



# wwPDB EM Validation Summary Report ⓘ

Mar 20, 2024 – 12:30 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev70  
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 : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

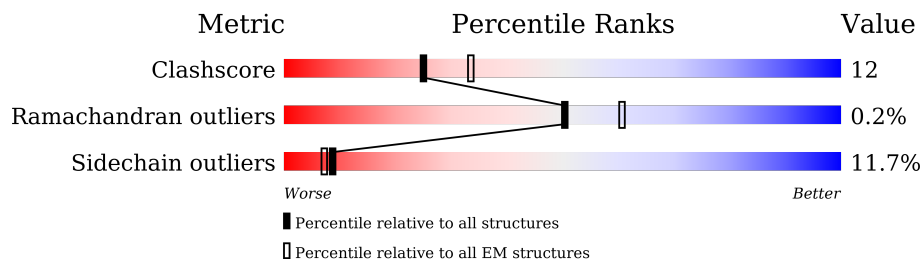
# 1 Overall quality at a glance i

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  $\geq 3$ , 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.

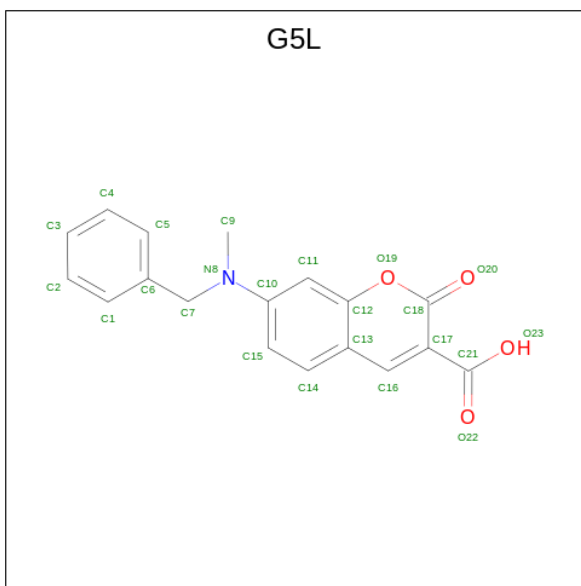
- Molecule 1 is a protein called Monocarboxylate transporter 1.

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

- Molecule 2 is a protein called Basigin.

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

- 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).

