIS
9	S	56	GLN
6	J	58	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	495/1540 (32%)	67 (13%)	6 (1%)

5 of 67 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	888	C
1	A	926	G
1	A	934	C
1	A	935	A
1	A	960	U

5 of 6 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1137	C
1	A	1225	A
1	A	1319	A
1	A	993	G
1	A	971	G

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

4 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	2MG	A	966	1,13	18,26,27	1.05	2 (11%)	16,38,41	0.66	0
1	4OC	A	1402	1	20,23,24	0.48	0	26,32,35	0.62	0
1	5MC	A	967	1	18,22,23	0.36	0	26,32,35	0.69	0
1	2MG	A	1207	1,10	18,26,27	1.00	1 (5%)	16,38,41	0.73	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	2MG	A	966	1,13	-	0/5/27/28	0/3/3/3
1	4OC	A	1402	1	-	0/9/29/30	0/2/2/2
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2
1	2MG	A	1207	1,10	-	0/5/27/28	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	966	2MG	C5-C6	-2.30	1.42	1.47
1	A	1207	2MG	C5-C6	-2.18	1.43	1.47
1	A	966	2MG	C8-N7	-2.06	1.31	1.35

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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 42 ligands modelled in this entry, 40 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
12	SCM	A	1603	-	23,25,25	0.35	0	26,39,39	0.81	0
11	U3B	A	1602	13	41,43,43	1.25	3 (7%)	48,69,69	1.48	9 (18%)

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
12	SCM	A	1603	-	-	0/4/57/57	0/3/3/3
11	U3B	A	1602	13	-	4/19/77/77	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1602	U3B	C25-N2	5.45	1.47	1.33
11	A	1602	U3B	C20-C21	-3.35	1.39	1.46
11	A	1602	U3B	C22-C21	2.35	1.40	1.36

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	1602	U3B	C20-C19-C18	3.81	114.35	109.88
11	A	1602	U3B	C19-C14-C15	3.41	116.30	111.64
11	A	1602	U3B	C25-C17-C16	3.10	124.56	120.87
11	A	1602	U3B	C12-C21-C22	-2.99	116.84	121.39
11	A	1602	U3B	C10-C9-N4	2.57	122.05	118.91

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	1602	U3B	C7-C6-N1-C5
11	A	1602	U3B	C4-C2-C5-N1
11	A	1602	U3B	C1-C2-C5-N1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	A	1602	U3B	C3-C2-C5-N1

There are no ring outliers.

No monomer is involved in short contacts.

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

Ligand SCM A 1603

Bond lengths

Bond angles

Torsions

Rings

Ligand U3B A 1602

Bond lengths

Bond angles

Torsions

Rings
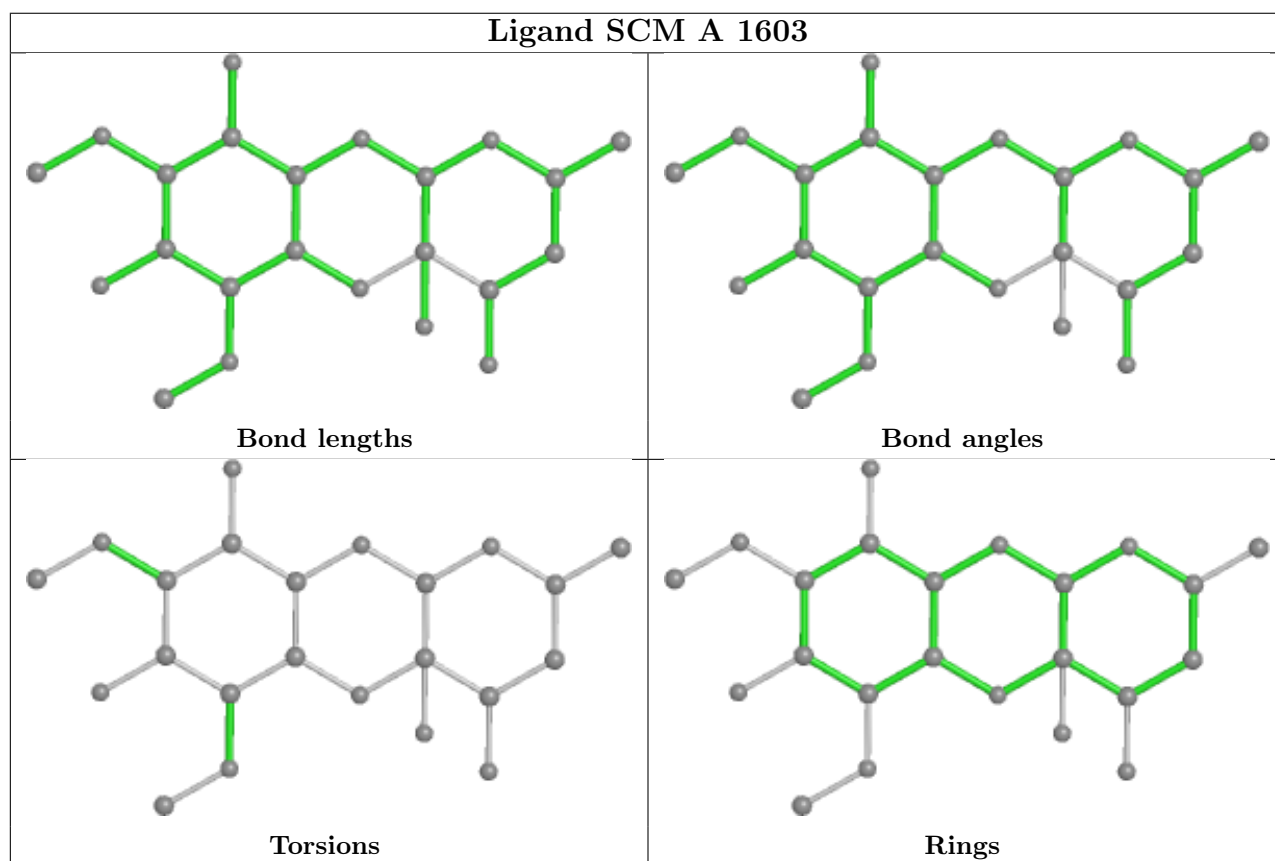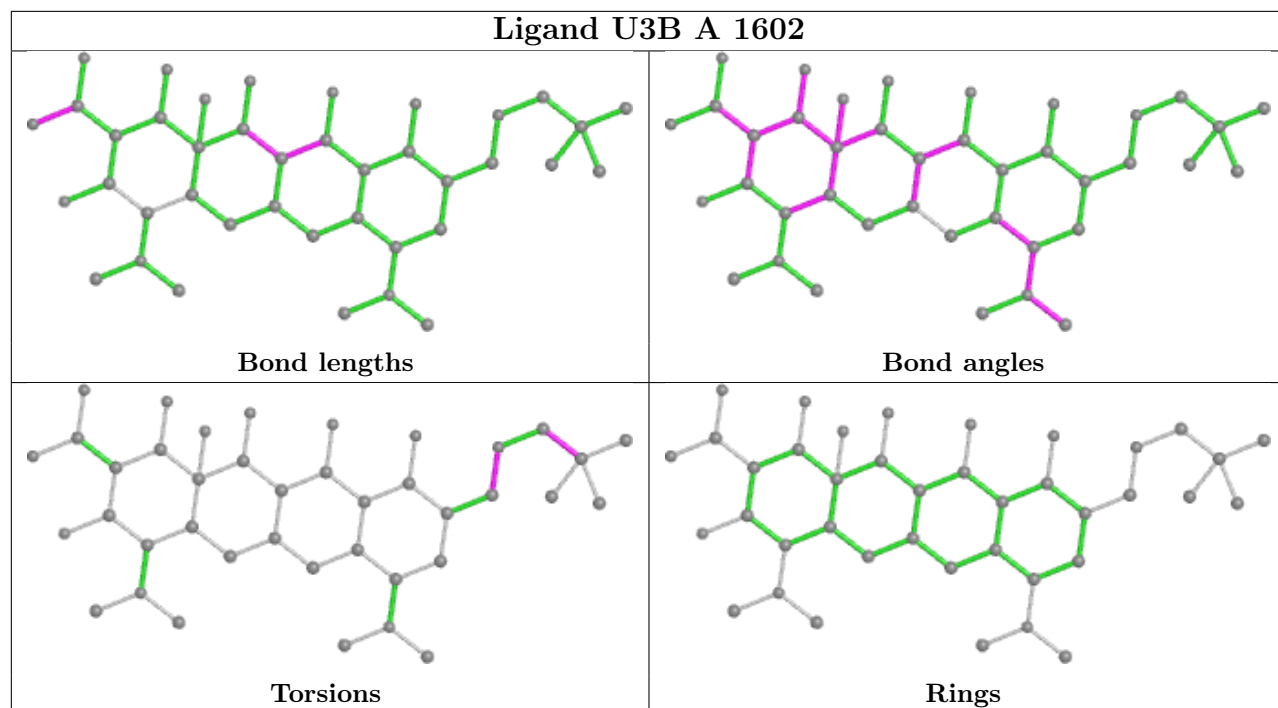
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-16520. 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 ⓘ
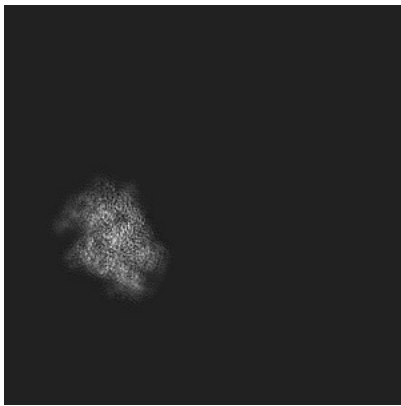
6.1.1 Primary map

