



wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 08:00 PM JST

PDB ID : 7CKO
EMDB ID : EMD-30389
Title : Cryo-EM structure of the human MCT1/Basigin-2 complex in the presence of anti-cancer drug candidate 7ACC2 in the inward-open conformation
Authors : Wang, N.; Jiang, X.; Zhang, S.; Zhu, A.; Yuan, Y.; Lei, J.; Yan, C.
Deposited on : 2020-07-18
Resolution : 2.95 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.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

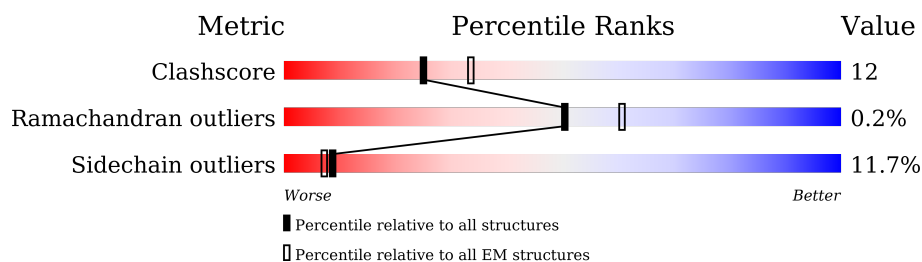
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.95 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	500	
2	B	269	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4029 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.

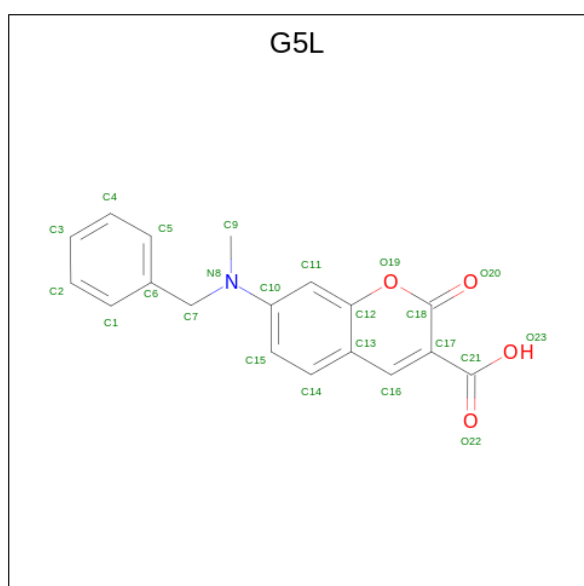
- Molecule 1 is a protein called Monocarboxylate transporter 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	375	Total	C	N	O	S	0	0
			2846	1896	452	473	25		

- Molecule 2 is a protein called Basigin.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	216	Total	C	N	O	0	0
			1160	710	228	222		

- Molecule 3 is 7-[methyl-(phenylmethyl)amino]-2-oxidanylidene-chromene-3-carboxylic acid (three-letter code: G5L) (formula: $C_{18}H_{15}NO_4$) (labeled as "Ligand of Interest" by depositor).

