



wwPDB EM Validation Summary Report ⓘ

Sep 23, 2025 – 02:16 PM JST

PDB ID : 9LG6 / pdb_00009lg6
EMDB ID : EMD-63055
Title : bovine ABCC1 bound to CDAS
Authors : Sun, P.P.; Liu, K.X.; Gao, P.
Deposited on : 2025-01-10
Resolution : 3.70 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.dev129
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

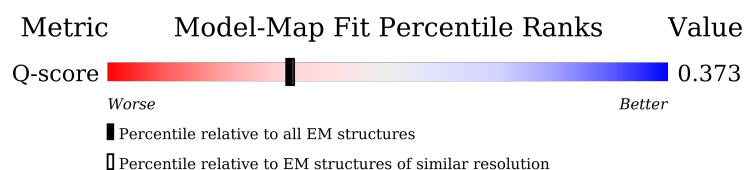
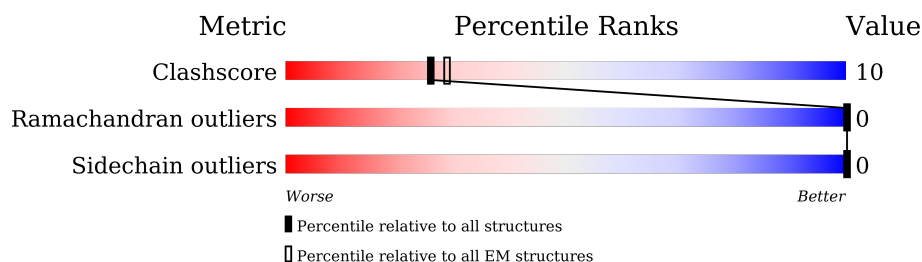
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	11569 (3.20 - 4.20)

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	1558	<div> <div>12%</div> <div>66%</div> <div>20%</div> <div>14%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10662 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.

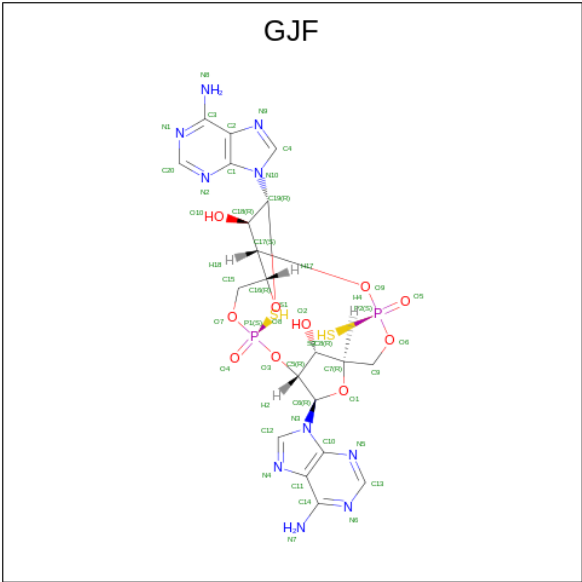
- Molecule 1 is a protein called Multidrug resistance-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1336	Total	C	N	O	S	0	0
			10618	6911	1762	1889	56		

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1531	LYS	-	expression tag	UNP Q8HXQ5
A	1532	LEU	-	expression tag	UNP Q8HXQ5
A	1533	GLY	-	expression tag	UNP Q8HXQ5
A	1534	SER	-	expression tag	UNP Q8HXQ5
A	1535	GLU	-	expression tag	UNP Q8HXQ5
A	1536	ASN	-	expression tag	UNP Q8HXQ5
A	1537	LEU	-	expression tag	UNP Q8HXQ5
A	1538	TYR	-	expression tag	UNP Q8HXQ5
A	1539	PHE	-	expression tag	UNP Q8HXQ5
A	1540	GLN	-	expression tag	UNP Q8HXQ5
A	1541	GLY	-	expression tag	UNP Q8HXQ5
A	1542	GLY	-	expression tag	UNP Q8HXQ5
A	1543	SER	-	expression tag	UNP Q8HXQ5
A	1544	GLY	-	expression tag	UNP Q8HXQ5
A	1545	GLY	-	expression tag	UNP Q8HXQ5
A	1546	SER	-	expression tag	UNP Q8HXQ5
A	1547	GLY	-	expression tag	UNP Q8HXQ5
A	1548	HIS	-	expression tag	UNP Q8HXQ5
A	1549	HIS	-	expression tag	UNP Q8HXQ5
A	1550	HIS	-	expression tag	UNP Q8HXQ5
A	1551	HIS	-	expression tag	UNP Q8HXQ5
A	1552	HIS	-	expression tag	UNP Q8HXQ5
A	1553	HIS	-	expression tag	UNP Q8HXQ5
A	1554	HIS	-	expression tag	UNP Q8HXQ5
A	1555	HIS	-	expression tag	UNP Q8HXQ5
A	1556	HIS	-	expression tag	UNP Q8HXQ5
A	1557	HIS	-	expression tag	UNP Q8HXQ5
A	1558	HIS	-	expression tag	UNP Q8HXQ5

- Molecule 2 is (1 {R},3 {S},6 {R},8 {R},9 {R},10 {S},12 {S},15 {R},17 {R},18 {R})-8,17-bis(6-aminopurin-9-yl)-3,12-bis(oxidanylidene)-3,12-bis(sulfanyl)-2,4,7,11,13,16-hexaoxa-3 λ ^5,12 λ ^5-diphosphatricyclo[13.2.1.0^6,10]octadecane-9,18-diol (CCD ID: GJF) (formula: C₂₀H₂₄N₁₀O₁₀P₂S₂) (labeled as "Ligand of Interest" by depositor).

