



## wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 11:20 PM JST

PDB ID : 7CQK  
EMDB ID : EMD-30442  
Title : Cryo-EM structure of the substrate-bound SPT-ORMDL3 complex  
Authors : Li, S.S.; Xie, T.; Wang, L.; Gong, X.  
Deposited on : 2020-08-11  
Resolution : 3.30 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.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

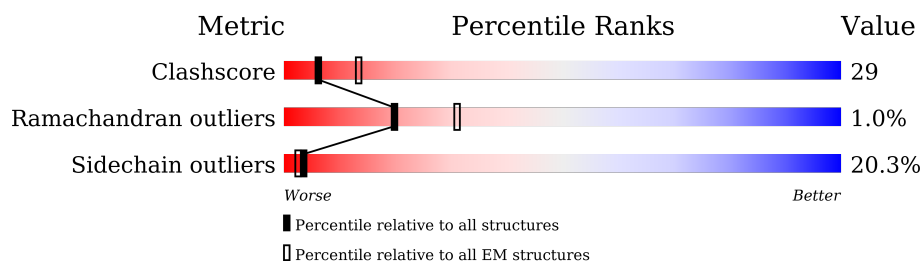
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.30 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	C	473	 95%
1	S	473	 59% 21% 8% 11%
2	T	562	 58% 22% 9% 12%
3	A	153	 7% 44% 25% 15% 15%
4	E	92	 21% 21% 9% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PLS	T	601	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8859 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 Serine palmitoyltransferase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	S	421	Total	C	N	O	S	0	0
			3268	2078	558	616	16		
1	C	22	Total	C	N	O		0	0
			177	125	26	26			

- Molecule 2 is a protein called Serine palmitoyltransferase 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	T	497	Total	C	N	O	S	0	0
			3907	2501	669	712	25		

- Molecule 3 is a protein called ORM1-like protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	130	Total	C	N	O	S	0	0
			1030	688	165	172	5		

- Molecule 4 is a protein called Serine palmitoyltransferase small subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	46	Total	C	N	O	S	0	0
			389	265	55	65	4		

There are 21 discrepancies between the modelled and reference sequences:

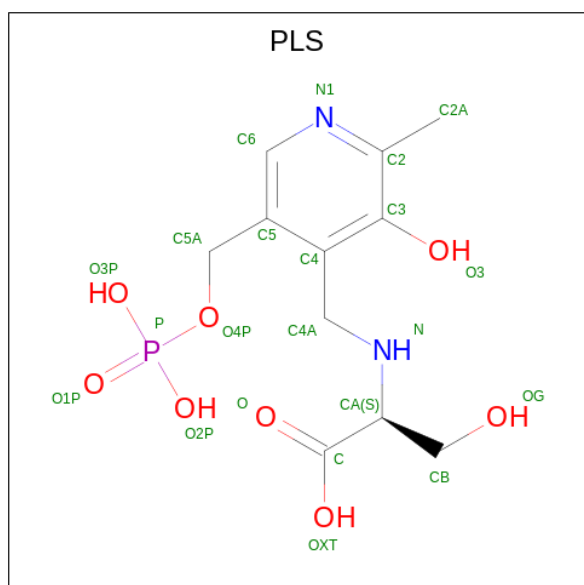
Chain	Residue	Modelled	Actual	Comment	Reference
E	-20	MET	-	initiating methionine	UNP Q969W0
E	-19	ALA	-	expression tag	UNP Q969W0
E	-18	ASP	-	expression tag	UNP Q969W0
E	-17	TYR	-	expression tag	UNP Q969W0
E	-16	LYS	-	expression tag	UNP Q969W0
E	-15	ASP	-	expression tag	UNP Q969W0
E	-14	ASP	-	expression tag	UNP Q969W0

