



wwPDB EM Validation Summary Report ⓘ

Mar 24, 2026 – 09:51 PM UTC

PDB ID : 8HW2 / pdb_00008hw2
EMDB ID : EMD-35049
Title : Cryo-EM structure of beta-estradiol 17-(beta-D-glucuronide)-bound human ABC transporter ABCC3 in nanodiscs
Authors : Wang, J.; Wang, F.F.; Chen, Y.X.; Zhou, C.Z.
Deposited on : 2022-12-28
Resolution : 3.65 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

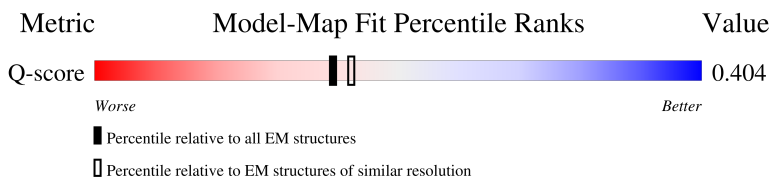
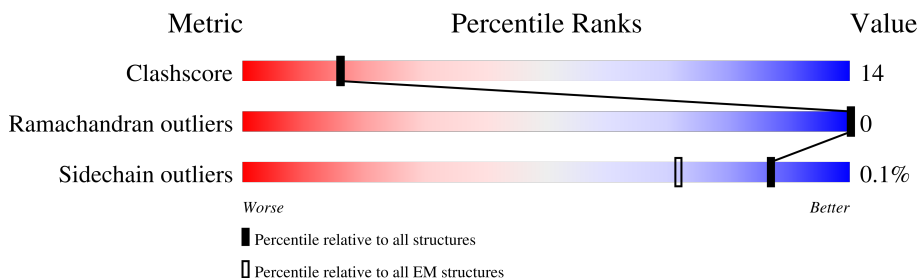
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.65 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	11564 (3.15 - 4.15)

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	1527	24% 63% 27% 10%

2 Entry composition [i](#)

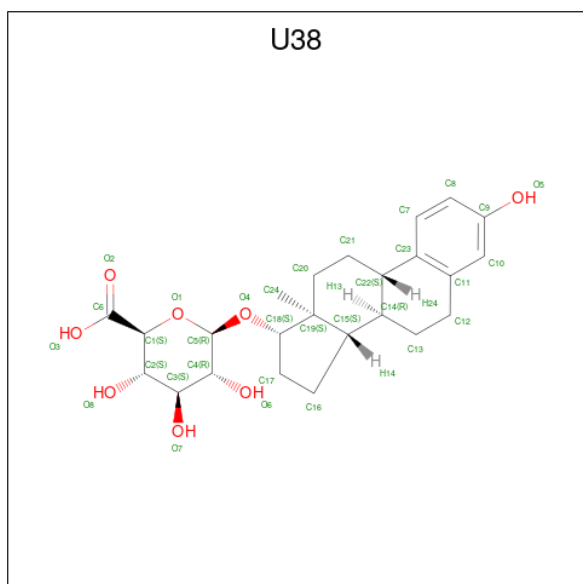
There are 2 unique types of molecules in this entry. The entry contains 10853 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ATP-binding cassette sub-family C member 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1375	10789	7015	1812	1905	57	0	0

- Molecule 2 is Estradiol-17beta-glucuronide (CCD ID: U38) (formula: $C_{24}H_{32}O_8$) (labeled as "Ligand of Interest" by depositor).

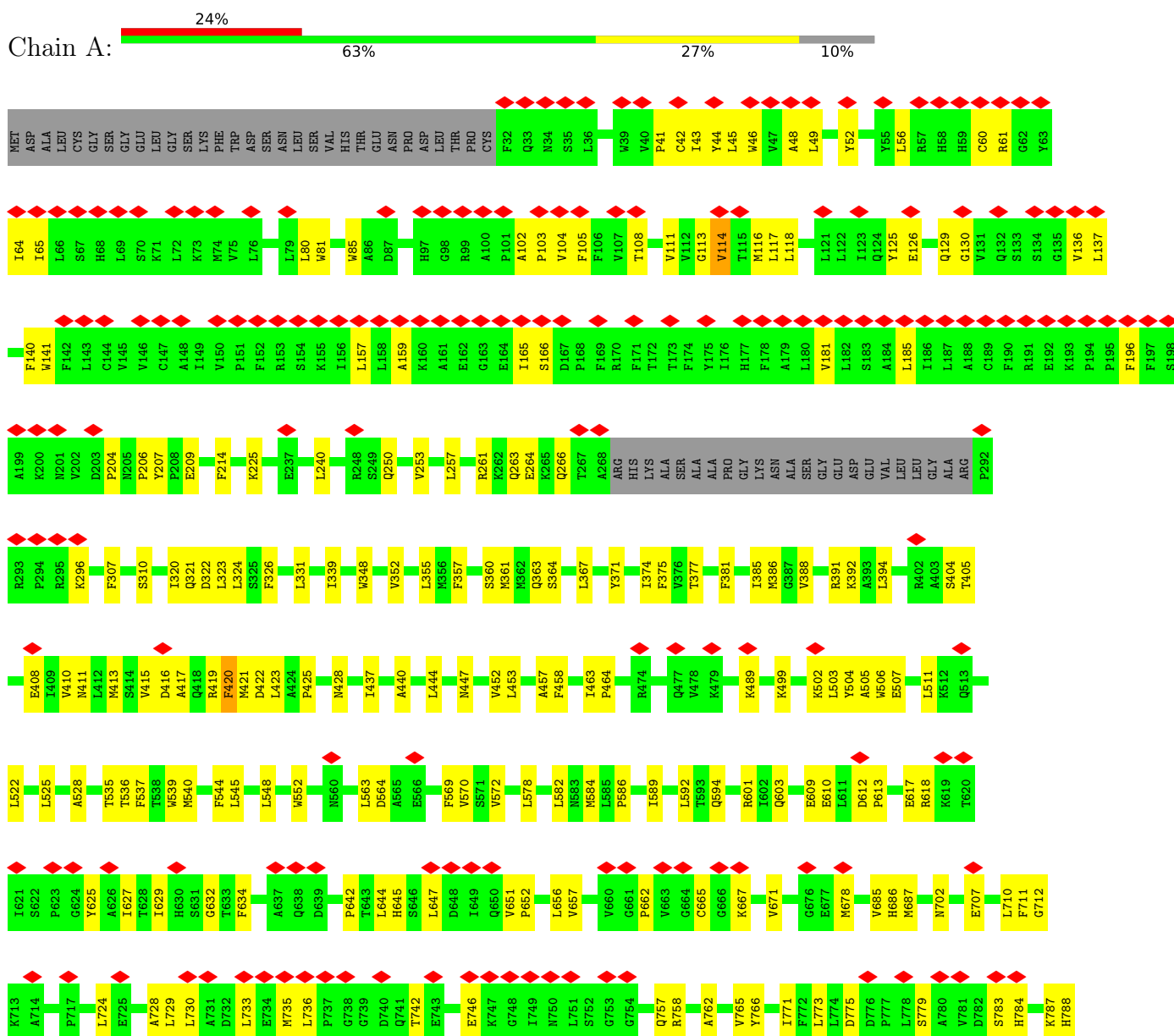


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
2	A	1	32	24	8	0
2	A	1	32	24	8	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: ATP-binding cassette sub-family C member 3