X
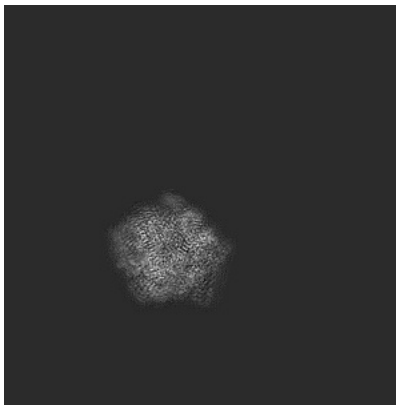
Y
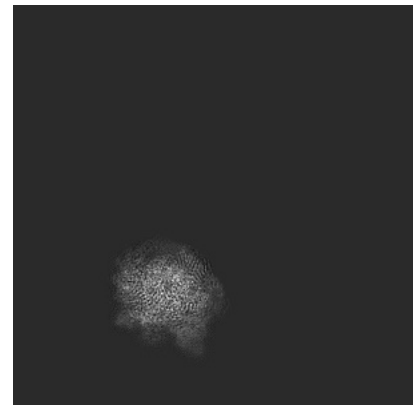
Z

6.1.2 Raw map

X

Y

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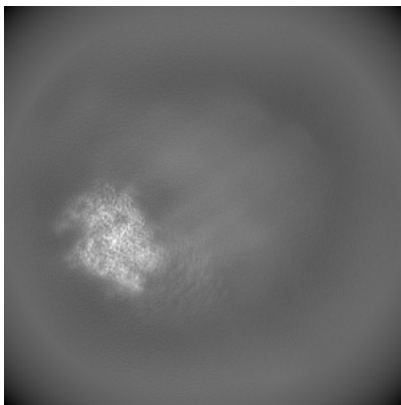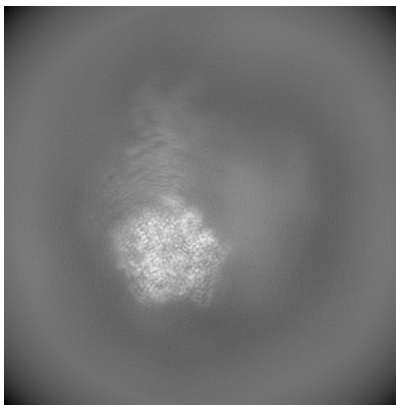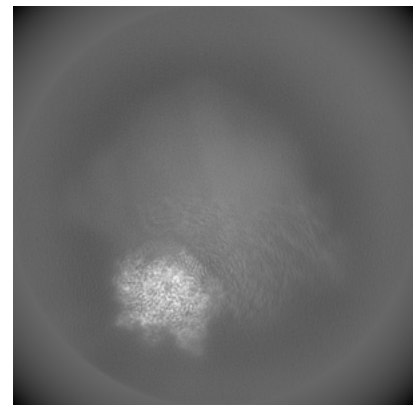
The images above show the map projected in three orthogonal directions.