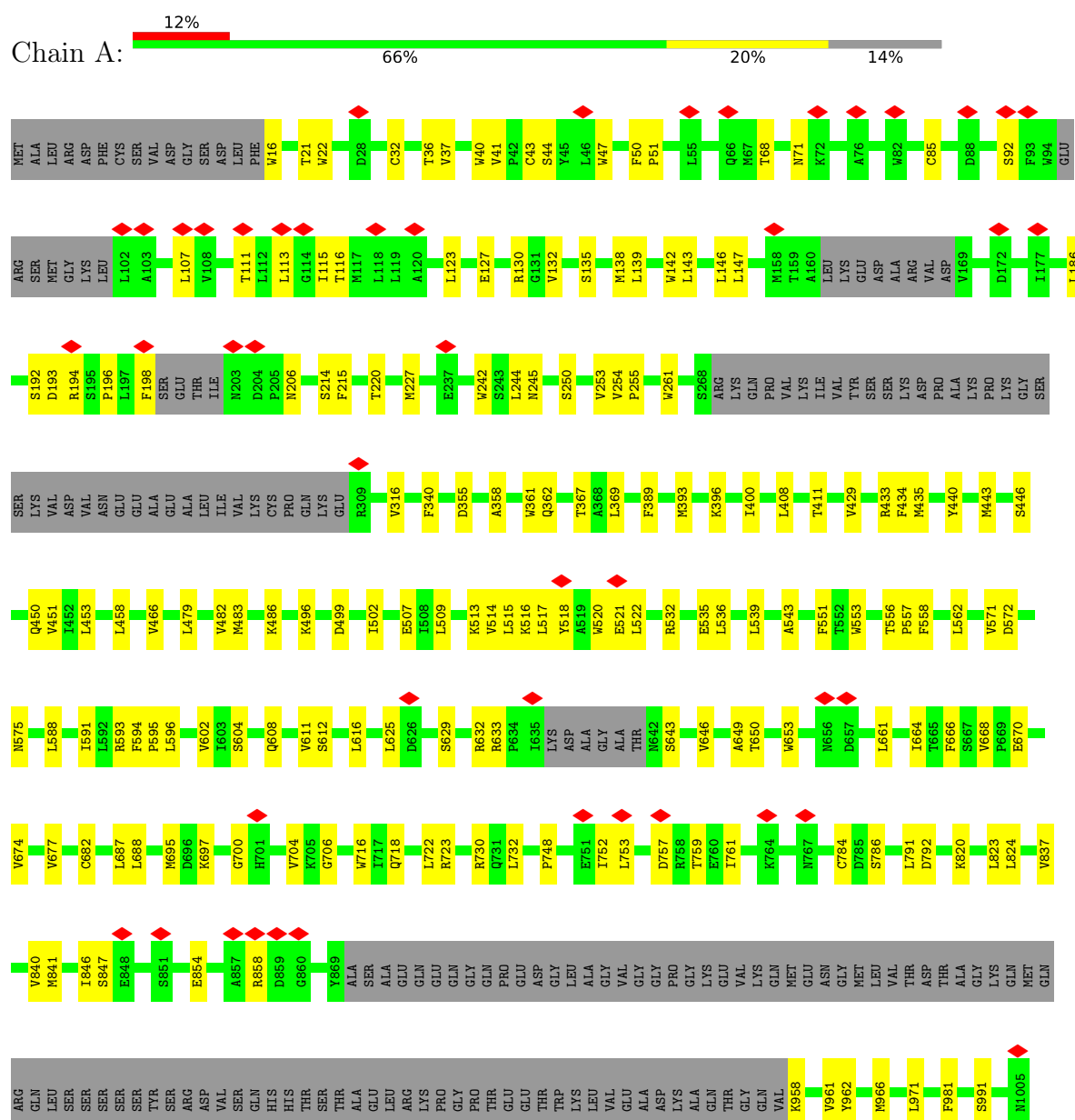


Mol	Chain	Residues	Atoms					AltConf	
2	A	1	Total	C	N	O	P	S	0
			44	20	10	10	2	2	

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: Multidrug resistance-associated protein 1



GLY	S1401	A1330	E1270	P1149	E1009
SER	L1402	G1331	K1271		
GLU	E1403	S1332	E1272	L1158	Y1018
ASN	L1404	S1333	A1273	G1159	G1019
LEU	A1405	S1334	P1274	G1160	G1022
TYR	H1406	L1335	W1275		I1023
PHE	H1407	T1336		I1164	
GLN	L1408	T1337			
GLY					
GLY	L1481	G1409	Q1278	F1167	V1029
SER	F1410	R1341	D1279		
GLY	V1411	I1342	M1280	F1173	Y1032
GLY	S1412	K1343	A1281	D1178	
SER	A1484	E1344	P1282		S1037
HIS	H1485	A1413	P1283	V1181	I1041
HIS	A1414	S1345	K1284	N1184	R1045
HIS	P1415	A1346	D1285	Q1185	R1046
HIS	D1416	E1347	W1286		
HIS	H1417	G1348	P1287	Y1188	L1056
HIS	L1418	E1349	Q1288	Y1189	
HIS	L1419	I1350	W1289	P1190	P1059
HIS	H1420	I1351	G1290	S1191	I1060
HIS	E1421	I1352	R1291	I1192	
HIS		D1353	V1292		R1065
		D1354	E1293	R1196	
	E1424	I1355	F1294	A1199	V1072
	G1425	M1356	R1295	V1200	M1073
	G1426	I1357	D1296	R1201	R1074
	E1427	A1358	Y1297	L1202	
	N1428	K1359	G1298	E1203	K1077
	L1429	I1360	Y1299	L1211	E1078
	S1430	G1361	R1300		L1079
		L1362	Y1301	F1216	V1082
			ARG	D1083	
	Q1433	L1365	GLU	R1221	
	R1434	R1366	ASP	H1222	P1087
	V1437	T1370	LEU	S1223	Q1088
		I1371		L1224	V1089
			D1306		I1090
	R1441	Q1374	L1307	S1236	K1091
		D1375	L1308	V1239	M1092
	R1445	P1376	V1309		F1093
	T1446	V1377	K1310	W1245	M1094
	K1447	V1377	H1311	L1246	
	K1448	L1378	I1312	V1247	F1098
	L1449	F1379	N1313	R1248	
	L1450	S1380	V1314	M1249	G1102
	V1451	G1381	T1315		I1105
	L1452	S1382	I1316	M1253	
	D1453	L1383			T1111
	E1454	R1384	D1317	E1261	Q1129
	A1455	L1387	G1318	R1262	
	THR		G1319	L1263	V1133
	ALA	Q1392	E1320	Y1266	
	ALA	Y1393	K1321		
	VAL	S1394	V1322		
	ALA	ASP	G1323		
	LEU	D1395	I1324		
	LYS	E1396	V1325		
	ASP	E1397	G1326		
	T1462	T1463	R1327		
	SER	D1464	T1328		
	GLY	LEU	G1329		
	VAL	D1465			
	VAL	L1466			
	LYS	I1467			
	LEU				

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	109497	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	2.790	Depositor
Minimum map value	-1.702	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.056	Depositor
Recommended contour level	0.42	Depositor
Map size (Å)	332.8, 332.8, 332.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.44	0/10856	0.61	1/14738 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	1289	VAL	N-CA-C	-6.36	107.66	113.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10618	0	10838	214	0
2	A	44	0	0	0	0
All	All	10662	0	10838	214	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 10.

The worst 5 of 214 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:674:VAL:HG22	1:A:837:VAL:HB	1.70	0.73
1:A:520:TRP:HH2	1:A:1441:ARG:HD2	1.54	0.72
1:A:451:VAL:HG23	1:A:595:PRO:HB2	1.72	0.71
1:A:543:ALA:HB1	1:A:1037:SER:HB3	1.73	0.70
1:A:192:SER:HB3	1:A:214:SER:HB3	1.73	0.69

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	1318/1558 (85%)	1280 (97%)	38 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1175/1358 (86%)	1175 (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. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	718	GLN
1	A	774	GLN
1	A	1386	ASN
1	A	1207	ASN
1	A	1363	HIS

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](#)

1 ligand is 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	GJF	A	1601	-	39,50,50	2.17	13 (33%)	46,78,78	2.00	7 (15%)

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	GJF	A	1601	-	-	13/18/62/62	0/6/7/7

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1601	GJF	P2-O9	5.17	1.66	1.57
2	A	1601	GJF	O1-C6	4.42	1.47	1.41
2	A	1601	GJF	C18-C17	-3.94	1.44	1.52
2	A	1601	GJF	O8-C19	3.94	1.46	1.41
2	A	1601	GJF	P2-O6	3.80	1.63	1.57

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1601	GJF	O6-P2-O9	6.62	120.74	102.22
2	A	1601	GJF	O3-P1-O7	5.93	118.81	102.22
2	A	1601	GJF	N5-C13-N6	-4.65	121.41	128.68
2	A	1601	GJF	N2-C20-N1	-4.27	122.00	128.68
2	A	1601	GJF	O8-C19-C18	-2.41	103.41	106.93

There are no chirality outliers.