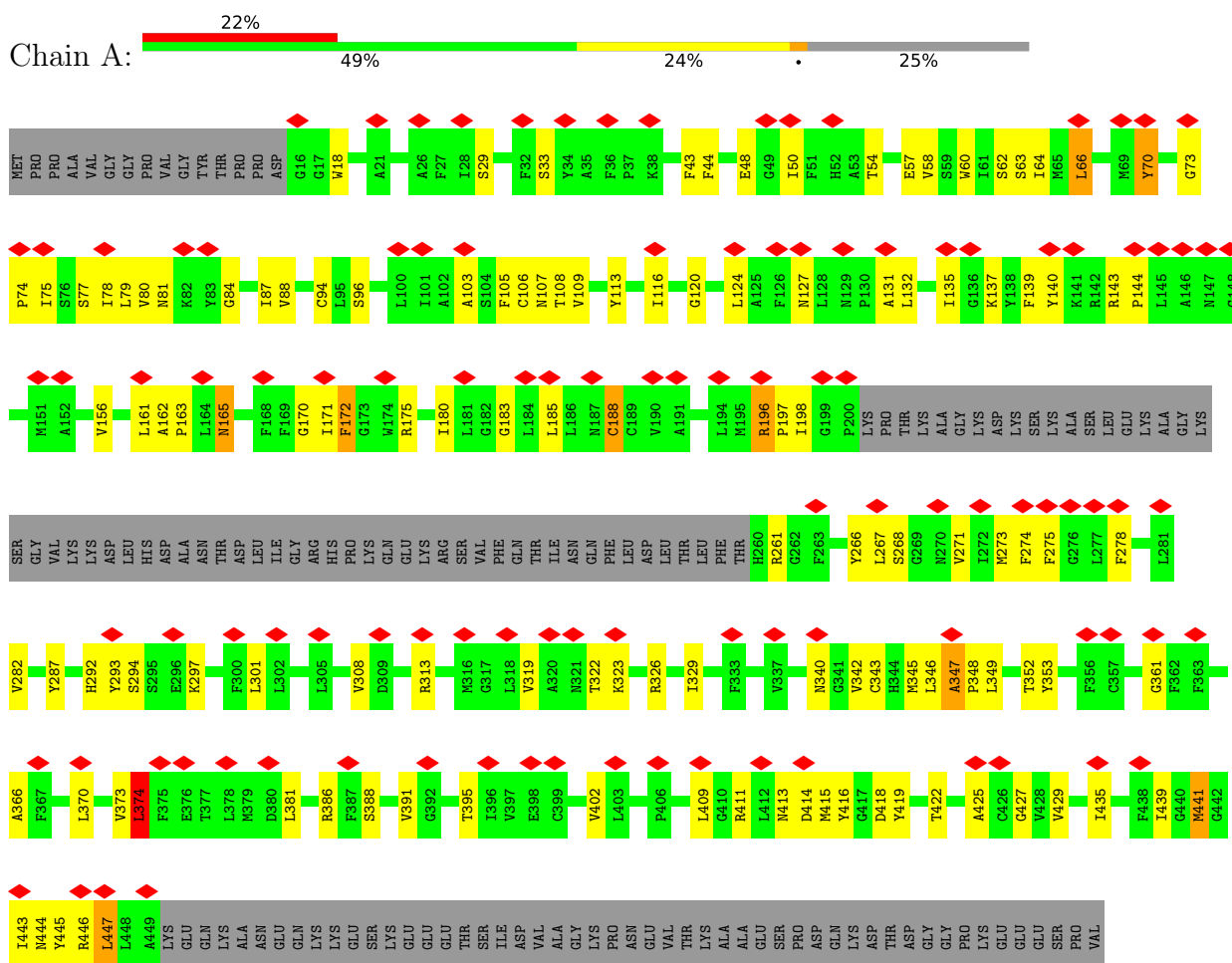


Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			23	18	1	4	

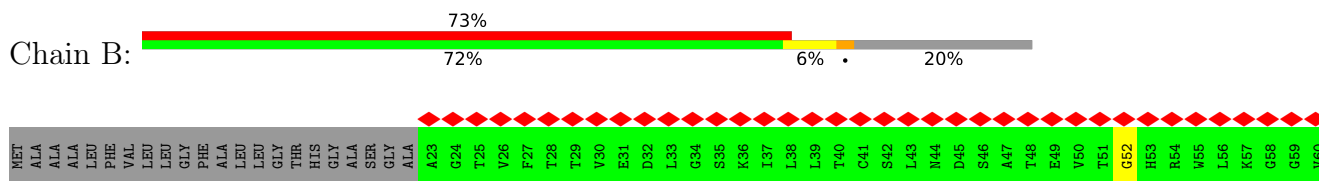
3 Residue-property plots

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: Monocarboxylate transporter 1



• Molecule 2: Basigin



ASP	G181	T121	V61
ALA	Q182	A122	L62
GLY	Y183	M123	K63
SER	ALA	L124	E64
ALA	R184	L125	D65
LEU	C185	C126	A66
LYS	M186	K127	L67
SER	G187	S128	P68
SER	T188	E129	G69
GLY	S189	S130	Q70
GLN	S190	V131	K71
HIS	K191	P132	T72
GLN	G192	P133	E73
ASN	S193	V134	F74
ASP	D194	T135	K75
LYS	Q195	D136	V76
LYS	A196	W137	V77
VAL	I197	A138	S78
ARG	I198	W139	D79
GLN	T199	Y140	D80
ARG	L200	K141	Q81
ASN	R201	I142	W82
SER	V202	T143	G83
	R203	D144	E84
	S204	S145	Y85
	H205	E146	S86
	L206	D147	C87
	A207	K148	V88
	A208	A149	F89
	L209	L150	L90
	GLY	M151	P91
	W210	M152	E92
	P211	G153	P93
	F212	S154	M94
	L213	E155	G95
	G214	S156	T96
	L215	R157	A97
	V216	F158	I99
		F159	Q100
	L220	V160	L101
	V221	S161	M102
	L222	S162	H102
	V223	S163	G103
	T224	Q164	P104
	L225	G165	P105
	T226	R166	R106
	F227	S167	V107
	L228	E168	K108
	V229	L169	A109
	E230	H170	V110
	K231	I171	K111
	R232	E172	S112
	R233	M173	S113
	K234	L174	E114
	P235	M175	H115
	E236	M176	I116
	D237	E177	M117
	V238	A178	E118
	LEU		G119
	ASP		F120
	ASP		
	ASP		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	533887	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	37.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.219	Depositor
Minimum map value	-2.767	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.070	Depositor
Recommended contour level	0.845	Depositor
Map size (\AA)	215.8848, 215.8848, 215.8848	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.8433, 0.8433, 0.8433	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: G5L

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	0.50	0/2926	0.56	3/3972 (0.1%)
2	B	0.53	0/1167	0.78	2/1617 (0.1%)
All	All	0.51	0/4093	0.63	5/5589 (0.1%)

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

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

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	91	PRO	CA-N-CD	-9.65	97.98	111.50
2	B	93	PRO	CA-N-CD	-8.89	99.06	111.50
1	A	374	LEU	CB-CG-CD1	7.16	123.17	111.00
1	A	66	LEU	CB-CG-CD1	5.87	120.97	111.00
1	A	66	LEU	CB-CG-CD2	5.59	120.50	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	347	ALA	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	2846	0	2901	77	0
2	B	1160	0	679	16	0
3	A	23	0	0	0	0
All	All	4029	0	3580	88	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 12.