V1501	A1502	E1503	F1504	D1505	S1506	P1507	A1508	N1509	L1510	I1511	A1512	A1513	R1514	G1515	I1516	F1517	Y1518	G1519	M1520	A1521	R1522	D1523	A1524	G1525	L1526	A1527																														
L1441	R1442	L1443	S1444	R1445	I1446	L1447	V1448	L1449	D1450	E1451	A1452	T1453	A1454	A1455	T1456	D1457	L1458	E1459	T1460	D1461	N1462	L1463	L1464	Q1465	A1466	T1467	I1468	R1469	T1470	Q1471	F1472	D1473	T1474	C1475	L1476	V1477	L1478																			
Q1371	D1372	P1373	I1374	L1375	F1376	S1377	R1381	M1382	N1383	L1384	G1388	S1389	Y1390	S1391	E1392	E1393	W1396	W1397	L1398	E1399	L1399	A1400	L1401	S1402	H1403	L1404	H1405	T1406	F1407	V1408	S1409	S1410	Q1411	P1412	A1413	D1416	F1417	Q1418	C1419	S1420	E1421	G1422	G1423	E1424	N1425	L1426	S1427	V1428	Q1429	L1430	V1431	Q1432	L1433	L1436	A1437	
L1302	D1303	L1304	V1305	L1306	R1307	D1308	L1309	S1310	L1311	H1312	V1313	H1314	G1315	V1319	G1320	T1321	V1322	G1323	R1324	T1325	G1326	A1327	G1328	K1329	S1330	S1331	M1332	C1335	L1336	F1337	R1338	I1339	L1340	E1341	A1342	A1343	K1344	G1345	E1346	I1347	R1348	G1351	L1352	N1353	V1354	A1355	L1356	T1357	G1358	L1359	H1360	R1363	I1368			
F1201	M1204	L1208	N1222	P1223	V1226	G1227	L1228	V1236	W1242	M1243	L1244	R1245	M1246	D1249	L1250	V1255	E1258	K1261	K1265	T1268	E1269	V1273	V1274	E1275	G1276	S1277	R1278	P1279	W1283	P1284	P1285	R1286	V1289	E1290	F1291	R1292	M1293	Y1294	S1295	V1296	R1297	P1300	G1301													
S1099	T1100	V1103	I1104	M1105	L1110	F1111	T1112	V1113	V1114	I1115	L1116	P1117	L1118	A1119	V1120	L1121	Y1122	V1125	Q1135	R1138	V1142	I1147	F1151	S1152	E1153	R1162	R1166	S1167	R1168	F1170	E1171	I1172	S1174	D1175	V1178	P1187	Y1188	I1189	N1192	R1193	W1194	L1195	E1200													
R1011	L1012	A1016	G1019	I1020	L1021	Q1022	G1023	F1024	L1025	V1026	M1027	L1028	A1029	M1033	I1038	Q1039	L1044	H1045	Q1046	H1050	M1051	K1052	I1053	R1054	D1061	F1064	R1067	I1068	L1069	N1070	C1071	D1075	I1076	Y1077	V1078	V1079	V1082	V1086	I1087	L1088	M1089	M1092	S1093	F1094	I1098											
TRP	THR	ALA	LEU	PRO	GLY	SER	GLU	LYS	ALA	GLU	ASP	GLN	VAL	THR	LEU	ASN	THR	GLN	GLU	LYS	ALA	ASP	ASN	ASP	PRO	VAL	THR	TYR	VAL	GLN	LYS	PHE	MET	ARG	GLN	LEU	SER	SER	ASP	GLY	GLY	GLN	GLY	ARG	PRO	VAL	PRO	ARG	ASP	GLN	GLY	HIS	LEU	GLU	ASP	SER
D791	H792	V793	E797	G798	L799	L800	R805	V808	S813	F814	L815	P816	Q817	T818	V823	L824	A825	D826	S830	E831	M832	Y835	P836	A837	L838	L839	Q840	R841	N842	G843	S844	F845	A846	N847	F848	L849	C850	N851	Y852	ALA	PRO	ASP	GLU	ASP	GLN	GLY	HIS	LEU	GLU	ASP	SER					

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	177500	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	54	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.165	Depositor
Minimum map value	-2.215	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.059	Depositor
Recommended contour level	0.447	Depositor
Map size (Å)	273.92, 273.92, 273.92	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: U38

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	0.17	0/11041	0.45	4/15014 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1026	VAL	N-CA-C	-6.30	107.72	113.71
1	A	114	VAL	N-CA-C	-5.38	107.58	112.96
1	A	420	PHE	CA-C-N	5.15	131.38	121.54
1	A	420	PHE	C-N-CA	5.15	131.38	121.54

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1245	ARG	Sidechain
1	A	1283	TRP	Peptide

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	10789	0	11029	312	0
2	A	64	0	0	25	0
All	All	10853	0	11029	312	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 14.

The worst 5 of 312 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:584:MET:HE2	2:A:1601:U38:C12	1.21	1.65
1:A:584:MET:CE	2:A:1601:U38:C12	1.97	1.42
1:A:584:MET:CE	2:A:1601:U38:C13	2.28	1.09
1:A:1192:ASN:ND2	2:A:1601:U38:O2	1.98	0.96
1:A:584:MET:HE2	2:A:1601:U38:C13	1.93	0.95

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	1369/1527 (90%)	1271 (93%)	98 (7%)	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	1176/1299 (90%)	1175 (100%)	1 (0%)	88 87

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1245	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1092	ASN
1	A	1312	HIS
1	A	447	ASN
1	A	519	GLN
1	A	591	ASN

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](#)

2 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	U38	A	1602	-	36,36,36	5.62	14 (38%)	54,56,56	2.59	15 (27%)
2	U38	A	1601	-	36,36,36	5.61	14 (38%)	54,56,56	2.84	20 (37%)

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	U38	A	1602	-	-	2/8/68/68	0/5/5/5
2	U38	A	1601	-	-	2/8/68/68	0/5/5/5

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1602	U38	C7-C23	17.37	1.60	1.39
2	A	1601	U38	C7-C23	17.29	1.60	1.39
2	A	1602	U38	C10-C11	13.56	1.60	1.39
2	A	1601	U38	C10-C11	13.48	1.60	1.39
2	A	1601	U38	C22-C14	11.92	1.68	1.54

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1601	U38	C20-C21-C22	9.71	124.91	112.34
2	A	1602	U38	C20-C21-C22	9.52	124.67	112.34
2	A	1601	U38	C10-C11-C23	-6.67	111.08	119.49
2	A	1602	U38	C10-C11-C23	-6.56	111.22	119.49
2	A	1601	U38	C23-C22-C14	-5.90	104.46	111.59

There are no chirality outliers.

All (4) torsion outliers are listed below:

