



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 05:21 PM UTC

PDB ID : 7OTG / pdb_00007otg
EMDB ID : EMD-13059
Title : Structure of ABCB1/P-glycoprotein in the presence of the CFTR potentiator ivacaftor
Authors : Ford, R.C.; Barbieri, A.; Thonghin, N.; Shafi, T.; Prince, S.M.; Collins, R.F.
Deposited on : 2021-06-10
Resolution : 5.40 Å(reported)

This is a Full wwPDB EM Validation 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

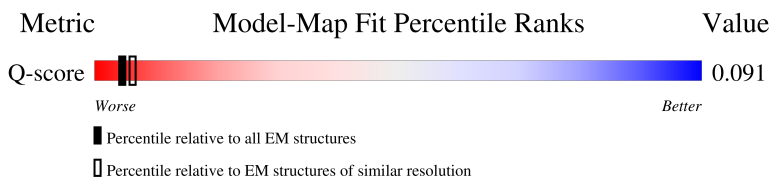
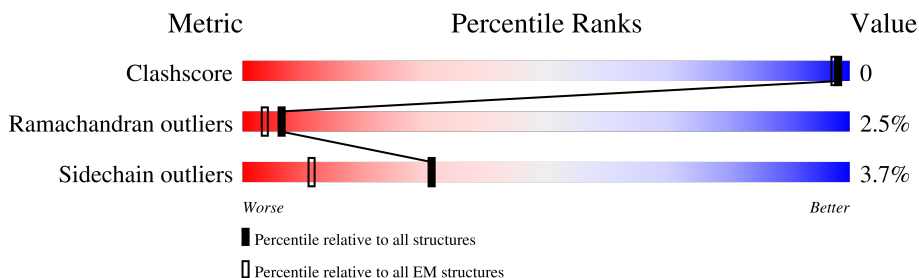
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.40 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	538 (4.90 - 5.90)

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	1284	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 9175 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.

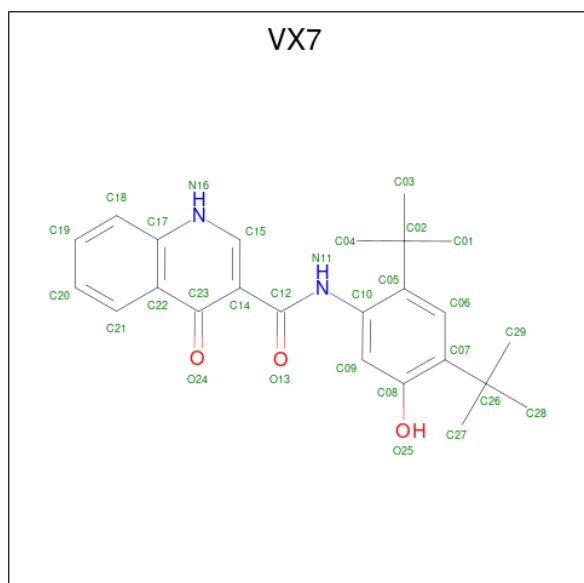
- Molecule 1 is a protein called Multidrug resistance protein 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1179	9146	5880	1549	1679	38	0	0

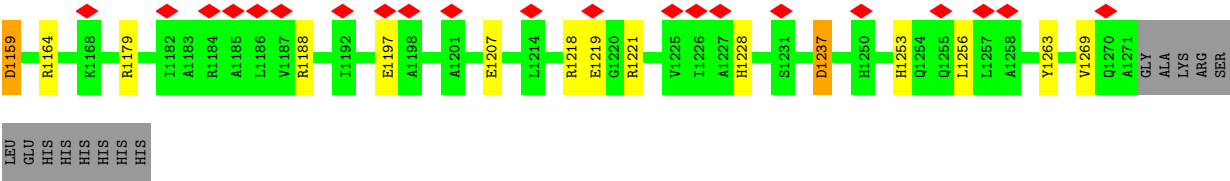
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1277	LEU	-	expression tag	UNP P21447
A	1278	GLU	-	expression tag	UNP P21447
A	1279	HIS	-	expression tag	UNP P21447
A	1280	HIS	-	expression tag	UNP P21447
A	1281	HIS	-	expression tag	UNP P21447
A	1282	HIS	-	expression tag	UNP P21447
A	1283	HIS	-	expression tag	UNP P21447
A	1284	HIS	-	expression tag	UNP P21447

- Molecule 2 is N-(2,4-di-tert-butyl-5-hydroxyphenyl)-4-oxo-1,4-dihydroquinoline-3-carboxamide (CCD ID: VX7) (formula: C₂₄H₂₈N₂O₃).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			29	24	2	3	



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	104000	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 ($e^-/\text{\AA}^2$)	64	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	4.332	Depositor
Minimum map value	-2.085	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.191	Depositor
Recommended contour level	0.67	Depositor
Map size ($\text{\AA}$)	229.45999, 229.45999, 229.45999	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.043, 1.043, 1.043	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: VX7

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	0.84	0/9314	1.43	30/12592 (0.2%)

