



wwPDB EM Validation Summary Report ⓘ

Mar 24, 2026 – 08:34 PM UTC

PDB ID : 8GMJ / pdb_00008gmj
EMDB ID : EMD-40227
Title : CryoEM structure of P-Glycoprotein in collapsed closed state under continuous turnover conditions with verapamil
Authors : Culbertson, A.; Liao, M.
Deposited on : 2023-03-26
Resolution : 4.40 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.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

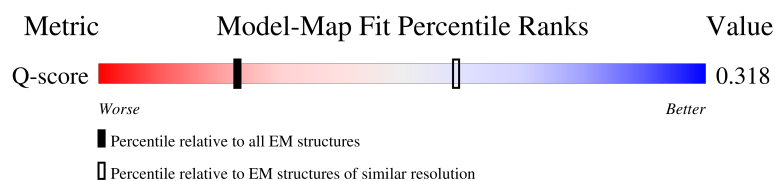
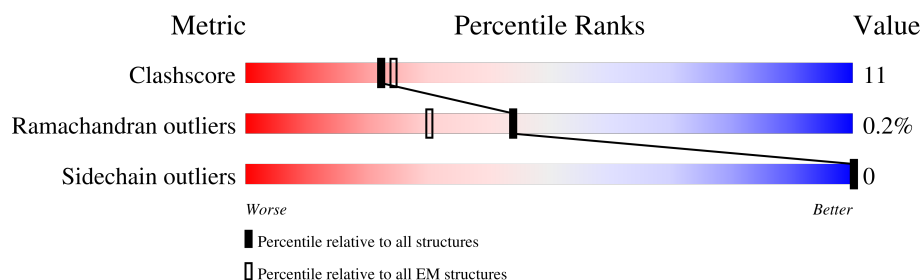
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 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	3132 (3.91 - 4.90)

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	1280	38% 80% 9% 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ATP	A	1304	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7960 atoms, of which 2194 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.

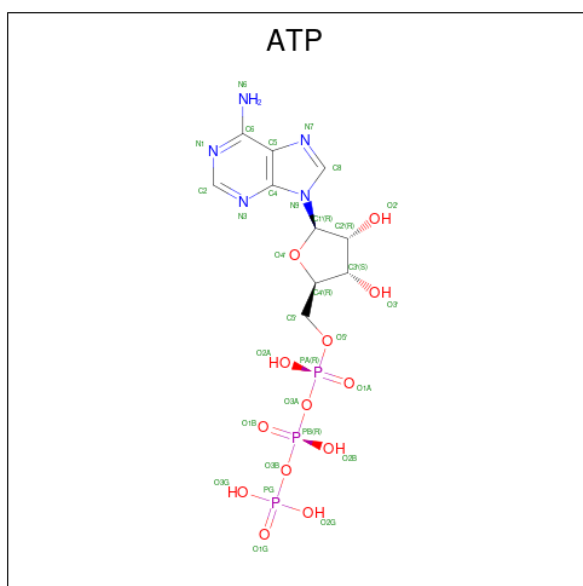
- Molecule 1 is a protein called ATP-dependent translocase ABCB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
1	A	1145	7872	3408	2170	1145	1149	0	0

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
2	A	2	Total	Mg	0
			2	2	

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
3	A	1	43	10	12	5	13	3	0
3	A	1	43	10	12	5	13	3	0

ALA	L1199	K748	A828	S931	A1001	L1082	L1199	L1199
GLY	D1200	K751	I829	L932	K1014	D1088	D1200	D1200
THR	E1201	S752	G830	R833	T1015	P1089	E1201	E1201
LYS	A1202	F755	A834	A935	P1016	L1090	A1202	A1202
ARG	S1204	S756	V835	H936	L1017	A1091	S1204	S1204
GLN	A1206	L757	I836	F937	I1018	G1092	A1206	A1206
	L1206	L758	Q838	F938	D1019	K1093	L1206	L1206
	D1207	F759	A841	S943	S1020	V1094	D1207	D1207
	T1208	L760	N842	F944	T1023	L1095	T1208	T1208
	K1220	A761	L843	T945	E1024	L1096	K1220	K1220
	A1221	L762	G844	Q946	G1025	D1097	A1221	A1221
	G1224	G763	T845	A947	L1026	G1098	G1224	G1224
	C1227	I764	G846	M948	M1027	K1099	C1227	C1227
	I1228	I765	I847	M949	P1028	E1100	I1228	I1228
	H1232	I766	I848	Y950	N1029	I1101	H1232	H1232
	R1233	F767	I849	F951	N1030	K1102	R1233	R1233
	L1234	I768	S850	Y952	L1031	R1103	L1234	L1234
	S1236	T769	F851	Y953	E1032	L1104	S1236	S1236
	T1236	F770	I852	A954	G1033	L1109	T1236	T1236
	N1239	F771	G854	Q955	N1034	R1110	N1239	N1239
	A1240	L772	W855	F957	V1035	A1111	A1240	A1240
	D1241	G773	Q856	R958	T1036	H1112	D1241	D1241
	L1242	G774	L857	F959	F1037	L1113	L1242	L1242
	I1243	F775	T858	Q960	V1040	V1116	I1243	I1243
	V1244	F776	L859	A961	V1041	S1117	V1244	V1244
	F1246	F777	L862	Y962	Y1044	Q1118	F1246	F1246
	Q1247	G778	A863	L963	P1045	E1119	Q1247	Q1247
	N1248	G781	I864	V964	T1046	P1120	N1248	N1248
	G1249	L784	V865	A965	P1047	F1123	G1249	G1249
	R1250	Y790	P866	H966	P1048	D1124	R1250	R1250
	V1251	D800	I867	L968	I1048	C1125	V1251	V1251
	K1252	V801	I868	M969	I1050	G1134	K1252	K1252
	E1253	D805	A869	S970	P1051	D1135	E1253	E1253
	H1254	P806	I870	F971	G1055	N1136	H1254	H1254
	G1255	P807	A871	E972	L1056	S1137	G1255	G1255
	T1256	K808	G881	A980	S1057	A1150	T1256	T1256
	H1257	N809	Q882	V981	L1058	E1151	H1257	H1257
	Q1258	T810	A883	V982	V1060	A1152	Q1258	Q1258
	Q1259	T811	L884	F983	K1061	L1161	Q1259	Q1259
	L1260	G812	K885	Q984	T1065	A1168	L1260	L1260
	L1261	A813	G894	A985	L1066	V1169	L1261	L1261
	A1262	L814	R905	M986	A1067	G1170	A1262	A1262
	Q1263	T815	Q922	N987	L1068	D1171	Q1263	Q1263
	K1264	T816	S923	A988	K1172	K1172	K1264	K1264
	G1265	A819	L924	Q989	V1069	G1173	G1265	G1265
	I1266	N820	Y928	V991	G1070	T1174	I1266	I1266
	S1269	A823	P927	S992	S1071	Q1175	S1269	S1269
	M1270	Q824	L924	A995	G1072	P1194	M1270	M1270
	V1271	V825	P927	P996	C1074	L1198	V1271	V1271
	S1272	K826	Y928	D997	G1075		S1272	S1272
	V1273	G827		Y998	K1076		V1273	V1273
				A999	T1078			GLN
				K1000				