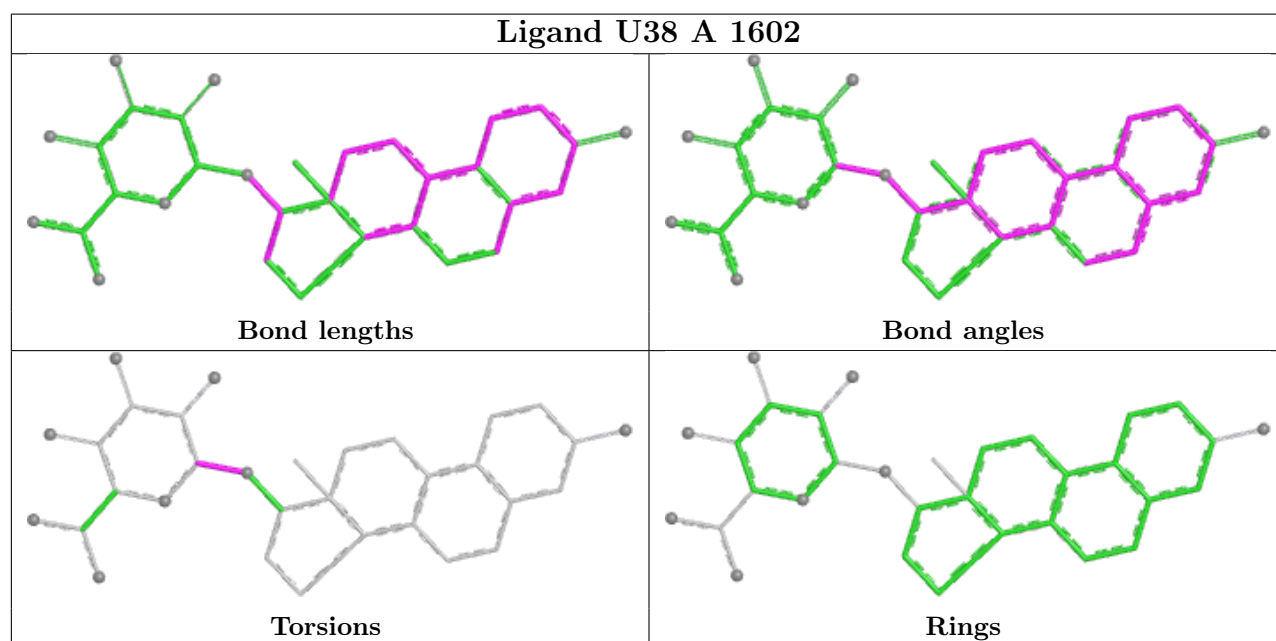
Mol	Chain	Res	Type	Atoms
2	A	1602	U38	O1-C5-O4-C18
2	A	1602	U38	C4-C5-O4-C18
2	A	1601	U38	O1-C5-O4-C18
2	A	1601	U38	C17-C18-O4-C5

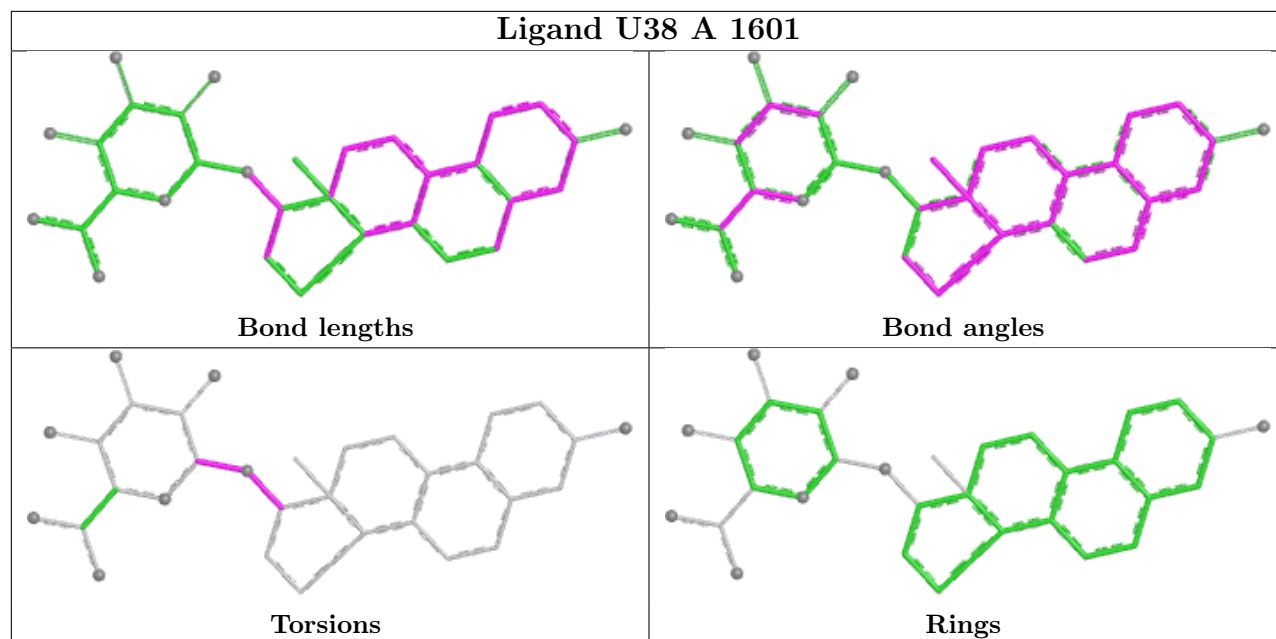
There are no ring outliers.

2 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1602	U38	12	0
2	A	1601	U38	13	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.

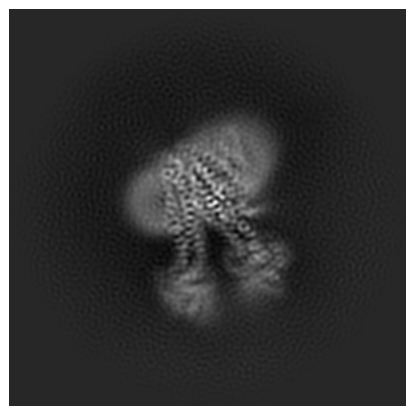
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35049. These allow visual inspection of the internal detail of the map and identification of artifacts.

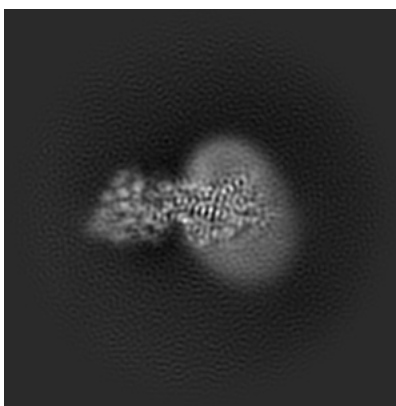
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

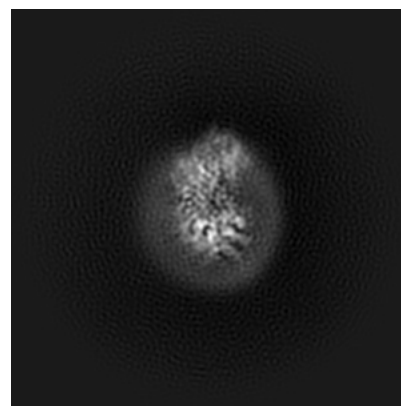
6.1.1 Primary map



X

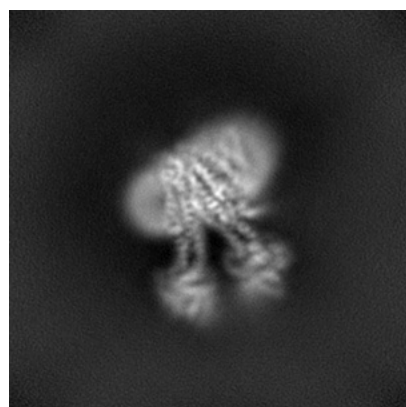


Y

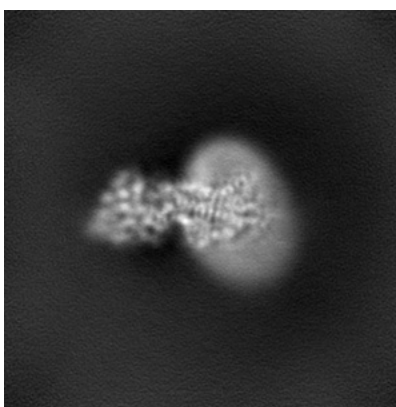


Z

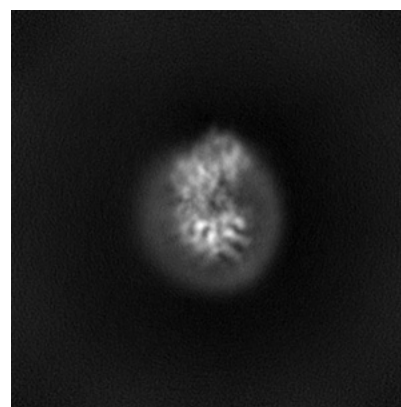
6.1.2 Raw map



X



Y

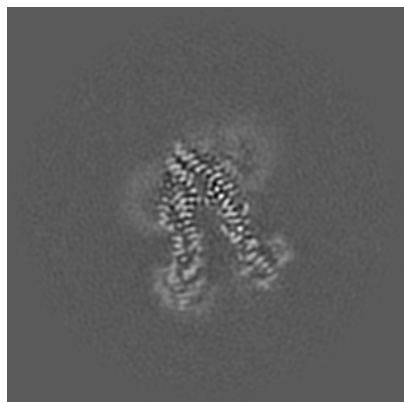


Z

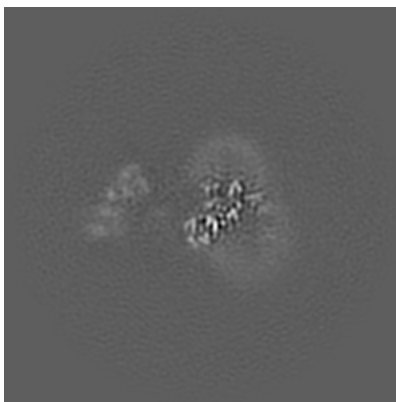
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