6.2   Central slices   ⓘ
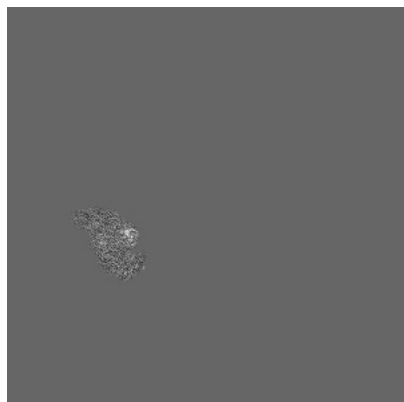
6.2.1   Primary map

X Index: 256   Y Index: 256   Z Index: 256

6.2.2   Raw map
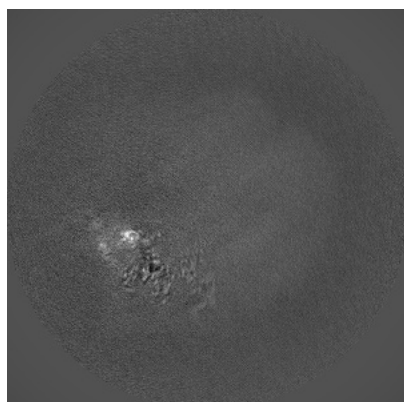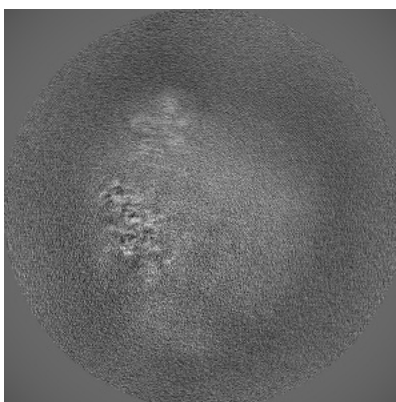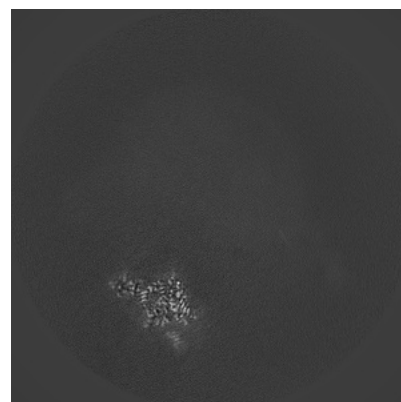
X Index: 256   Y Index: 256   Z Index: 256

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

6.3　Largest variance slices (i)

6.3.1　Primary map
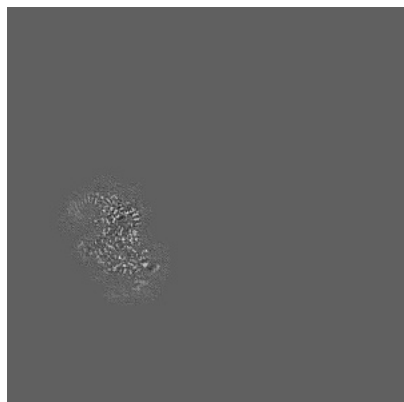
| X Index: 210 | Y Index: 140 | Z Index: 192 |
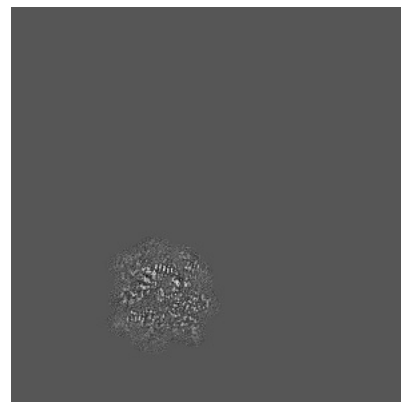
6.3.2　Raw map
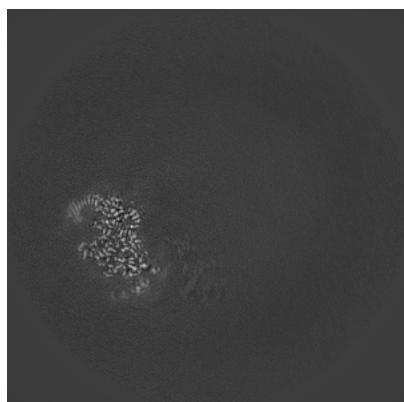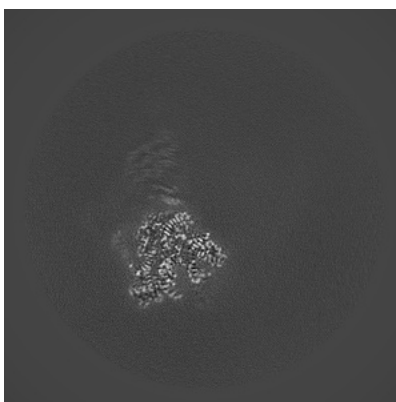
| X Index: 211 | Y Index: 140 | Z Index: 192 |
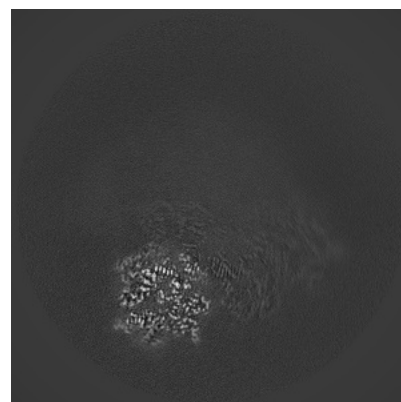
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map
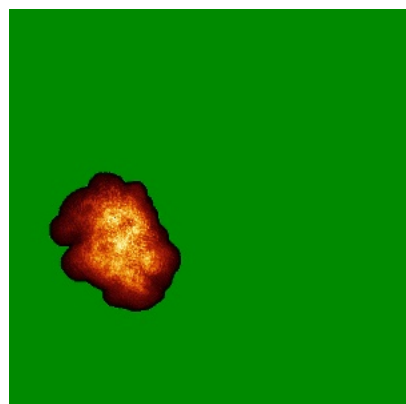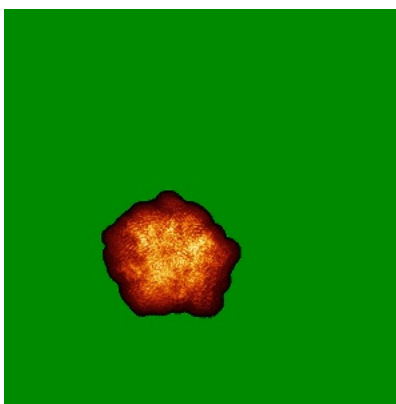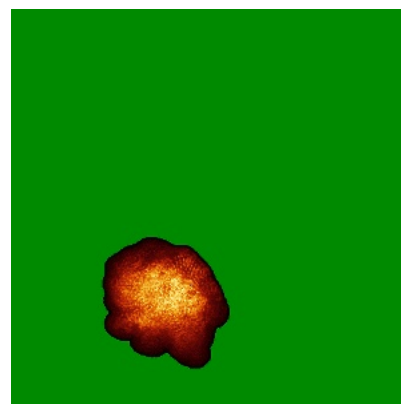
X Y Z