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	18

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	592	ASP	CA-CB-CG	8.16	120.76	112.60
1	A	551	ASP	CA-CB-CG	8.11	120.71	112.60
1	A	724	PHE	CA-CB-CG	6.77	120.57	113.80
1	A	1093	ASP	CA-CB-CG	6.69	119.29	112.60
1	A	372	ASP	CA-CB-CG	6.62	119.22	112.60
1	A	374	PHE	CA-CB-CG	6.61	120.41	113.80
1	A	362	PHE	CA-CB-CG	6.16	119.96	113.80
1	A	39	PHE	CA-CB-CG	6.08	119.88	113.80
1	A	689	PRO	N-CA-C	5.79	117.76	110.70
1	A	1237	ASP	CA-CB-CG	5.68	118.28	112.60
1	A	740	PRO	N-CA-C	5.66	117.60	110.70
1	A	113	TYR	CA-CB-CG	5.60	123.98	113.90
1	A	367	ASN	CA-CB-CG	5.48	118.08	112.60
1	A	870	VAL	CA-C-N	5.45	127.84	120.38
1	A	870	VAL	C-N-CA	5.45	127.84	120.38
1	A	383	ASN	CA-C-N	5.38	131.65	121.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	383	ASN	C-N-CA	5.38	131.65	121.97
1	A	955	PHE	CA-CB-CG	5.37	119.17	113.80
1	A	801	ASP	CA-CB-CG	5.35	117.95	112.60
1	A	1228	HIS	CB-CG-CD2	-5.30	124.31	131.20
1	A	544	ASN	CB-CA-C	5.29	115.68	110.71
1	A	183	GLY	CA-C-N	5.27	127.60	120.38
1	A	183	GLY	C-N-CA	5.27	127.60	120.38
1	A	325	GLY	CA-C-N	5.24	127.56	120.38
1	A	325	GLY	C-N-CA	5.24	127.56	120.38
1	A	1134	ARG	CD-NE-CZ	5.24	131.73	124.40
1	A	310	PHE	CA-CB-CG	5.20	119.00	113.80
1	A	773	PHE	CA-CB-CG	5.09	118.89	113.80
1	A	159	PHE	CA-CB-CG	5.07	118.87	113.80
1	A	1253	HIS	CB-CG-CD2	-5.04	124.64	131.20

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1017	TYR	Sidechain
1	A	1082	PHE	Peptide
1	A	1118	LEU	Peptide
1	A	113	TYR	Sidechain
1	A	1164	ARG	Sidechain
1	A	1179	ARG	Sidechain
1	A	1218	ARG	Sidechain
1	A	1221	ARG	Sidechain
1	A	153	ASN	Peptide
1	A	319	SER	Peptide
1	A	359	TYR	Sidechain
1	A	397	TYR	Sidechain
1	A	412	LYS	Peptide
1	A	417	GLN	Peptide
1	A	543	ARG	Sidechain
1	A	695	ARG	Sidechain
1	A	963	GLN	Peptide
1	A	993	ASP	Peptide

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	9146	0	9323	7	0
2	A	29	0	0	0	0
All	All	9175	0	9323	7	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 0.

All (7) 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:44:TRP:CG	1:A:45:LEU:H	2.25	0.54
1:A:1139:GLU:CD	1:A:1139:GLU:H	2.26	0.43
1:A:418:THR:H	1:A:592:ASP:CG	2.27	0.43
1:A:1256:LEU:HB3	1:A:1263:TYR:CD2	2.55	0.42
1:A:382:ASP:C	1:A:384:ILE:H	2.28	0.41
1:A:316:LEU:HD12	1:A:320:LYS:HE2	2.02	0.41
1:A:1028:GLU:CD	1:A:1028:GLU:H	2.29	0.41

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	1175/1284 (92%)	1043 (89%)	103 (9%)	29 (2%)	4 25

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	324	ILE
1	A	384	ILE
1	A	601	VAL
1	A	319	SER
1	A	356	GLY
1	A	385	GLN
1	A	525	ALA
1	A	1269	VAL
1	A	1197	GLU
1	A	523	ARG
1	A	694	TRP
1	A	742	GLU
1	A	1067	SER
1	A	1159	ASP
1	A	1219	GLU
1	A	93	GLU
1	A	318	ILE
1	A	383	ASN
1	A	574	GLU
1	A	577	THR
1	A	799	TRP
1	A	838	ASN
1	A	964	LEU
1	A	1093	ASP
1	A	207	GLY
1	A	958	TYR
1	A	1149	ASN
1	A	1046	ILE
1	A	408	GLY

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	973/1065 (91%)	937 (96%)	36 (4%)	30	51

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ASP
1	A	96	LYS
1	A	131	PHE
1	A	146	LYS
1	A	166	GLU
1	A	176	SER
1	A	275	ASN
1	A	320	LYS
1	A	321	GLU
1	A	360	GLU
1	A	372	ASP
1	A	380	LYS
1	A	444	ASP
1	A	452	GLN
1	A	509	ILE
1	A	551	ASP
1	A	579	ILE
1	A	592	ASP
1	A	605	GLN
1	A	608	HIS
1	A	609	ASP
1	A	614	GLU
1	A	745	ARG
1	A	778	GLU
1	A	795	GLN
1	A	852	GLN
1	A	913	GLU
1	A	921	GLN
1	A	1028	GLU
1	A	1037	VAL
1	A	1106	ARG
1	A	1117	ILE
1	A	1159	ASP
1	A	1188	ARG
1	A	1207	GLU
1	A	1237	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
1	A	385	GLN
1	A	452	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	744	GLN
1	A	910	GLN
1	A	932	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	VX7	A	2000	-	31,31,31	1.37	5 (16%)	47,48,48	0.96	1 (2%)

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	VX7	A	2000	-	-	4/20/20/20	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2000	VX7	C15-N16	3.95	1.39	1.33
2	A	2000	VX7	C14-C23	2.62	1.50	1.44
2	A	2000	VX7	C10-C05	2.50	1.43	1.40
2	A	2000	VX7	C06-C05	2.21	1.42	1.39
2	A	2000	VX7	C06-C07	2.12	1.42	1.39

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2000	VX7	C15-C14-C23	-3.13	117.35	119.45

There are no chirality outliers.