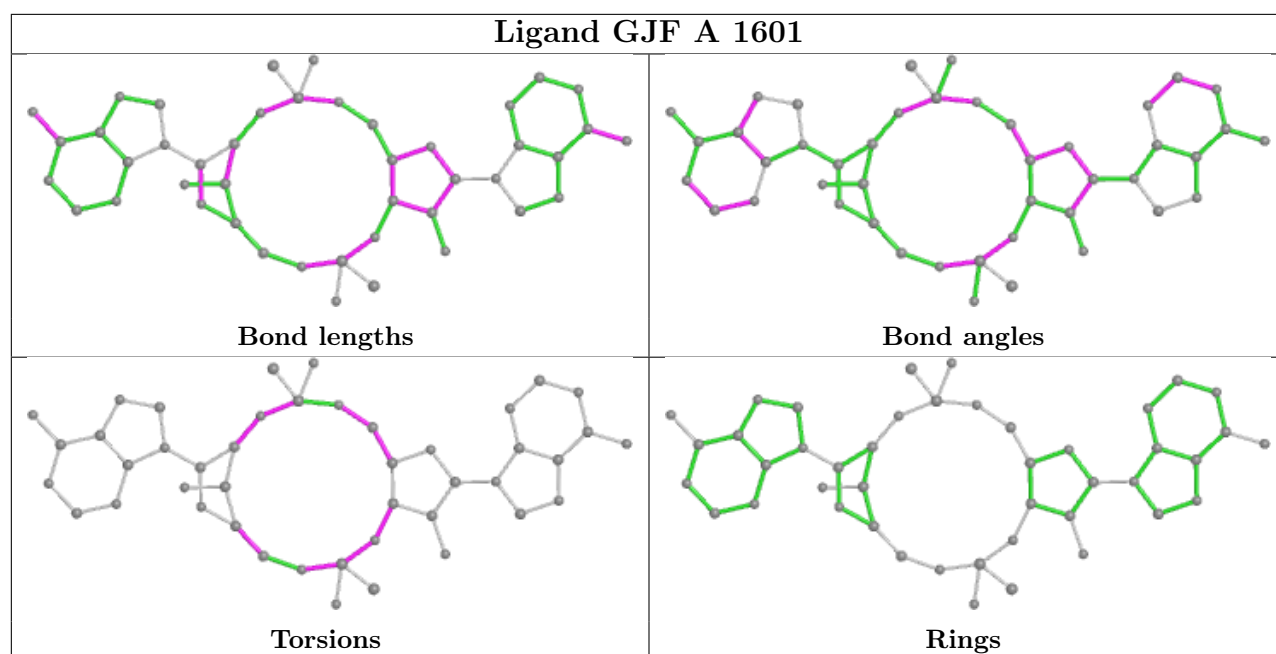
5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1601	GJF	C17-O9-P2-O5
2	A	1601	GJF	C17-O9-P2-O6
2	A	1601	GJF	C16-C17-O9-P2
2	A	1601	GJF	O1-C7-C9-O6
2	A	1601	GJF	C9-O6-P2-O5

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

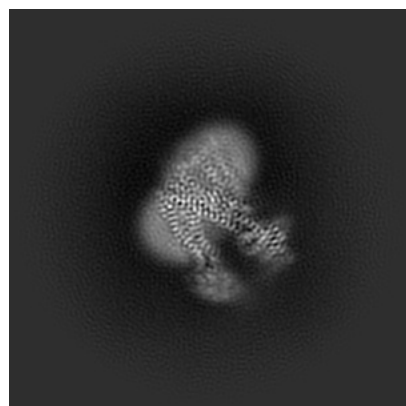
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63055. These allow visual inspection of the internal detail of the map and identification of artifacts.

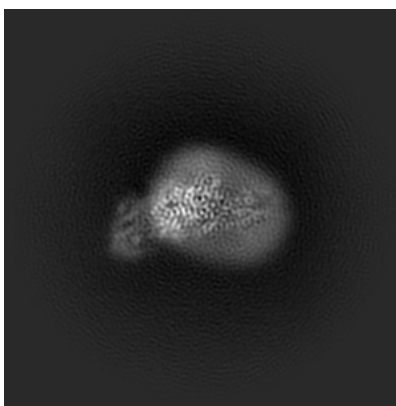
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

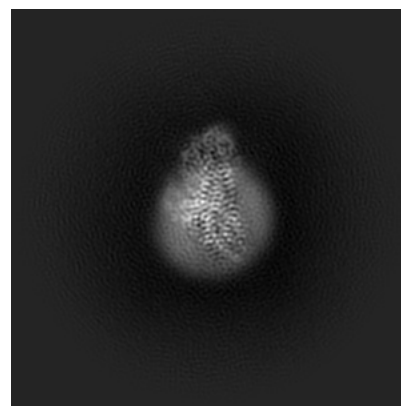
6.1.1 Primary map



X

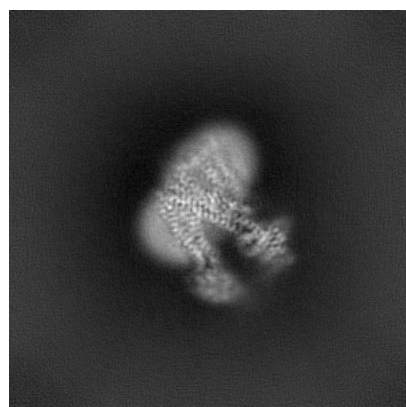


Y

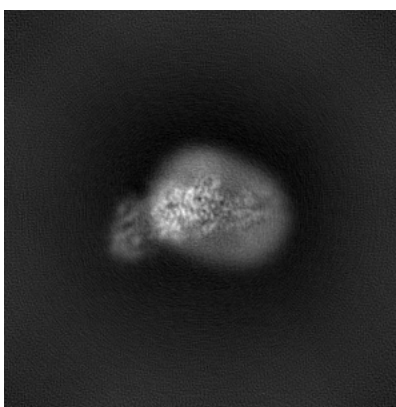


Z

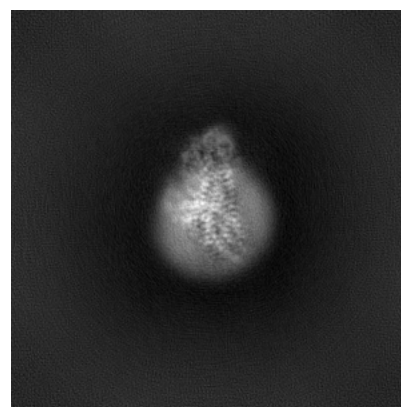
6.1.2 Raw map



X



Y

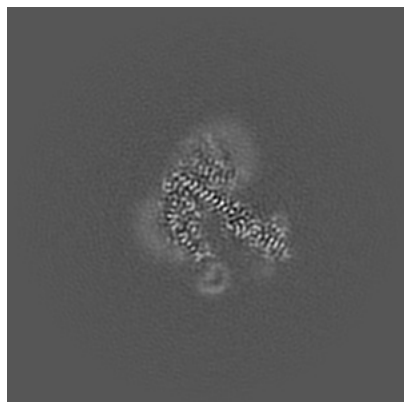


Z

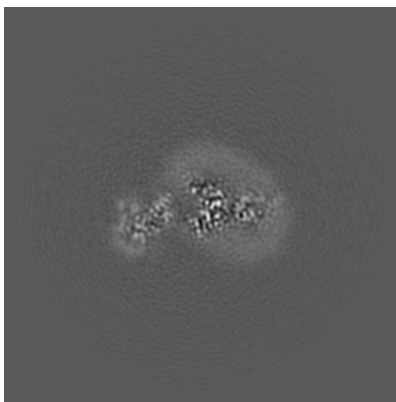
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