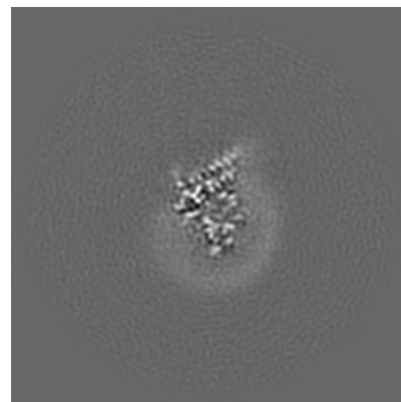
6.2.1 Primary map



X Index: 128

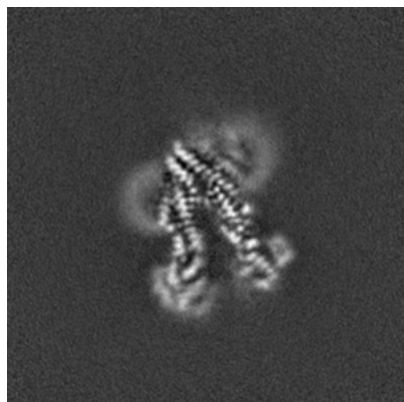


Y Index: 128

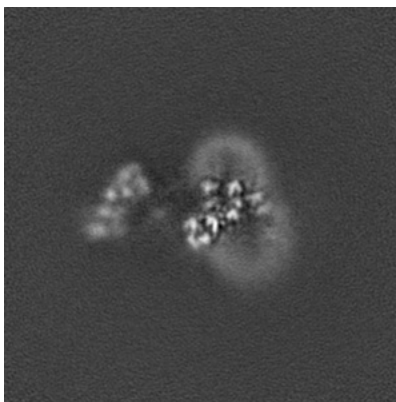


Z Index: 128

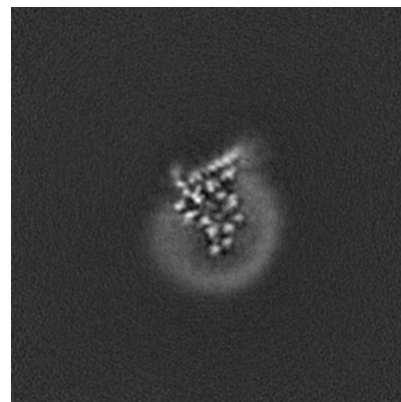
6.2.2 Raw map



X Index: 128



Y Index: 128

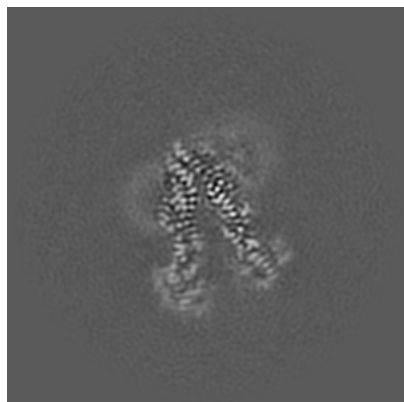


Z Index: 128

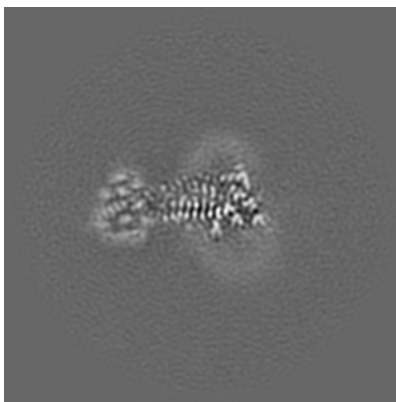
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

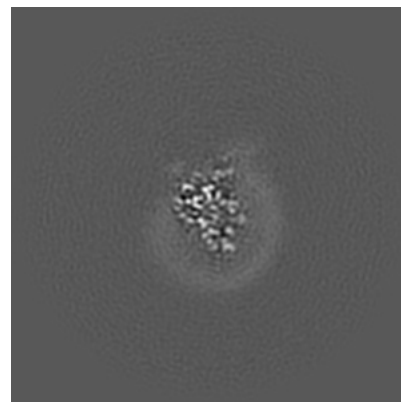
6.3.1 Primary map



X Index: 127

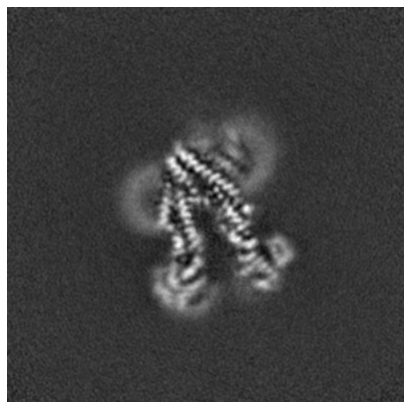


Y Index: 116

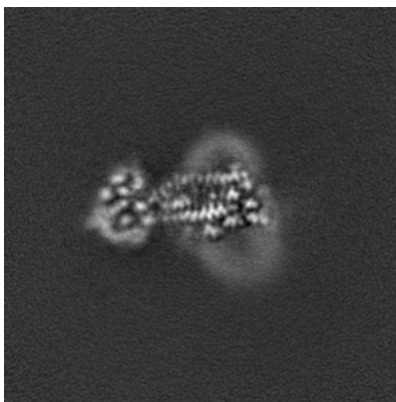


Z Index: 131

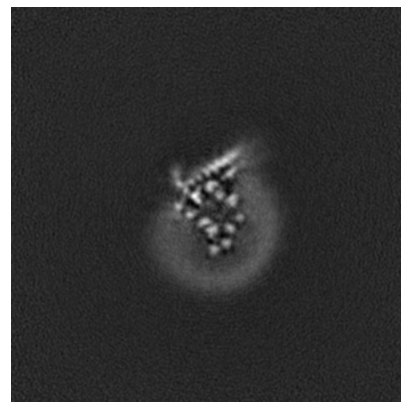
6.3.2 Raw map



X Index: 129



Y Index: 118

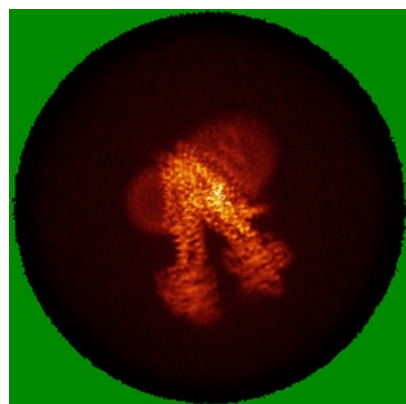


Z Index: 127

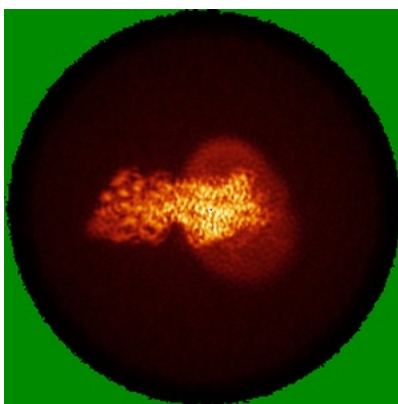
The images above show the largest variance slices of the map in three orthogonal directions.