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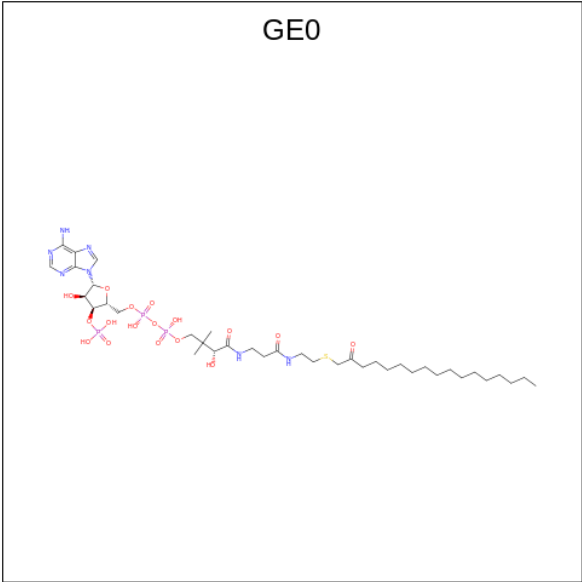
Chain	Residue	Modelled	Actual	Comment	Reference
E	-13	ASP	-	expression tag	UNP Q969W0
E	-12	ASP	-	expression tag	UNP Q969W0
E	-11	LYS	-	expression tag	UNP Q969W0
E	-10	SER	-	expression tag	UNP Q969W0
E	-9	GLY	-	expression tag	UNP Q969W0
E	-8	PRO	-	expression tag	UNP Q969W0
E	-7	ASP	-	expression tag	UNP Q969W0
E	-6	GLU	-	expression tag	UNP Q969W0
E	-5	VAL	-	expression tag	UNP Q969W0
E	-4	ASP	-	expression tag	UNP Q969W0
E	-3	ALA	-	expression tag	UNP Q969W0
E	-2	SER	-	expression tag	UNP Q969W0
E	-1	GLY	-	expression tag	UNP Q969W0
E	0	ARG	-	expression tag	UNP Q969W0

- Molecule 5 is [3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-YL METHYL]-SERINE (three-letter code: PLS) (formula: C<sub>11</sub>H<sub>17</sub>N<sub>2</sub>O<sub>8</sub>P).



Mol	Chain	Residues	Atoms					AltConf
5	T	1	Total	C	N	O	P	0
			22	11	2	8	1	

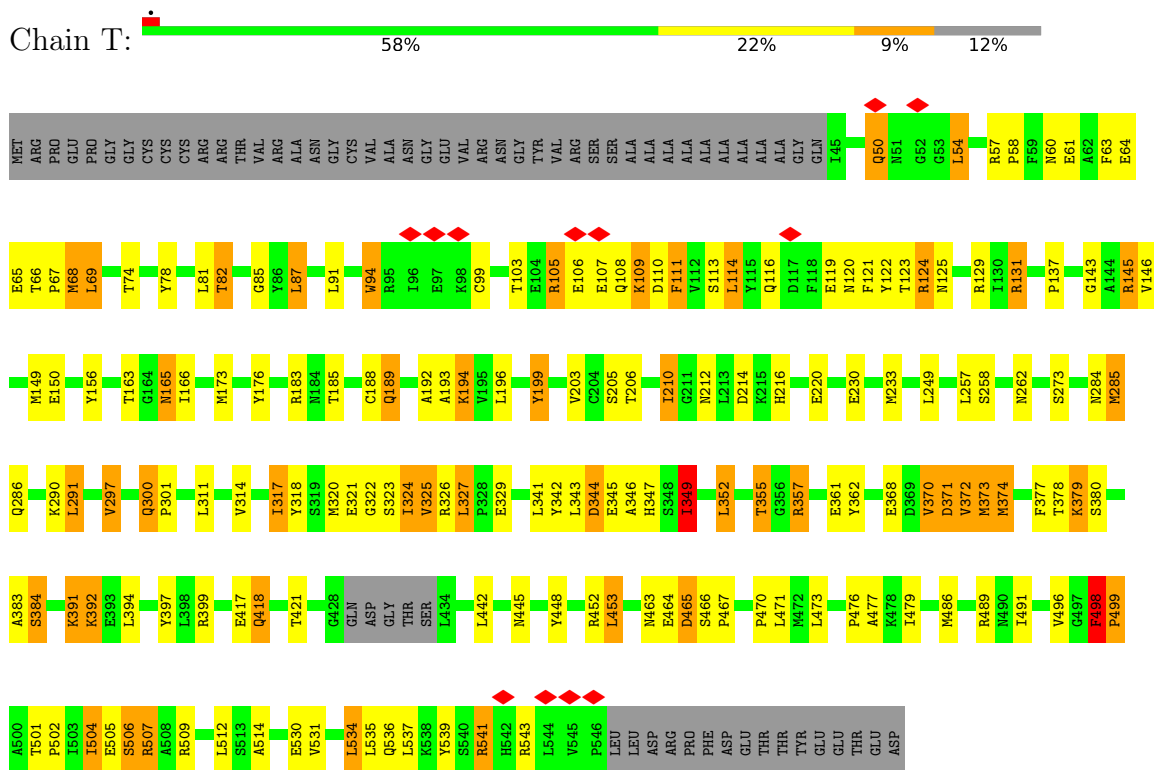
- Molecule 6 is [[(2R,3S,4R,5R)-5-(6-aminopurin-9-yl)-4-oxidanyl-3-phosphonooxy-oxolan-2-yl]methoxy-oxidanyl-phosphoryl] [(3R)-2,2-dimethyl-3-oxidanyl-4-oxidanylidene-4-[[3-oxidanylidene-3-[2-(2-oxidanylideneheptadecylsulfanyl)ethylamino]propyl]amino]butyl] hydrogen phosphate (three-letter code: GE0) (formula: C<sub>38</sub>H<sub>68</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>S) (labeled as "Ligand of Interest" by depositor).