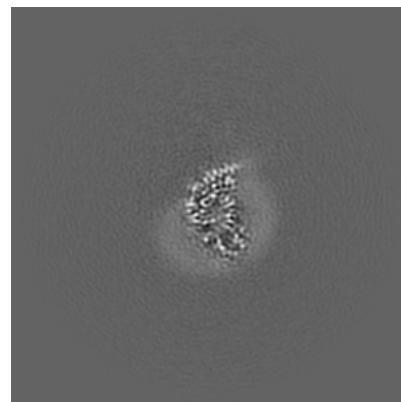
6.2.1 Primary map



X Index: 160

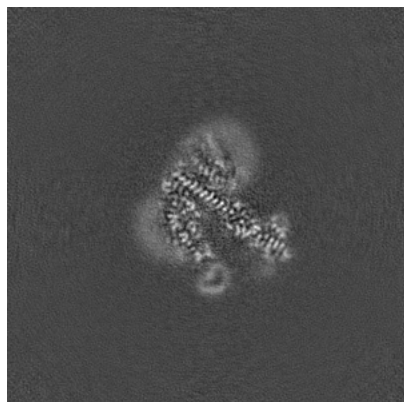


Y Index: 160

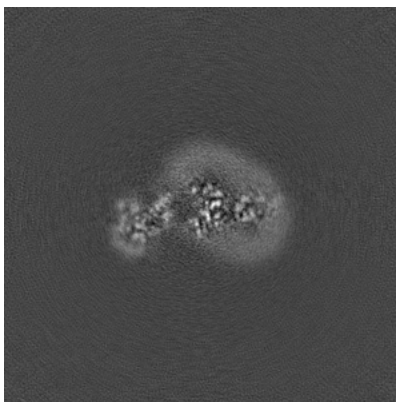


Z Index: 160

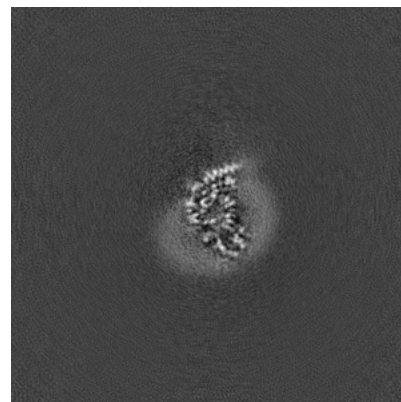
6.2.2 Raw map



X Index: 160



Y Index: 160

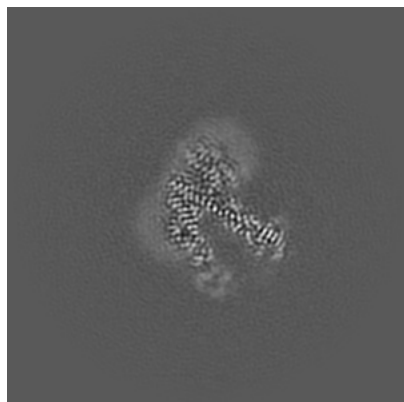


Z Index: 160

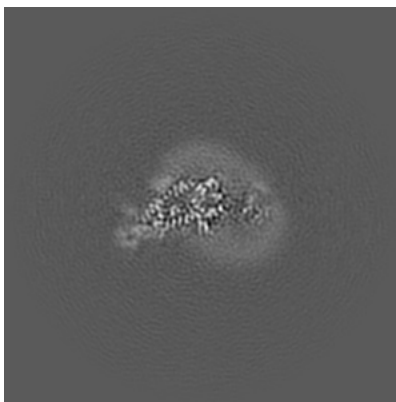
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

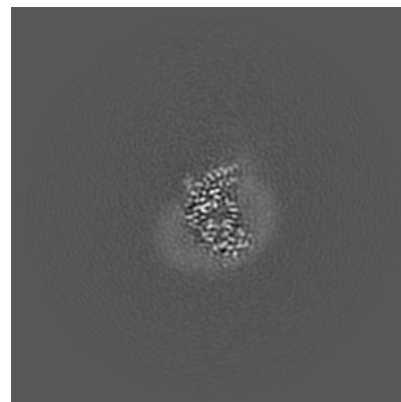
6.3.1 Primary map



X Index: 156

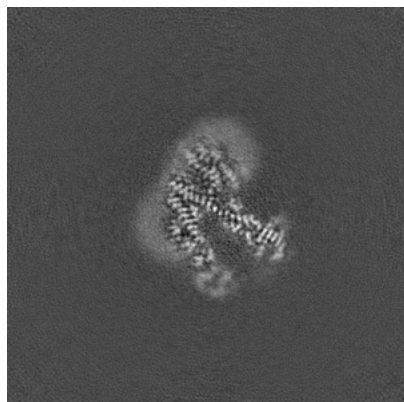


Y Index: 152

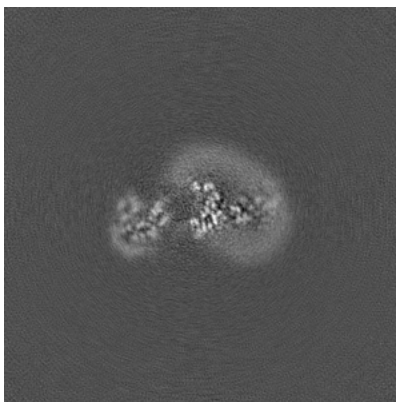


Z Index: 162

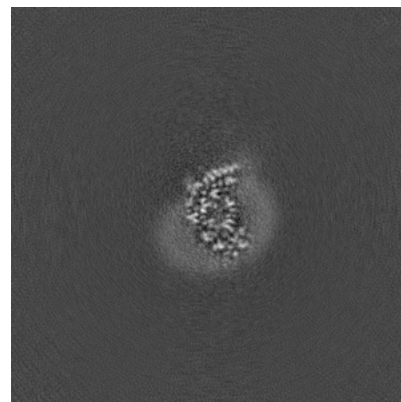
6.3.2 Raw map



X Index: 156



Y Index: 162

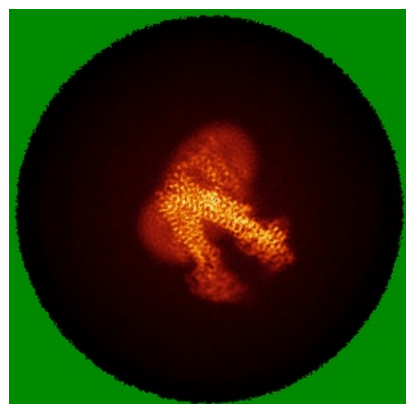


Z Index: 161

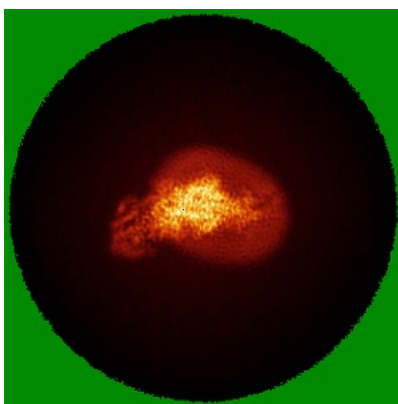
The images above show the largest variance slices of the map in three orthogonal directions.