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	33409	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 ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.133	Depositor
Minimum map value	-0.068	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.049	Depositor
Map size ($\text{\AA}$)	128.26, 126.13999, 155.81999	wwPDB
Map dimensions	121, 119, 147	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.38	0/5727	0.60	0/7978

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	5702	2170	2848	98	0
2	A	2	0	0	0	0
3	A	62	24	24	12	0
All	All	5766	2194	2872	98	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 11.

The worst 5 of 98 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:1077:SER:HB2	3:A:1304:ATP:PA	2.16	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:726:PRO:HB3	1:A:846:GLY:HA2	1.58	0.83
1:A:726:PRO:HG3	1:A:845:THR:C	2.02	0.83
1:A:996:PRO:HD2	1:A:997:ASP:H	1.48	0.79
1:A:62:GLY:HA3	1:A:195:GLN:O	1.83	0.78

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
1	A	1139/1280 (89%)	1091 (96%)	46 (4%)	2 (0%)	43 77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	184	GLU
1	A	187	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	30/1064 (3%)	30 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 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	$\# Z > 2$
3	ATP	A	1303	2	32,33,33	0.64	2 (6%)	48,52,52	0.74	2 (4%)
3	ATP	A	1304	2	32,33,33	0.56	0	48,52,52	0.65	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
3	ATP	A	1303	2	-	5/22/38/38	0/3/3/3
3	ATP	A	1304	2	-	5/22/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1303	ATP	PA-O3A	-2.37	1.56	1.59
3	A	1303	ATP	PB-O3B	-2.04	1.57	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1303	ATP	O3'-C3'-C2'	-2.19	104.79	111.82
3	A	1303	ATP	O2'-C2'-C3'	-2.19	104.80	111.82

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

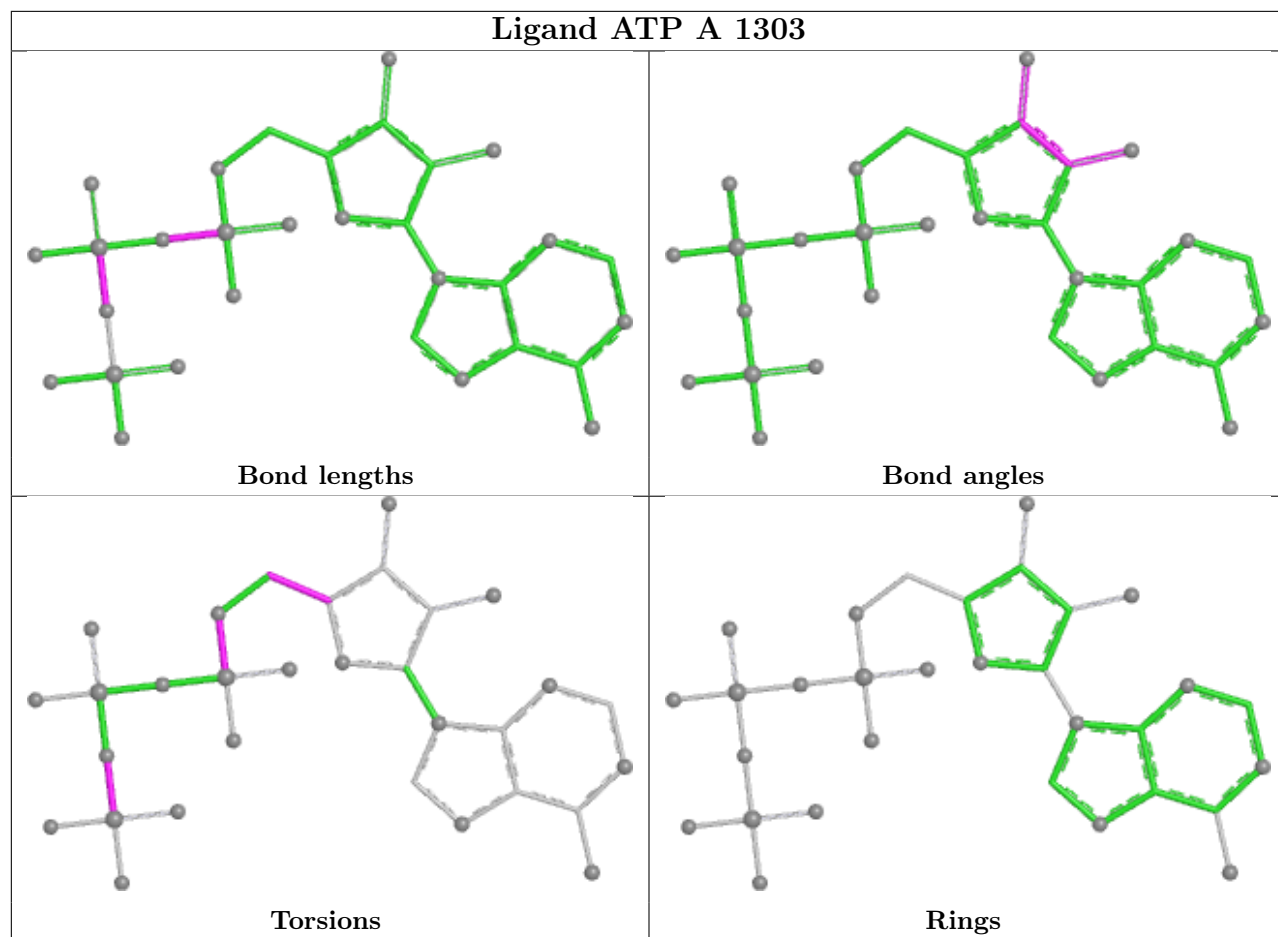
Mol	Chain	Res	Type	Atoms
3	A	1303	ATP	PB-O3B-PG-O3G
3	A	1303	ATP	C5'-O5'-PA-O1A
3	A	1303	ATP	C5'-O5'-PA-O3A
3	A	1304	ATP	PB-O3B-PG-O2G
3	A	1304	ATP	PA-O3A-PB-O3B