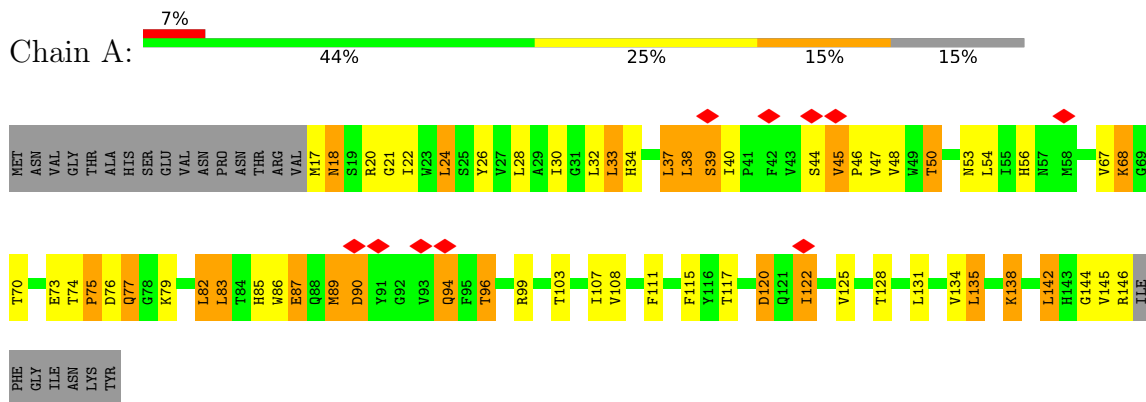
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
6	A	1	66	38	7	17	3	1	0



- Molecule 2: Serine palmitoyltransferase 2



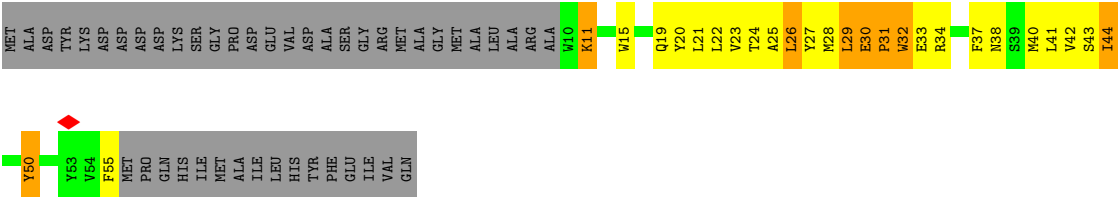
- Molecule 3: ORM1-like protein 3



- Molecule 4: Serine palmitoyltransferase small subunit A







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	106196	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 ( $e^-/\text{\AA}^2$ )	50	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	0.191	Depositor
Minimum map value	-0.120	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.03	Depositor
Map size ( $\text{\AA}$ )	276.48, 276.48, 276.48	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.08, 1.08, 1.08	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: GE0, PLS

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	C	0.26	0/181	0.54	0/247
1	S	0.39	0/3329	0.60	2/4501 (0.0%)
2	T	0.43	0/3989	0.67	8/5387 (0.1%)
3	A	0.30	0/1060	0.55	0/1451
4	E	0.35	0/402	0.45	0/547
All	All	0.40	0/8961	0.62	10/12133 (0.1%)