6.4.2 Raw map

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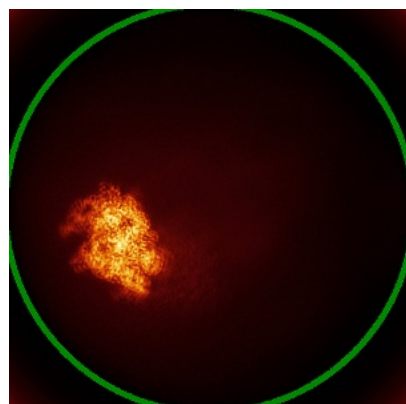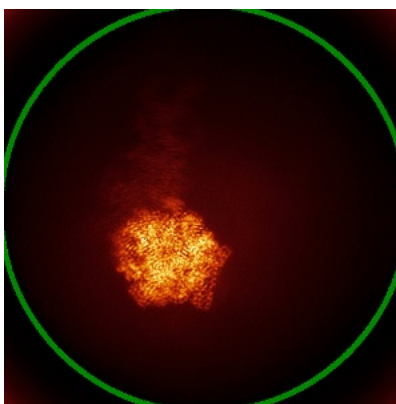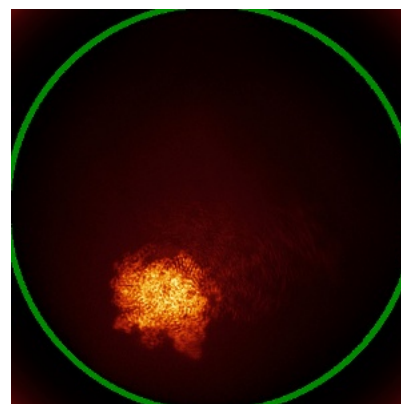
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ

6.5.1 Primary map

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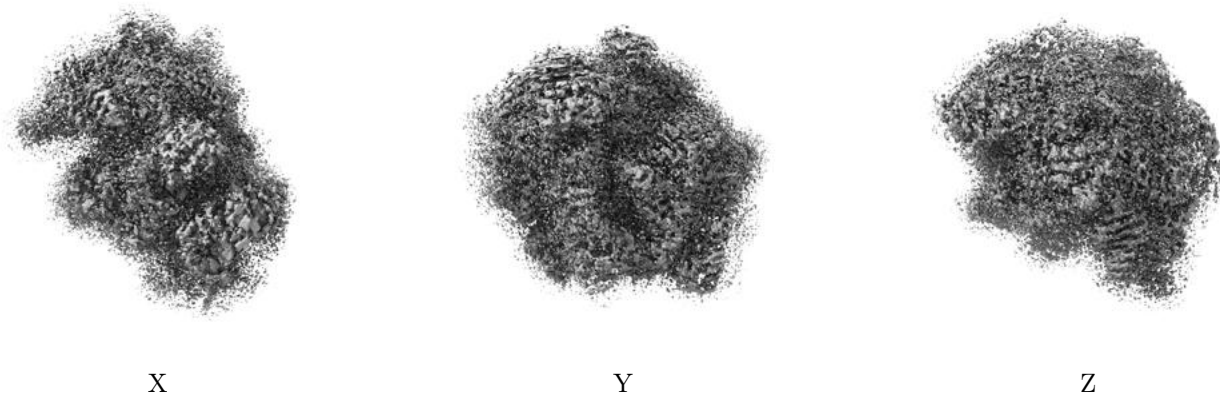
The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

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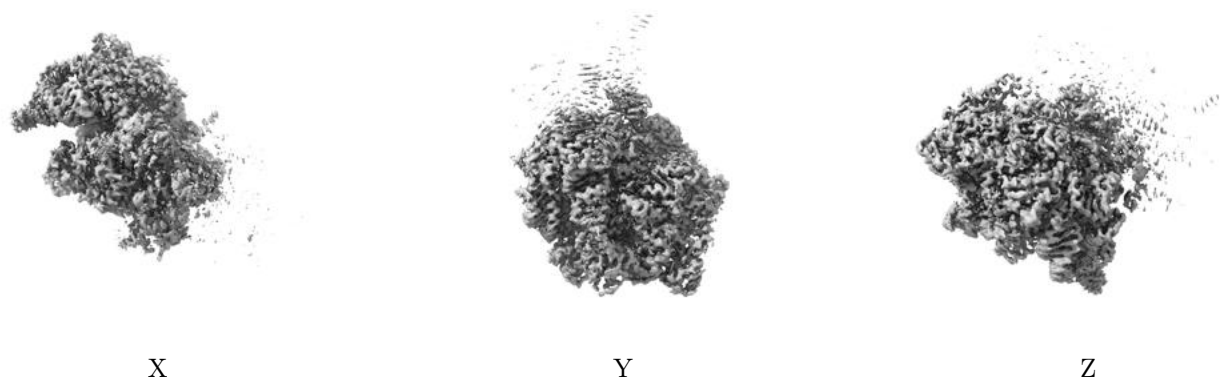
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation ⓘ