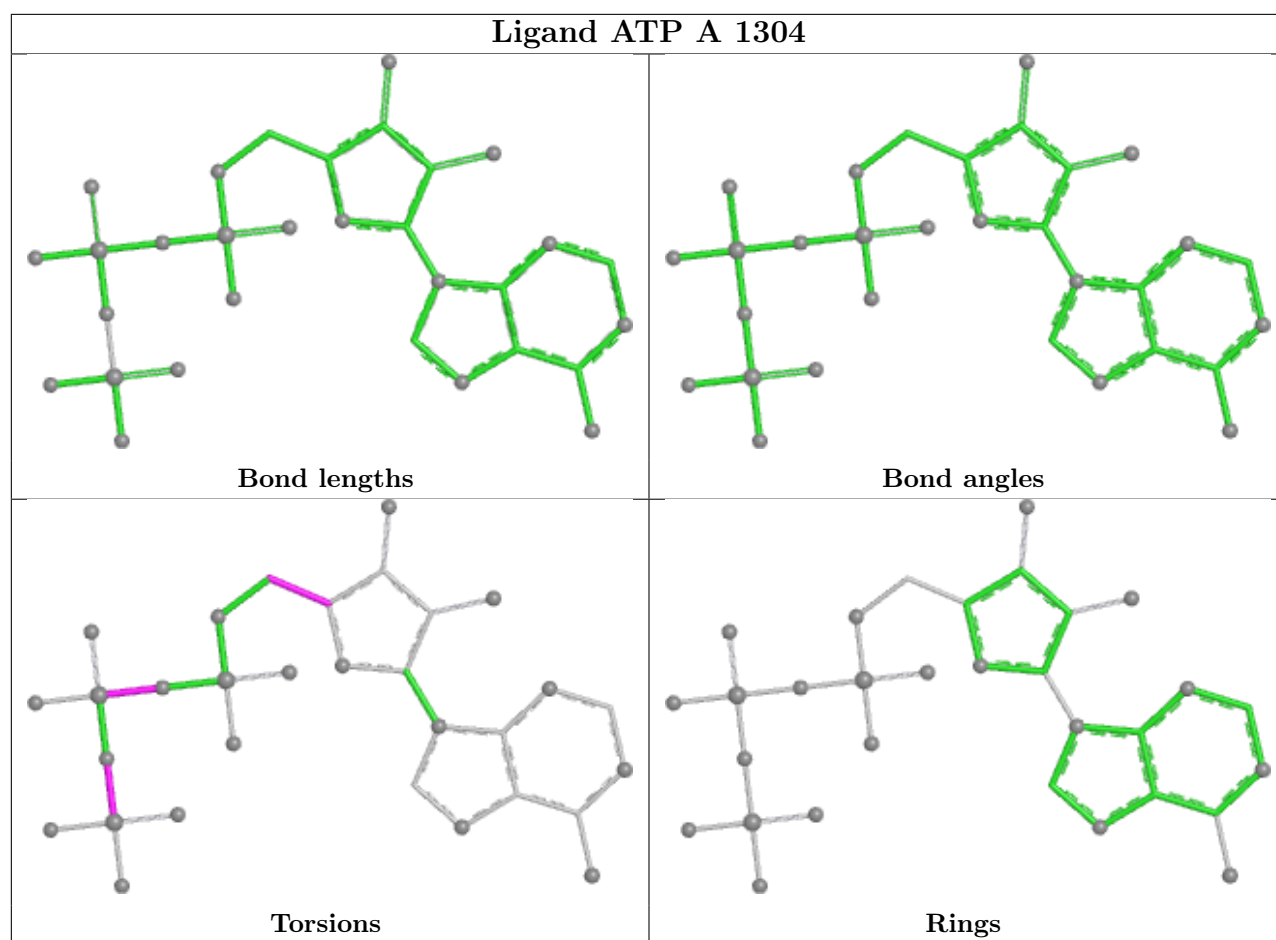
There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1303	ATP	3	0
3	A	1304	ATP	9	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

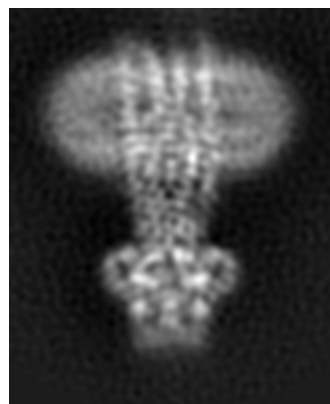
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40227. These allow visual inspection of the internal detail of the map and identification of artifacts.

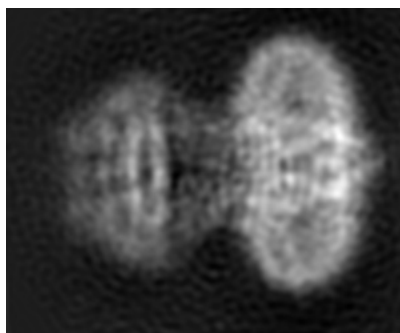
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