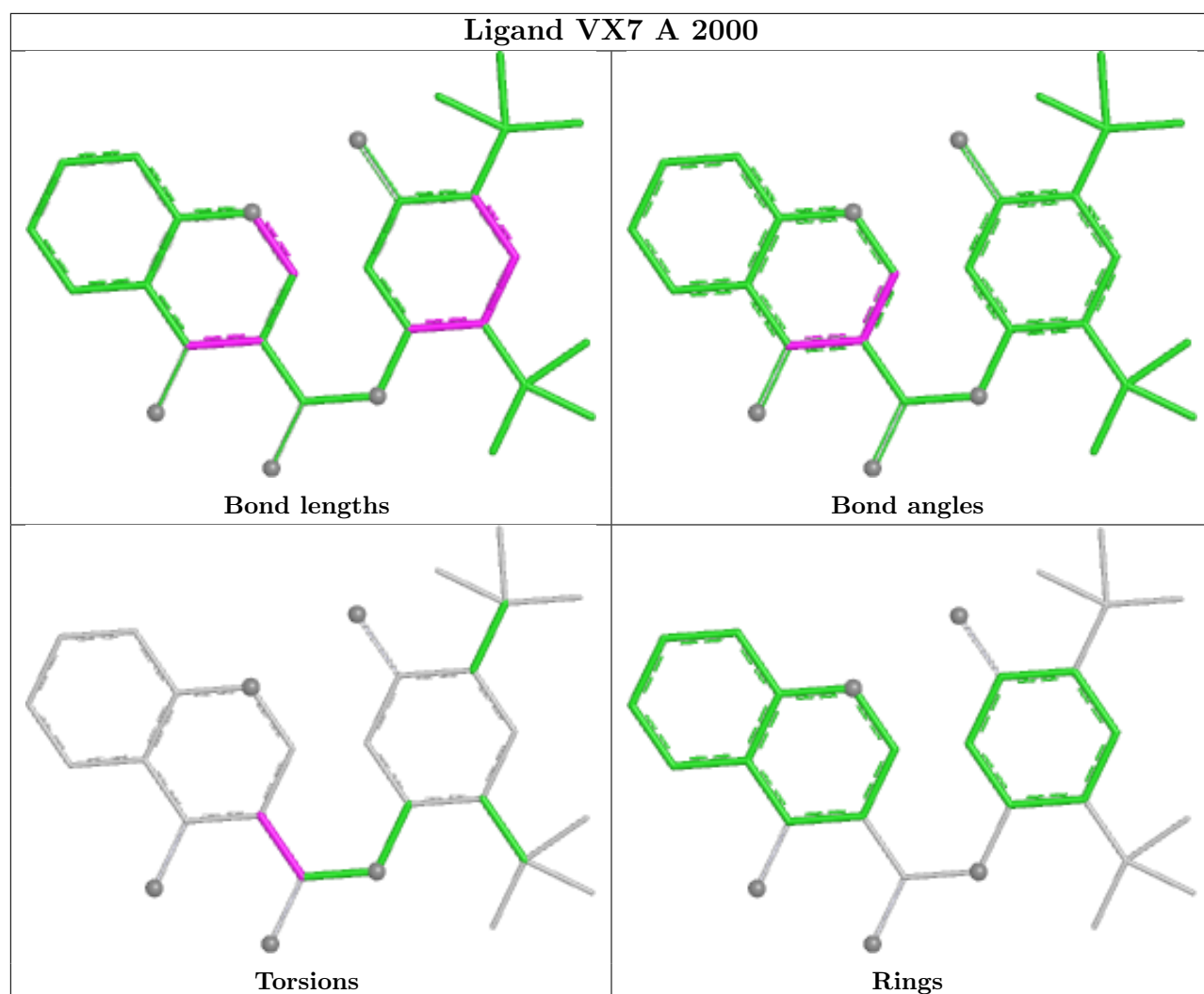
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2000	VX7	O13-C12-C14-C23
2	A	2000	VX7	N11-C12-C14-C23
2	A	2000	VX7	O13-C12-C14-C15
2	A	2000	VX7	N11-C12-C14-C15

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.

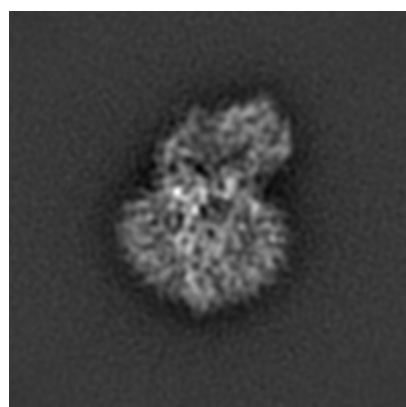
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13059. These allow visual inspection of the internal detail of the map and identification of artifacts.