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

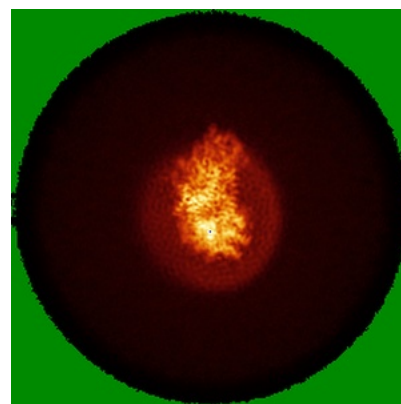
6.4.1 Primary map



X

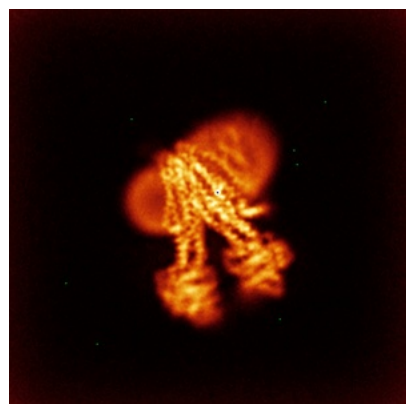


Y

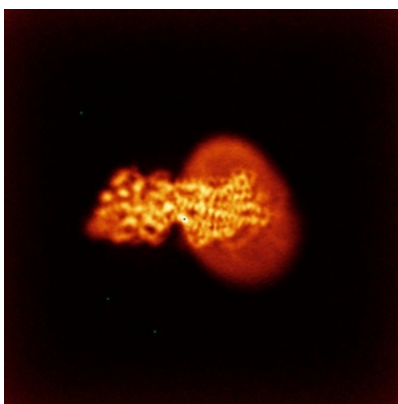


Z

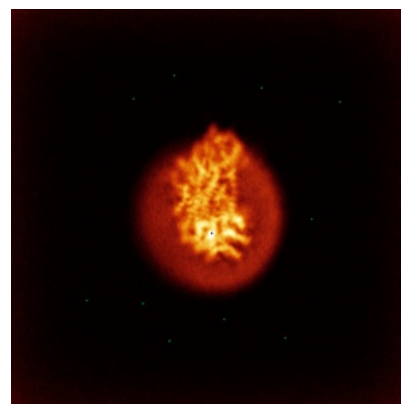
6.4.2 Raw map



X



Y

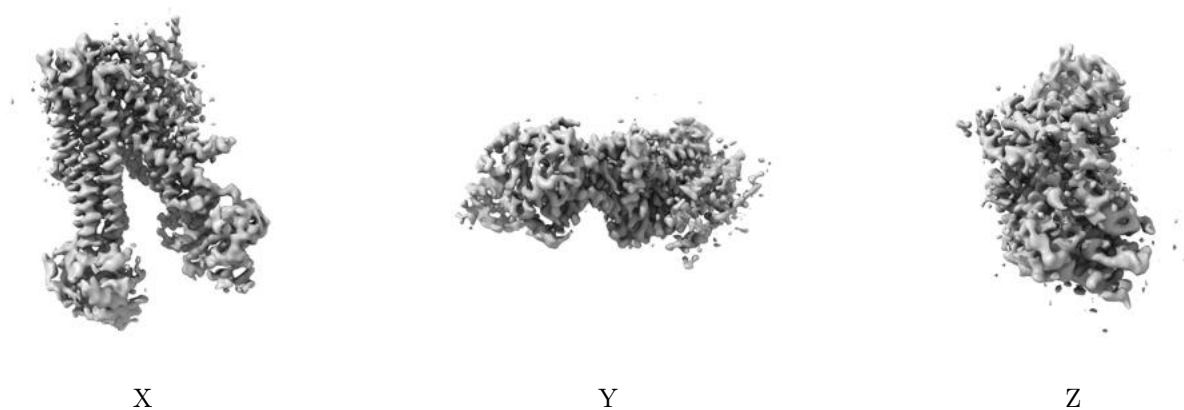


Z

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.

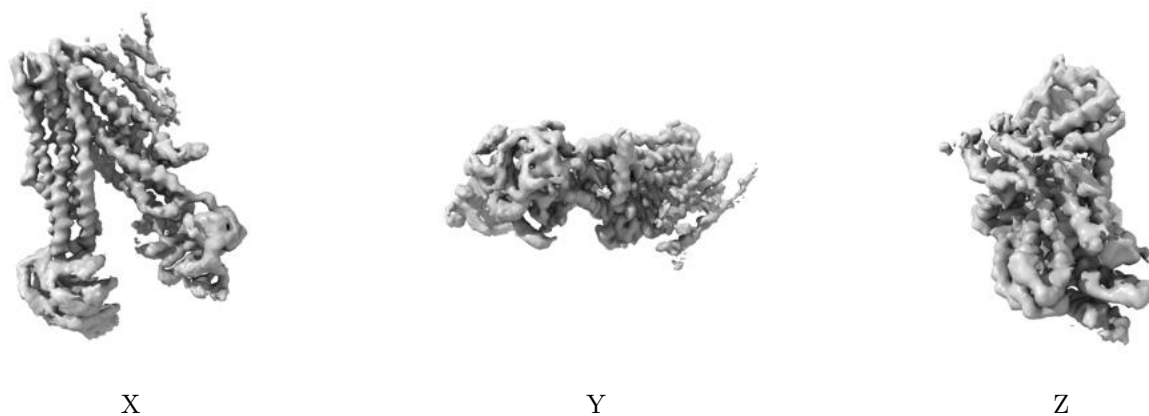
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.447. 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.