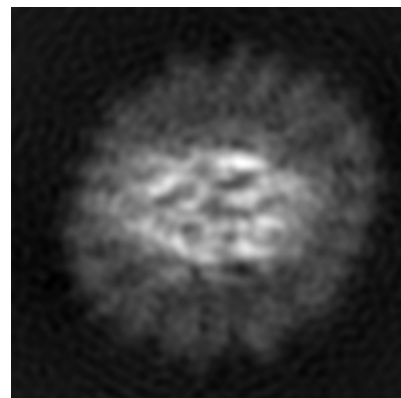
6.1.1 Primary map



X

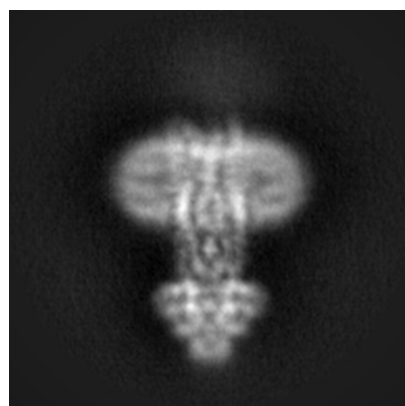


Y

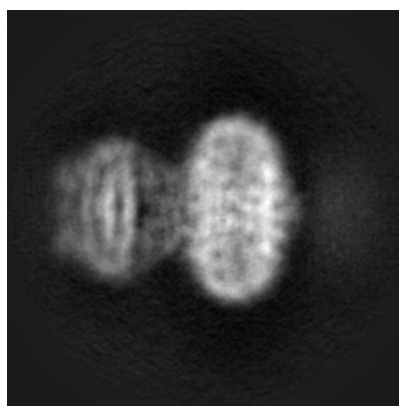


Z

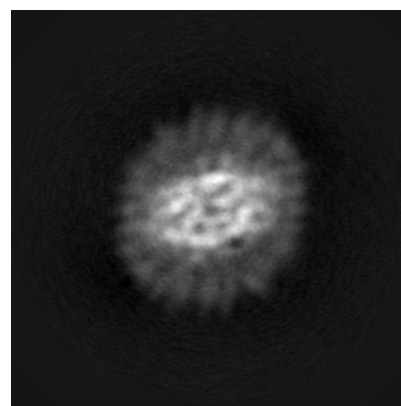
6.1.2 Raw map



X



Y



Z

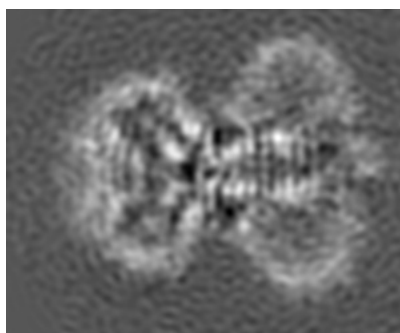
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

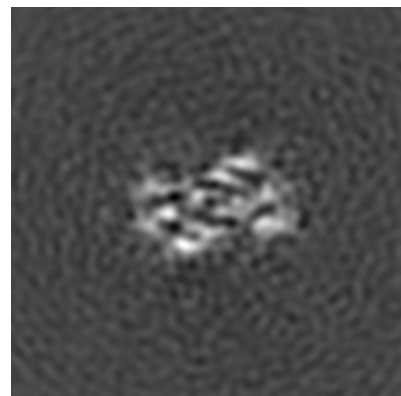
6.2.1 Primary map



X Index: 60

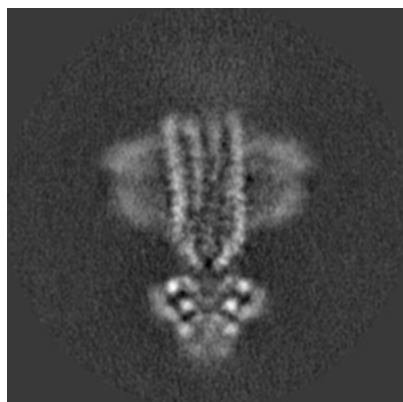


Y Index: 59

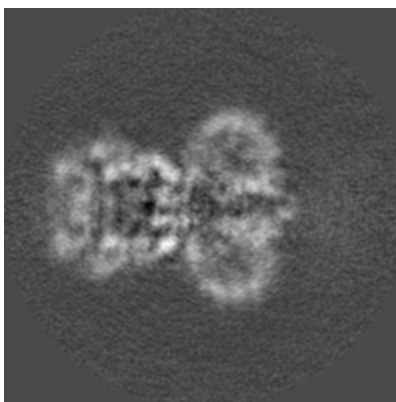


Z Index: 73

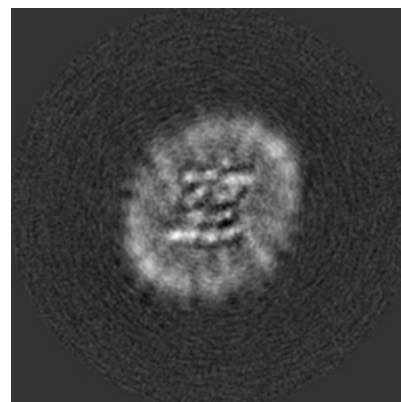
6.2.2 Raw map



X Index: 96



Y Index: 96

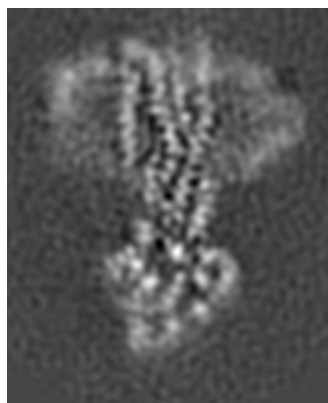


Z Index: 96

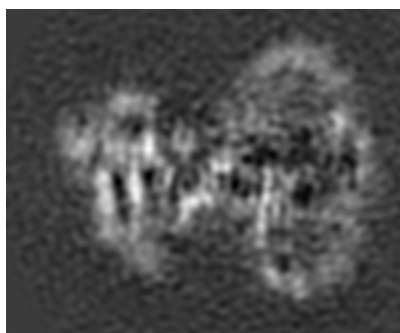
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