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

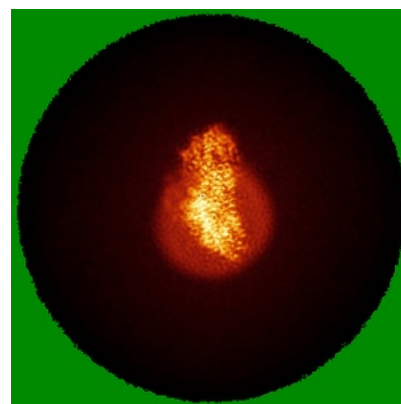
6.4.1 Primary map



X

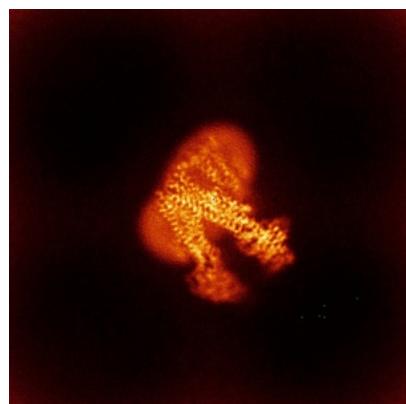


Y

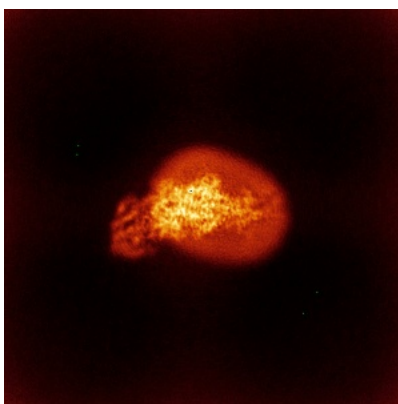


Z

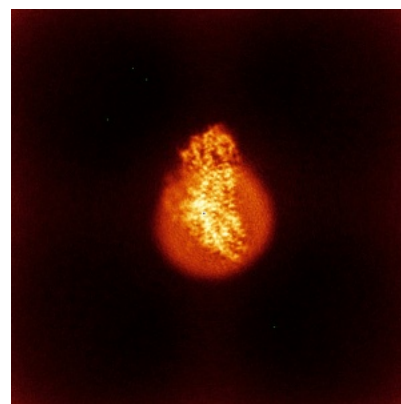
6.4.2 Raw map



X



Y

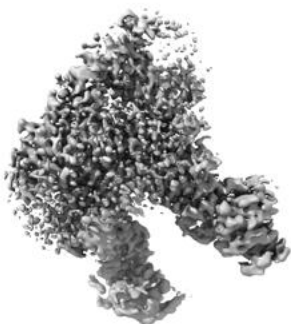


Z

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 0.42. 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.

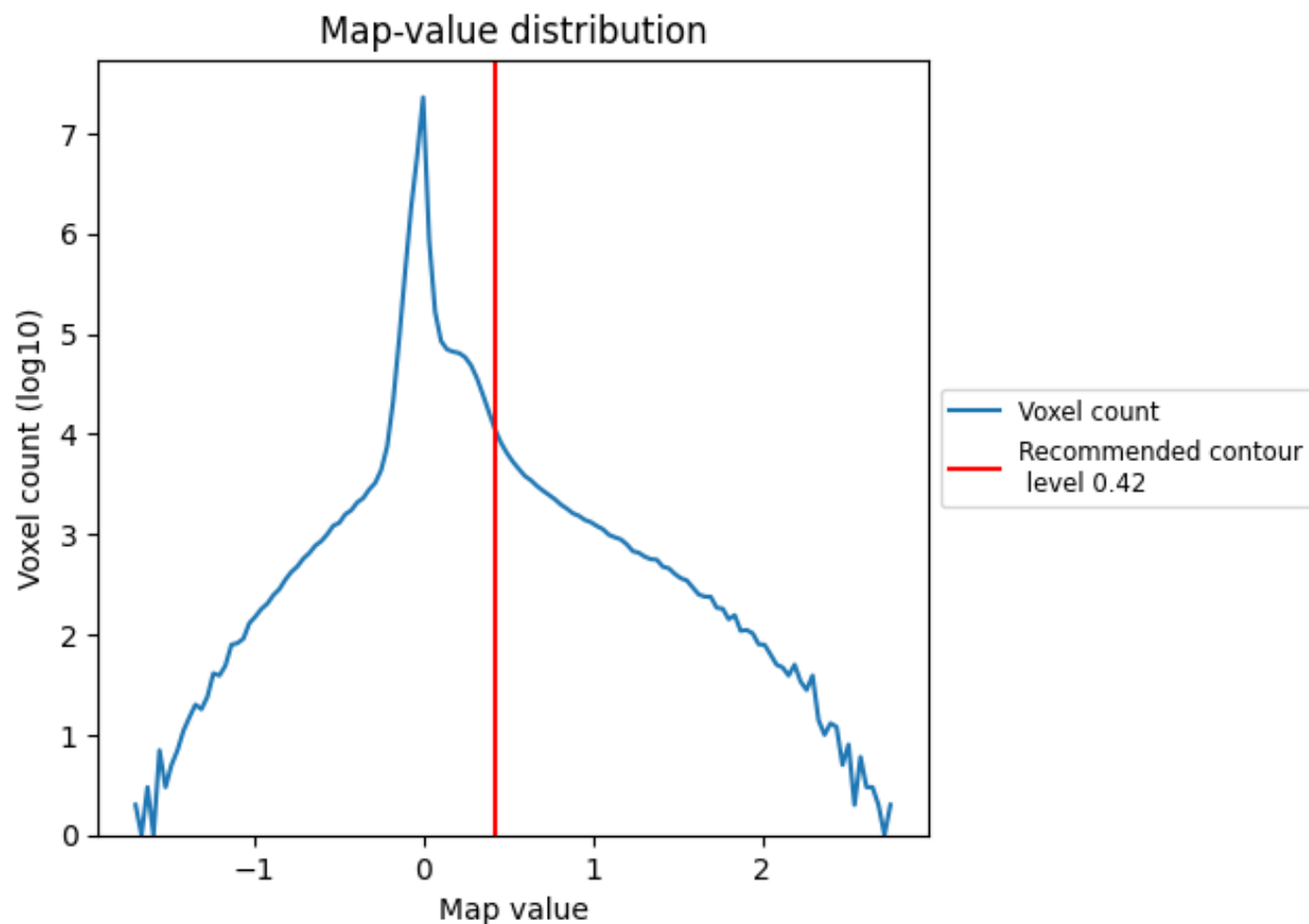
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