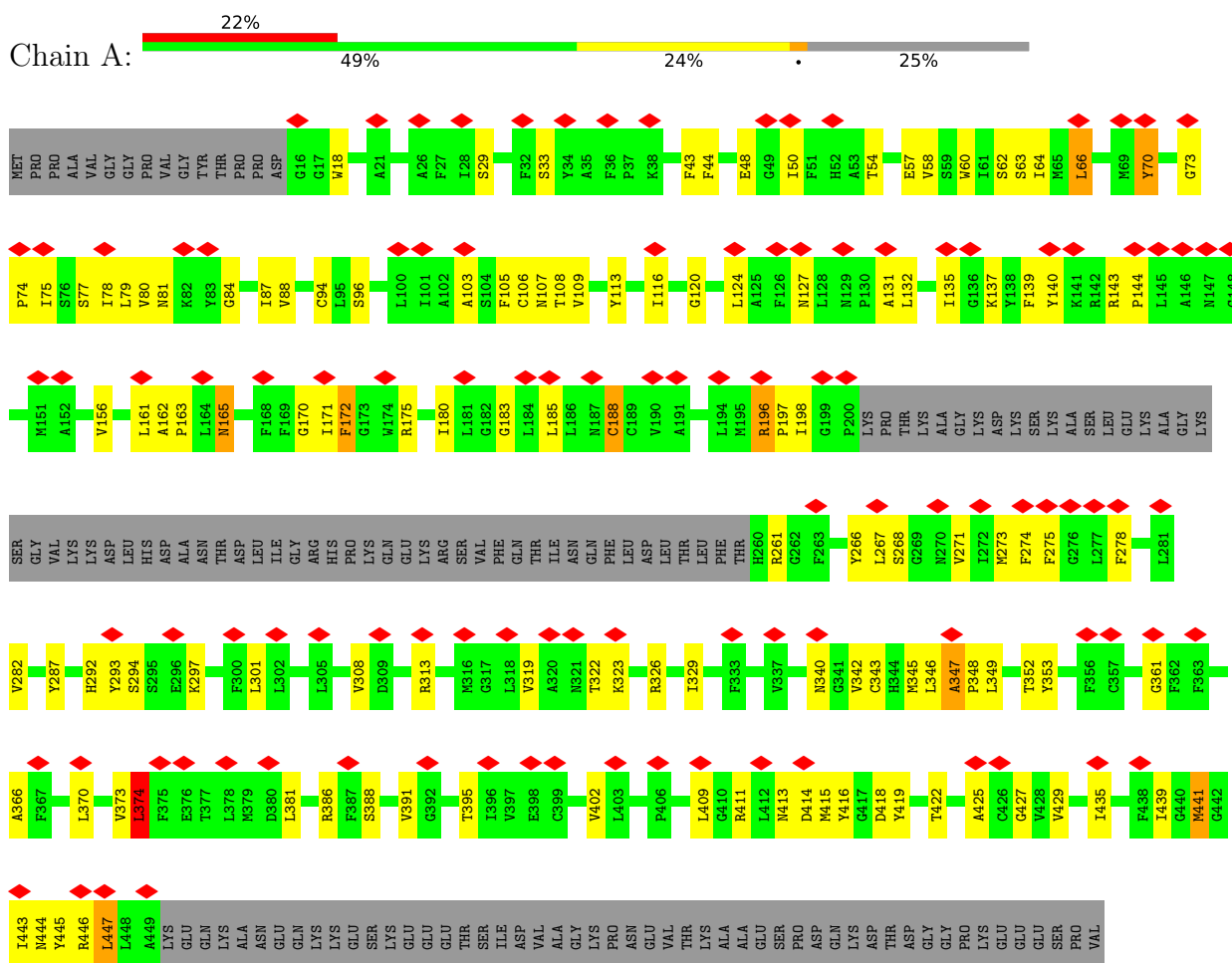


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	A	1	23	18	1	4	0

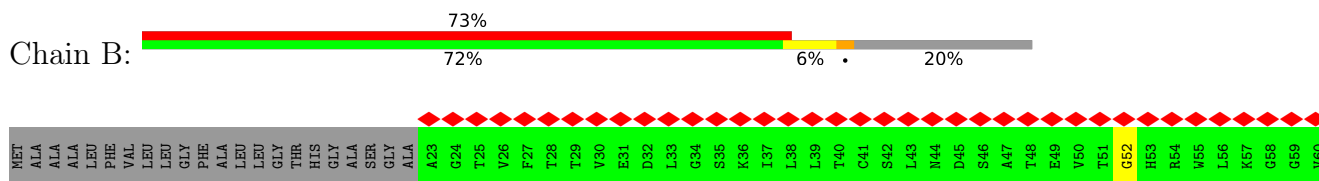
### 3 Residue-property plots

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: Monocarboxylate transporter 1



- Molecule 2: Basigin



V61	L62	K63	E64	D65	A66	L67	P68	G69	Q70	K71	T72	E73	F74	K75	V76	D77	S78	D79	D80	Q81	W82	G83	E84	Y85	S86	C87	V88	F89	L90	P91	E92	P93	M94	G95	T96	A97	N98	I99	Q100	L101	H102	G103	P104	P105	R106	V107	K108	A109	V110	K111	S112	S113	E114	H115	I116	N117	E118	G119	E120
T121	A122	M123	L124	V125	C126	K127	S128	E129	S130	V131	P132	E133	V134	T135	D136	W137	A138	W139	Y140	K141	I142	T143	D144	S145	E146	D147	K148	A149	L150	M151	N152	G153	S154	E155	S156	R157	F158	F159	V160	S161	S162	S163	Q164	G165	R166	S167	E168	L169	H170	I171	E172	N173	L174	N175	M176	E177	A178	D179	P180
G181	Q182	Y183	R184	C185	N186	G187	T188	S189	S190	K191	G192	S193	D194	Q195	A196	I197	I198	T199	L200	R201	V202	R203	S204	H205	L206	A207	A208	L209	W210	P211	F212	L213	G214	I215	V216	L220	V221	L222	V223	T224	I225	I226	F227	I228	Y229	E230	K231	R232	R233	K234	P235	E236	D237	V238	LEU	ASP	ASP	ASP	
ASP	ALA	GLY	SER	ALA	PRO	LEU	LYS	SER	SER	GLN	ASN	ASP	LYS	GLY	LYS	ASN	VAL	ARG	GLN	ARG	ASN	SER	SER																																				

## 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 ( $\text{\AA}$ )	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 ( $\text{\AA}$ )	0.8433, 0.8433, 0.8433	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: 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 [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	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 [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 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.