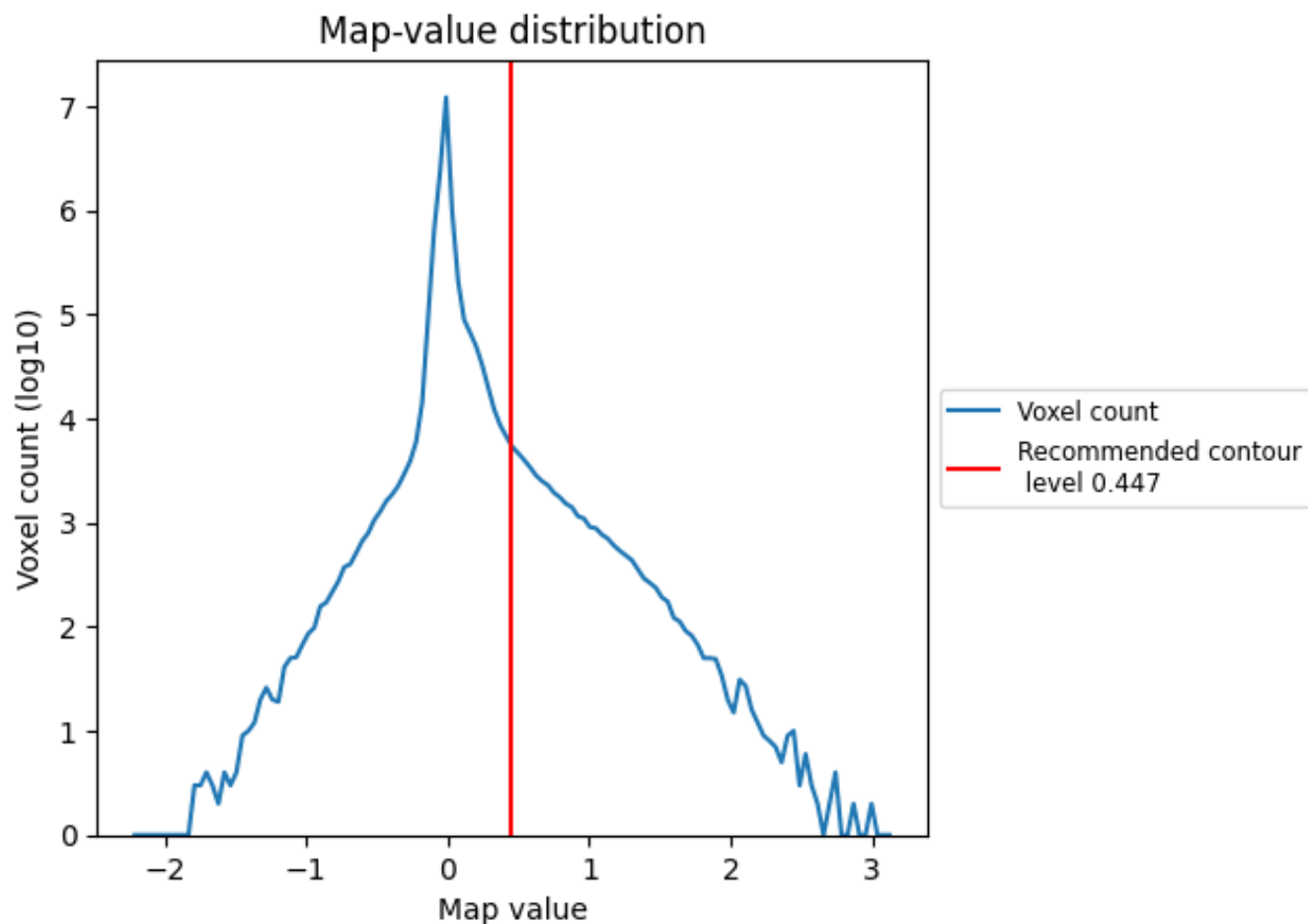
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

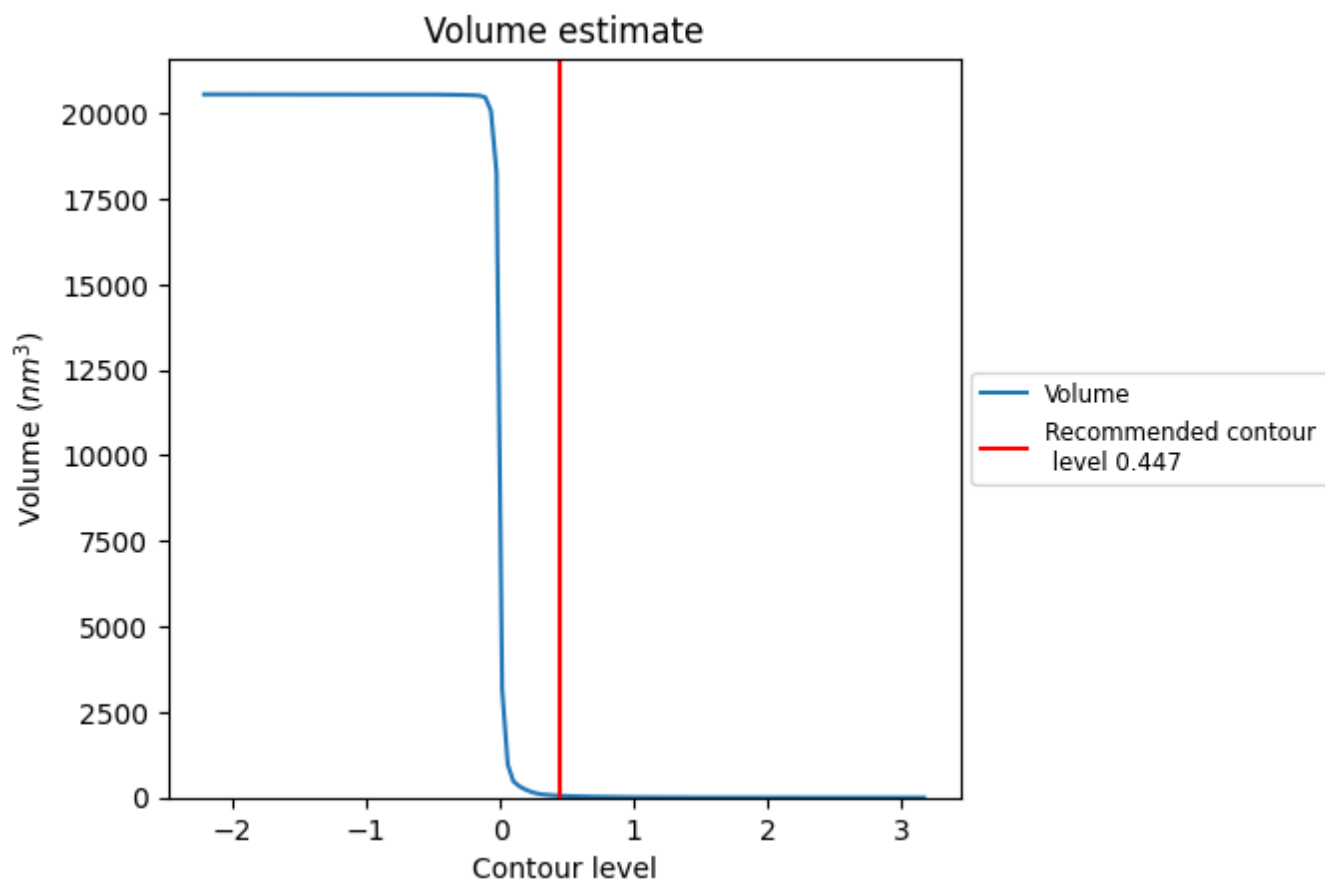
This section contains the results of statistical analysis of the map.

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.