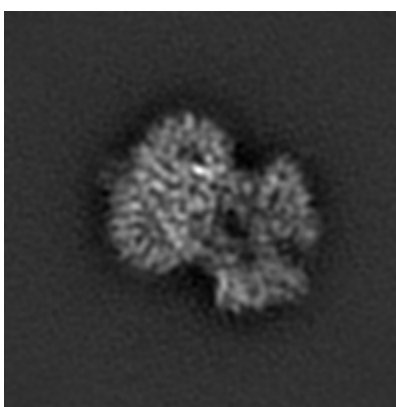
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

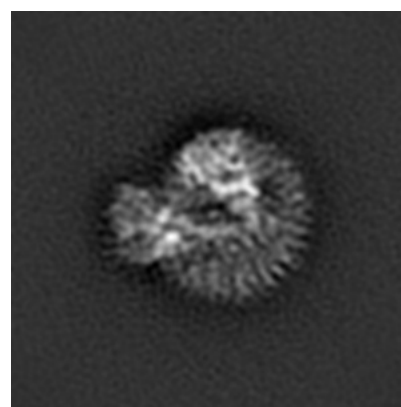
6.1.1 Primary map



X



Y

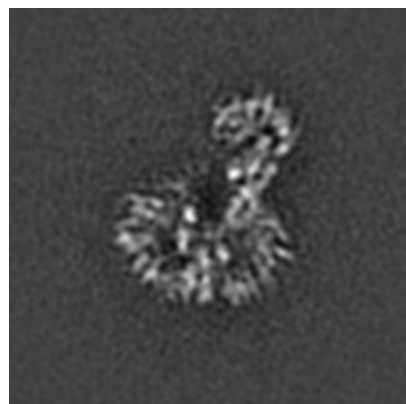


Z

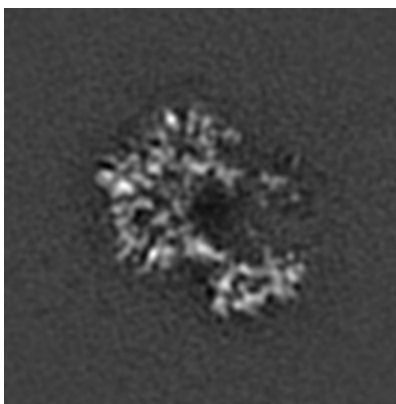
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

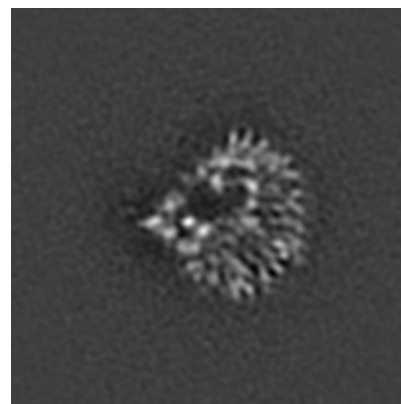
6.2.1 Primary map



X Index: 110



Y Index: 110

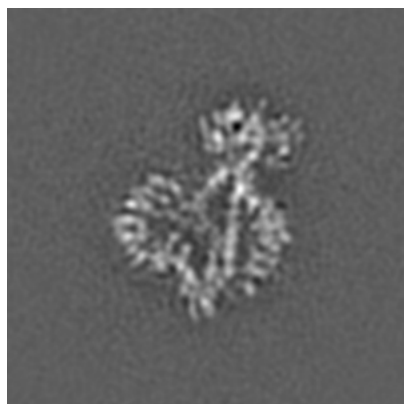


Z Index: 110

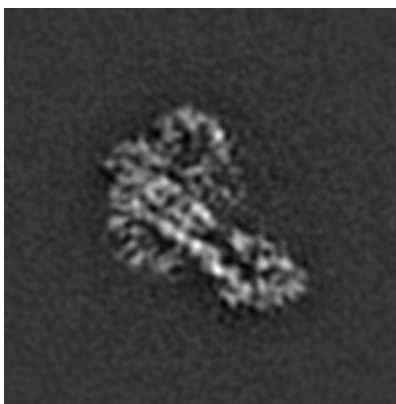
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

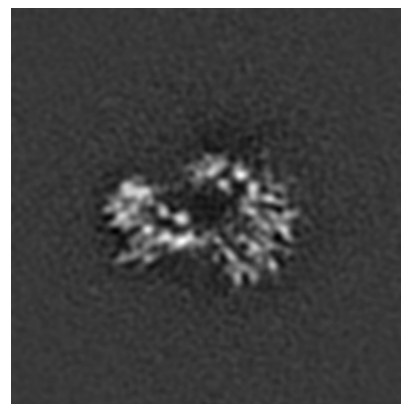
6.3.1 Primary map



X Index: 126



Y Index: 98

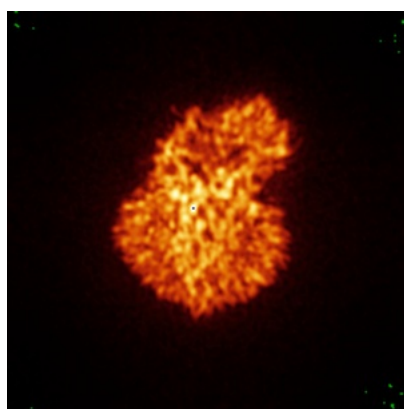


Z Index: 119

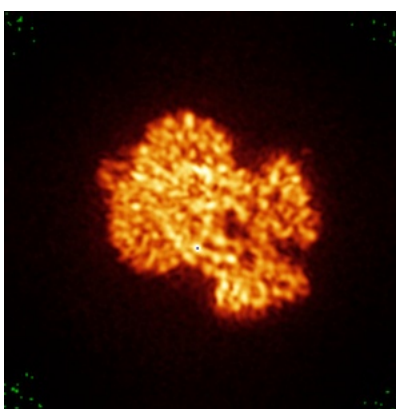
The images above show the largest variance slices of the map in three orthogonal directions.