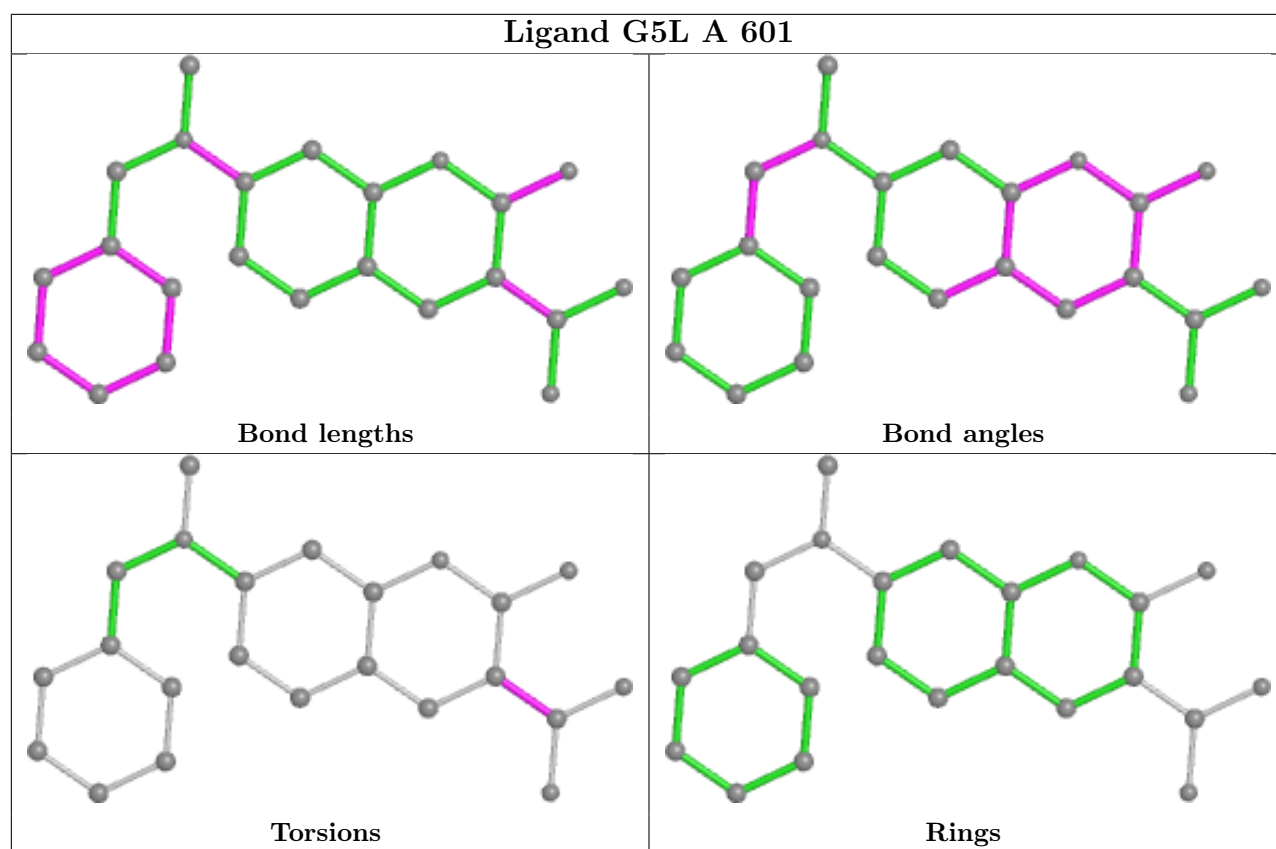
All (4) torsion outliers are listed below:

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.

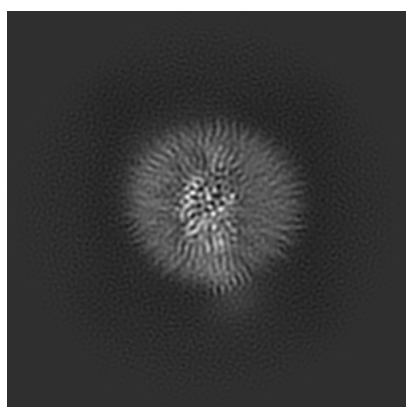
## 6 Map visualisation [i](#)

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.

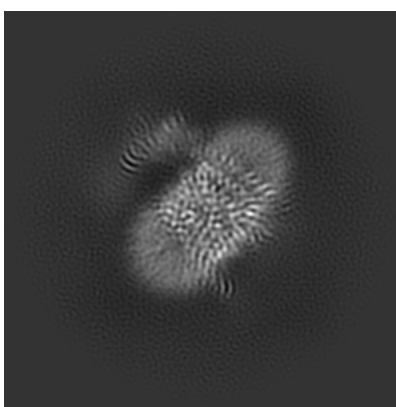
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

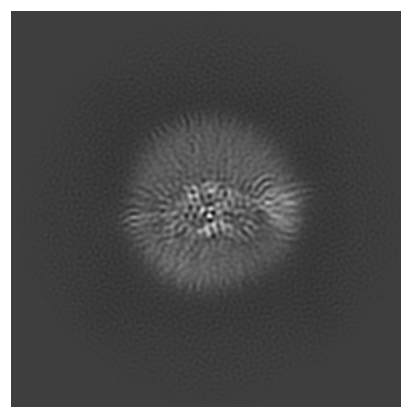
#### 6.1.1 Primary map



X



Y

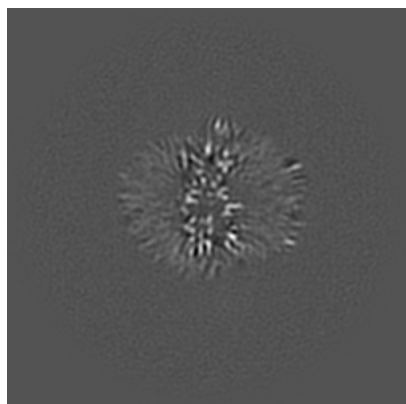


Z

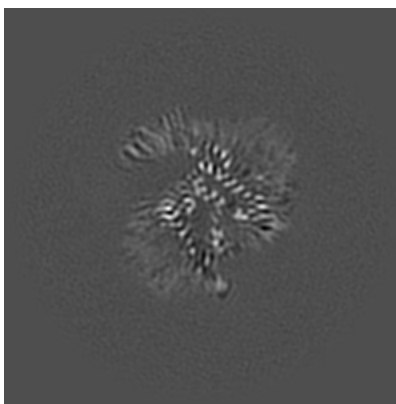
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