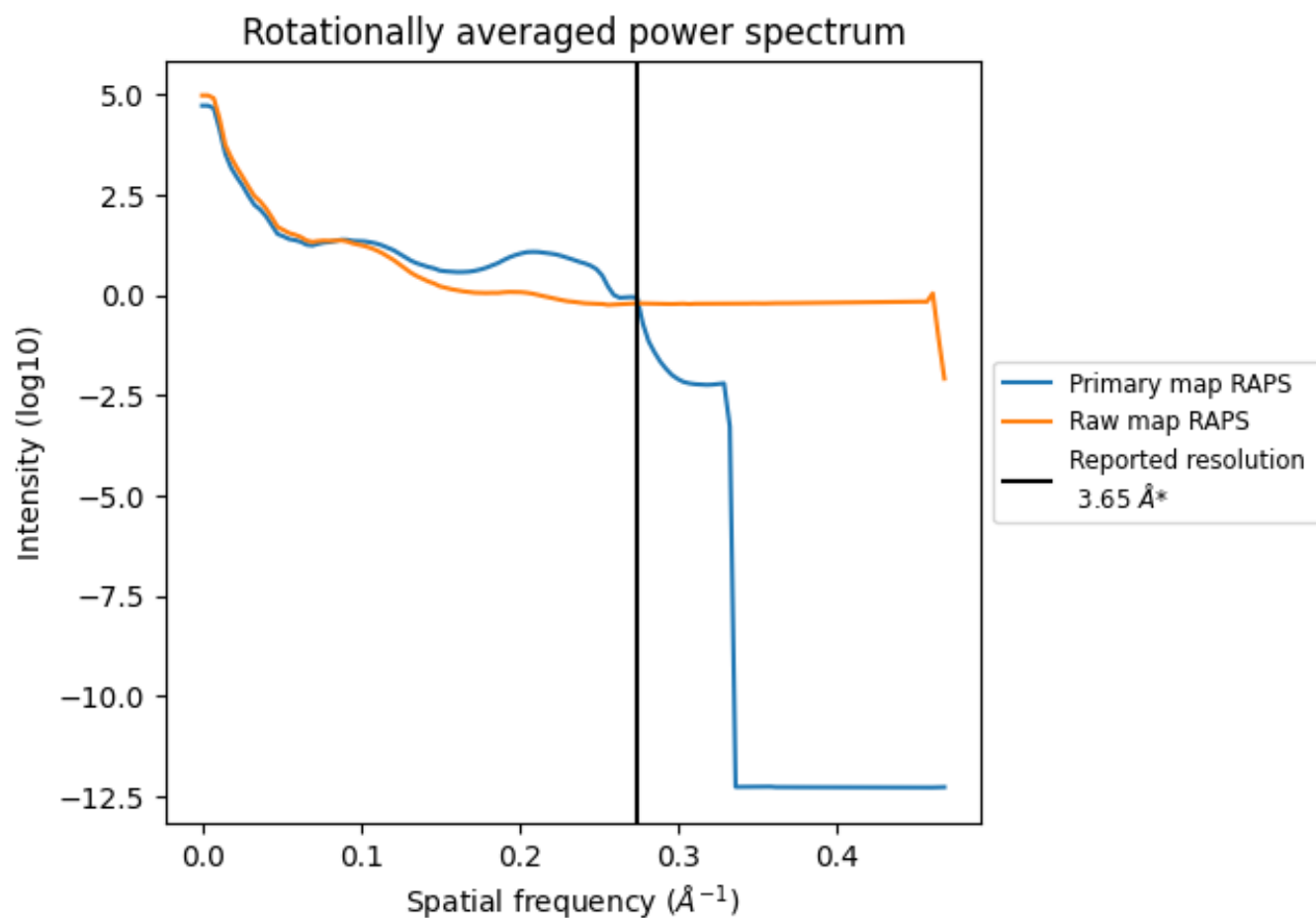
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 52 nm³; this corresponds to an approximate mass of 47 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 ⓘ

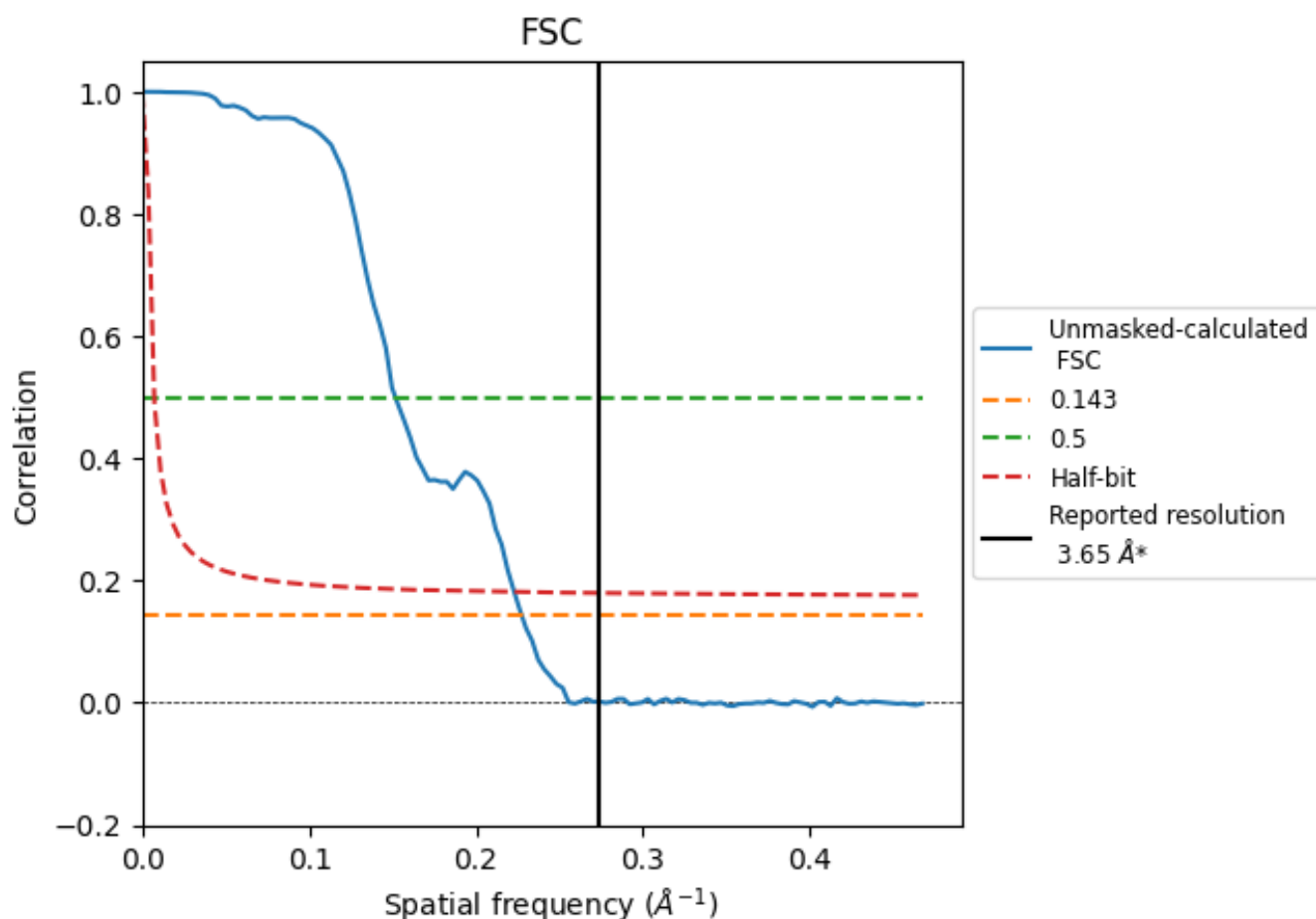


*Reported resolution corresponds to spatial frequency of 0.274 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.274 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

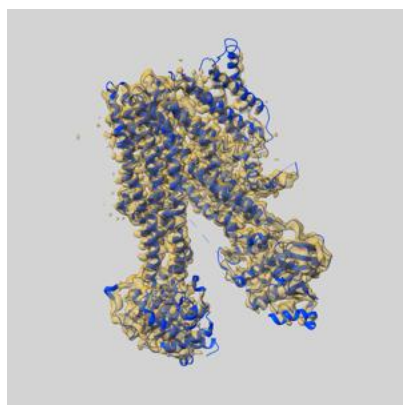
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.65	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.40	6.59	4.49

*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 4.40 differs from the reported value 3.65 by more than 10 %

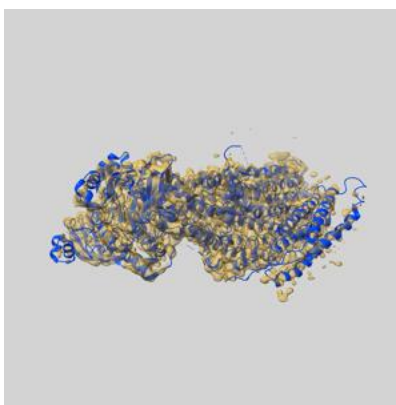
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-35049 and PDB model 8HW2. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

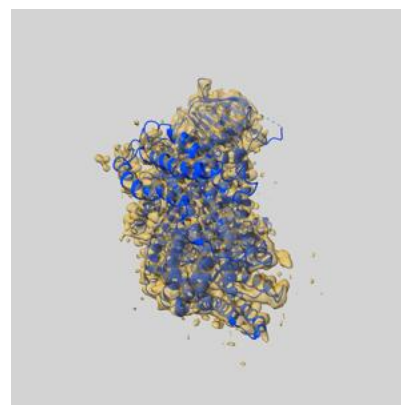
9.1 Map-model overlay [i](#)