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

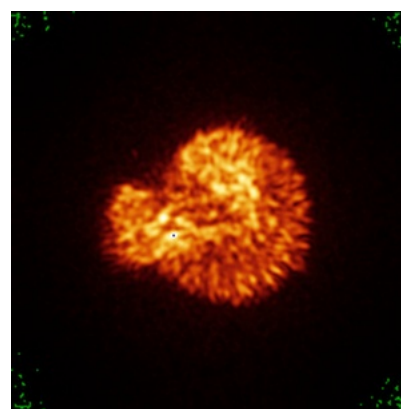
6.4.1 Primary map



X



Y

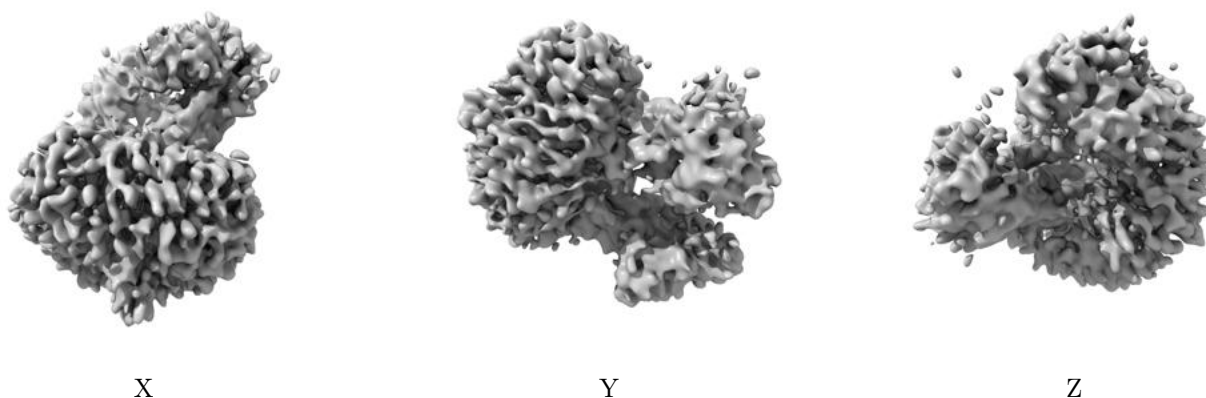


Z

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 0.67. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

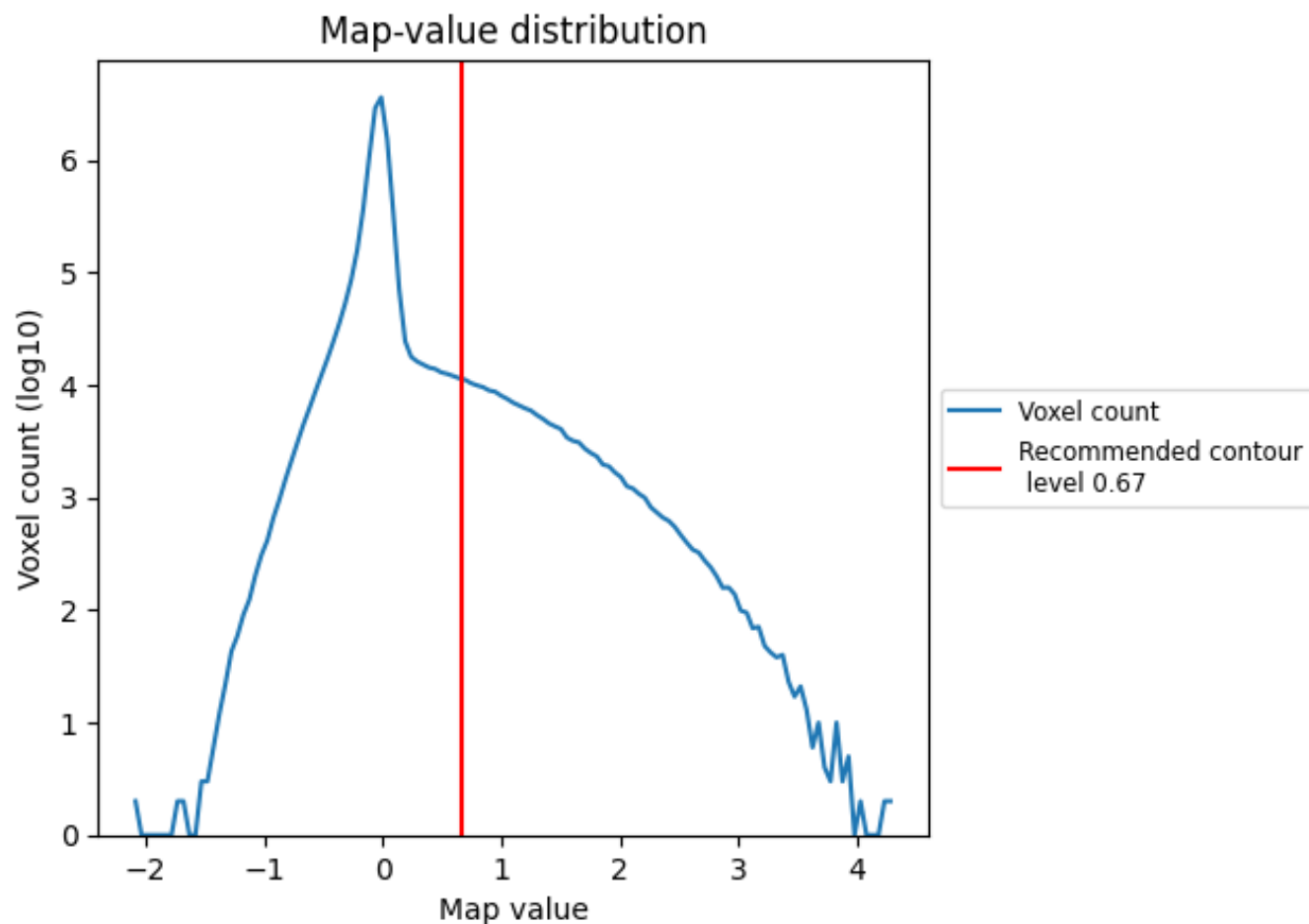
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