The worst 5 of 88 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:196:ARG:NH2	1:A:197:PRO:O	1.96	0.98
1:A:48:GLU:HG2	1:A:58:VAL:HG21	1.45	0.97
1:A:44:PHE:O	1:A:48:GLU:HG3	1.76	0.85
1:A:329:ILE:HD11	1:A:373:VAL:HG13	1.60	0.82
1:A:266:TYR:OH	1:A:374:LEU:HD13	1.86	0.76

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	371/500 (74%)	334 (90%)	37 (10%)	0	100	100
2	B	214/269 (80%)	197 (92%)	16 (8%)	1 (0%)	29	64
All	All	585/769 (76%)	531 (91%)	53 (9%)	1 (0%)	50	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	104	PRO

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	299/405 (74%)	269 (90%)	30 (10%)	7	26
2	B	27/225 (12%)	19 (70%)	8 (30%)	0	1
All	All	326/630 (52%)	288 (88%)	38 (12%)	9	20

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	446	ARG
2	B	216	VAL
1	A	447	LEU
2	B	206	LEU
2	B	230	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	GLN
1	A	127	ASN
1	A	260	HIS
1	A	292	HIS

5.3.3 RNA ⓘ

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 monosaccharides 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$
3	G5L	A	601	-	25,25,25	3.18	9 (36%)	33,35,35	1.74	7 (21%)

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	G5L	A	601	-	-	4/12/12/12	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	G5L	O20-C18	8.91	1.40	1.21
3	A	601	G5L	C2-C1	6.69	1.53	1.38
3	A	601	G5L	C5-C6	6.50	1.52	1.38
3	A	601	G5L	C4-C3	5.55	1.52	1.38
3	A	601	G5L	C4-C5	-3.41	1.31	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	G5L	C6-C7-N8	-4.56	108.14	113.81
3	A	601	G5L	O19-C18-O20	3.15	120.38	116.22
3	A	601	G5L	C12-O19-C18	-3.00	119.32	122.23
3	A	601	G5L	C12-C13-C16	2.95	120.34	118.04
3	A	601	G5L	C13-C16-C17	-2.80	119.40	122.10

There are no chirality outliers.

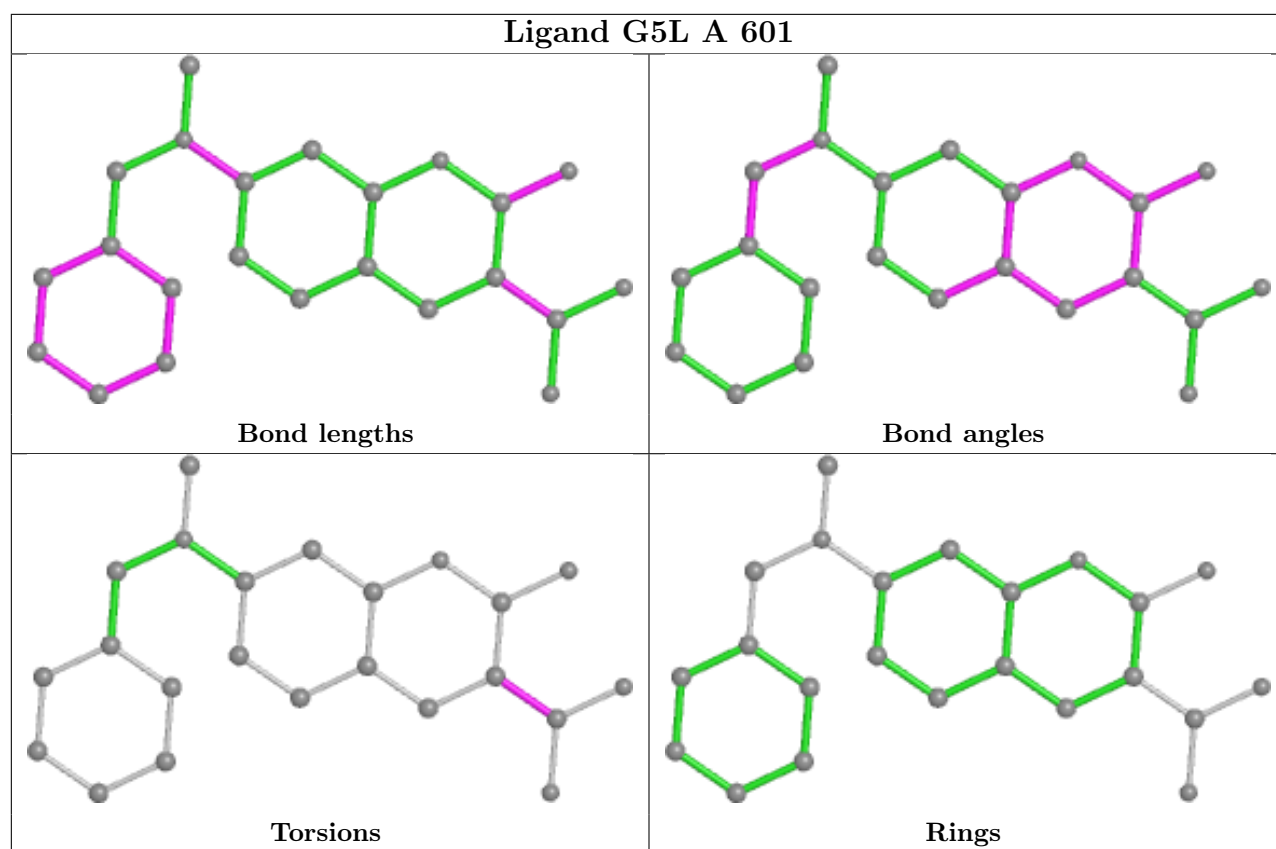
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	G5L	C18-C17-C21-O22
3	A	601	G5L	C18-C17-C21-O23
3	A	601	G5L	C16-C17-C21-O22
3	A	601	G5L	C16-C17-C21-O23

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.