X



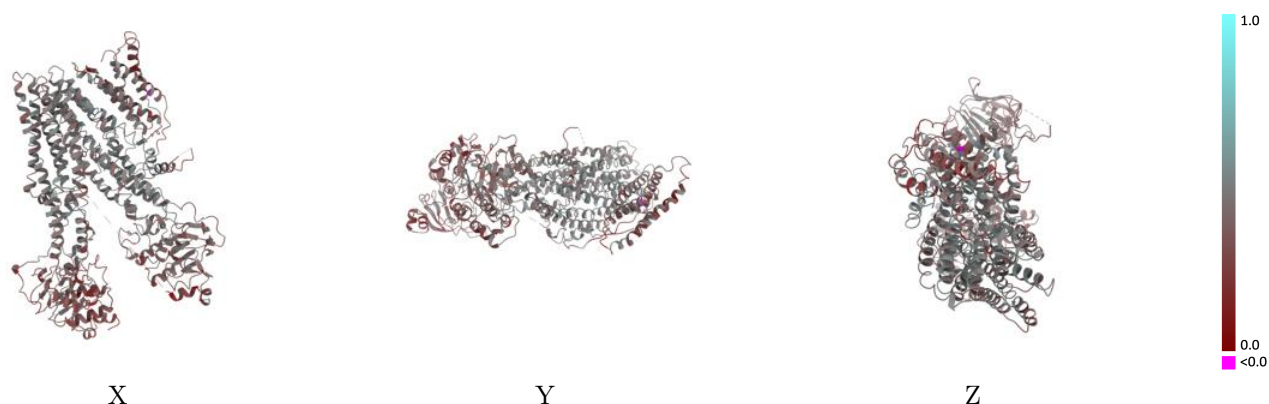
Y



Z

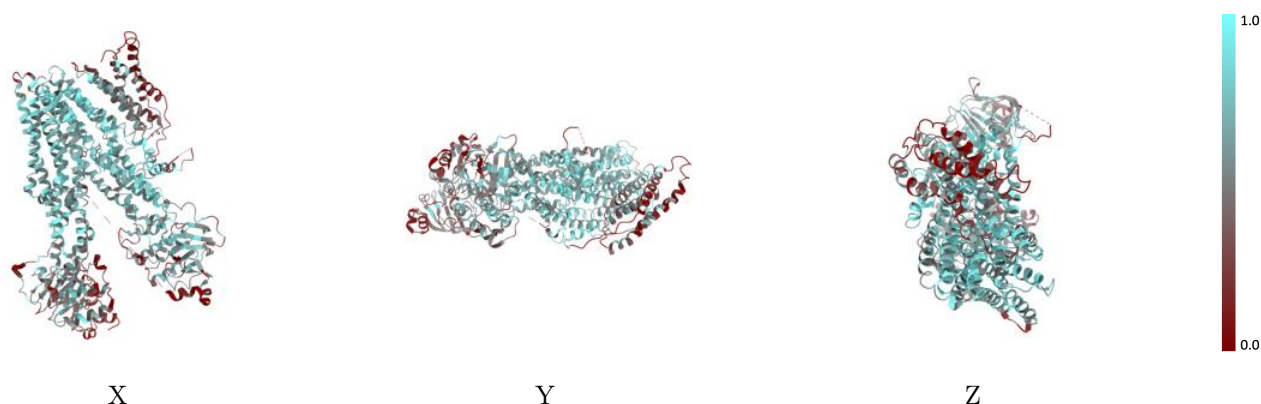
The images above show the 3D surface view of the map at the recommended contour level 0.447 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



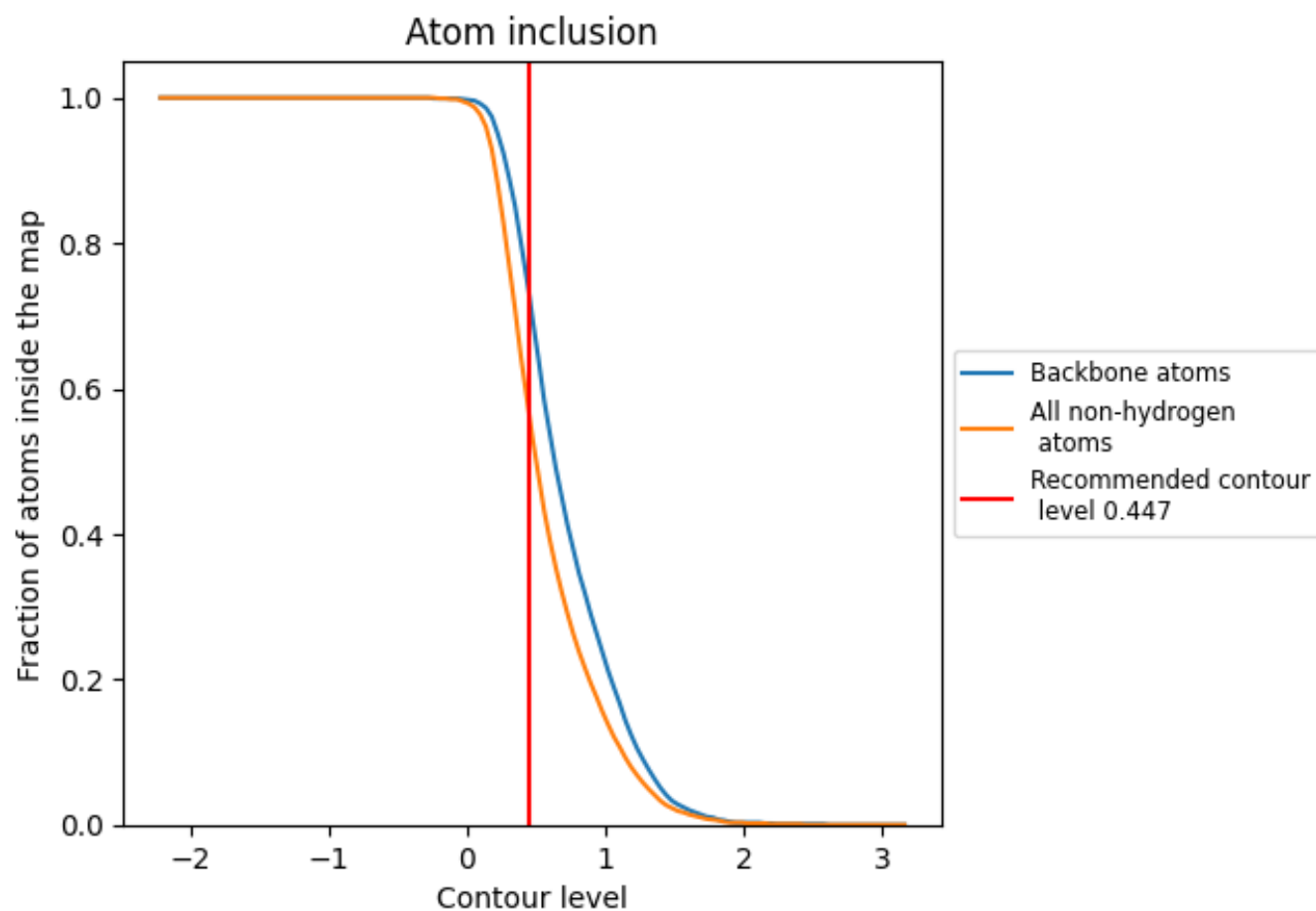
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.447).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 57% 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 (0.447) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5690	0.4040
A	0.5690	0.4040