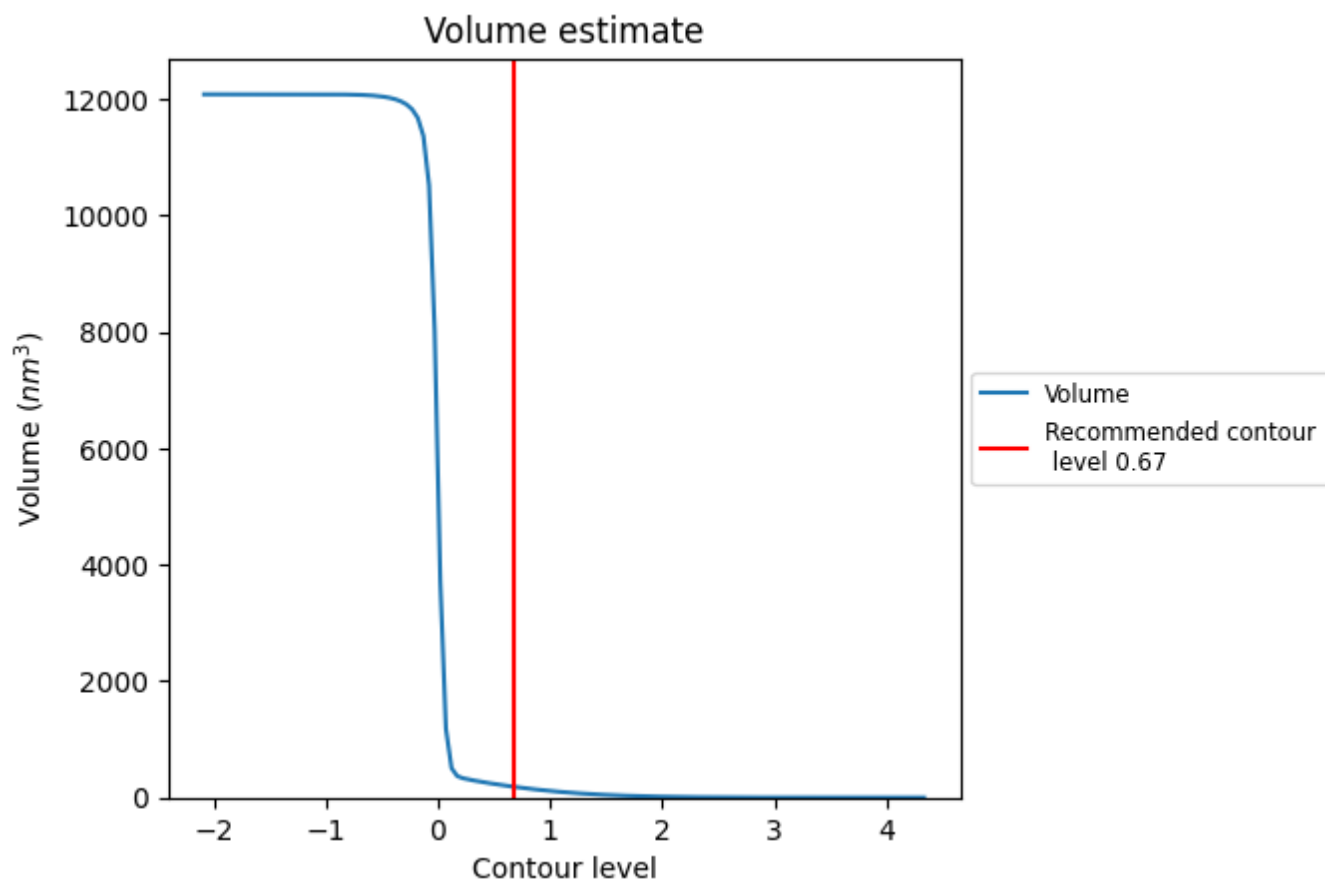
This section contains the results of statistical analysis of the map.

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.

