wwPDB EM Validation Summary Report

Aug 10, 2026 – 12:31 PM JST

PDB ID	:	9U58 / pdb_00009u58
EMDB ID	:	EMD-63866
Title	:	Cryo-EM structure of AZ-GS bound AtABCC2
Authors	:	Dong, J.; Yang, T.-L.; Yang, G.-F.
Deposited on	:	2025-03-20
Resolution	:	3.36 Å(reported)

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:

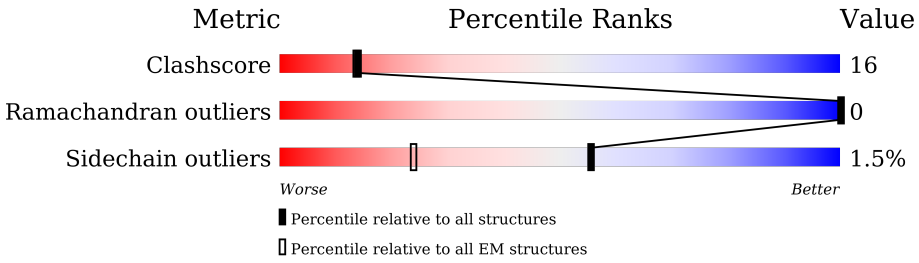
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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)	:	2.50

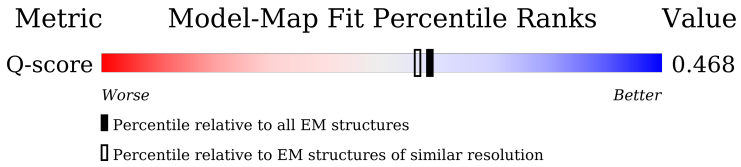
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.36 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	-
Q-score	-	25397	14332 (2.86 - 3.86)

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	1464	64% 30% • 6%

2 Entry composition

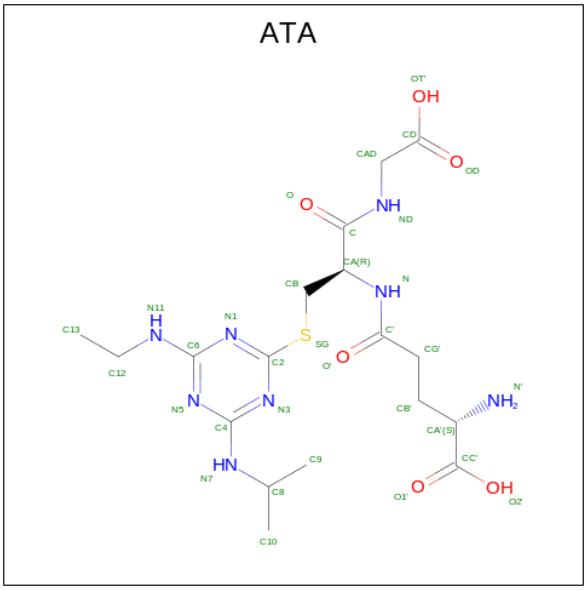
There are 3 unique types of molecules in this entry. The entry contains 11144 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called ABC transporter C family member 2.

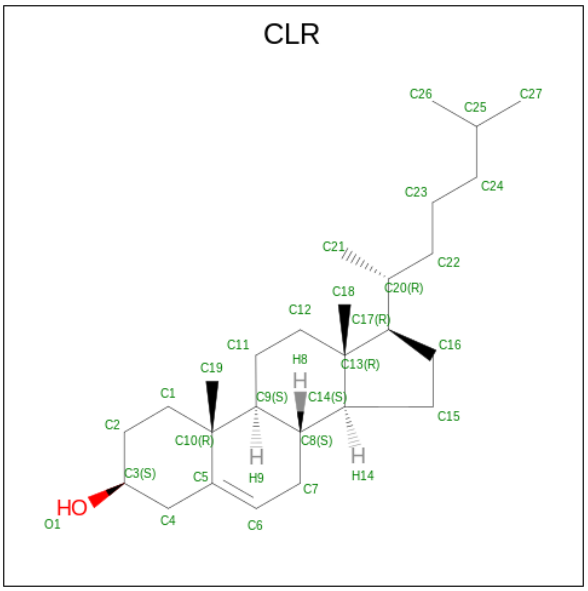
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1379	10915	7068	1839	1956	52	0	0

- Molecule 2 is ATRAZINE GLUTATHIONE CONJUGATE (CCD ID: ATA) (formula: $C_{18}H_{30}N_8O_6S$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
2	A	1	33	18	8	6	1	0

- Molecule 3 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total C O 28 27 1	0
3	A	1	Total C O 28 27 1	0
3	A	1	Total C O 28 27 1	0
3	A	1	Total C O 28 27 1	0
3	A	1	Total C O 28 27 1	0
3	A	1	Total C O 28 27 1	0
3	A	1	Total C O 28 27 1	0

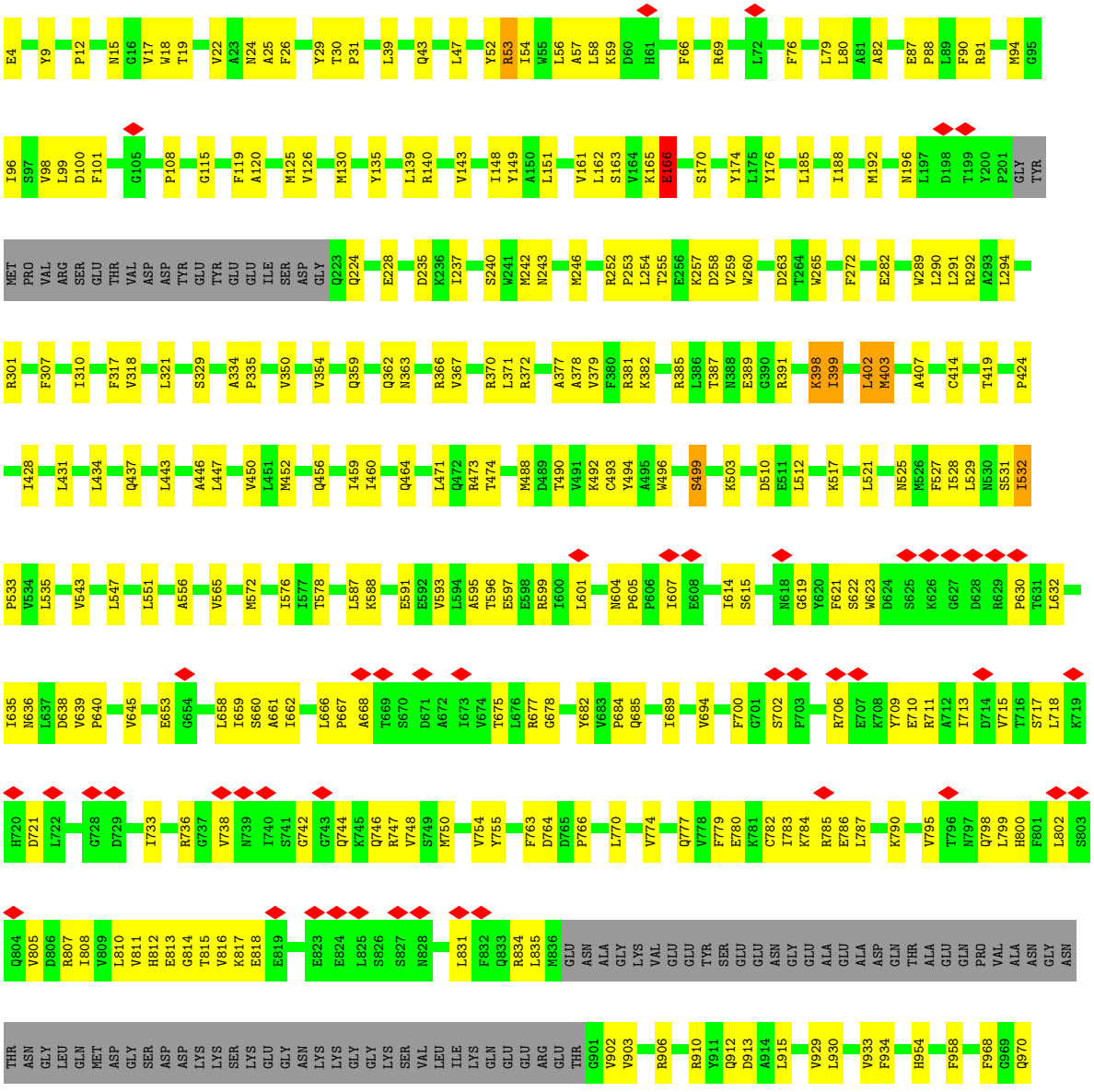
3 Residue-property plots (i)