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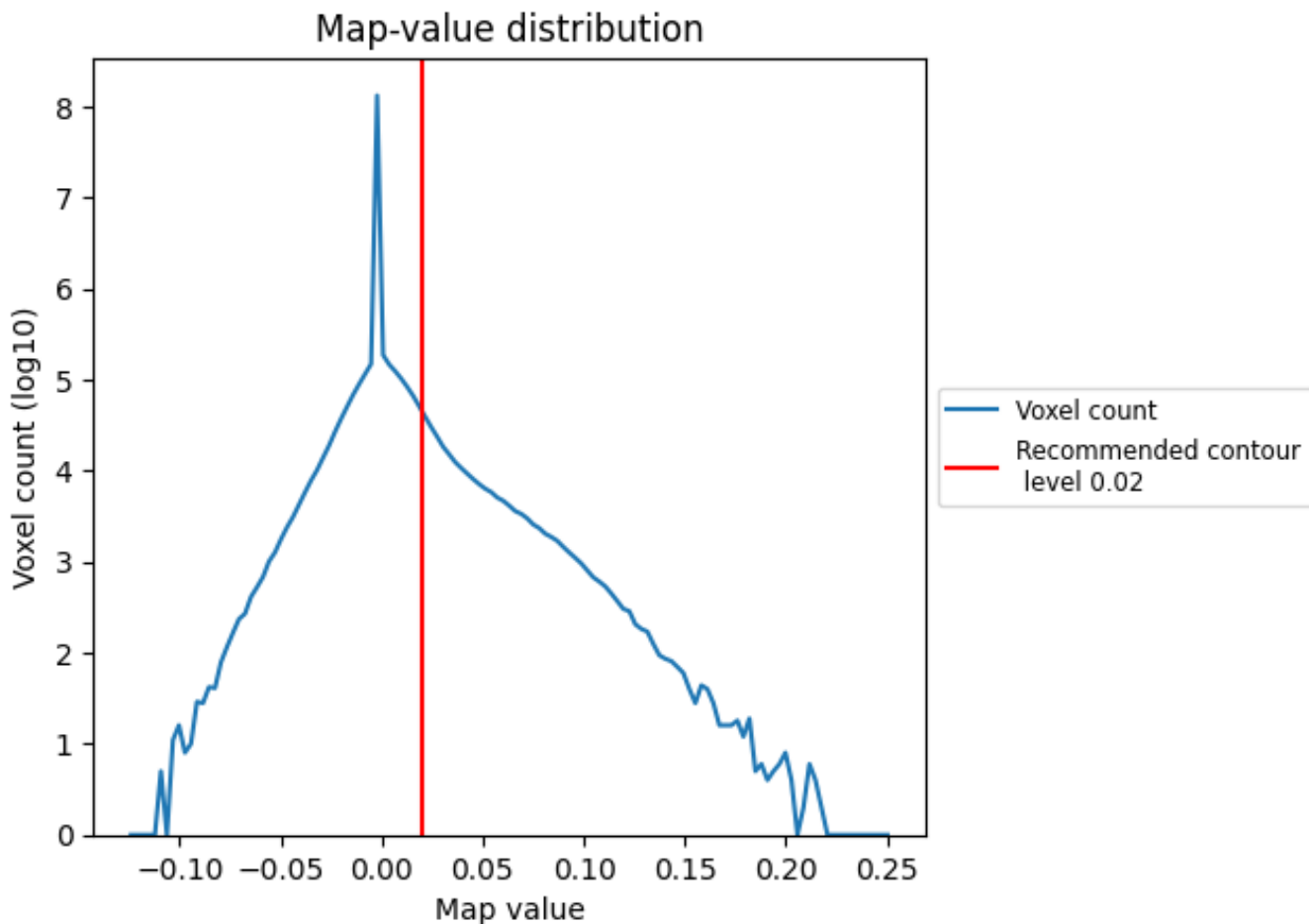
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2   Volume estimate ⓘ
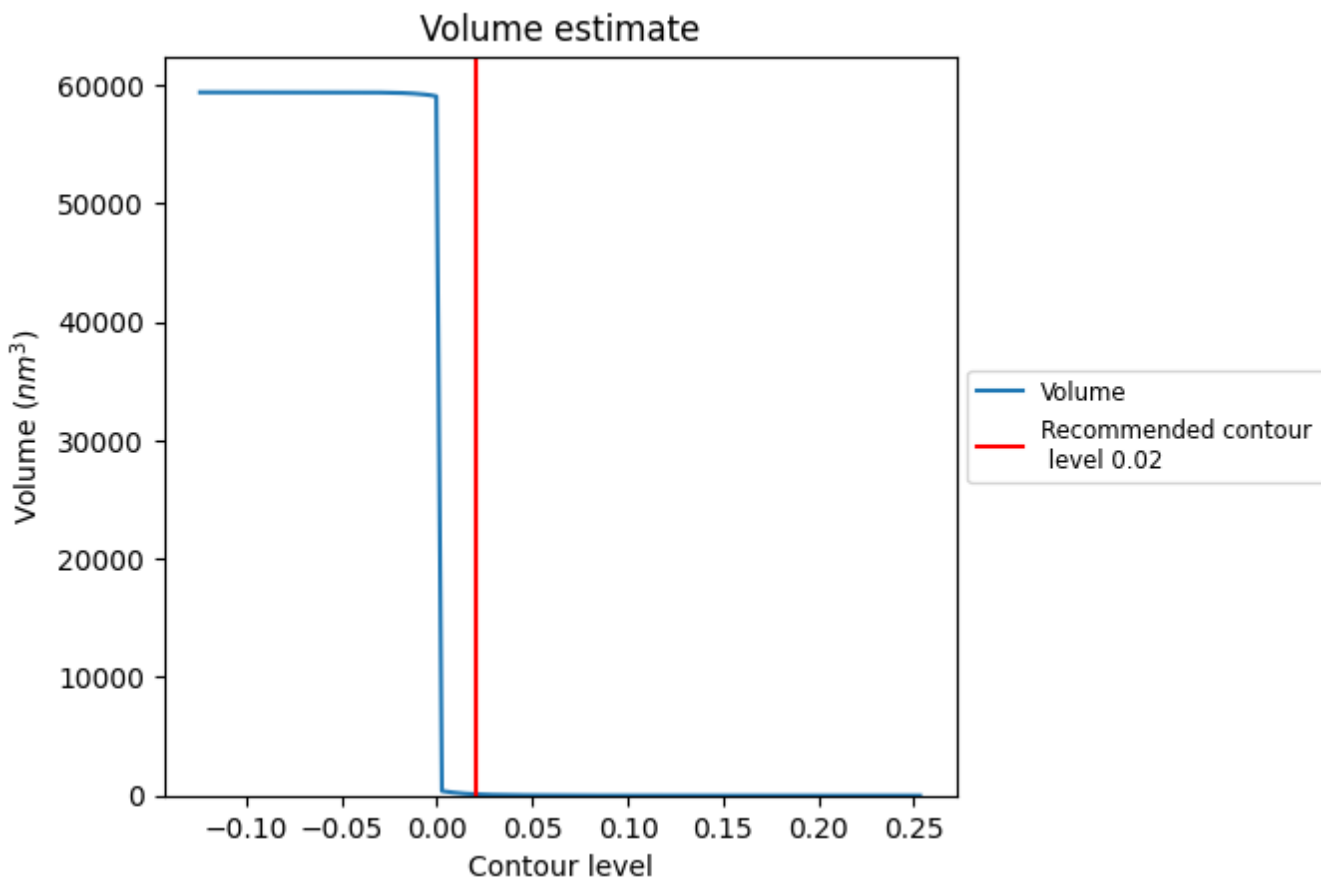
The volume at the recommended contour level is 114 nm^3; this corresponds to an approximate mass of 103 kDa.