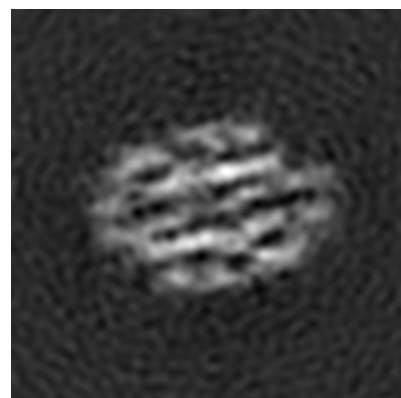
6.3.1 Primary map



X Index: 72

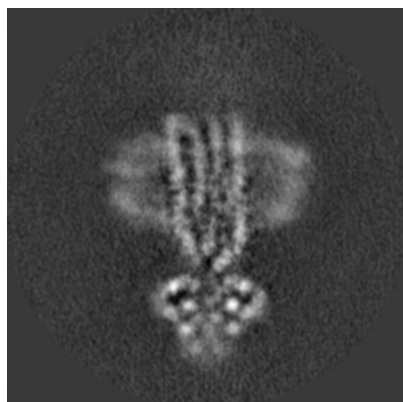


Y Index: 48

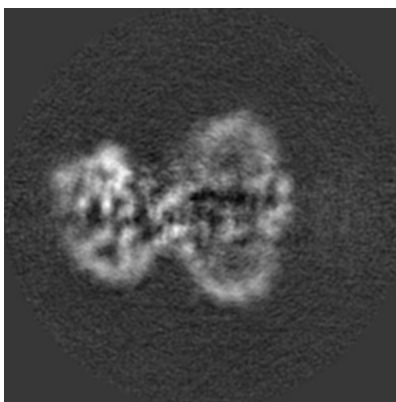


Z Index: 47

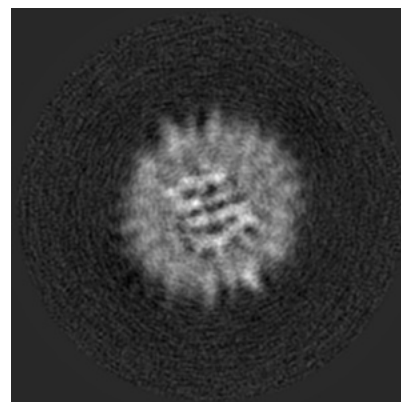
6.3.2 Raw map



X Index: 98



Y Index: 87

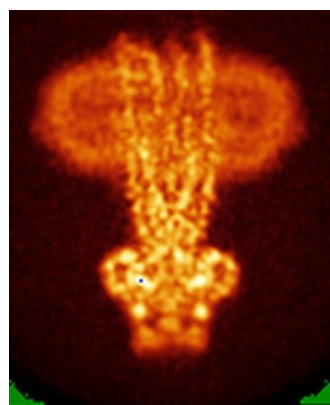


Z Index: 124

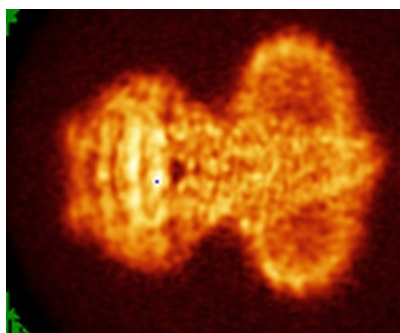
The images above show the largest variance slices of the map in three orthogonal directions.

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

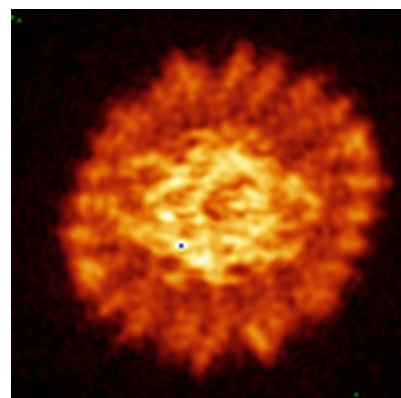
6.4.1 Primary map



X



Y

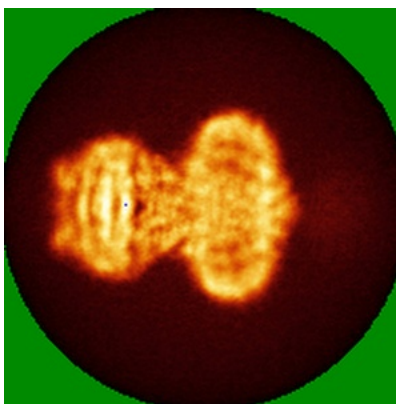


Z

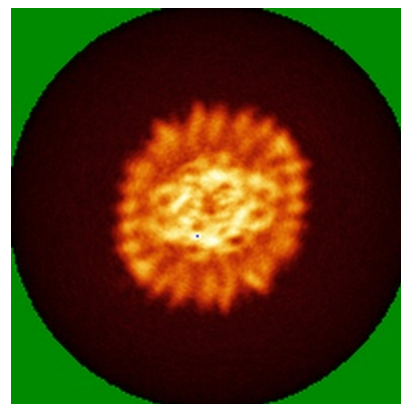
6.4.2 Raw map



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.

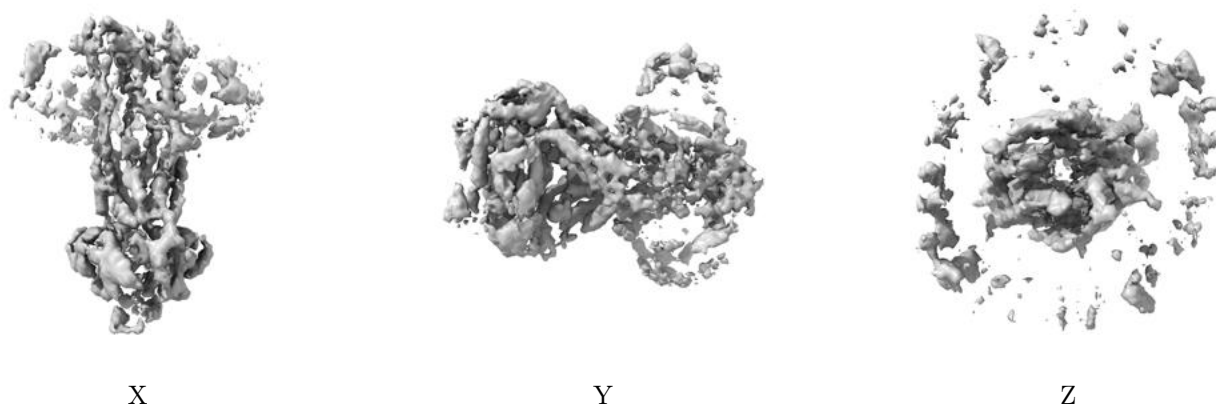
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.049. 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



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.