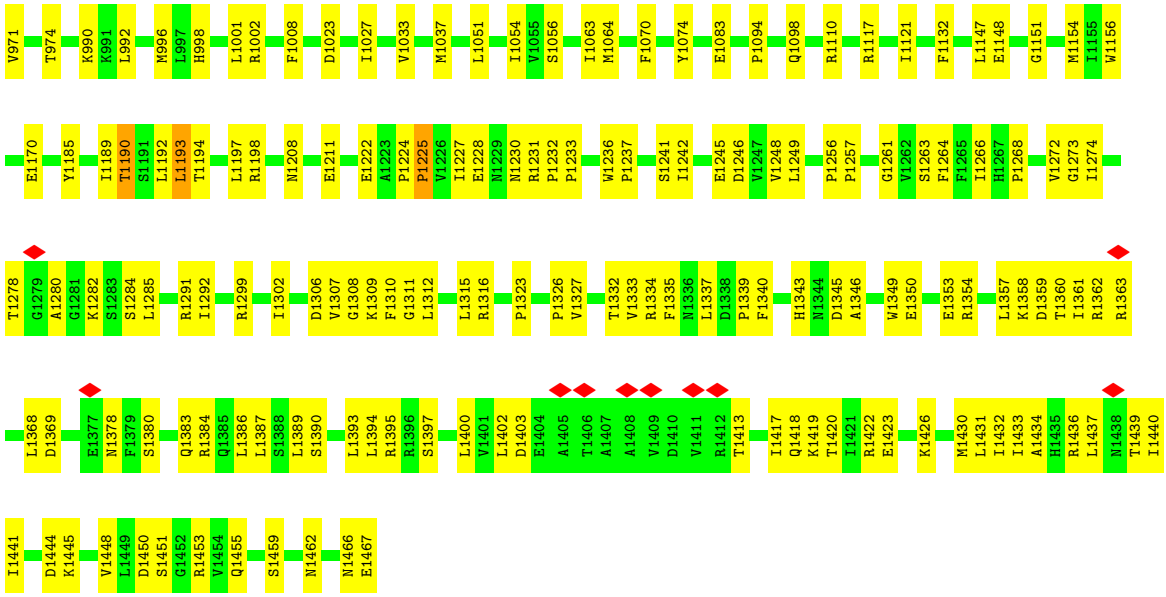
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: ABC transporter C family member 2

Chain A:






V971 T974 K990 K991 L992 M996 L997 H998 L1001 R1002 F1008 D1023 I1027 V1033 M1037 L1051 I1054 V1055 S1056 I1063 M1064 F1070 Y1074 E1083 P1094 Q1098 R1110 R1117 I1121 F1132 L1147 E1148 G1151 M1154 I1155 W1156
E1170 Y1185 I1189 T1190 S1191 L1192 L1193 T1194 L1197 R1198 N1208 E1211 E1222 A1223 P1224 P1225 V1226 I1227 E1228 N1229 N1230 R1231 P1232 P1233 W1236 P1237 S1241 I1242 E1245 D1246 V1247 V1248 L1249 P1256 P1257 G1261 V1262 S1263 F1264 F1265 I1266 H1267 P1268 V1272 G1273 I1274
T1278 G1279 A1280 G1281 K1282 S1283 S1284 L1285 R1291 I1292 R1299 I1302 D1306 V1307 G1308 K1309 F1310 G1311 L1312 L1315 R1316 P1323 P1326 V1327 T1332 V1333 R1334 F1335 N1336 L1337 D1338 P1339 F1340 H1343 N1344 D1345 A1346 W1349 E1350 E1353 R1354 L1357 K1358 D1359 T1360 I1361 R1362 R1363
L1368 D1369 E1377 N1378 F1379 S1380 Q1383 R1384 Q1385 L1386 L1387 S1388 L1389 S1390 L1393 L1394 R1395 R1396 S1397 L1400 V1401 L1402 D1403 E1404 A1405 T1406 A1407 A1408 V1409 D1410 V1411 R1412 T1413 I1417 Q1418 K1419 T1420 I1421 R1422 E1423 K1426 M1430 L1431 I1432 I1433 A1434 H1435 R1436 L1437 N1438 T1439 I1440
I1441 D1444 K1445 V1448 L1449 D1450 S1451 G1452 R1453 V1454 Q1455 S1459 N1462 N1466 E1467

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	135841	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 ($e^-/Å^2$)	49.79	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.088	Depositor
Minimum map value	-1.215	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	296.0, 296.0, 296.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.74, 0.74, 0.74	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATA, CLR

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	0.60	1/11160 (0.0%)	0.70	9/15159 (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
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	499	SER	CA-C	-5.15	1.45	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1339	PRO	CA-N-CD	-11.31	96.16	112.00
1	A	1225	PRO	N-CA-CB	-6.59	96.33	103.25
1	A	166	GLU	CA-C-N	-6.10	114.08	123.17
1	A	166	GLU	C-N-CA	-6.10	114.08	123.17
1	A	503	LYS	N-CA-C	-5.63	108.20	114.62

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	53	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	10915	0	11098	345	0
2	A	33	0	28	1	0
3	A	196	0	322	28	0
All	All	11144	0	11448	355	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 16.

The worst 5 of 355 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:929:VAL:HG22	3:A:1505:CLR:C26	1.38	1.48
1:A:929:VAL:CG2	3:A:1505:CLR:H262	1.73	1.18
1:A:929:VAL:CG2	3:A:1505:CLR:C26	2.23	1.13
1:A:929:VAL:HA	3:A:1505:CLR:H263	1.41	0.99
1:A:82:ALA:HA	1:A:125:MET:HE2	1.52	0.92

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1373/1464 (94%)	1259 (92%)	114 (8%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1193/1264 (94%)	1175 (98%)	18 (2%)	57 68

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1190	THR
1	A	1222	GLU
1	A	1194	THR
1	A	403	MET
1	A	1189	ILE

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

Mol	Chain	Res	Type
1	A	456	GLN
1	A	773	HIS
1	A	1383	GLN
1	A	1205	ASN
1	A	230	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands 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	$\#\|Z\| > 2$
2	ATA	A	1501	-	32,33,33	2.54	7 (21%)	41,43,43	5.36	13 (31%)
3	CLR	A	1508	-	31,31,31	0.31	0	48,48,48	0.45	0
3	CLR	A	1505	-	31,31,31	0.32	0	48,48,48	0.64	0
3	CLR	A	1504	-	31,31,31	0.34	0	48,48,48	0.79	1 (2%)
3	CLR	A	1507	-	31,31,31	0.32	0	48,48,48	0.42	0
3	CLR	A	1502	-	31,31,31	0.33	0	48,48,48	0.56	0
3	CLR	A	1503	-	31,31,31	0.29	0	48,48,48	0.43	0
3	CLR	A	1506	-	31,31,31	0.30	0	48,48,48	0.50	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
2	ATA	A	1501	-	-	13/34/34/34	0/1/1/1
3	CLR	A	1508	-	-	8/10/68/68	0/4/4/4
3	CLR	A	1505	-	-	9/10/68/68	0/4/4/4
3	CLR	A	1504	-	-	9/10/68/68	0/4/4/4
3	CLR	A	1507	-	-	10/10/68/68	0/4/4/4
3	CLR	A	1502	-	-	8/10/68/68	0/4/4/4
3	CLR	A	1503	-	-	8/10/68/68	0/4/4/4
3	CLR	A	1506	-	-	2/10/68/68	0/4/4/4

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1501	ATA	C4-N7	7.75	1.44	1.34
2	A	1501	ATA	C6-N11	7.48	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1501	ATA	C'-N	5.01	1.44	1.34
2	A	1501	ATA	C-ND	4.77	1.44	1.33
2	A	1501	ATA	C2-SG	3.24	1.81	1.75

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1501	ATA	C2-N1-C6	29.84	130.65	113.85
2	A	1501	ATA	N1-C6-N5	-7.95	113.66	126.23
2	A	1501	ATA	N3-C2-N1	-7.02	114.08	126.95
2	A	1501	ATA	C4-N7-C8	-6.13	119.50	124.53
2	A	1501	ATA	C2-N3-C4	5.64	117.03	113.85

There are no chirality outliers.

5 of 67 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1501	ATA	N5-C6-N11-C12
2	A	1501	ATA	N1-C6-N11-C12
2	A	1501	ATA	N1-C2-SG-CB
2	A	1501	ATA	N3-C2-SG-CB
2	A	1501	ATA	N5-C4-N7-C8

There are no ring outliers.