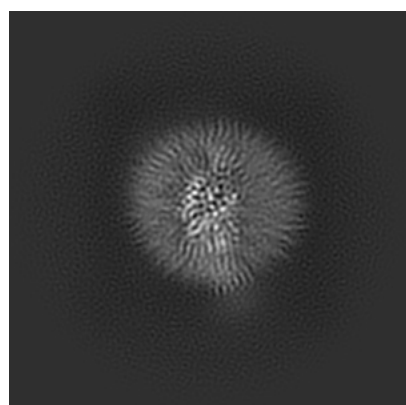
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30389. These allow visual inspection of the internal detail of the map and identification of artifacts.

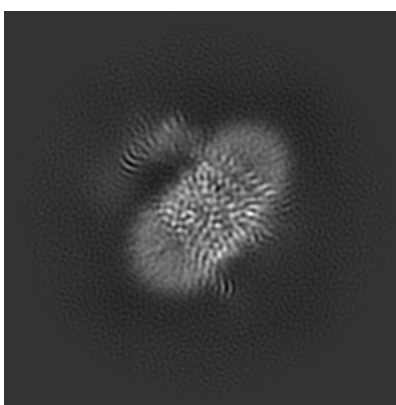
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

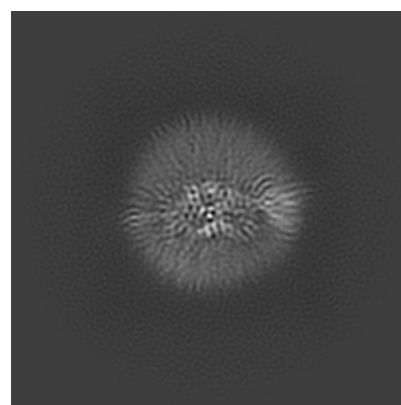
6.1.1 Primary map



X



Y

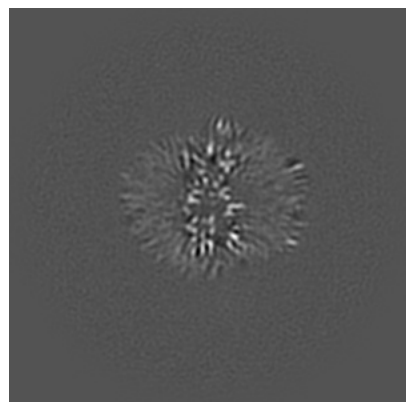


Z

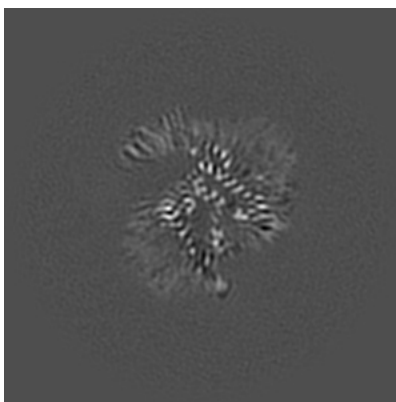
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

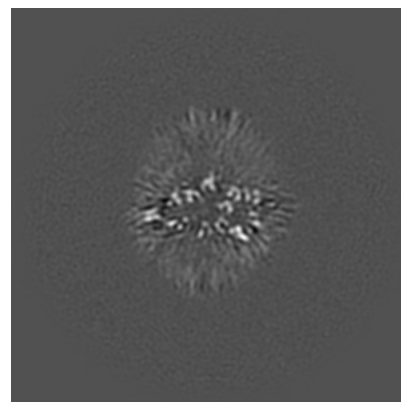
6.2.1 Primary map



X Index: 128



Y Index: 128

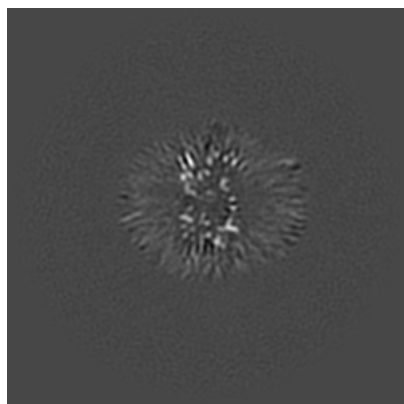


Z Index: 128

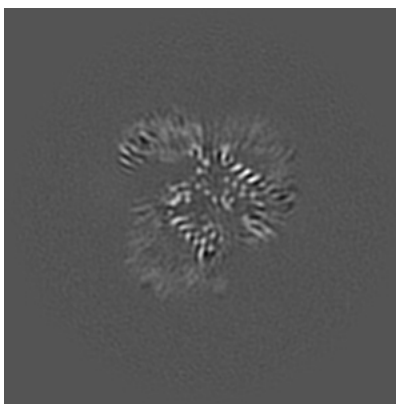
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

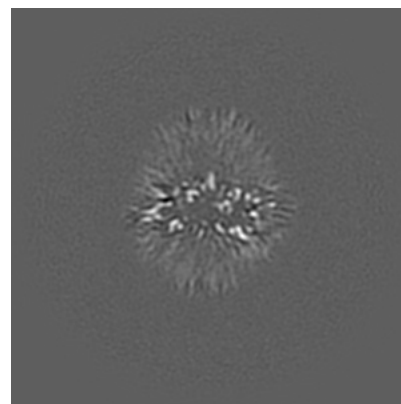
6.3.1 Primary map



X Index: 125



Y Index: 132

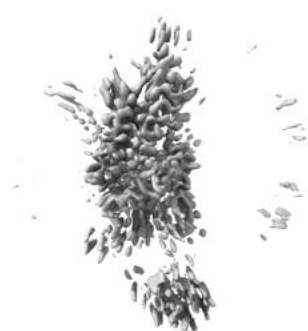


Z Index: 129

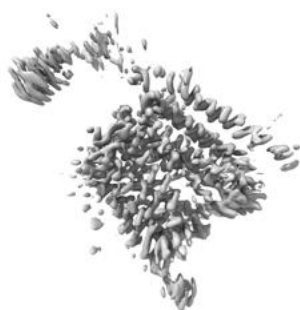
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.845. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