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	291	LEU	CA-CB-CG	6.61	130.49	115.30
2	T	311	LEU	CA-CB-CG	6.30	129.79	115.30
2	T	471	LEU	CA-CB-CG	6.09	129.30	115.30
2	T	210	ILE	CG1-CB-CG2	-5.91	98.39	111.40
2	T	257	LEU	CA-CB-CG	5.57	128.12	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	177	0	194	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	S	3268	0	3291	182	0
2	T	3907	0	3897	219	0
3	A	1030	0	1049	87	0
4	E	389	0	379	48	0
5	T	22	0	13	12	0
6	A	66	0	0	18	0
All	All	8859	0	8823	514	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 29.

The worst 5 of 514 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:S:254:ILE:HD11	1:S:390:LEU:CD1	1.34	1.54
2:T:67:PRO:HB3	2:T:541:ARG:NH1	1.27	1.46
3:A:117:THR:HG22	3:A:120:ASP:CG	1.36	1.43
2:T:498:PHE:HB3	2:T:499:PRO:CD	1.42	1.42
2:T:196:LEU:CG	2:T:417:GLU:OE1	1.73	1.32

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	C	20/473 (4%)	19 (95%)	1 (5%)	0	100	100
1	S	419/473 (89%)	370 (88%)	46 (11%)	3 (1%)	22	54
2	T	493/562 (88%)	425 (86%)	63 (13%)	5 (1%)	15	46
3	A	128/153 (84%)	113 (88%)	13 (10%)	2 (2%)	9	36
4	E	44/92 (48%)	41 (93%)	2 (4%)	1 (2%)	6	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1104/1753 (63%)	968 (88%)	125 (11%)	11 (1%)	20	46

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	S	78	PRO
2	T	349	ILE
2	T	498	PHE
2	T	499	PRO
2	T	199	TYR

### 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	C	18/401 (4%)	12 (67%)	6 (33%)	0	1
1	S	353/401 (88%)	286 (81%)	67 (19%)	1	6
2	T	411/466 (88%)	336 (82%)	75 (18%)	1	7
3	A	114/140 (81%)	85 (75%)	29 (25%)	0	2
4	E	41/78 (53%)	28 (68%)	13 (32%)	0	1
All	All	937/1486 (63%)	747 (80%)	190 (20%)	3	5

5 of 190 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	T	355	THR
3	A	18	ASN
2	T	372	VAL
2	T	465	ASP
3	A	40	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
2	T	445	ASN
3	A	18	ASN
2	T	536	GLN
3	A	53	ASN
1	S	413	GLN

### 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](#)

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$
6	GE0	A	201	-	60,68,68	1.35	7 (11%)	72,94,94	1.31	4 (5%)
5	PLS	T	601	-	22,22,22	2.50	3 (13%)	27,31,31	1.33	2 (7%)

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
6	GE0	A	201	-	-	25/63/83/83	0/3/3/3
5	PLS	T	601	-	-	9/17/17/17	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	T	601	PLS	C3-C2	8.01	1.48	1.40
5	T	601	PLS	C5-C4	5.90	1.48	1.40
5	T	601	PLS	C3-C4	5.43	1.48	1.40
6	A	201	GE0	C2-N3	4.89	1.40	1.32
6	A	201	GE0	PAY-OBA	3.37	1.61	1.50

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	201	GE0	N3-C2-N1	-6.88	117.92	128.68
6	A	201	GE0	PAS-OAR-PAQ	-4.01	119.07	132.83
5	T	601	PLS	C4A-N-CA	3.16	119.90	113.92
6	A	201	GE0	C5-C6-N6	-2.58	116.44	120.35
6	A	201	GE0	O4'-C1'-C2'	-2.47	103.31	106.93

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	T	601	PLS	C-CA-N-C4A
5	T	601	PLS	C5A-O4P-P-O2P
5	T	601	PLS	C5A-O4P-P-O3P
6	A	201	GE0	SAA-CAB-CAC-NAD
6	A	201	GE0	CAI-CAJ-CAL-CAO