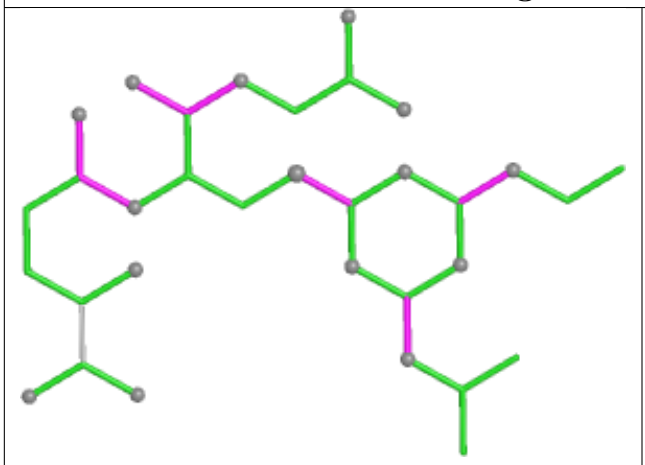
7 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1501	ATA	1	0
3	A	1508	CLR	5	0
3	A	1505	CLR	13	0
3	A	1507	CLR	5	0
3	A	1502	CLR	2	0
3	A	1503	CLR	3	0
3	A	1506	CLR	3	0

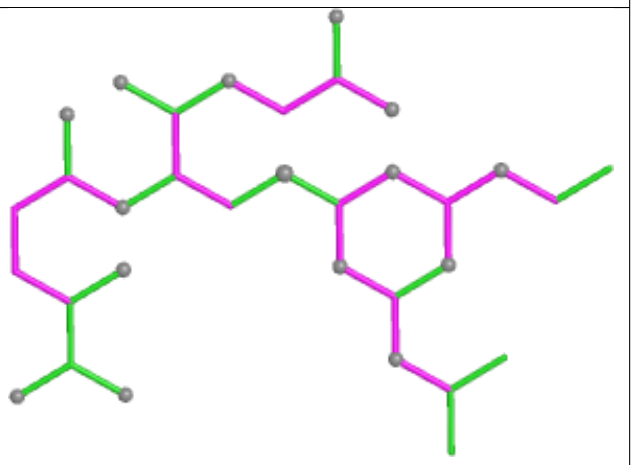
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