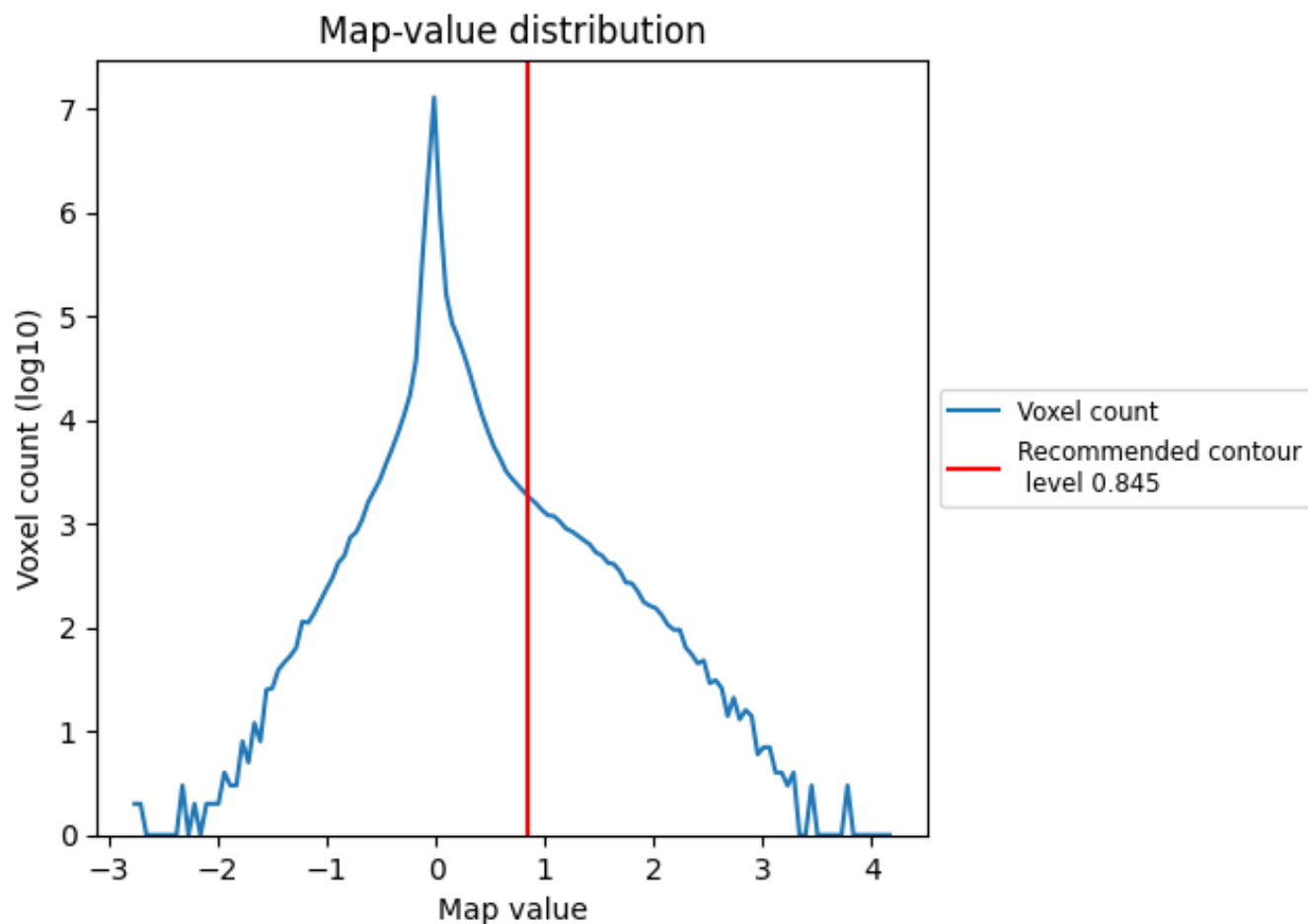
6.5 Mask visualisation

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

7 Map analysis [i](#)

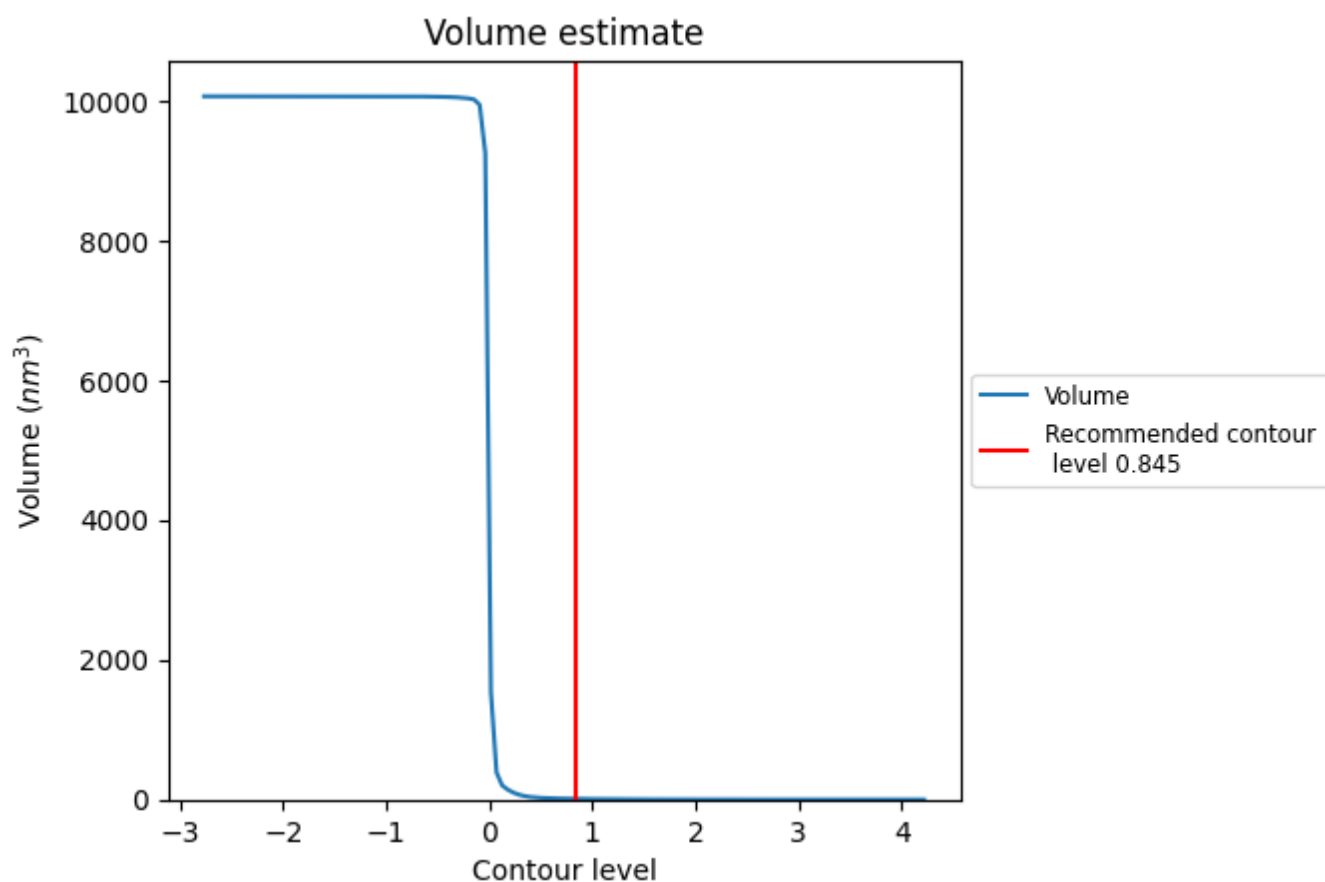
This section contains the results of statistical analysis of the map.