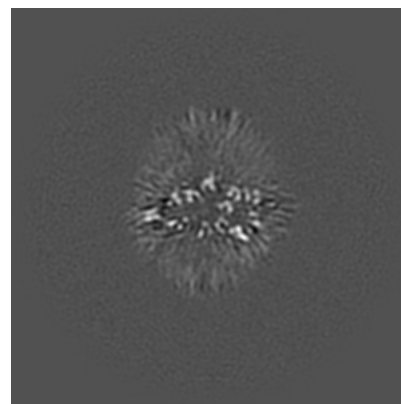
#### 6.2.1 Primary map



X Index: 128



Y Index: 128

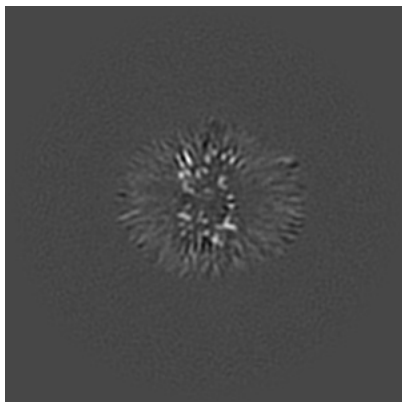


Z Index: 128

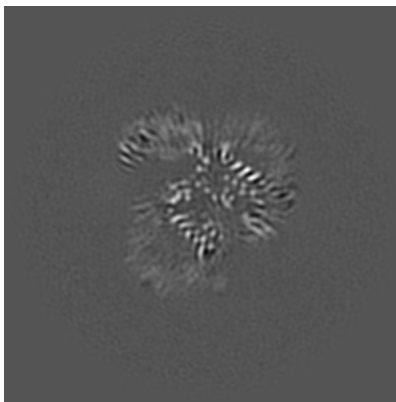
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

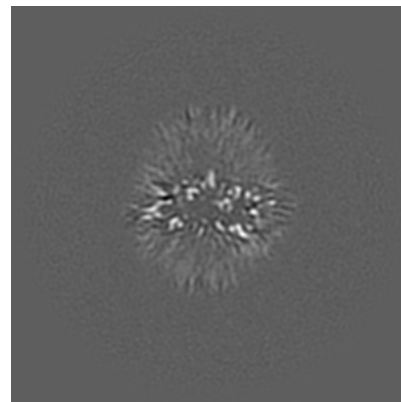
### 6.3.1 Primary map



X Index: 125



Y Index: 132

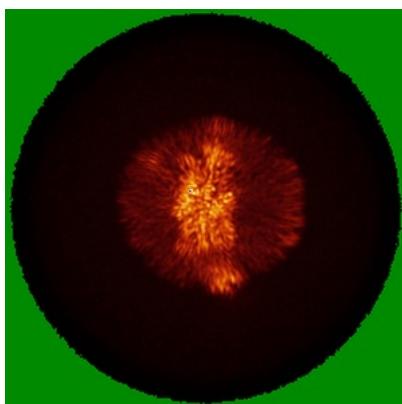


Z Index: 129

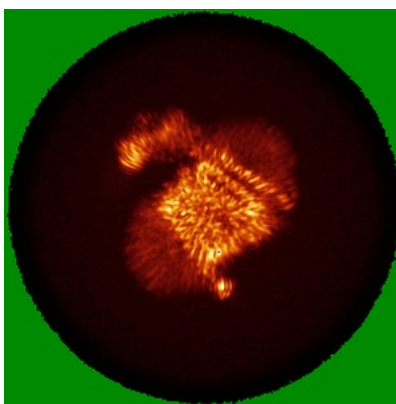
The images above show the largest variance slices of the map in three orthogonal directions.