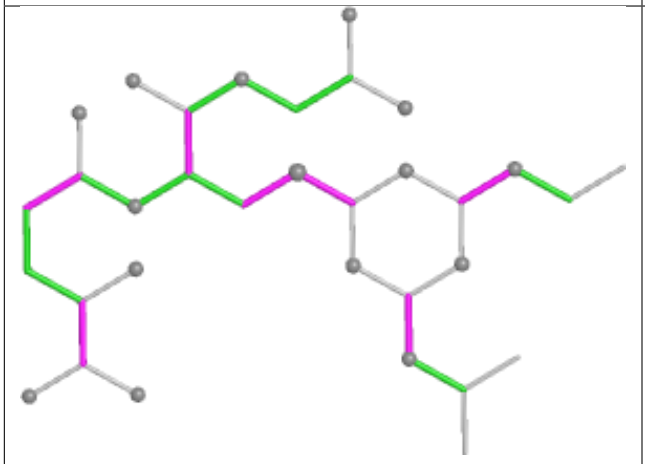
Ligand ATA A 1501



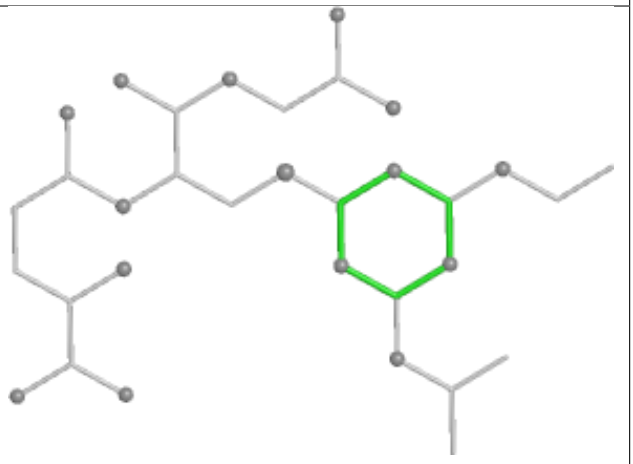
Bond lengths



Bond angles

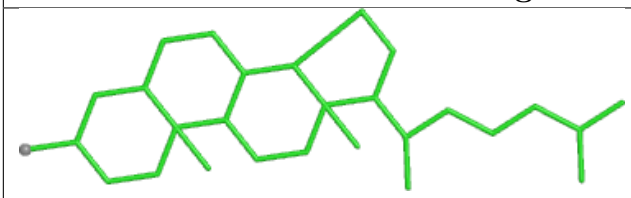


Torsions

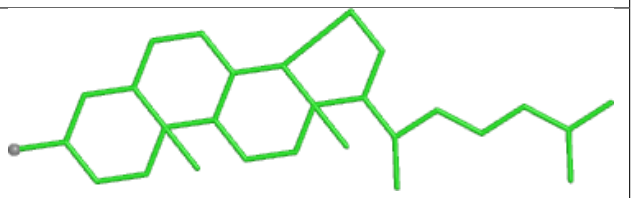


Rings

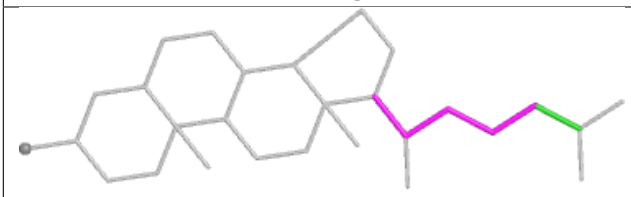
Ligand CLR A 1508



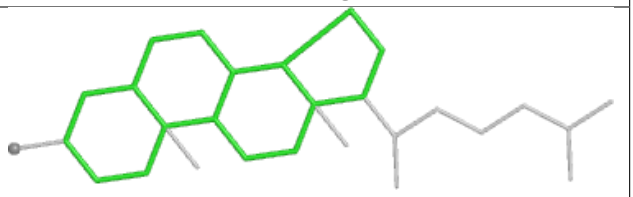
Bond lengths



Bond angles

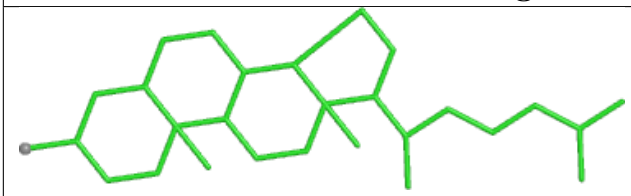


Torsions

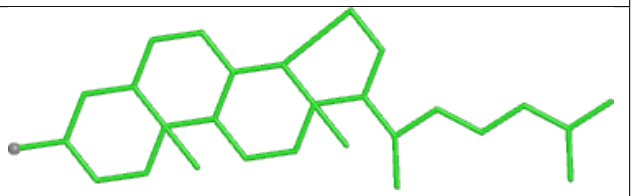


Rings

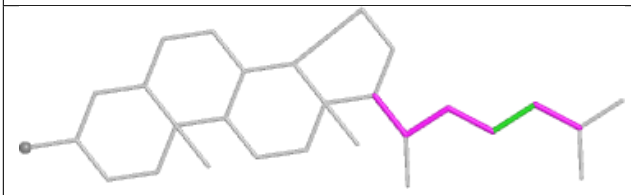
Ligand CLR A 1505



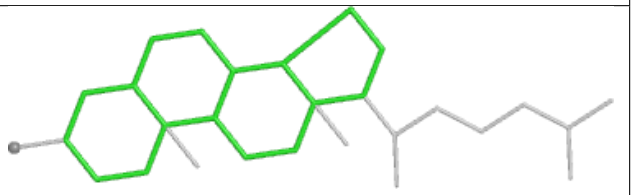
Bond lengths



Bond angles

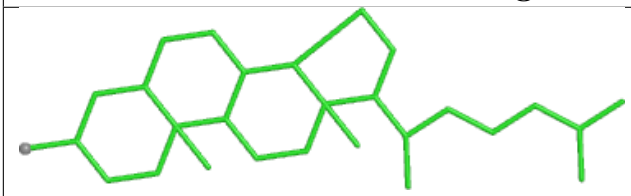


Torsions

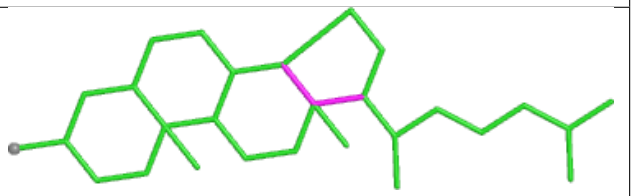


Rings

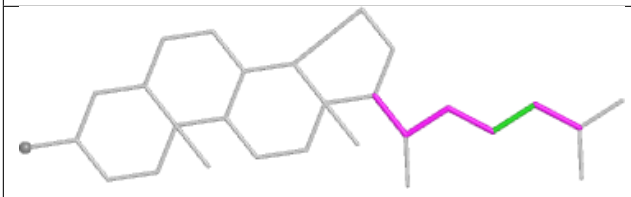
Ligand CLR A 1504



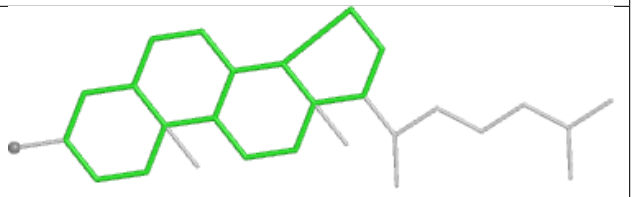
Bond lengths



Bond angles

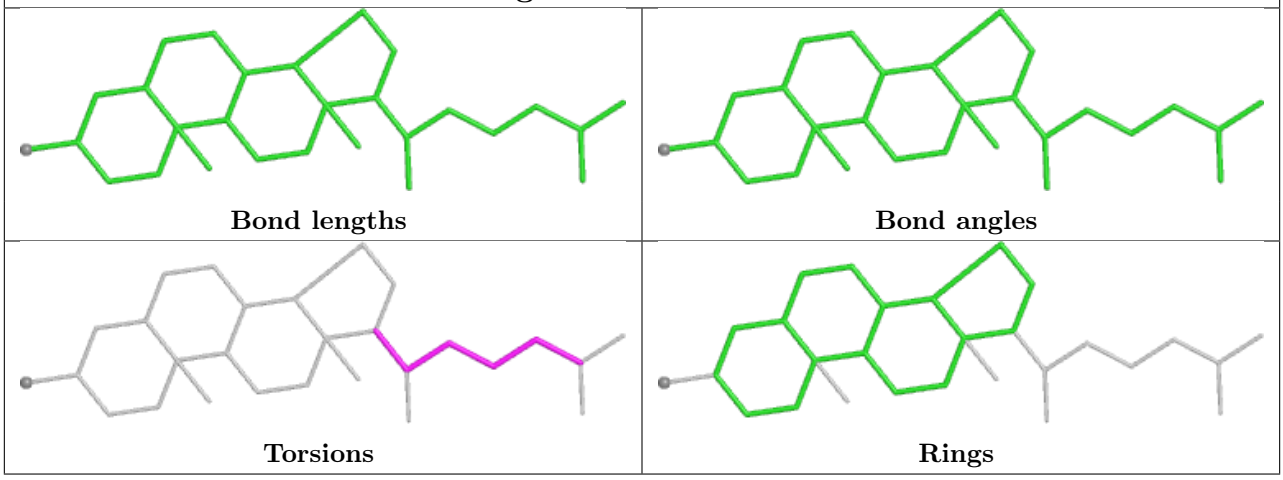


Torsions

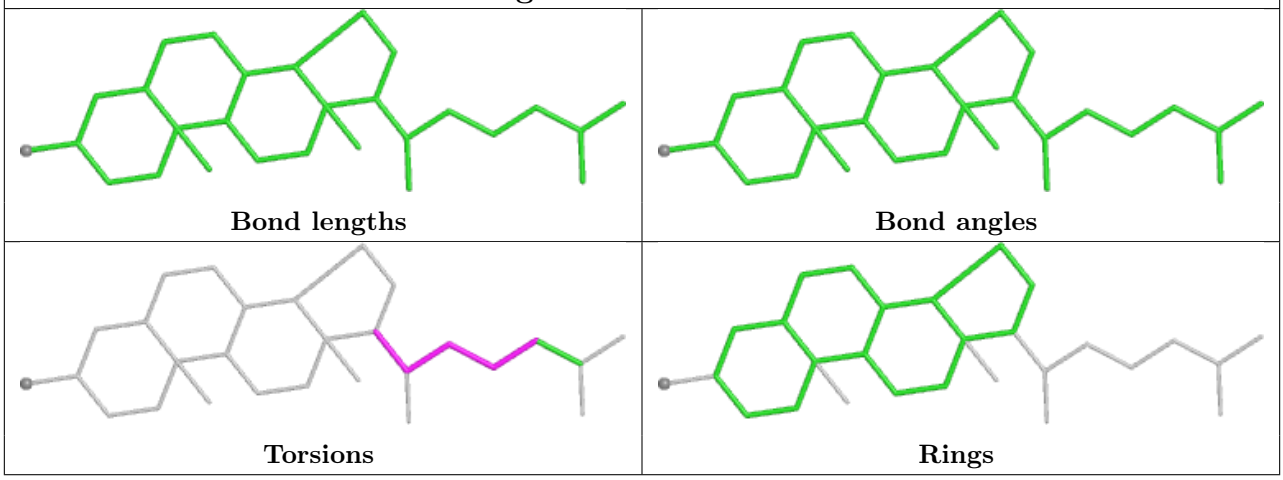


Rings

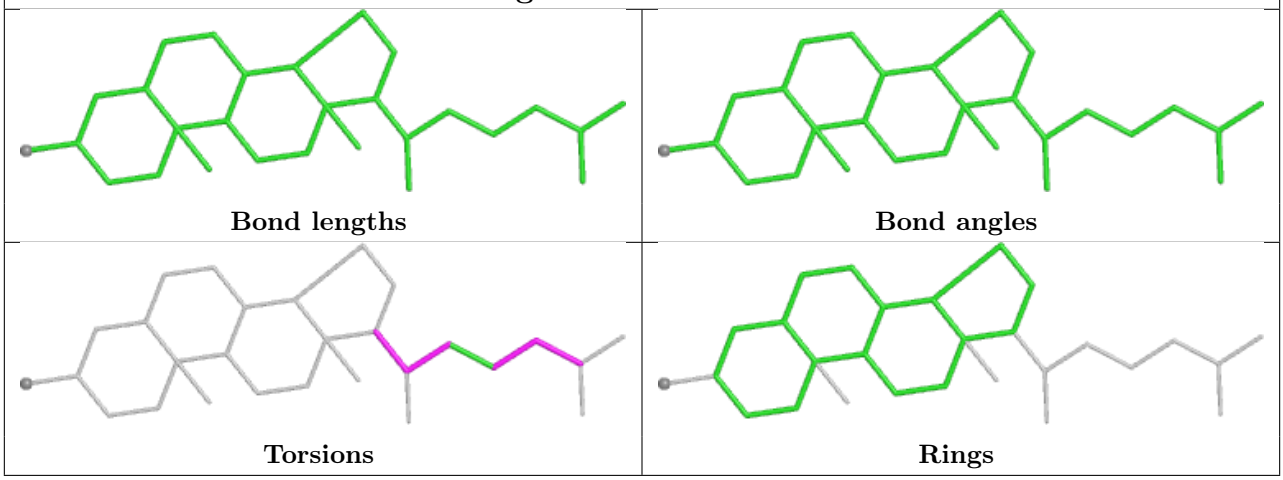
Ligand CLR A 1507

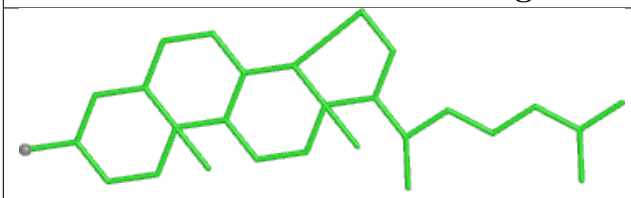
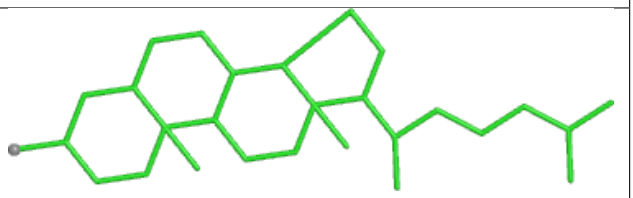
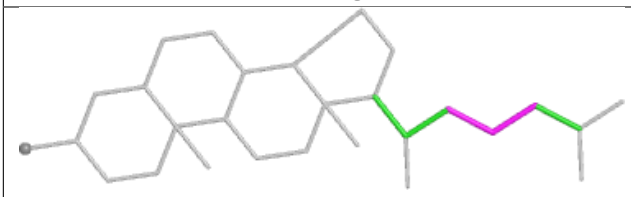
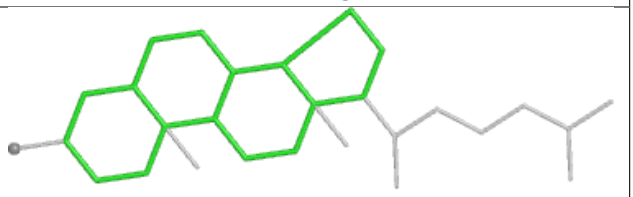


Ligand CLR A 1502



Ligand CLR A 1503



Ligand CLR A 1506	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

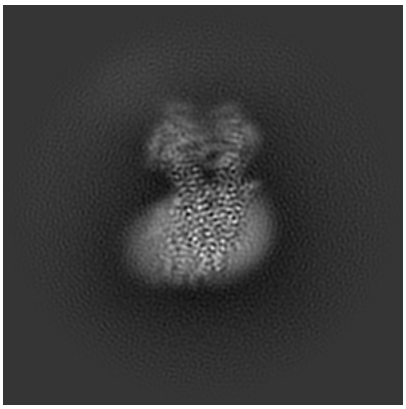
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-63866. These allow visual inspection of the internal detail of the map and identification of artifacts.