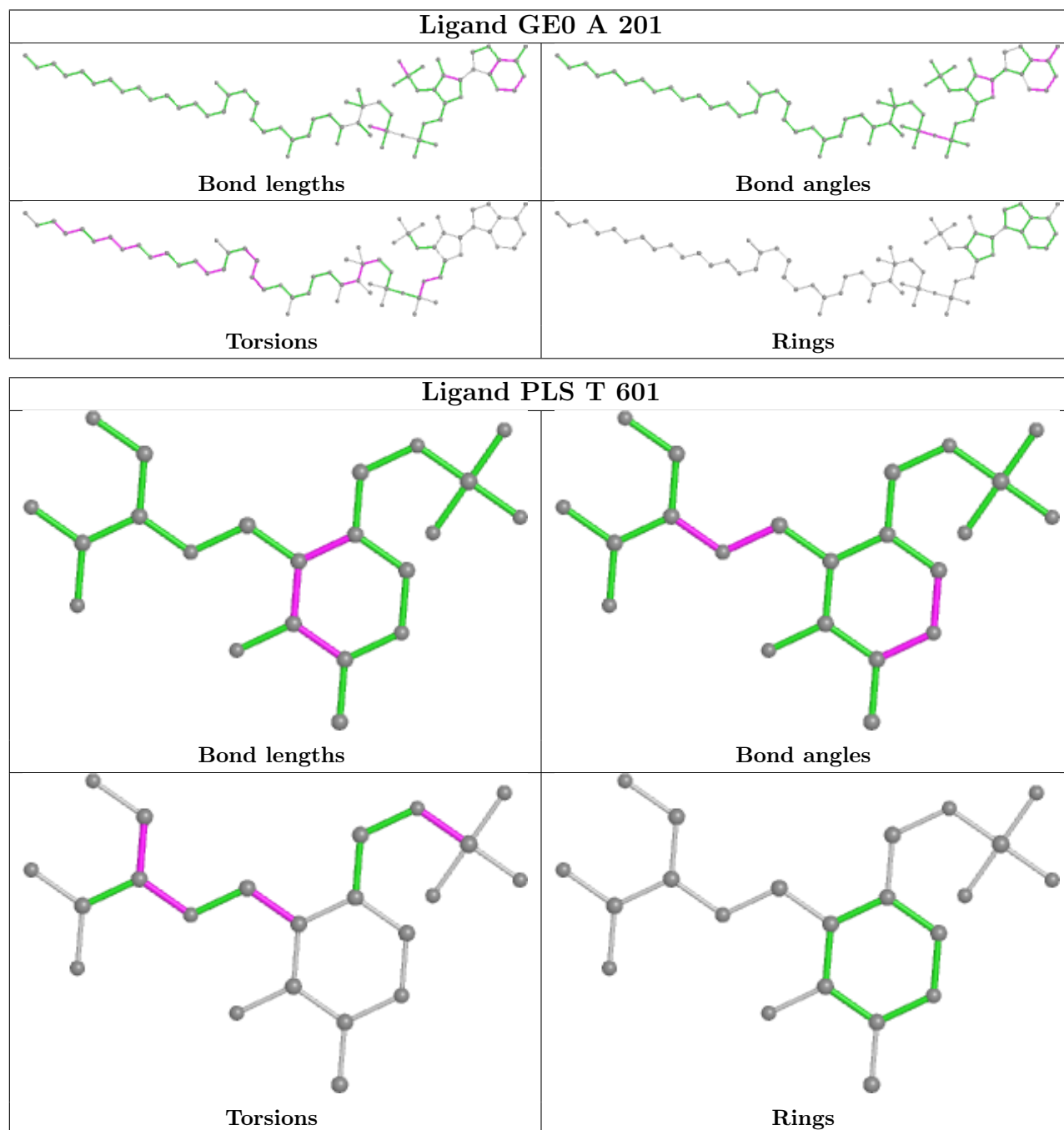
There are no ring outliers.

2 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	201	GE0	18	0
5	T	601	PLS	12	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.

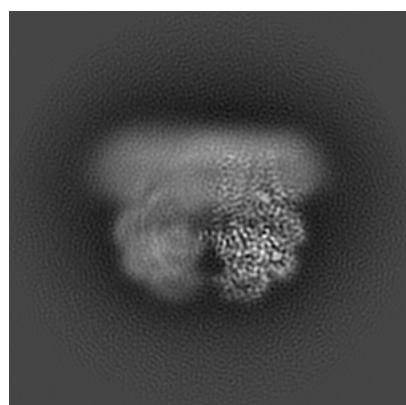
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30442. These allow visual inspection of the internal detail of the map and identification of artifacts.