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 ⓘ
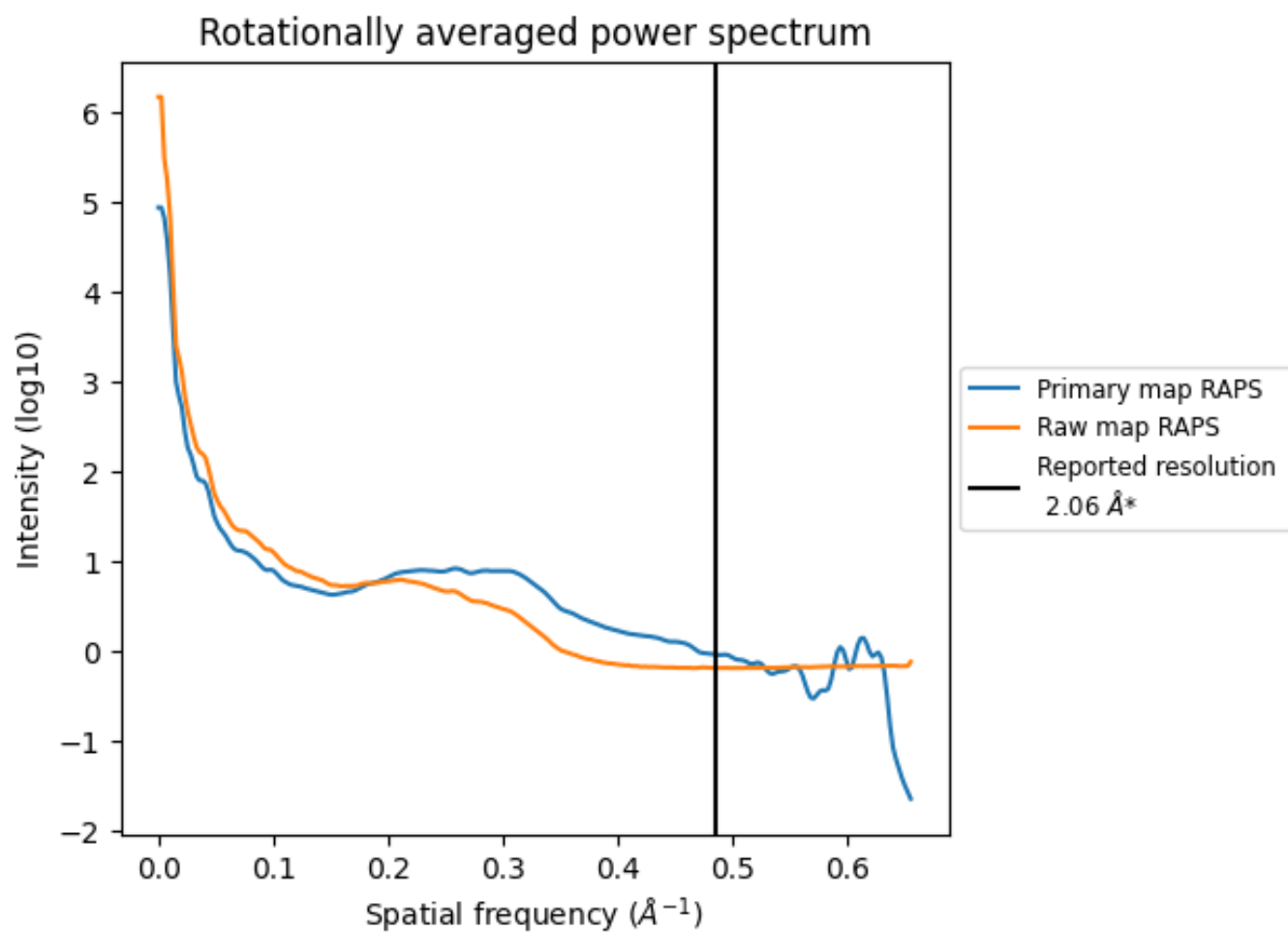
*Reported resolution corresponds to spatial frequency of 0.485 Å^{-1}