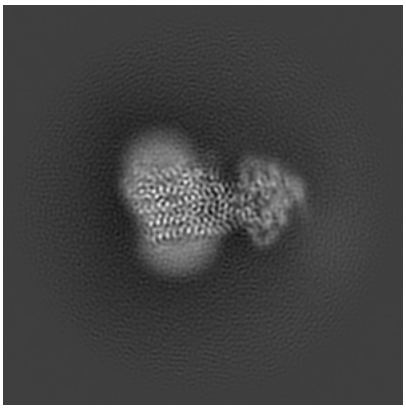
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

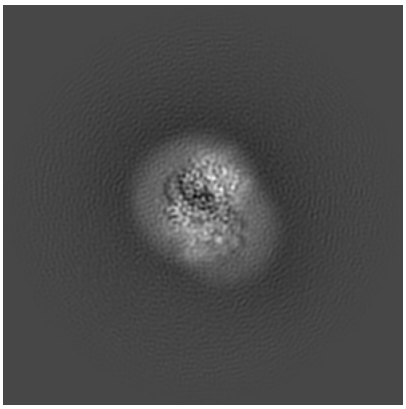
6.1.1 Primary map



X

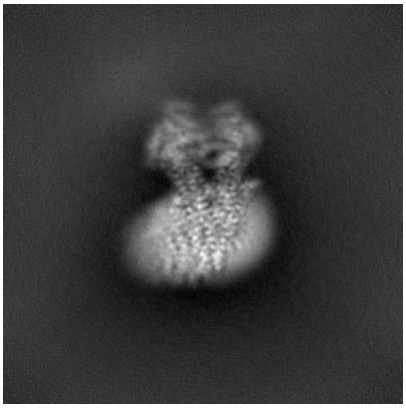


Y

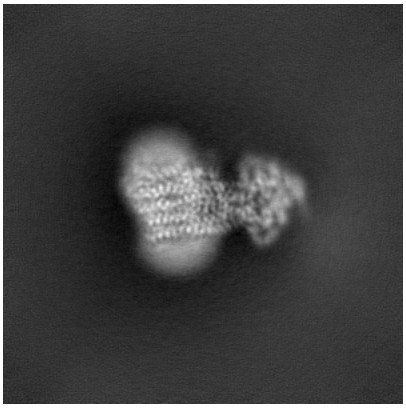


Z

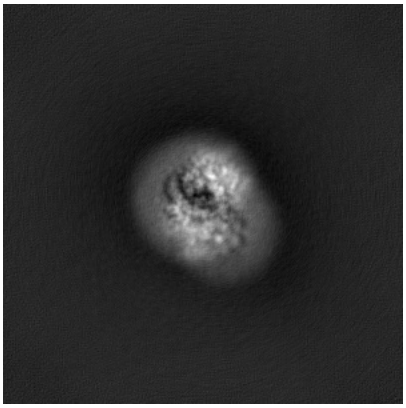
6.1.2 Raw map



X



Y

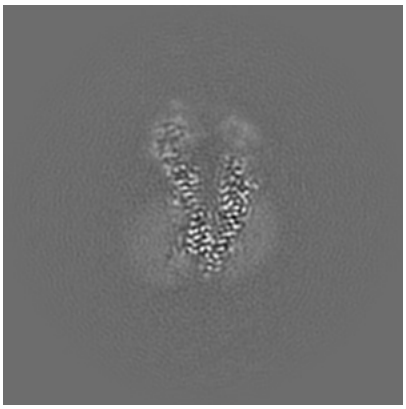


Z

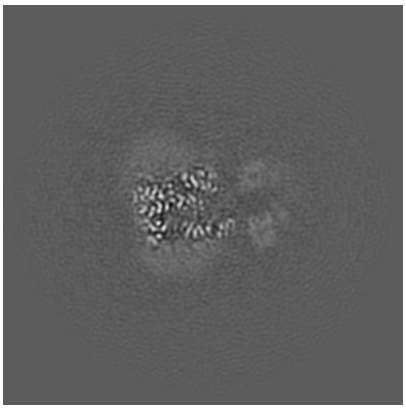
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

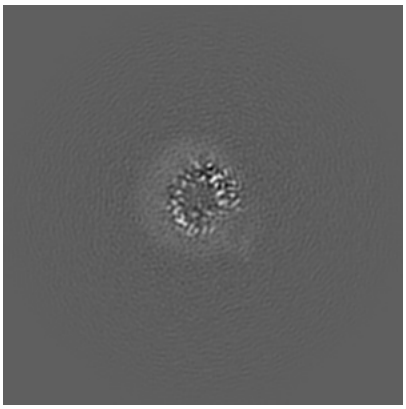
6.2.1 Primary map



X Index: 200

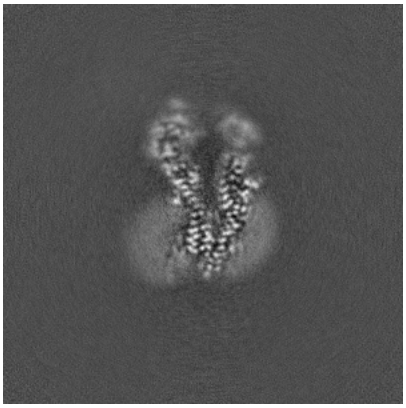


Y Index: 200

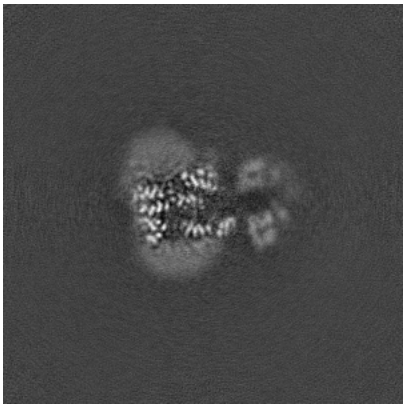


Z Index: 200

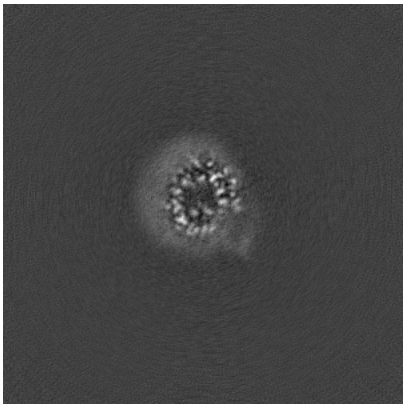
6.2.2 Raw map



X Index: 200



Y Index: 200

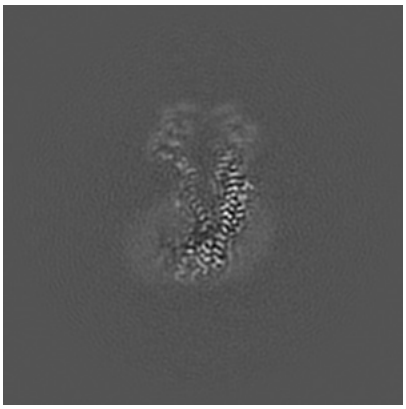


Z Index: 200

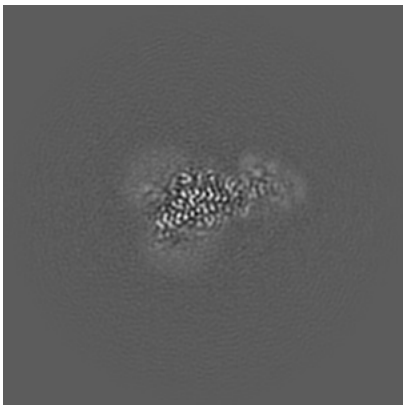
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

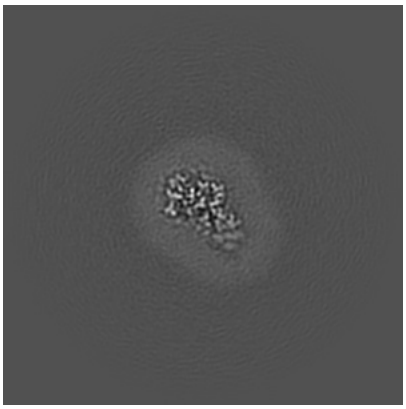
6.3.1 Primary map



X Index: 208

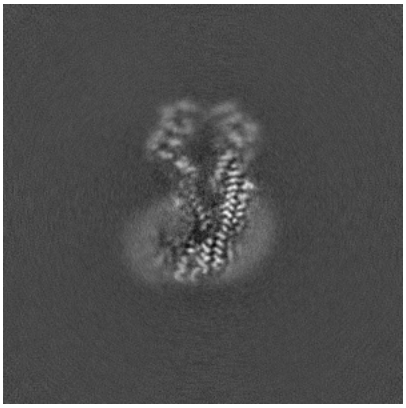


Y Index: 225

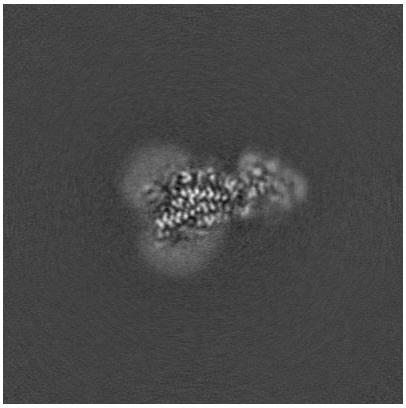


Z Index: 157

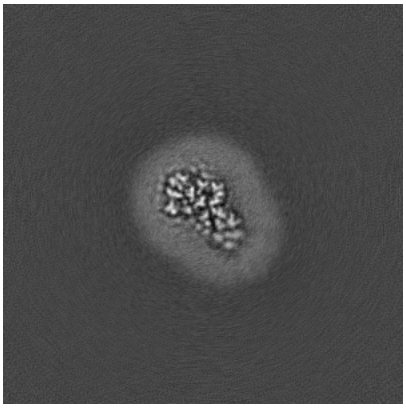
6.3.2 Raw map



X Index: 208



Y Index: 225

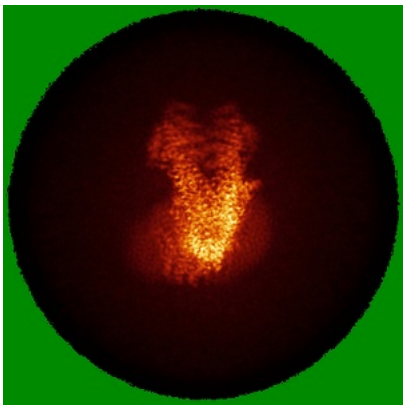


Z Index: 157

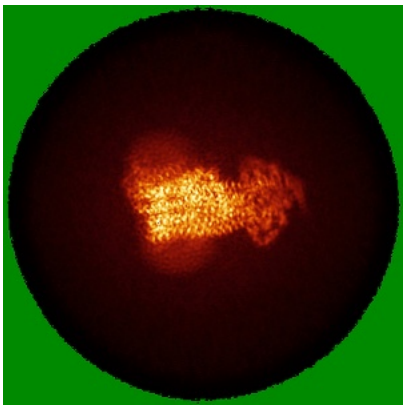
The images above show the largest variance slices of the map in three orthogonal directions.