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

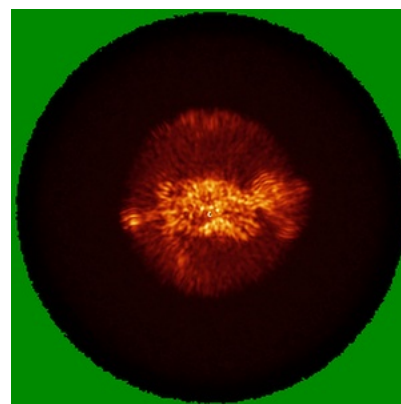
### 6.4.1 Primary map



X



Y

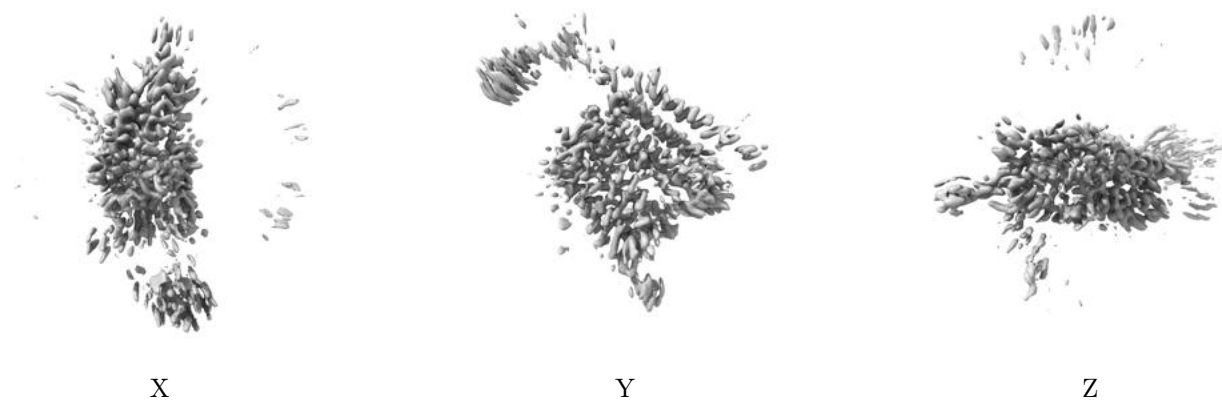


Z

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

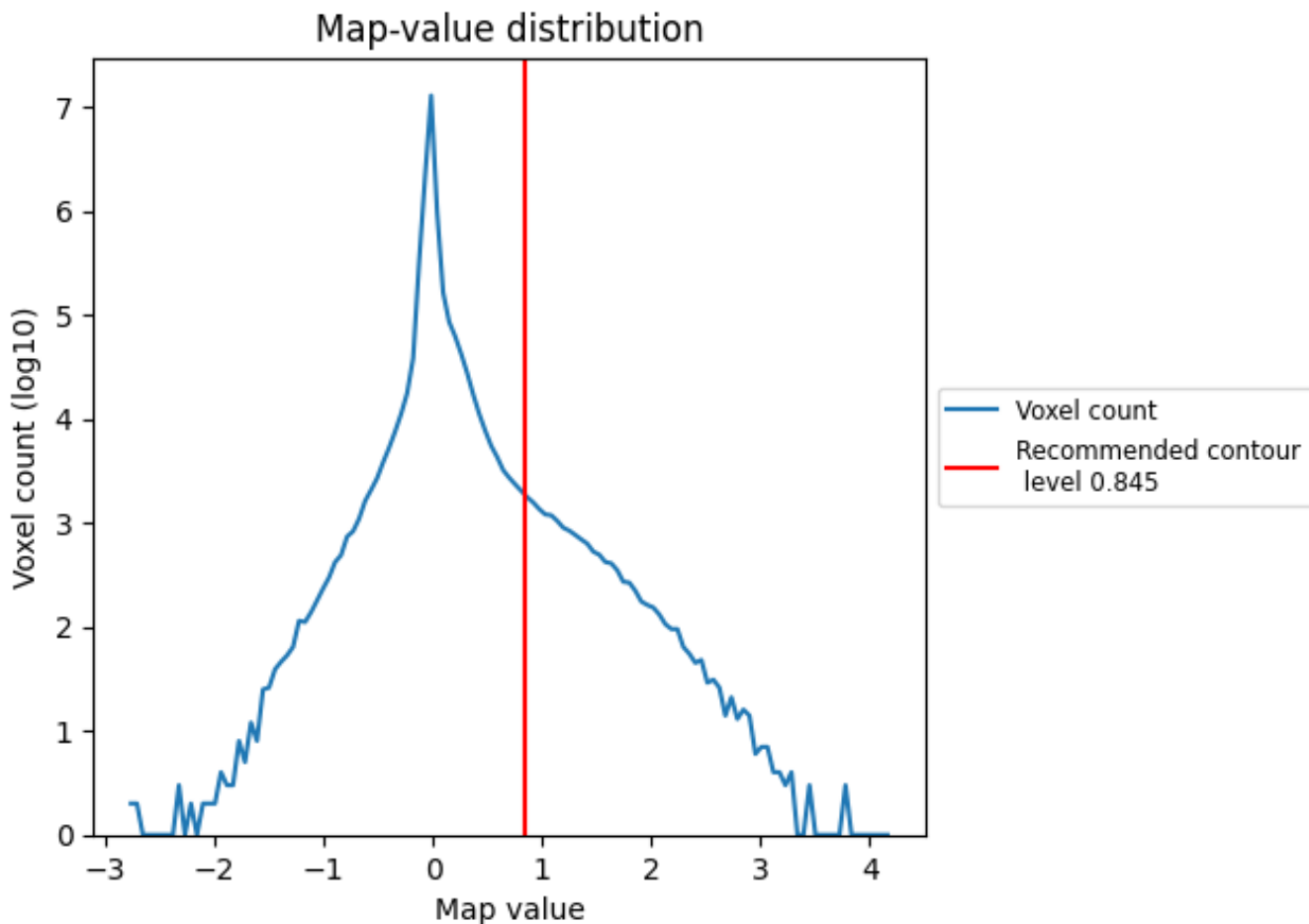
## 6.6 Mask visualisation [i](#)

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.