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.

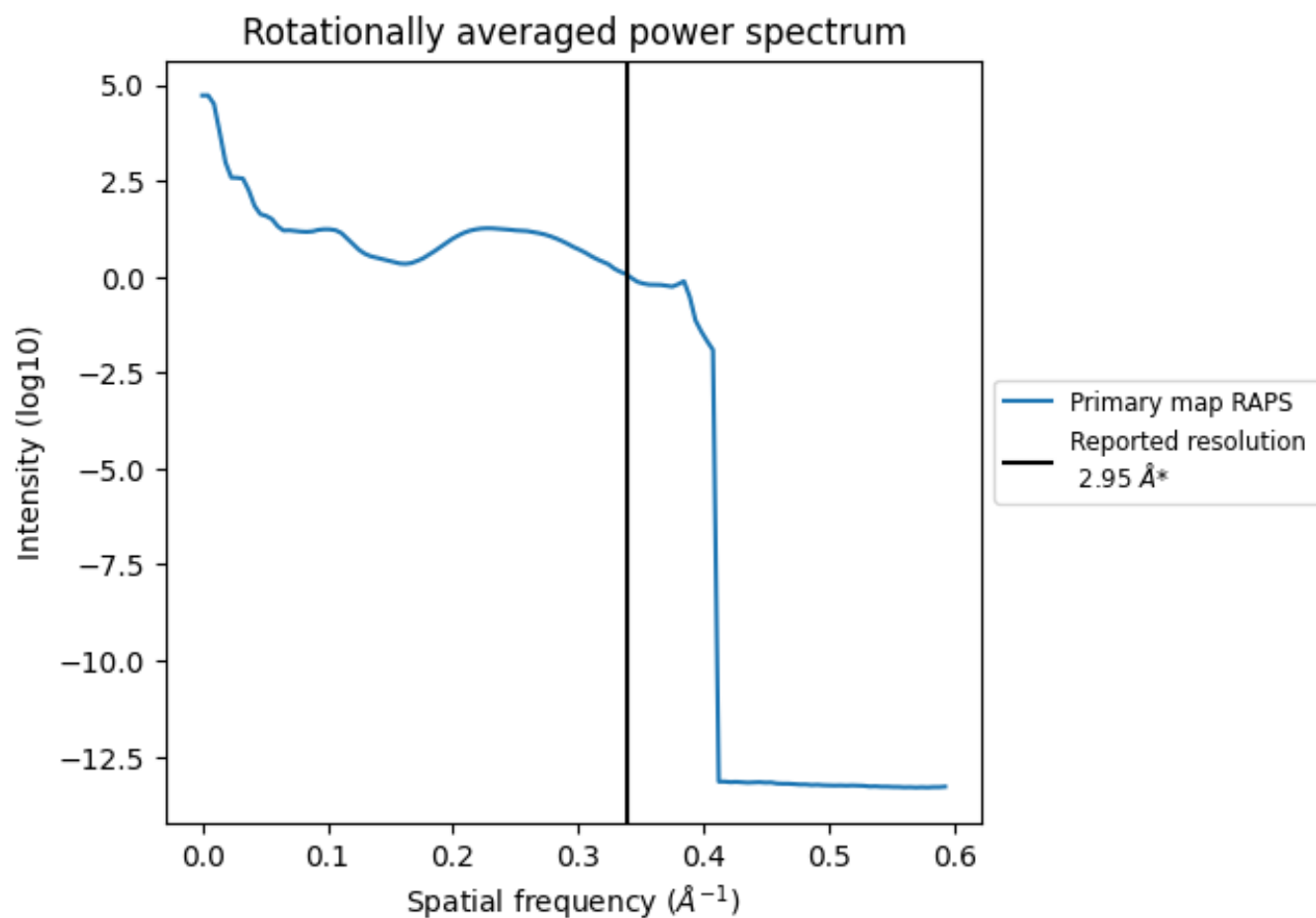
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 10 nm³; this corresponds to an approximate mass of 9 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 0.339 Å⁻¹