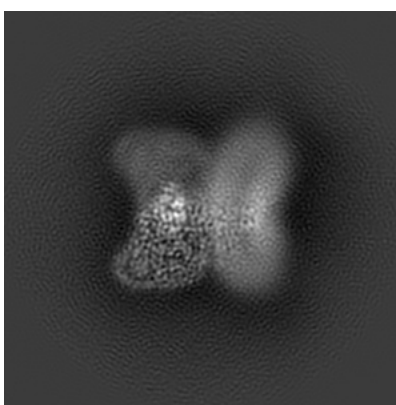
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

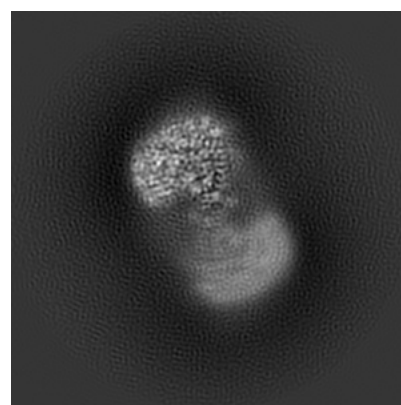
#### 6.1.1 Primary map



X



Y

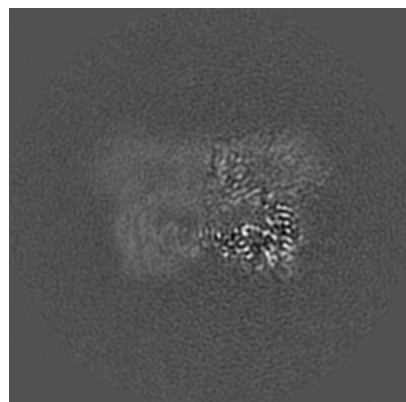


Z

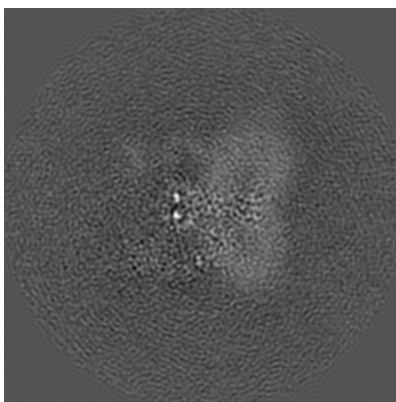
The images above show the map projected in three orthogonal directions.

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

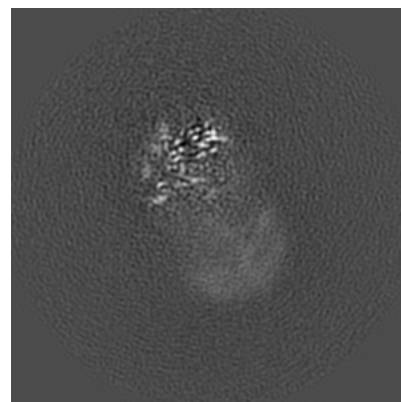
#### 6.2.1 Primary map



X Index: 128



Y Index: 128

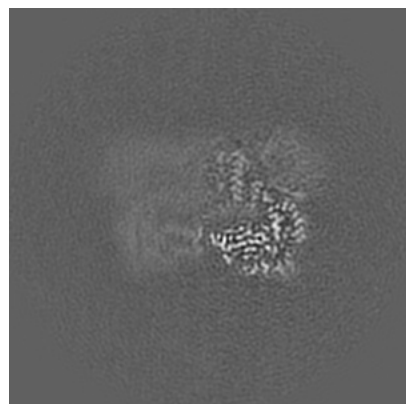


Z Index: 128

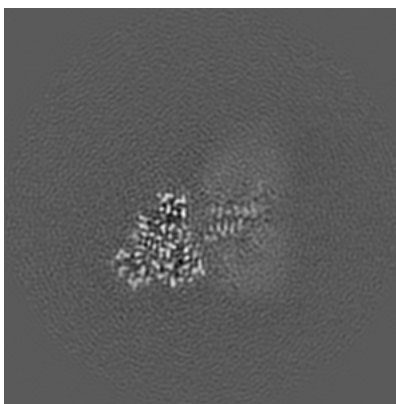
The images above show central slices of the map in three orthogonal directions.