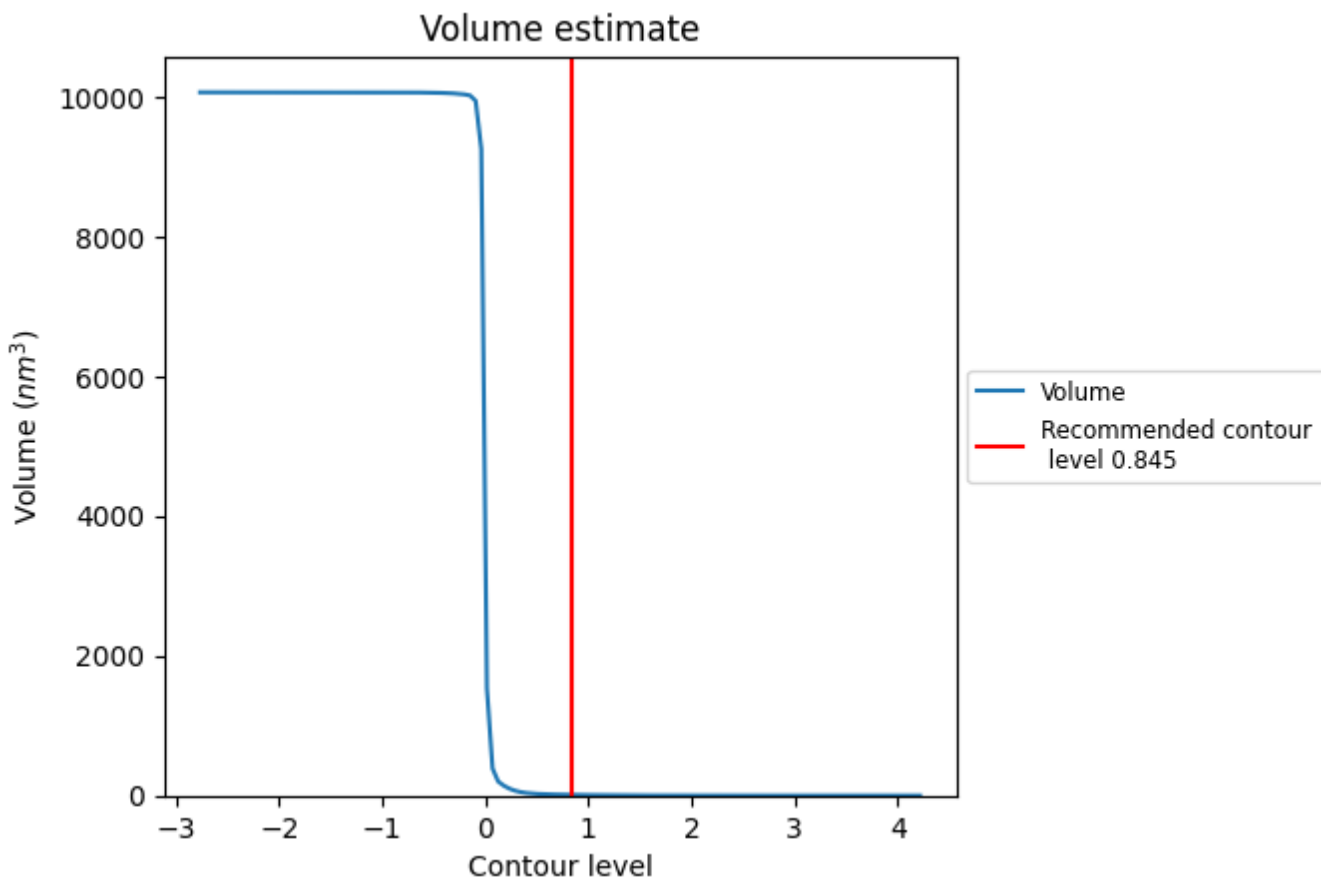
### 7.1 Map-value distribution [i](#)



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.



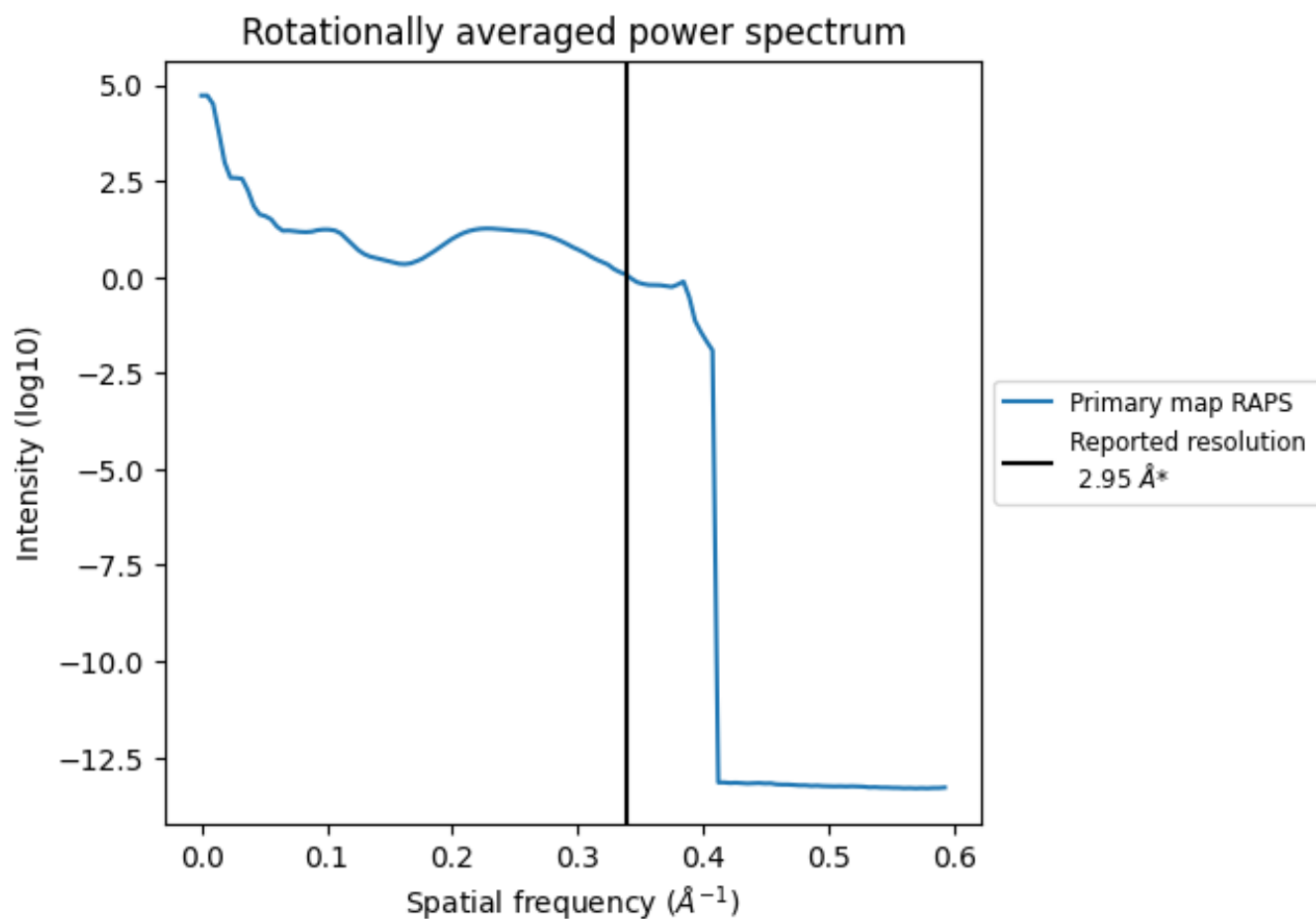
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 10 nm<sup>3</sup>; 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 [\(i\)](#)