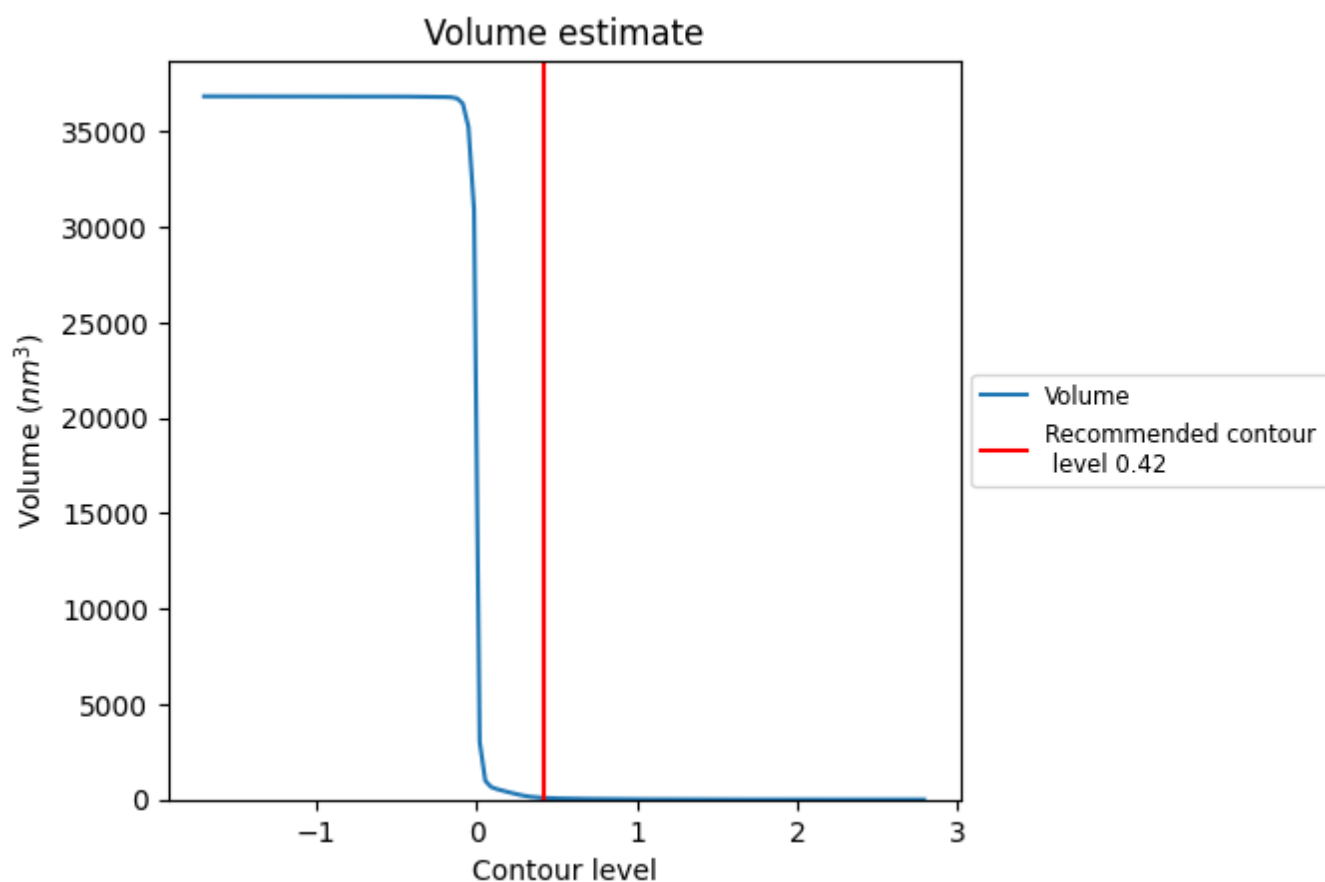
This section contains the results of statistical analysis of the map.

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.

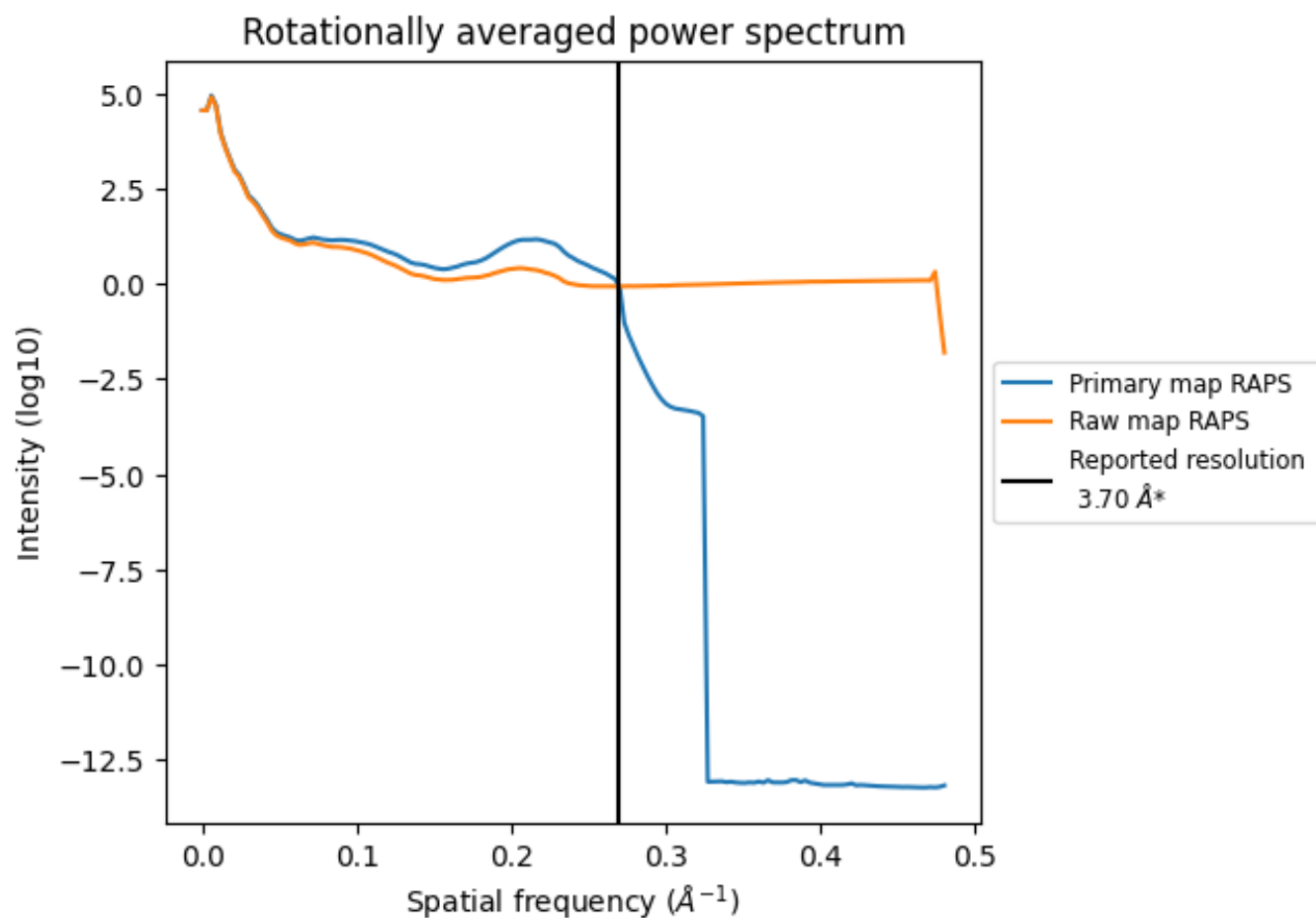
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 87 nm³; this corresponds to an approximate mass of 79 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 ⓘ