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 ⓘ
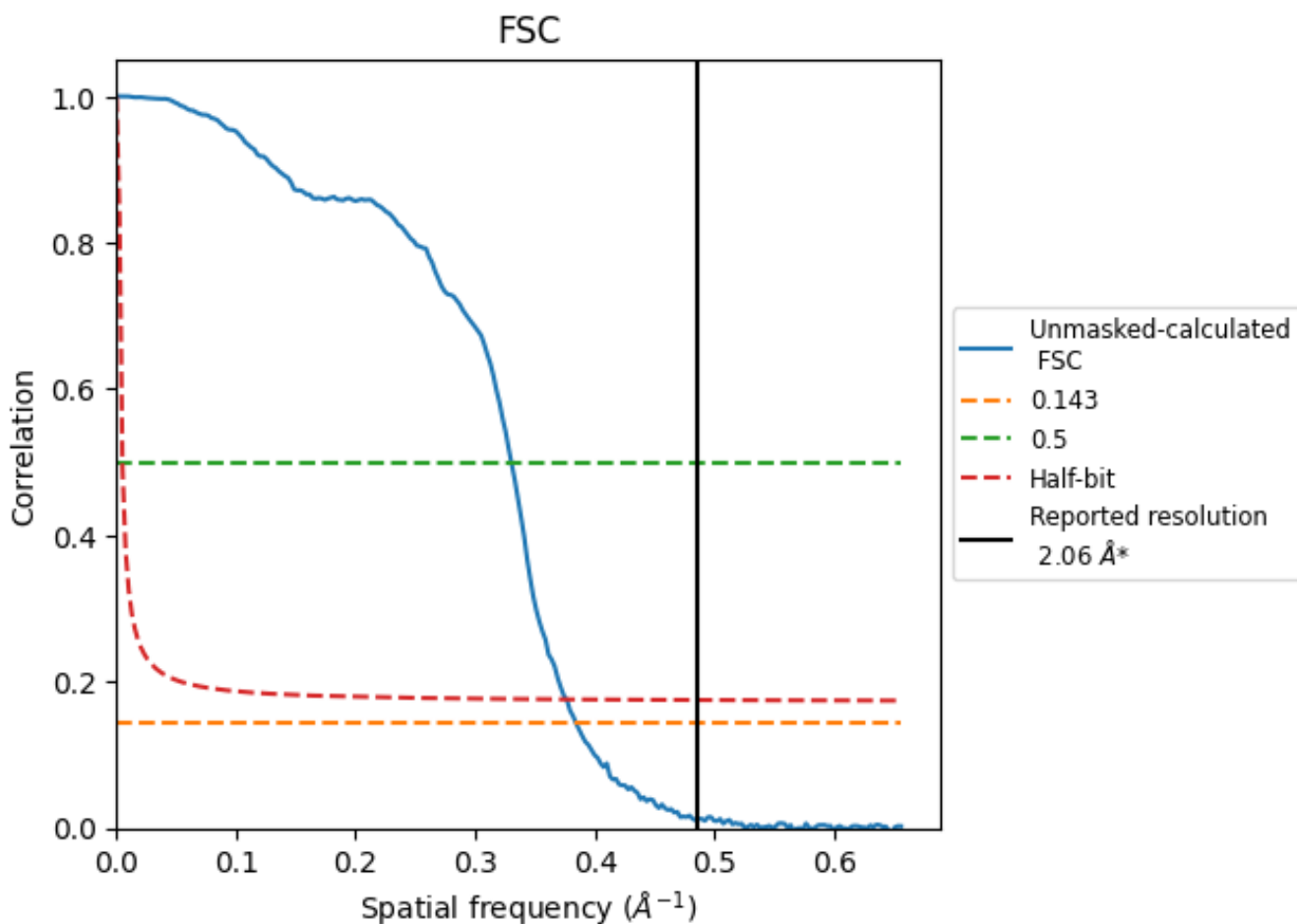
*Reported resolution corresponds to spatial frequency of 0.485 Å^{-1}

8.2   Resolution estimates ⓘ

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.06	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.60	3.03	2.66

*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 2.60 differs from the reported value 2.06 by more than 10 %

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-16520 and PDB model 8CA7. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay ⓘ

| X | Y | Z |
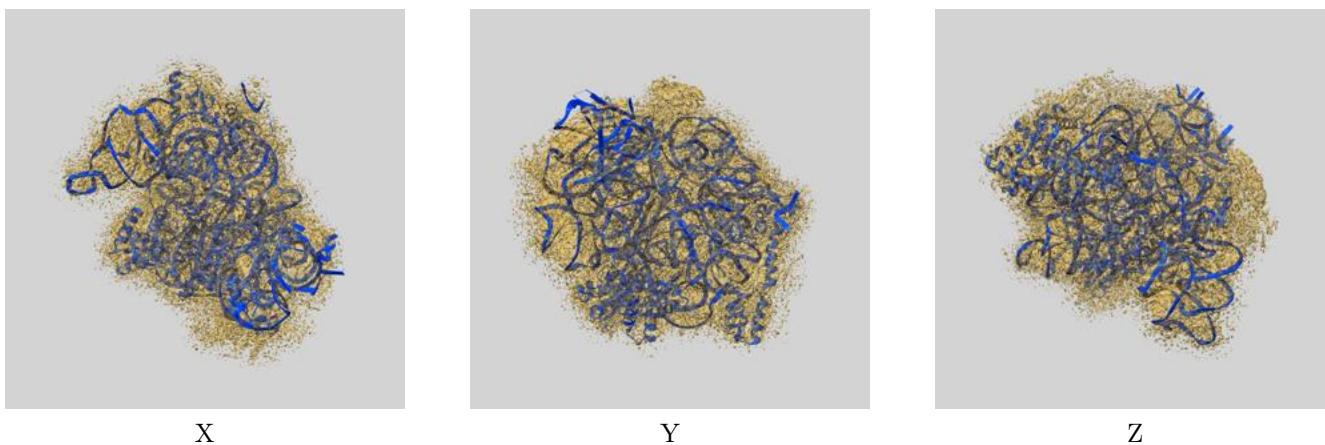
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model ⓘ

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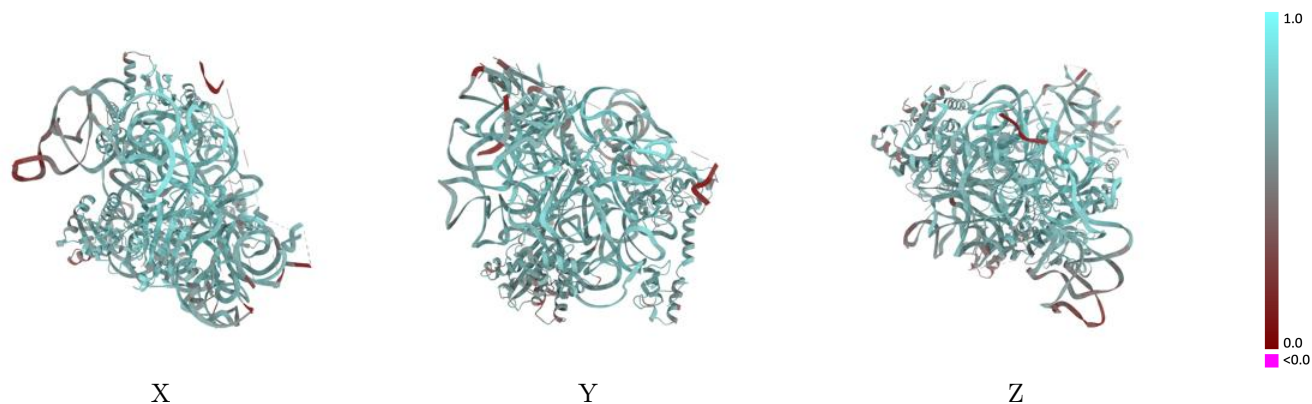
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3   Atom inclusion mapped to coordinate model ⓘ