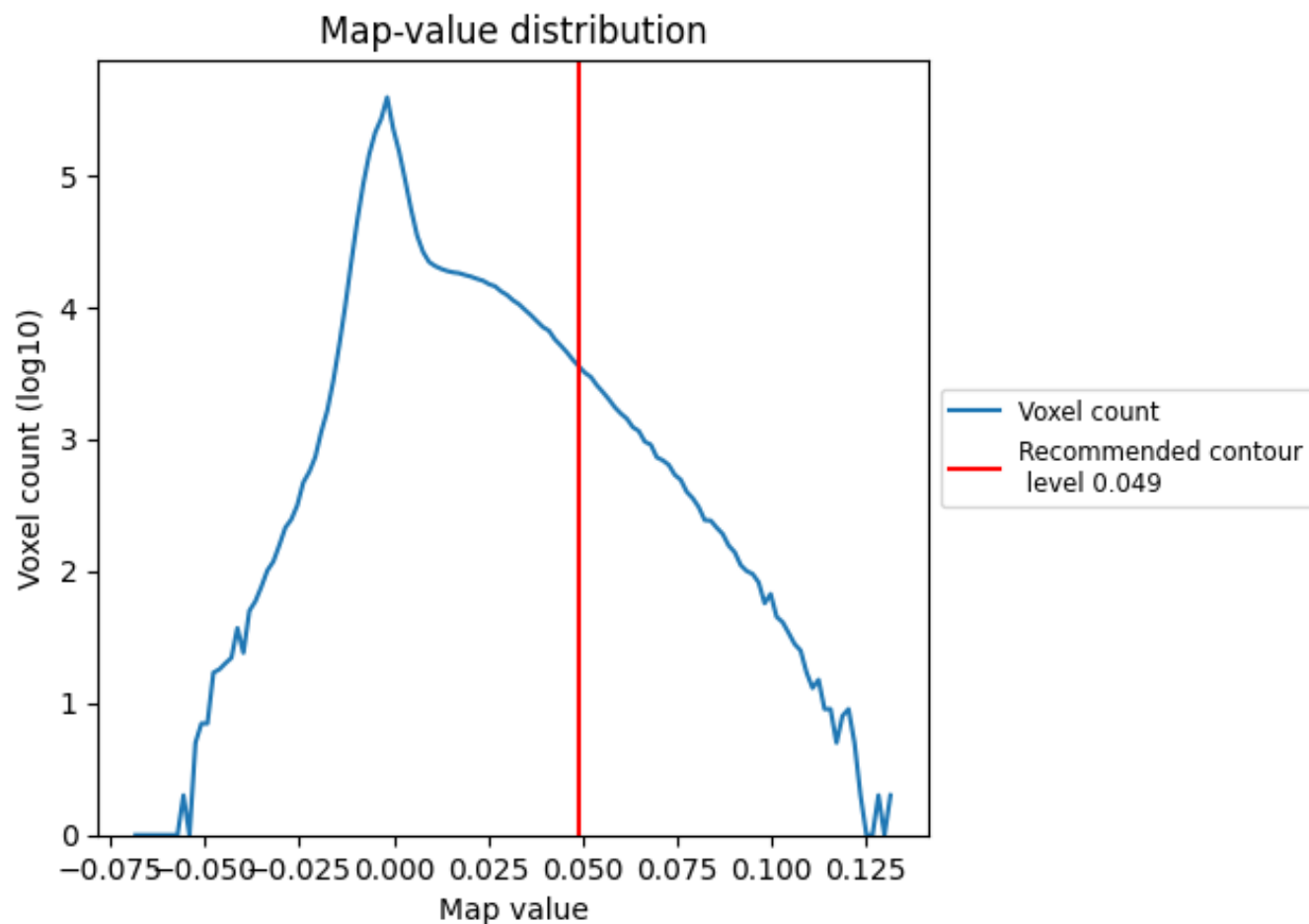
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

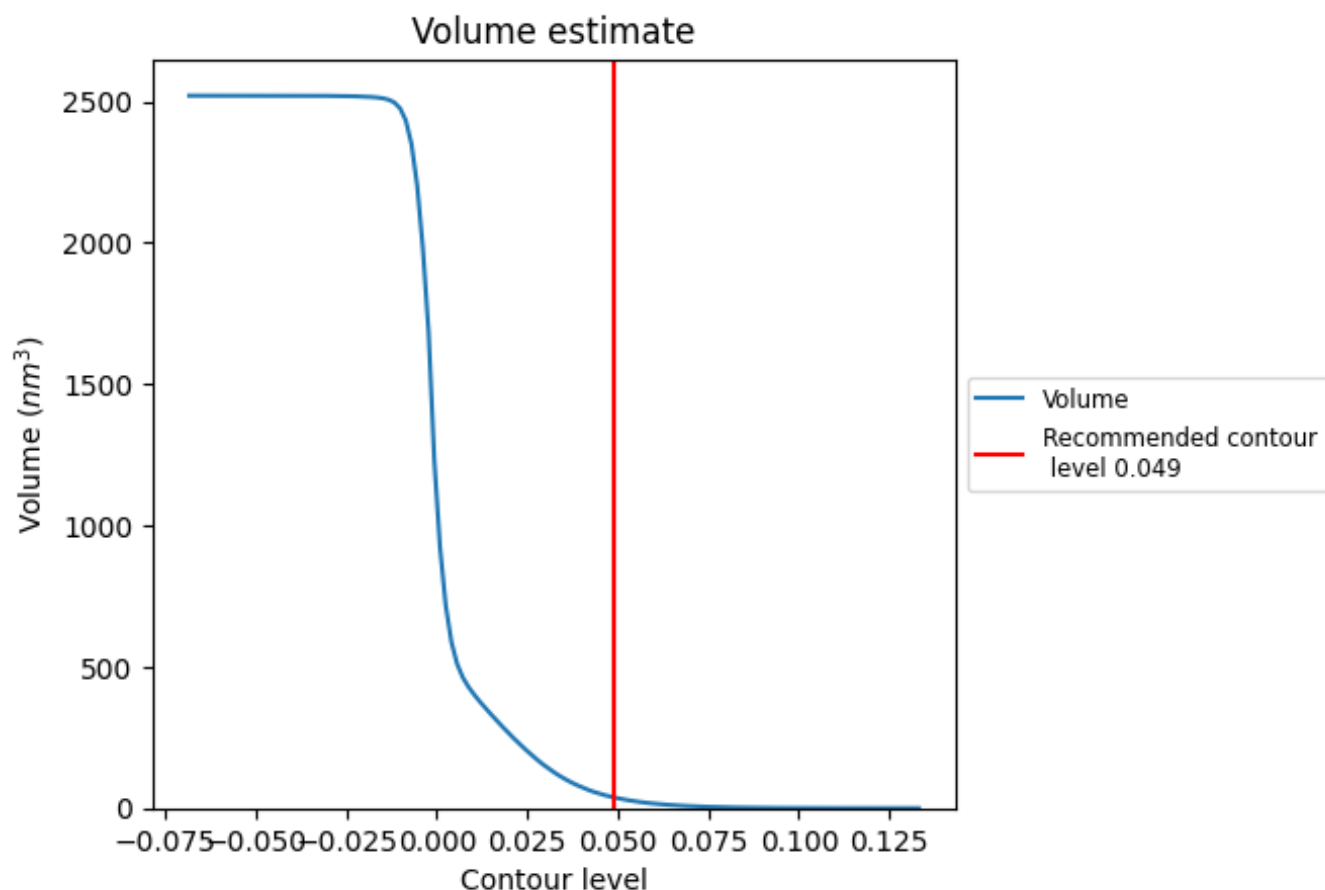
This section contains the results of statistical analysis of the map.

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 38 nm³; this corresponds to an approximate mass of 34 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.