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

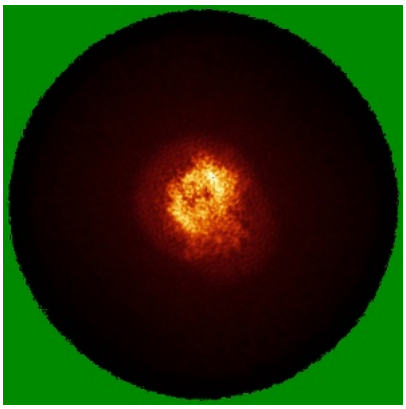
6.4.1 Primary map



X

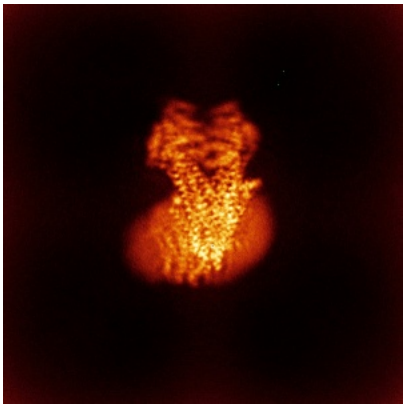


Y

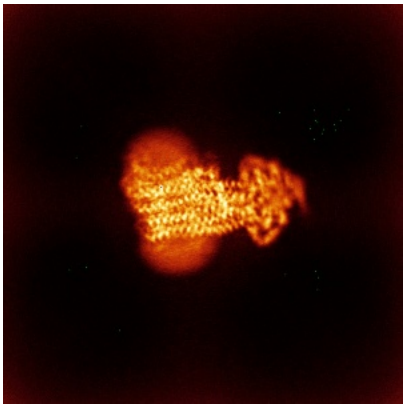


Z

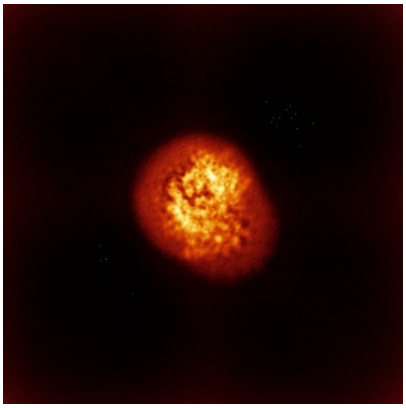
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. 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.

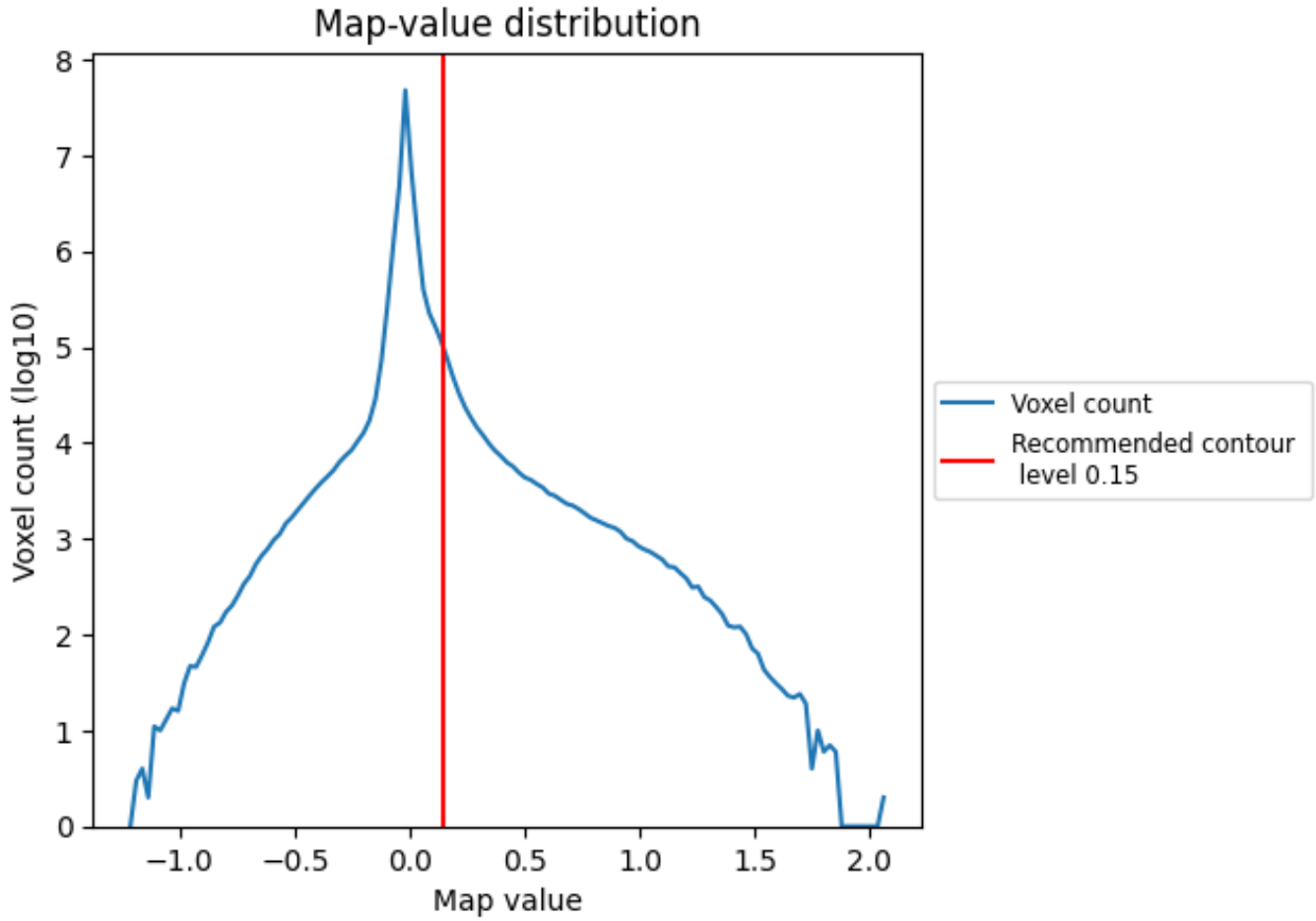
6.6 Mask visualisation (i)

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

7 Map analysis

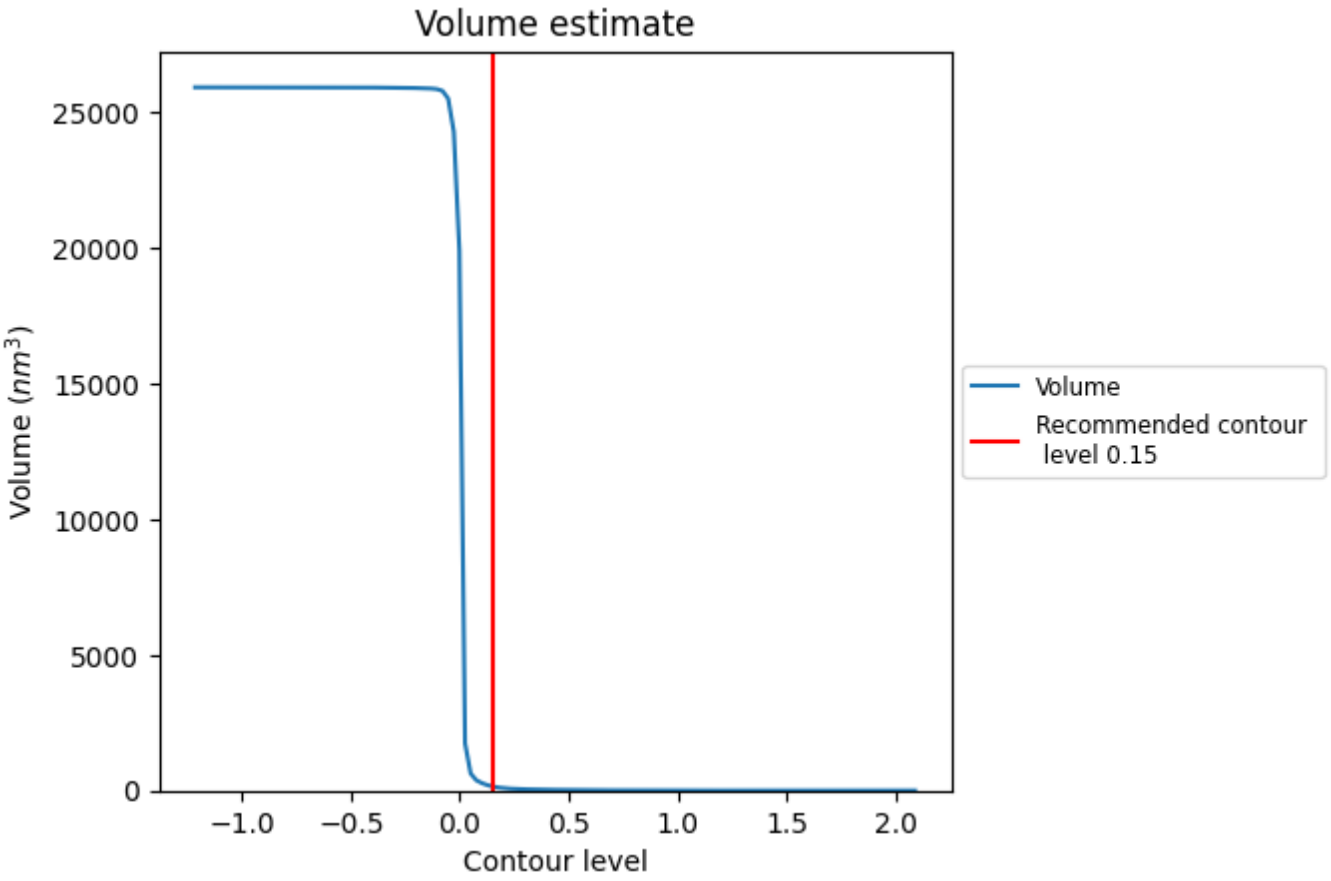
This section contains the results of statistical analysis of the map.