X   Y   Z
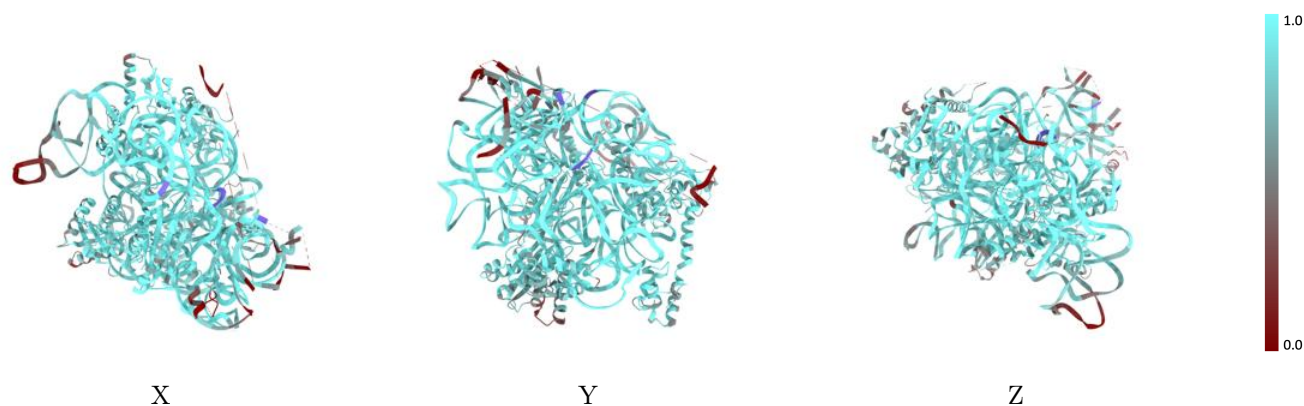
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4   Atom inclusion (i)
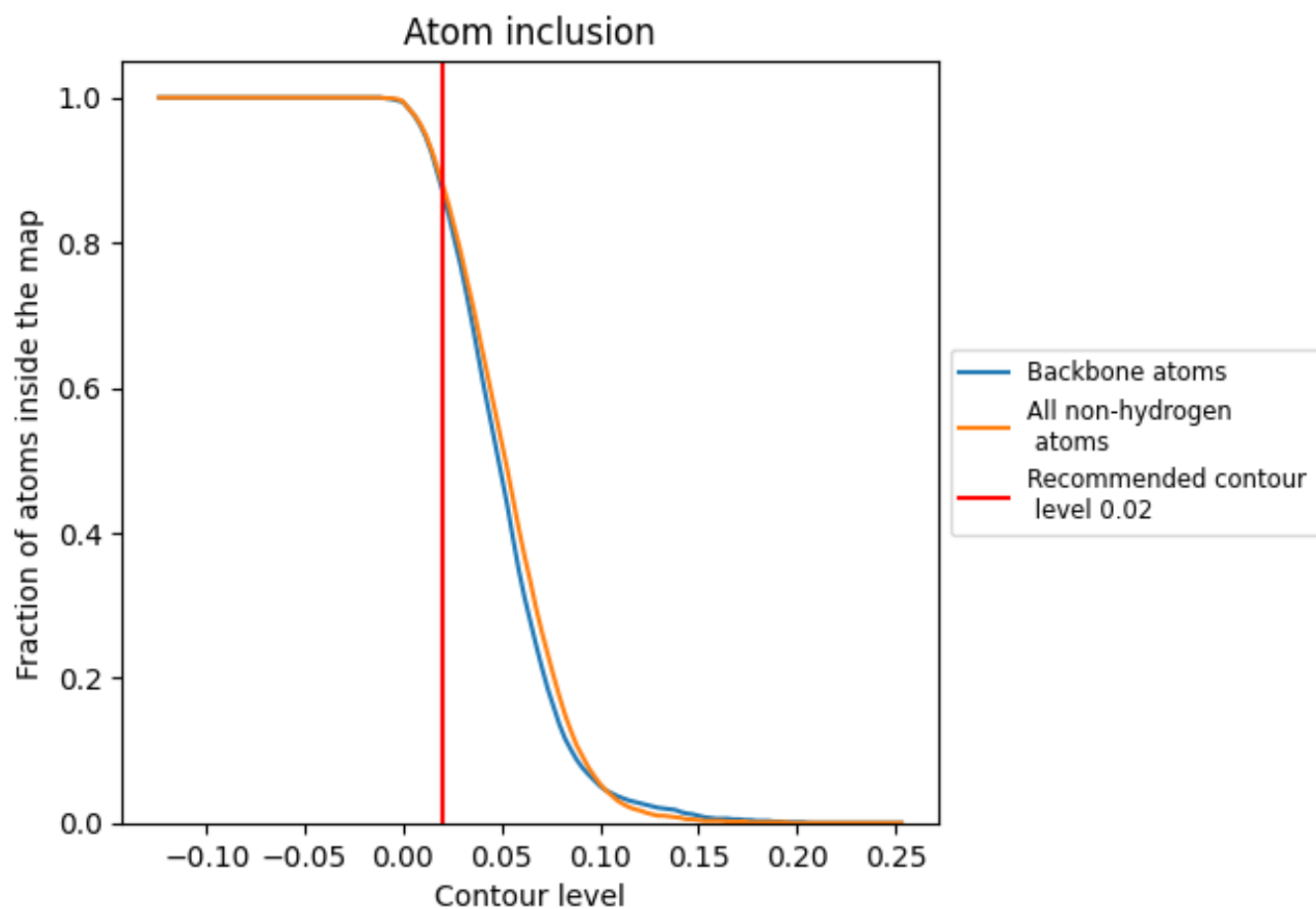
At the recommended contour level, 87% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8810	0.6660
A	0.9000	0.6690
C	0.9120	0.7100
E	0.5550	0.5720
G	0.7500	0.5970
I	0.8630	0.6410
J	0.8260	0.6240
M	0.8580	0.6510
N	0.9200	0.6990
S	0.9050	0.6780

1.0

0.0
<0.0