\*Reported resolution corresponds to spatial frequency of  $0.339 \text{ \AA}^{-1}$

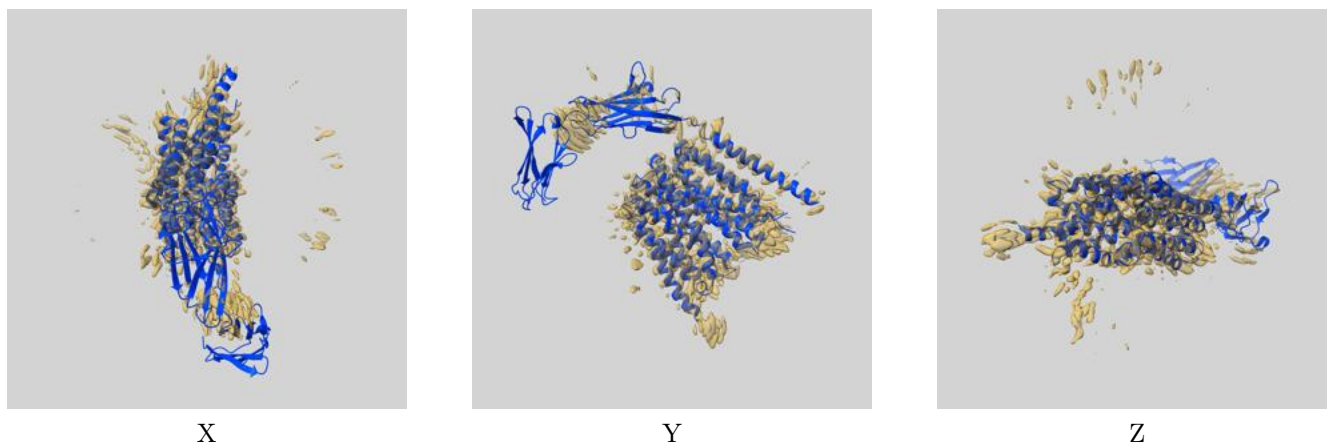
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

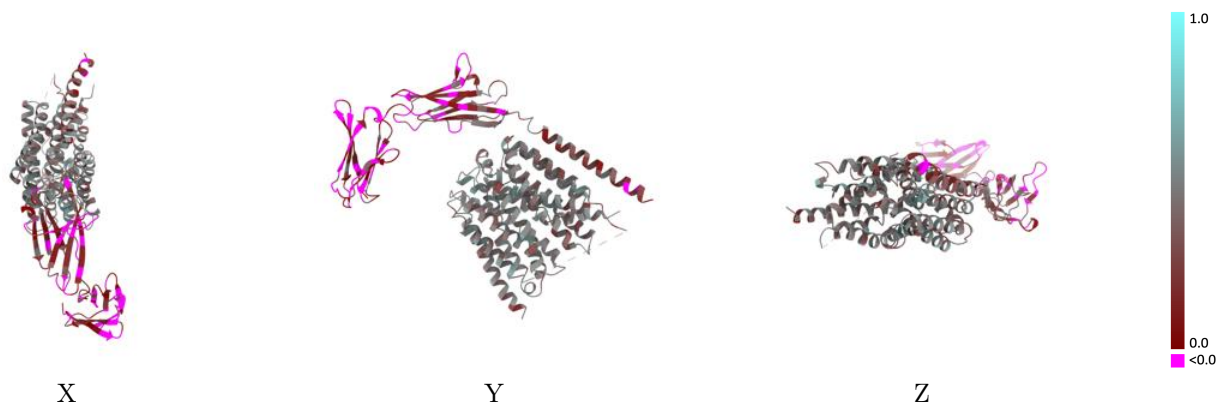
This section contains information regarding the fit between EMDB map EMD-30389 and PDB model 7CKO. Per-residue inclusion information can be found in section [3](#) on page [4](#).