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.

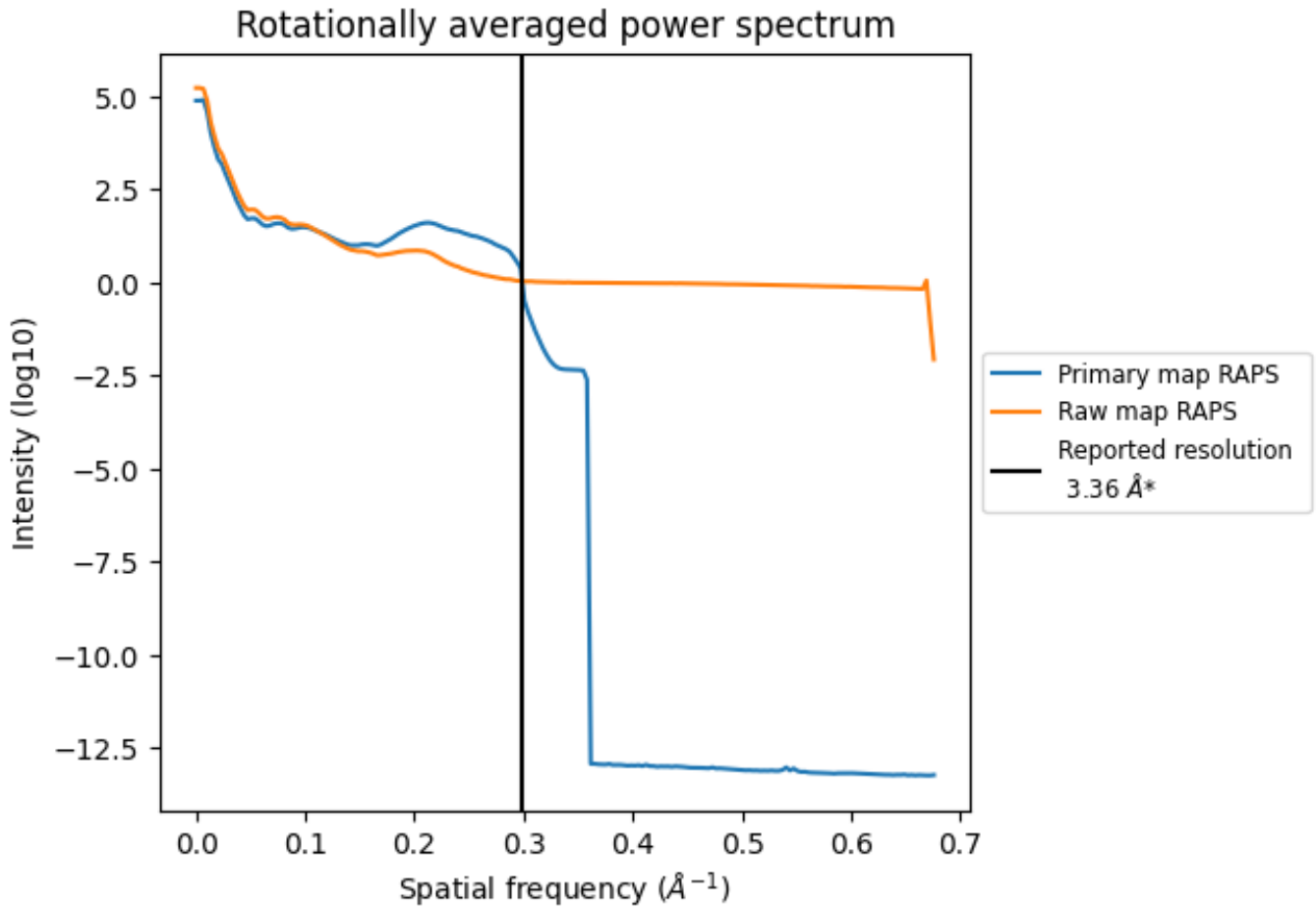
7.2 Volume estimate (i)



The volume at the recommended contour level is 152 nm^3; this corresponds to an approximate mass of 137 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)

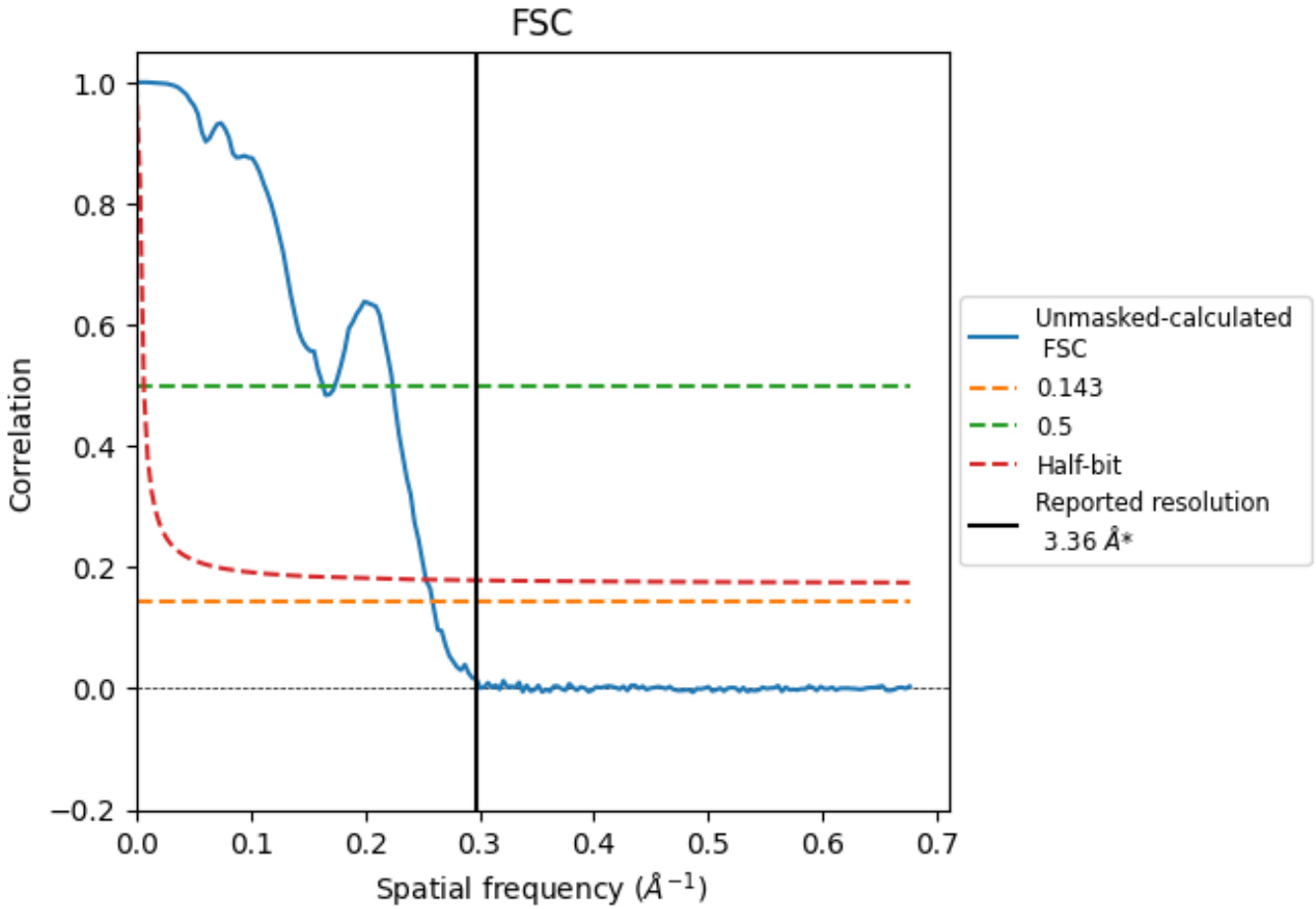


*Reported resolution corresponds to spatial frequency of 0.298 Å^{-1}

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 0.298 Å^{-1}

8.2 Resolution estimates (i)

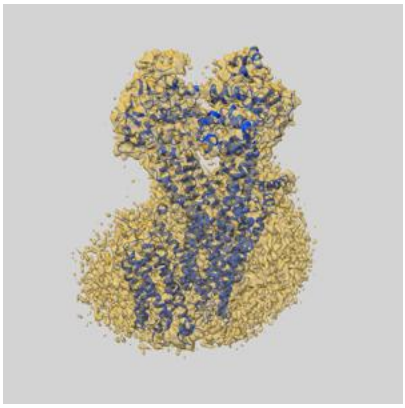
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.36	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.86	6.13	3.95