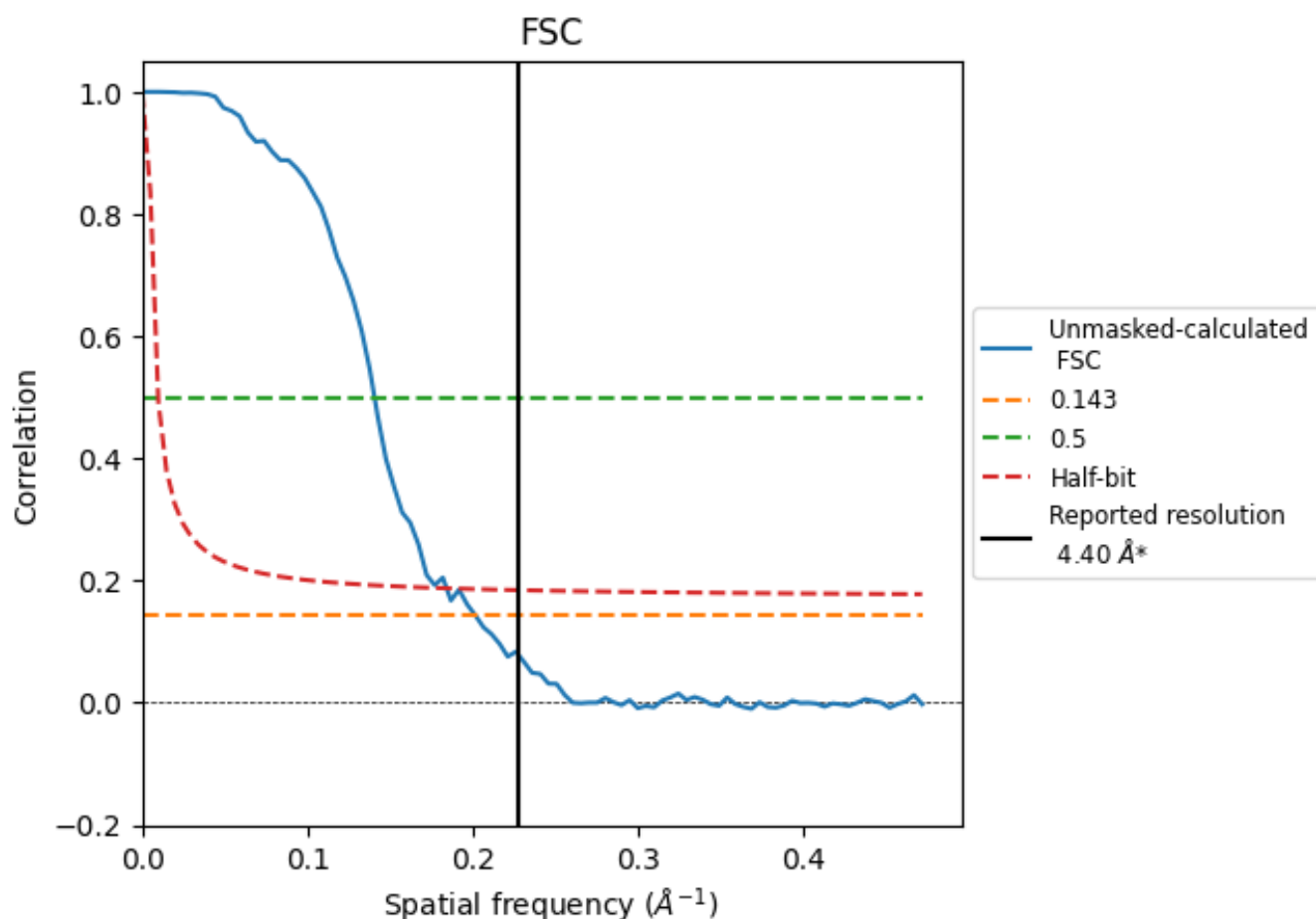
7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

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 0.227 Å⁻¹

8.2 Resolution estimates [i](#)

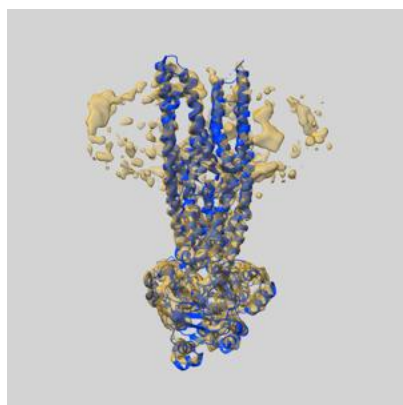
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.97	7.12	5.43

*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 4.97 differs from the reported value 4.4 by more than 10 %

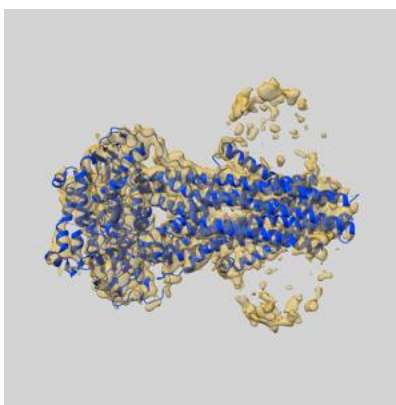
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-40227 and PDB model 8GMJ. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

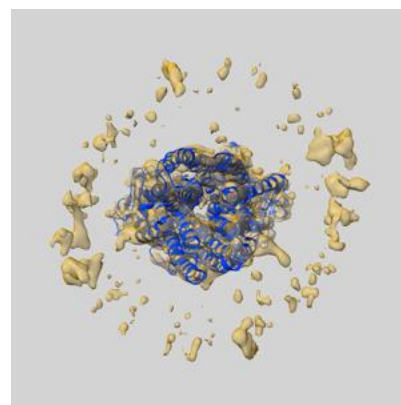
9.1 Map-model overlay [i](#)