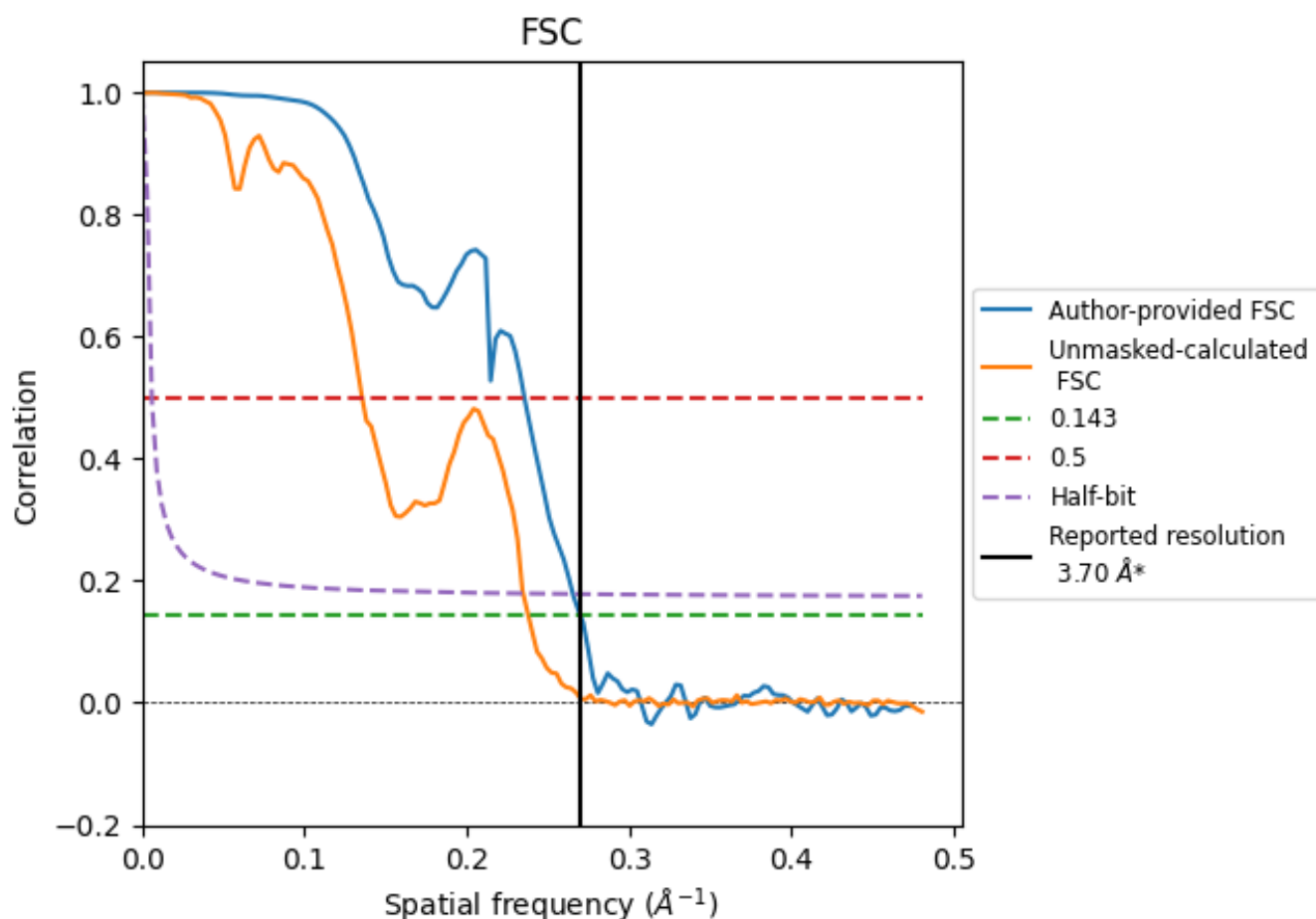


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

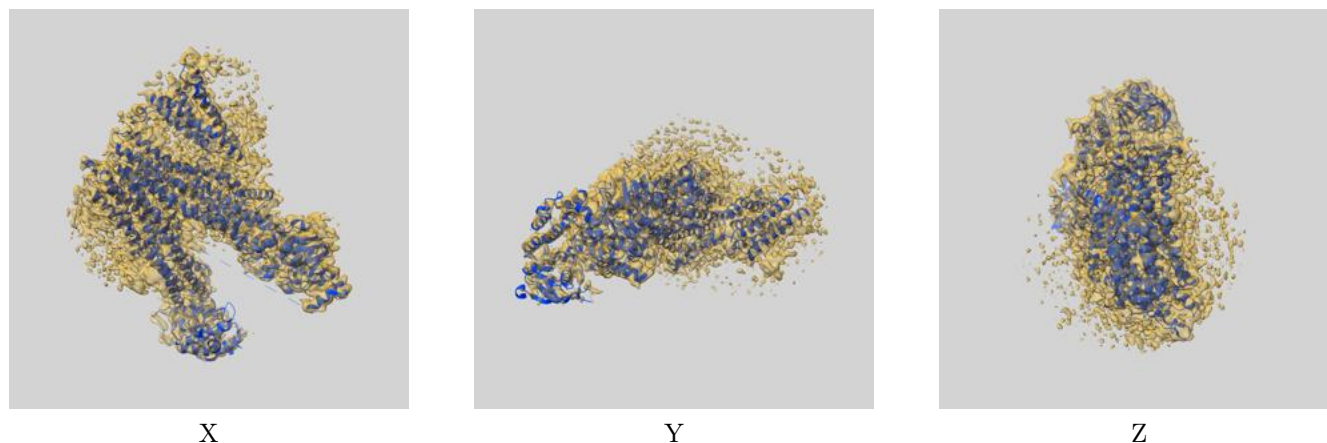
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.70	4.24	3.77
Unmasked-calculated*	4.20	7.37	4.26

*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 4.20 differs from the reported value 3.7 by more than 10 %