*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 3.86 differs from the reported value 3.36 by more than 10 %

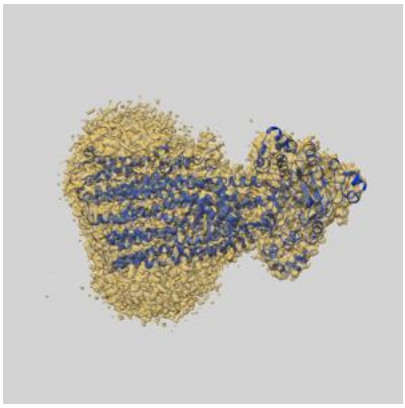
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-63866 and PDB model 9U58. Per-residue inclusion information can be found in section 3 on page 5.

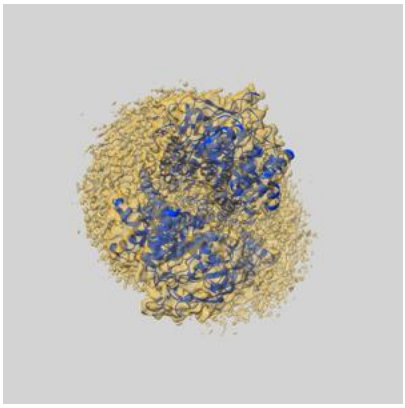
9.1 Map-model overlay



X



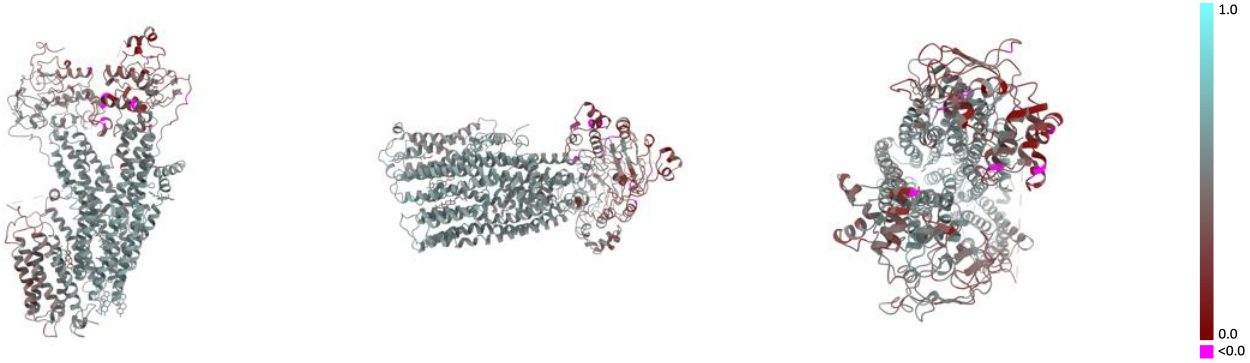
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15 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.

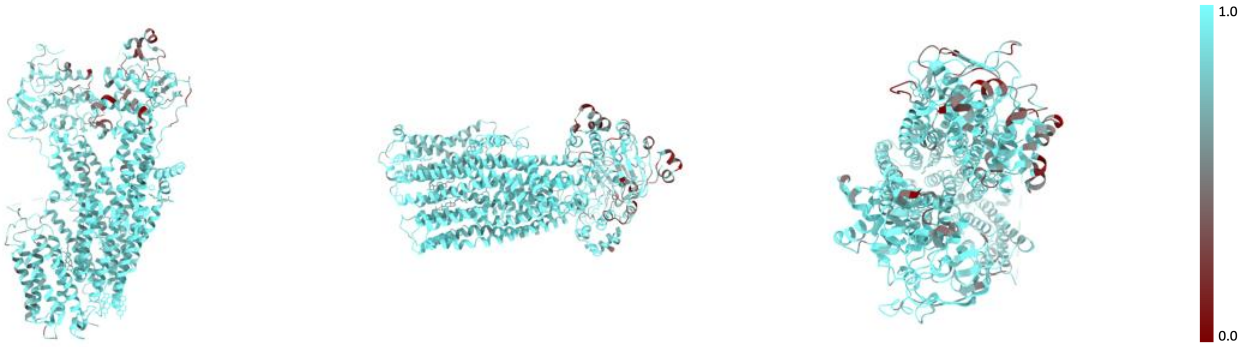
9.2 Q-score mapped to coordinate model (i)



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.

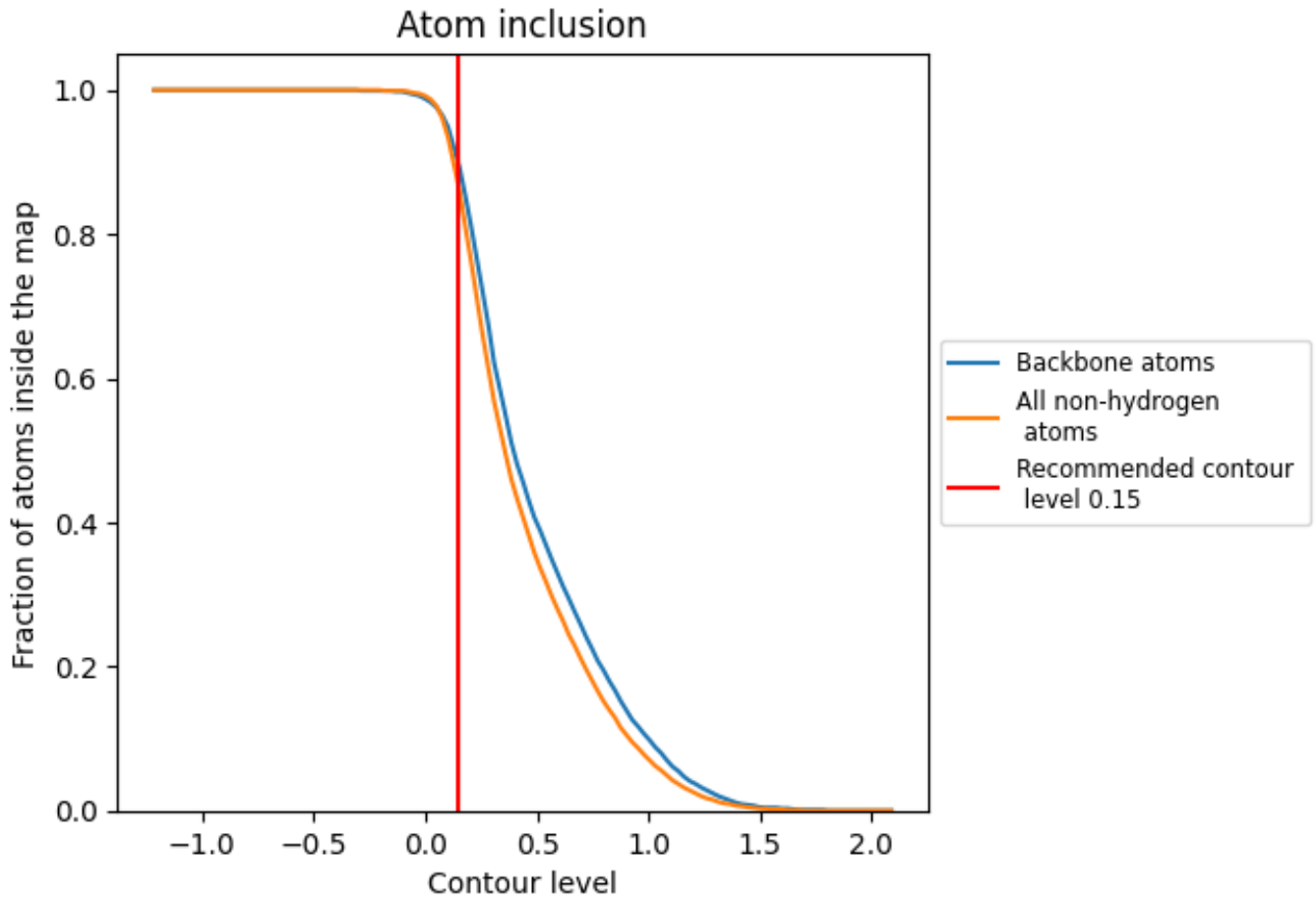
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.15).

9.4 Atom inclusion (i)



At the recommended contour level, 90% 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 (0.15) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.8660	0.4680
A	0.8660	0.4680