X



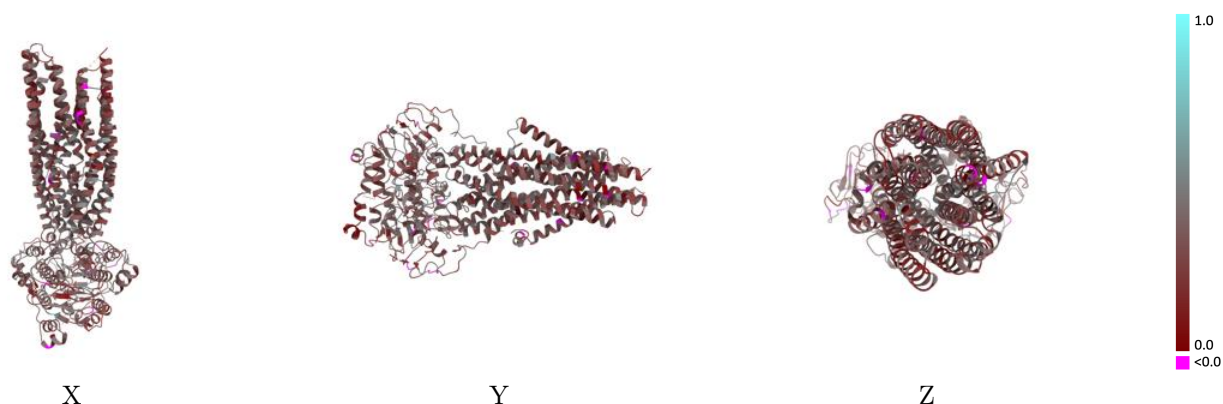
Y



Z

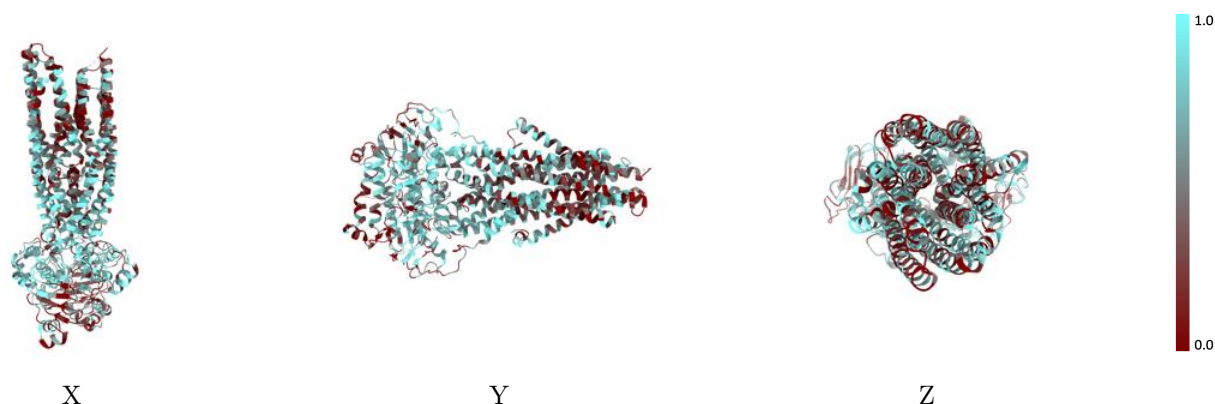
The images above show the 3D surface view of the map at the recommended contour level 0.049 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



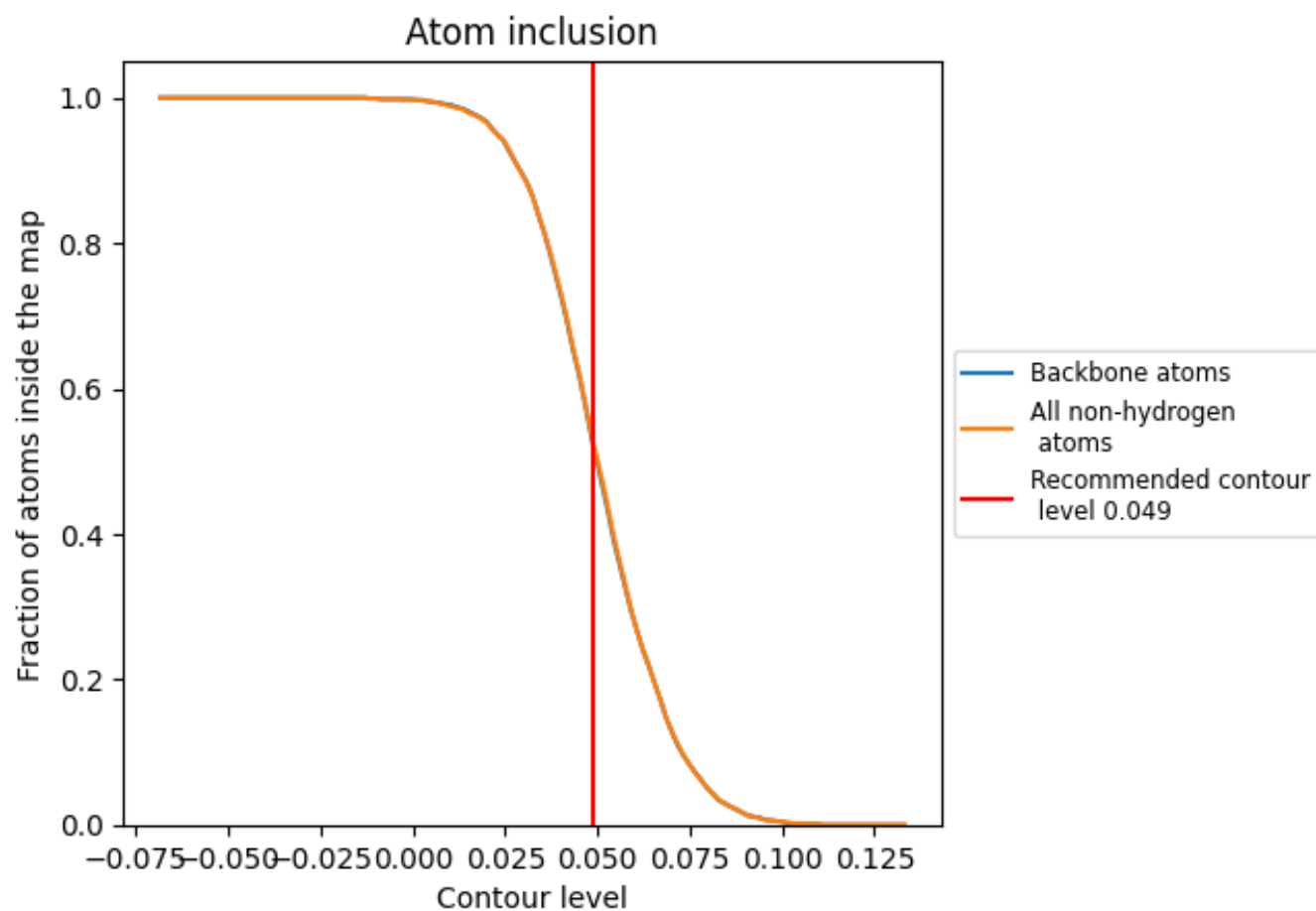
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.049).

9.4 Atom inclusion [i](#)



At the recommended contour level, 52% of all backbone atoms, 52% 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 (0.049) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5210	0.3180
A	0.5270	0.3180