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

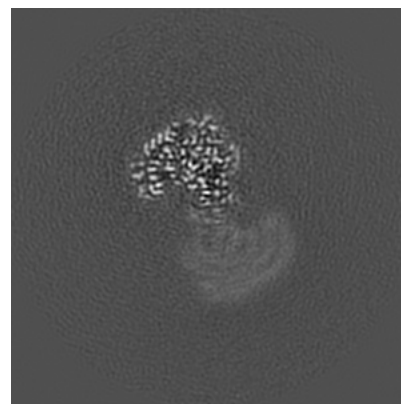
### 6.3.1 Primary map



X Index: 125



Y Index: 148



Z Index: 107

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

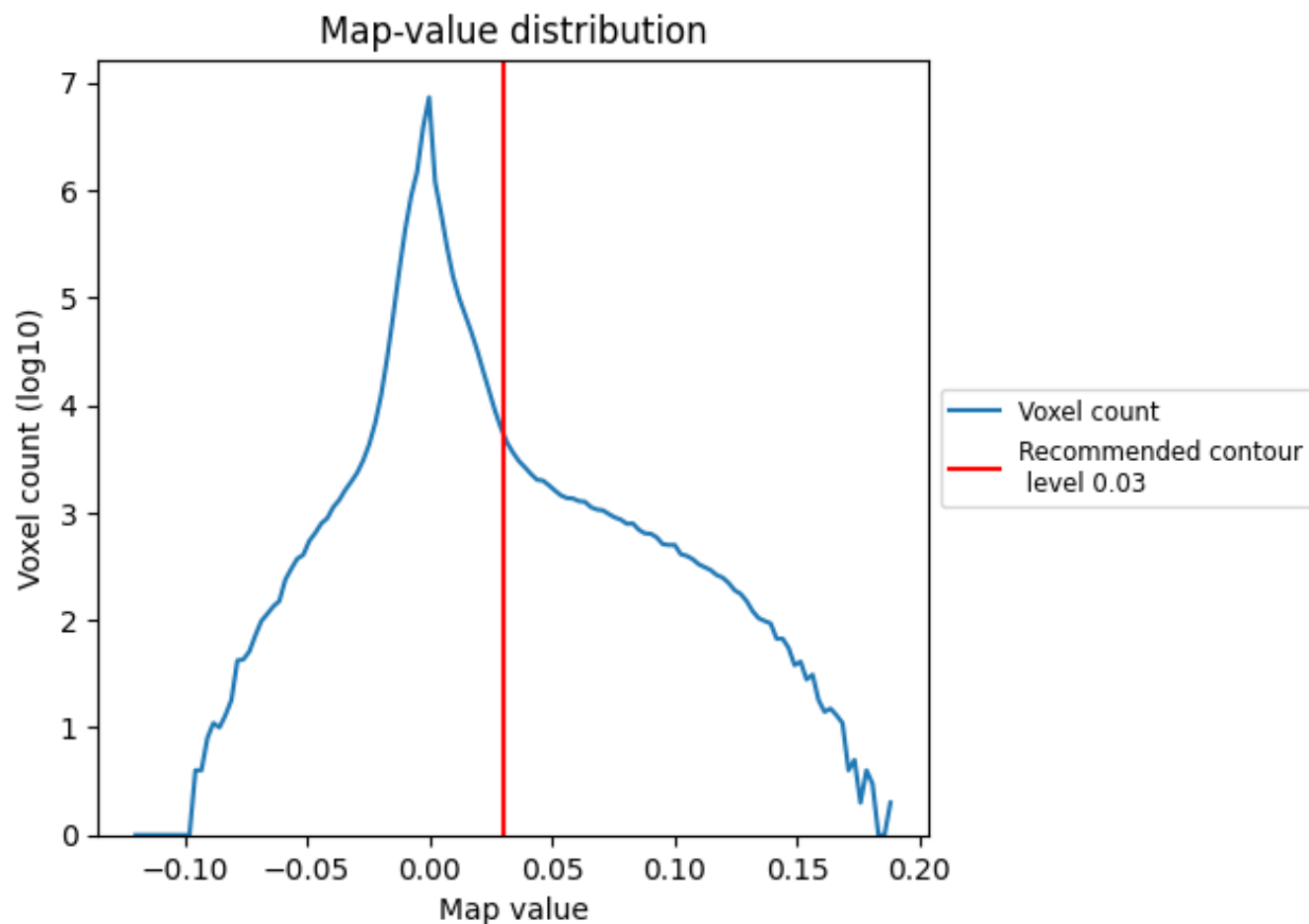
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