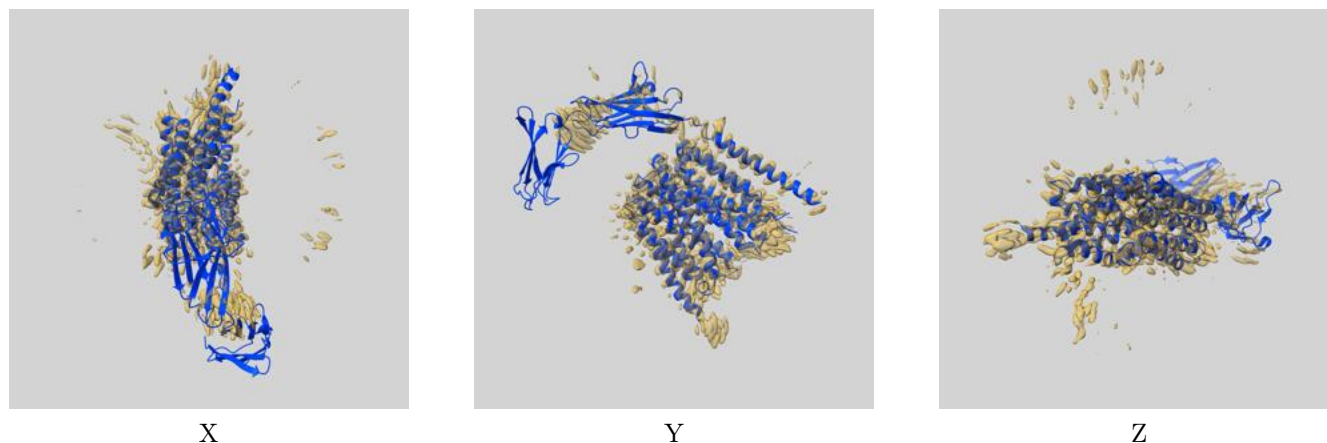
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

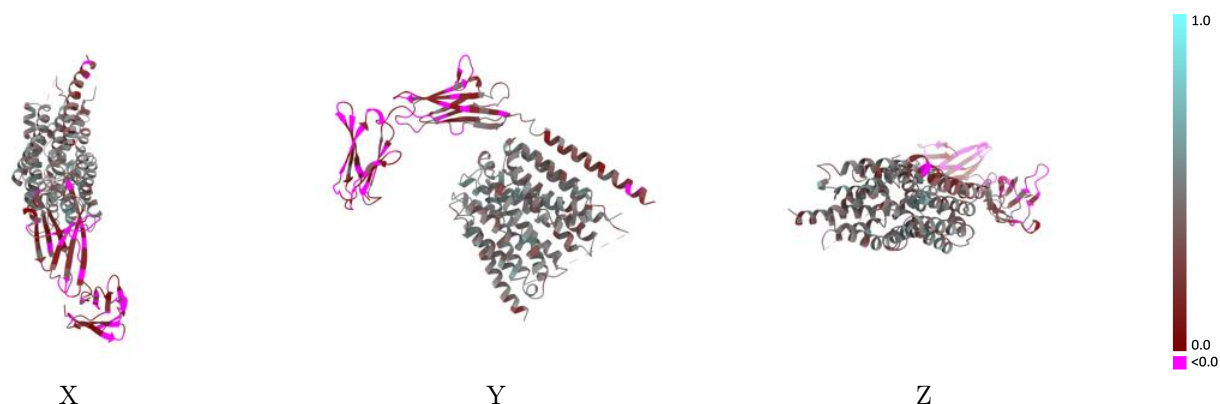
This section contains information regarding the fit between EMDB map EMD-30389 and PDB model 7CKO. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