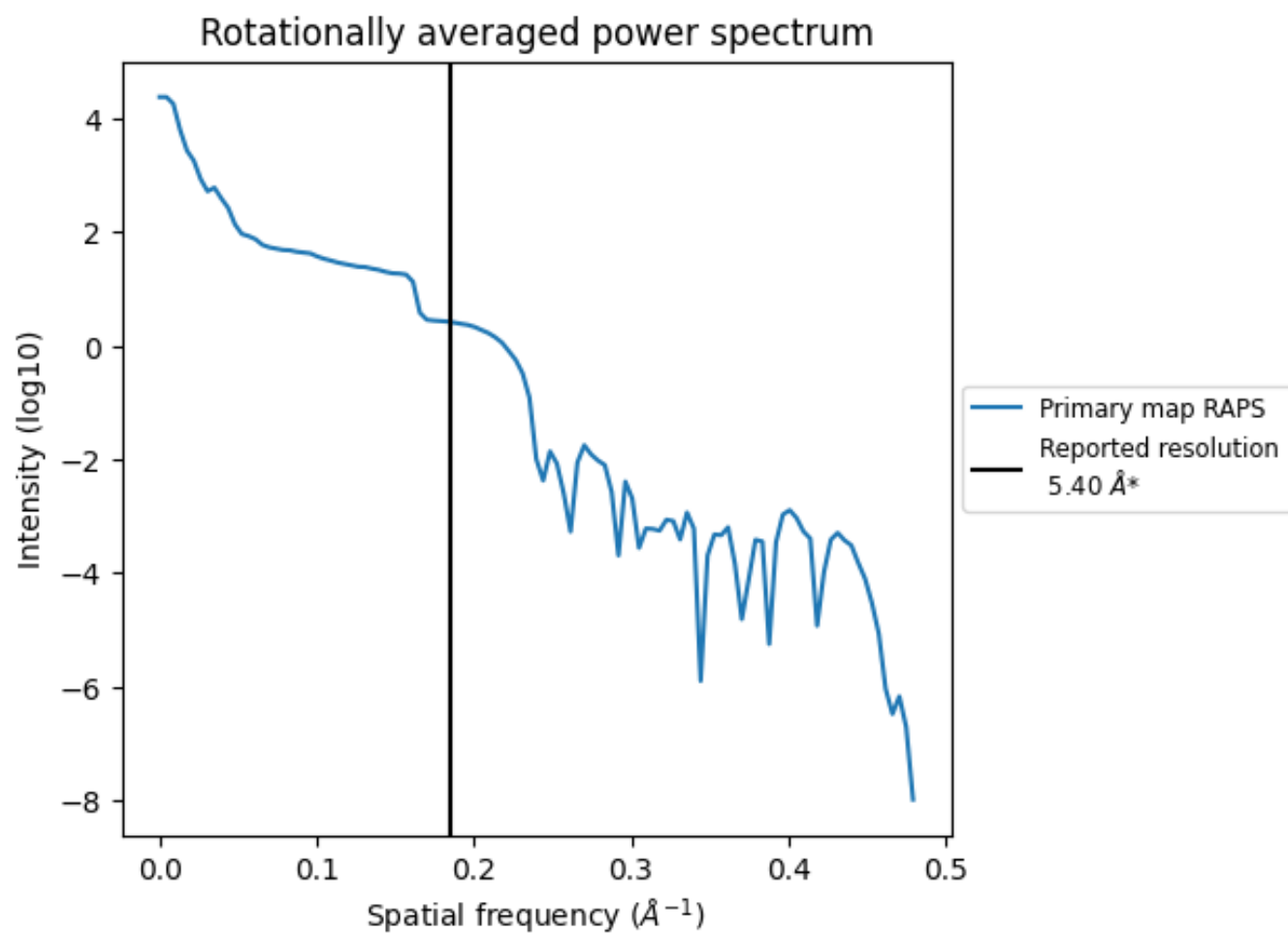
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 187 nm³; this corresponds to an approximate mass of 169 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 0.185 Å⁻¹

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

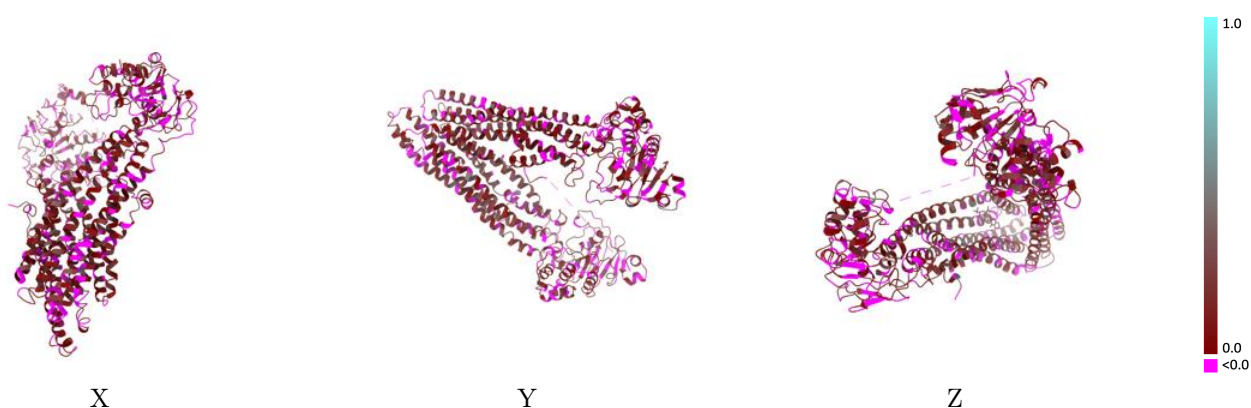
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13059 and PDB model 7OTG. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)