9 Map-model fit [i](#)

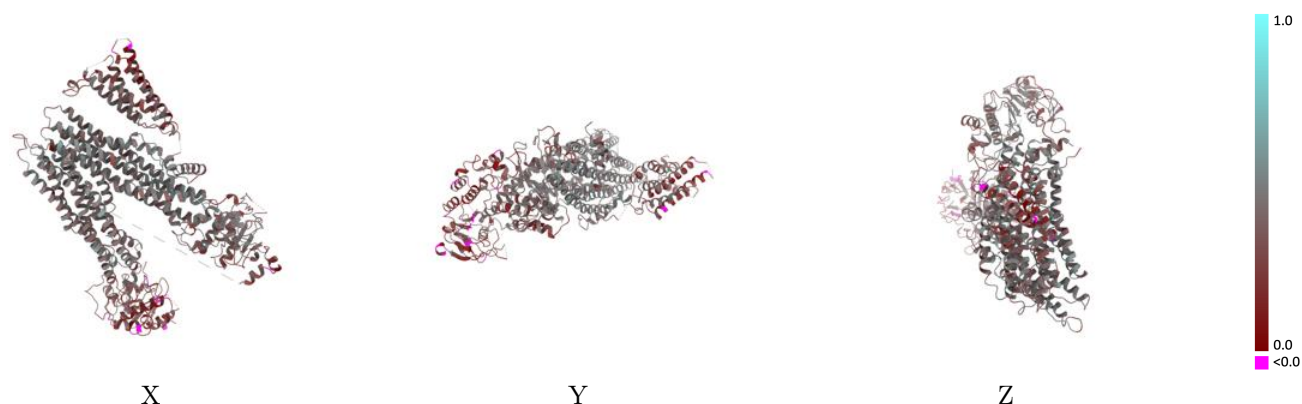
This section contains information regarding the fit between EMDB map EMD-63055 and PDB model 9LG6. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



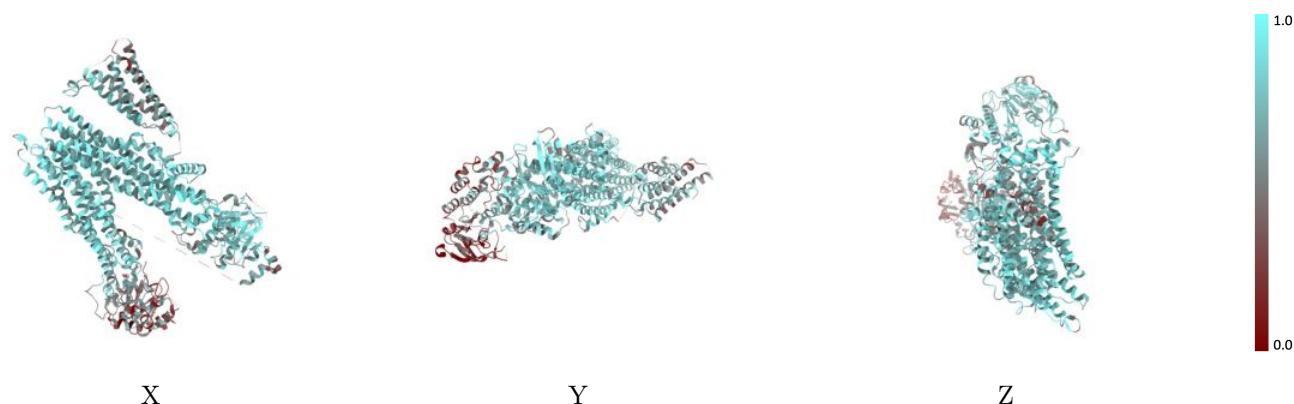
The images above show the 3D surface view of the map at the recommended contour level 0.42 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



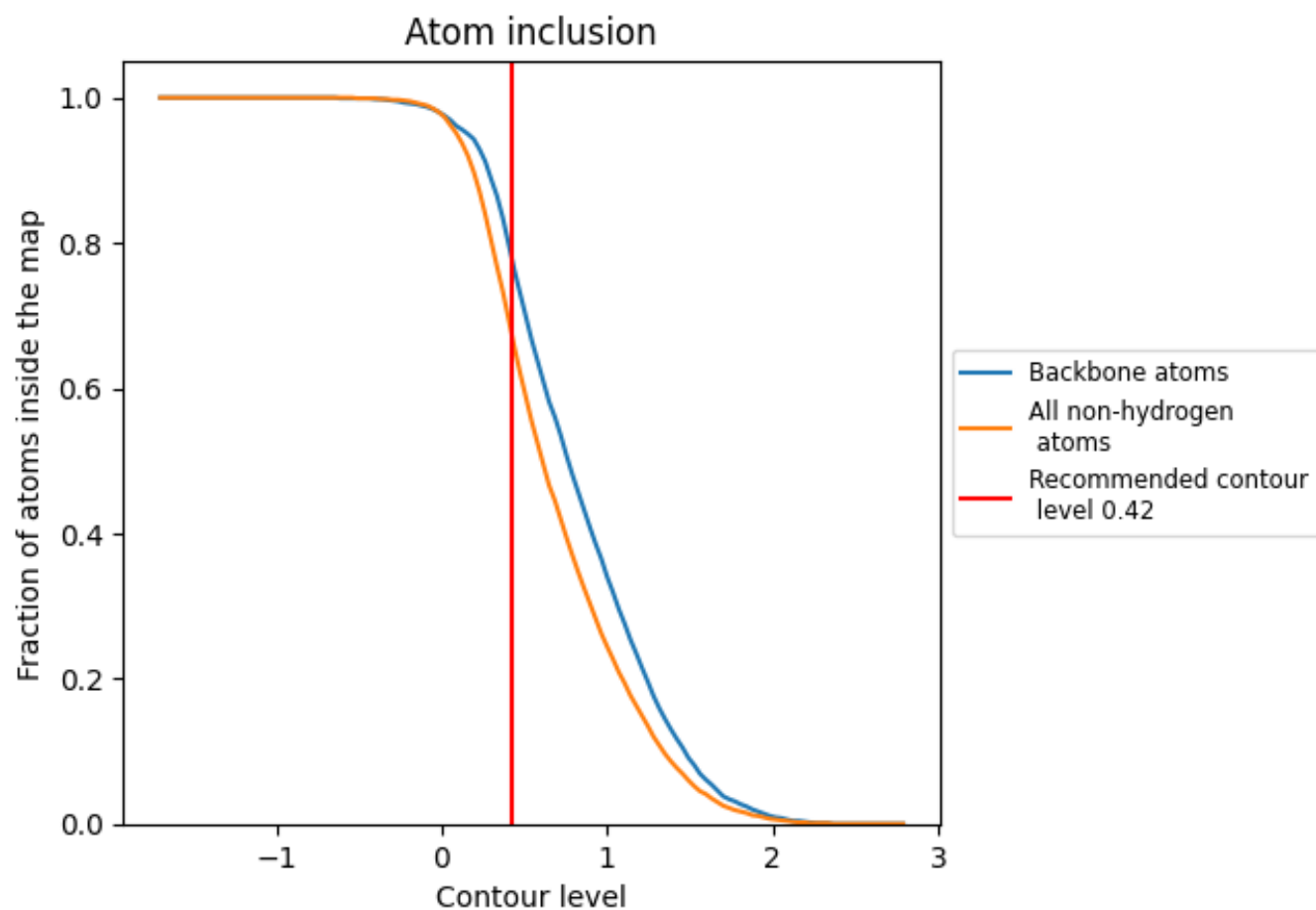
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.42).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 68% 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 (0.42) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6780	<div></div> 0.3730
A	<div></div> 0.6780	<div></div> 0.3730