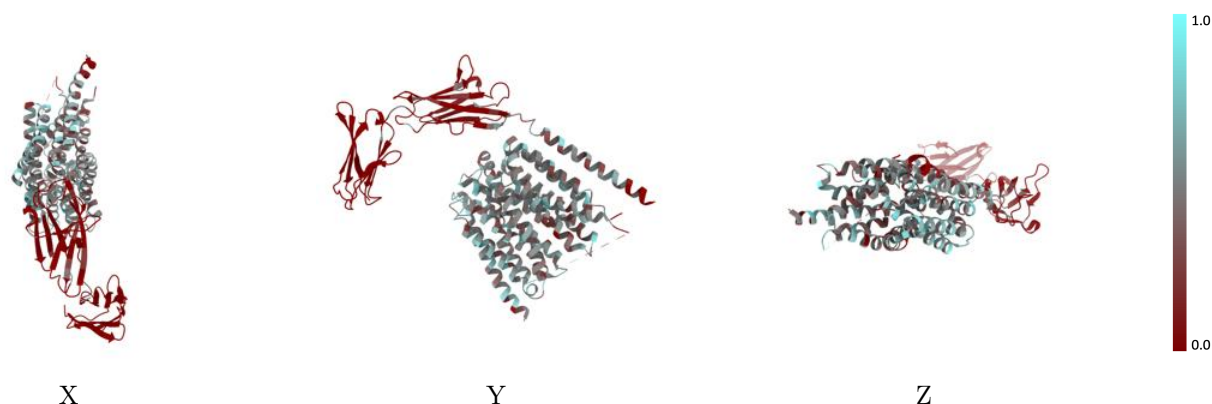
The images above show the 3D surface view of the map at the recommended contour level 0.845 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



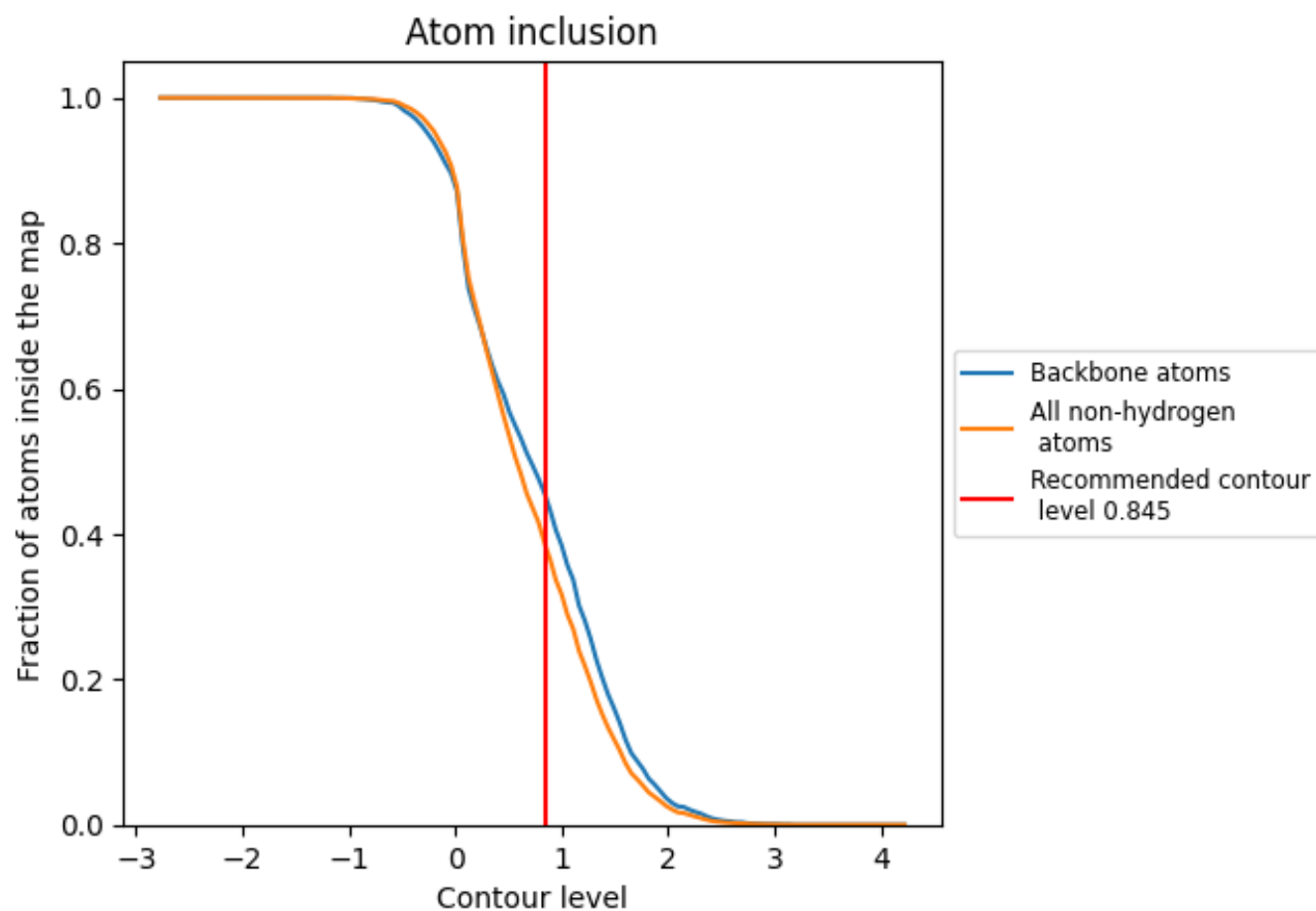
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.845).

9.4 Atom inclusion [i](#)



At the recommended contour level, 45% of all backbone atoms, 38% 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 (0.845) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.3842	<div></div> 0.3620
A	<div></div> 0.4924	<div></div> 0.4530
B	<div></div> 0.1197	<div></div> 0.1370