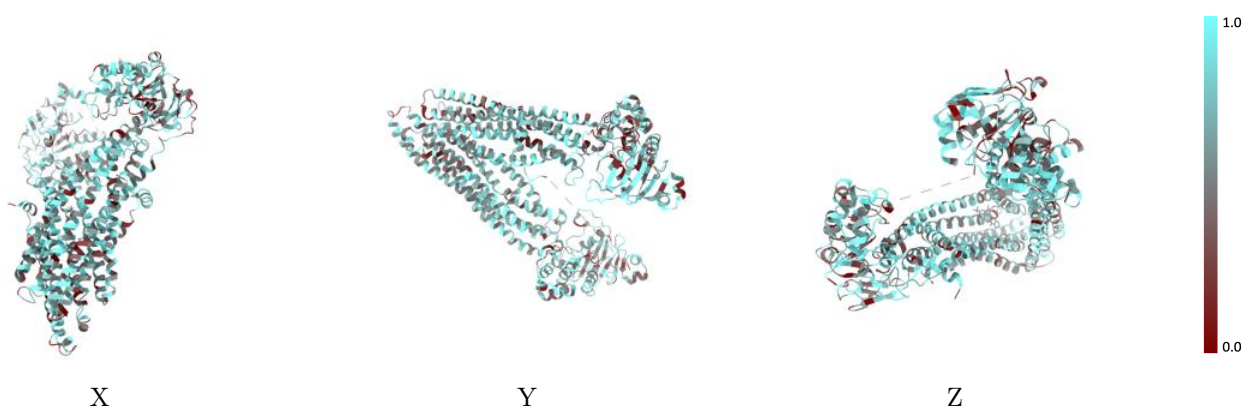
This section was not generated.

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



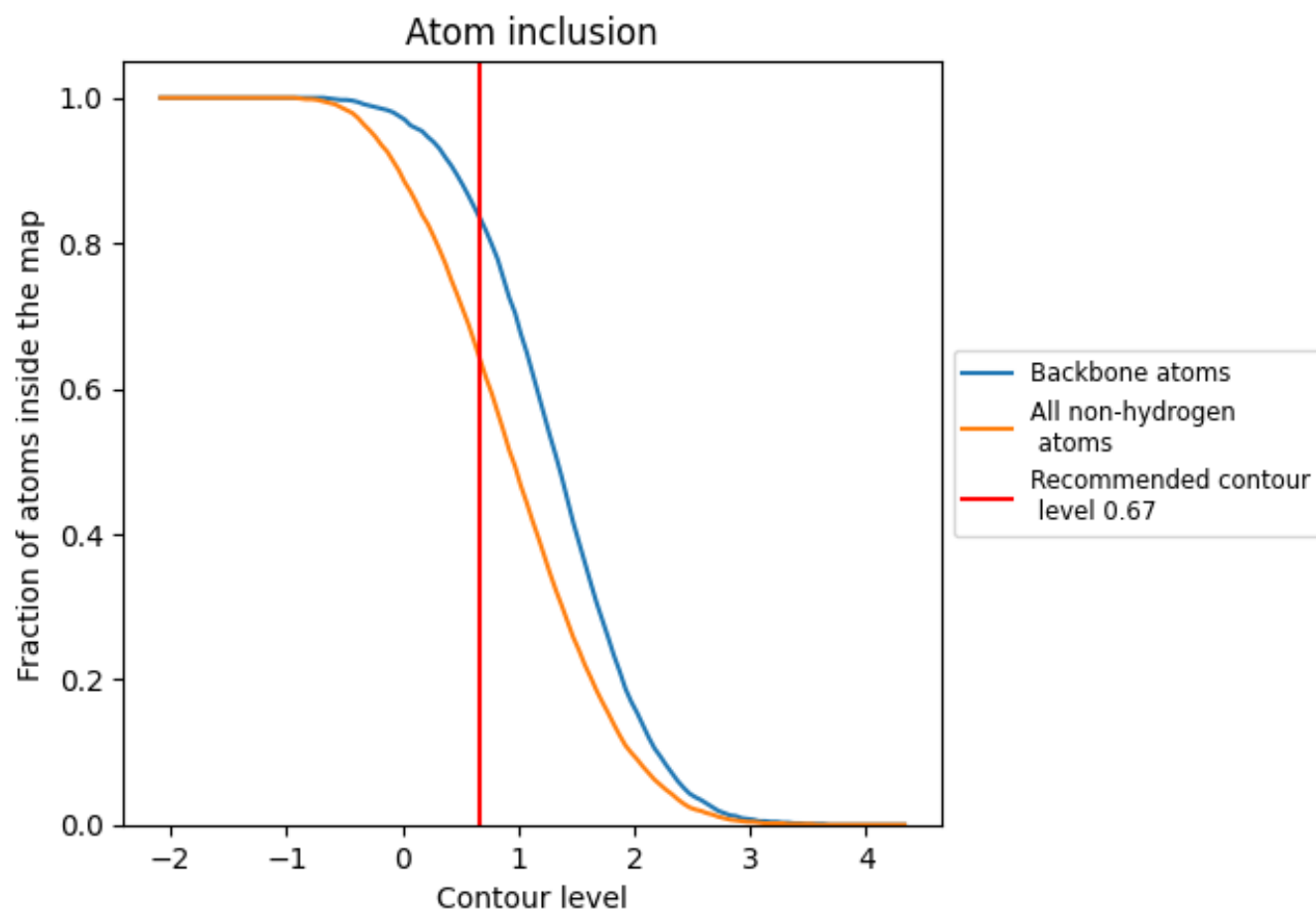
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.67).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 64% 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 (0.67) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6410	0.0910
A	0.6410	0.0910