### 9.1 Map-model overlay [i](#)



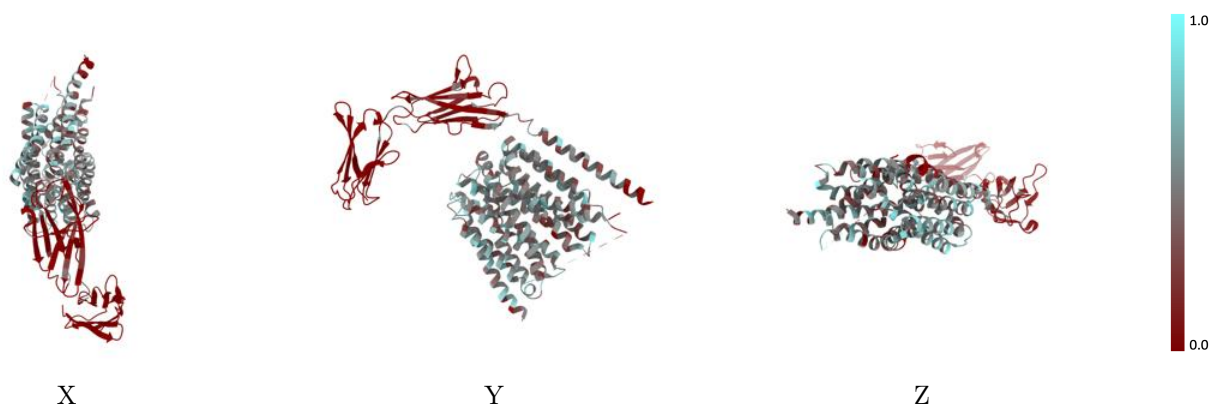
The images above show the 3D surface view of the map at the recommended contour level 0.845 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



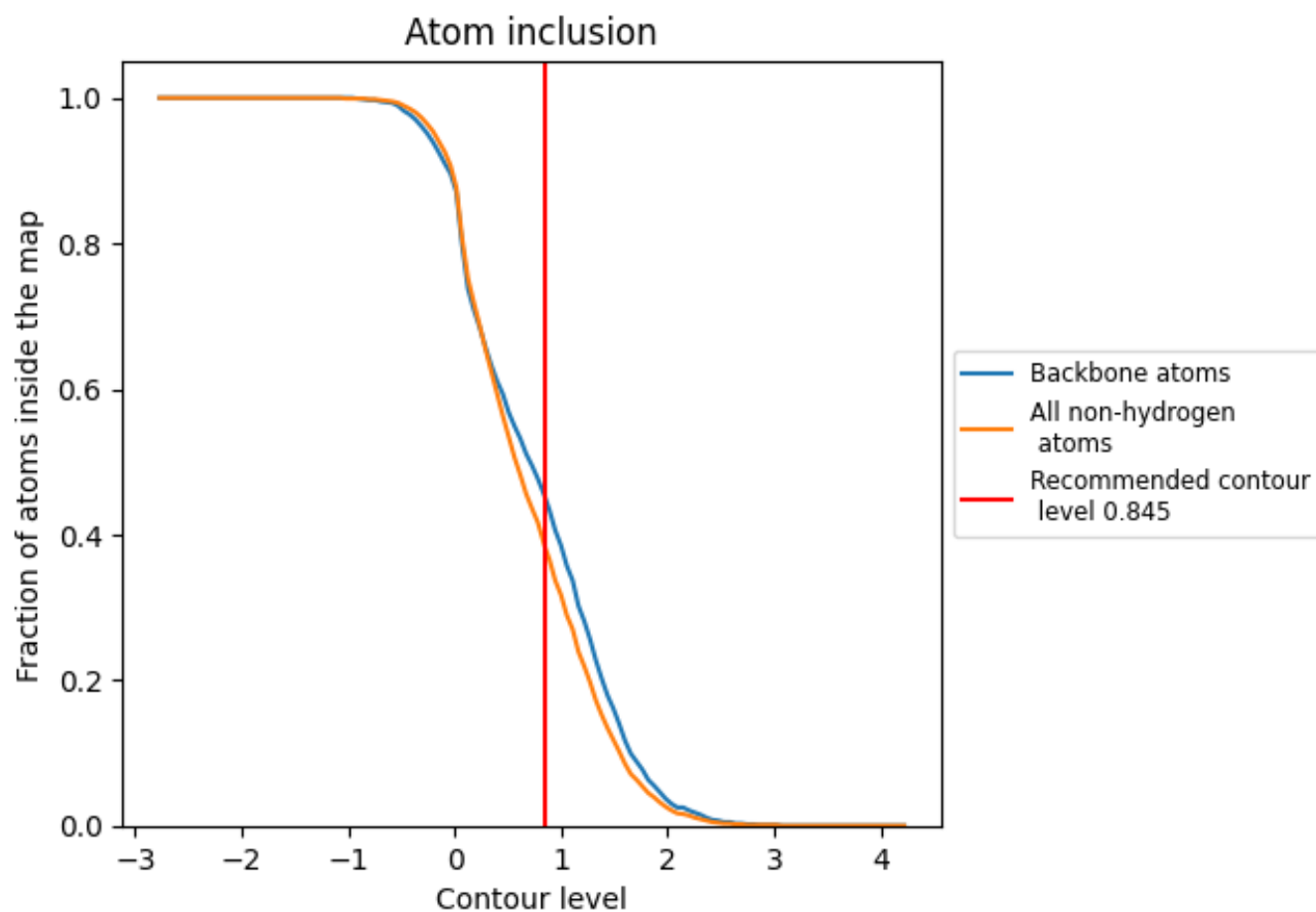
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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	 0.3840	 0.3620
A	 0.4920	 0.4530
B	 0.1200	 0.1370