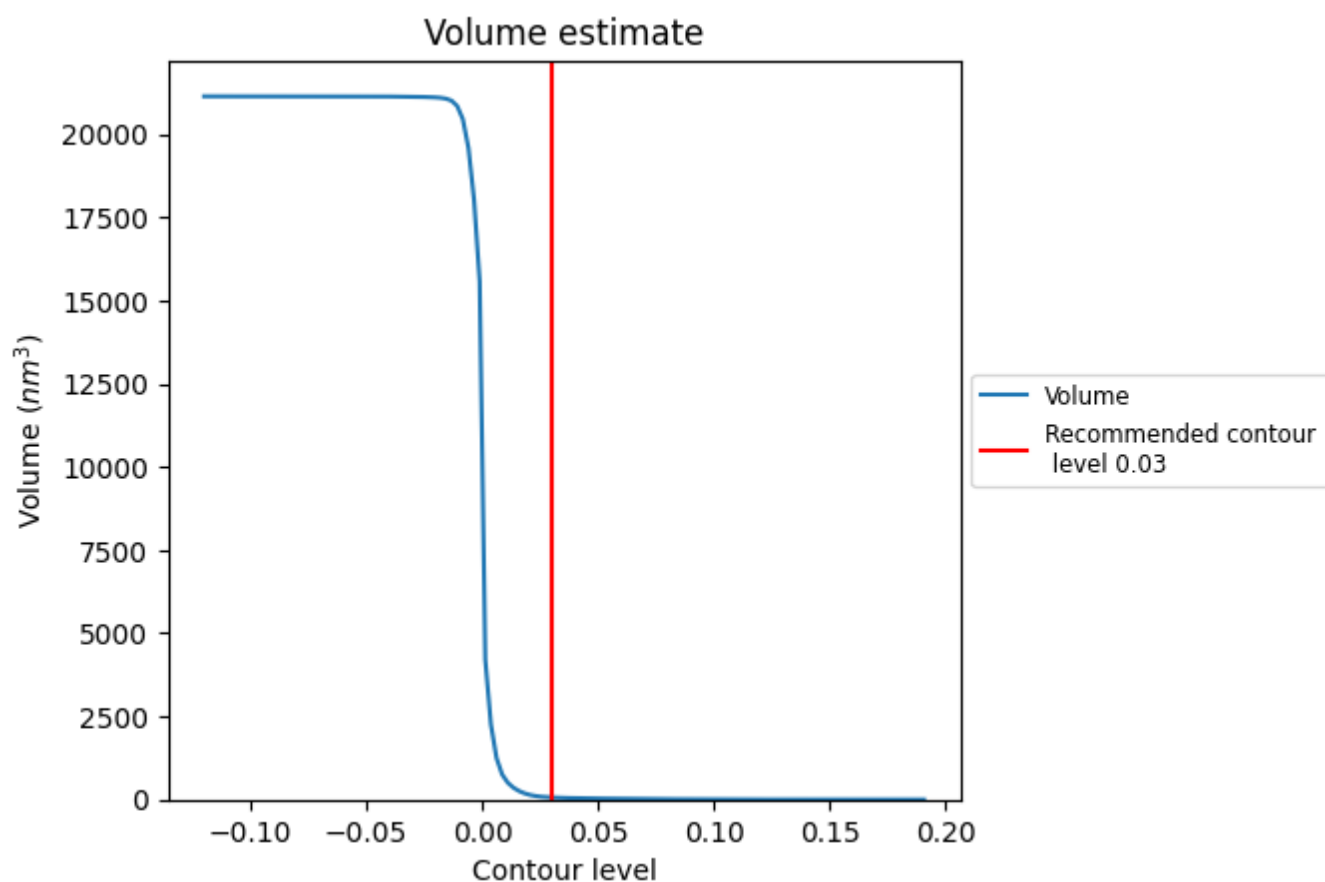
This section contains the results of statistical analysis of the map.

### 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.

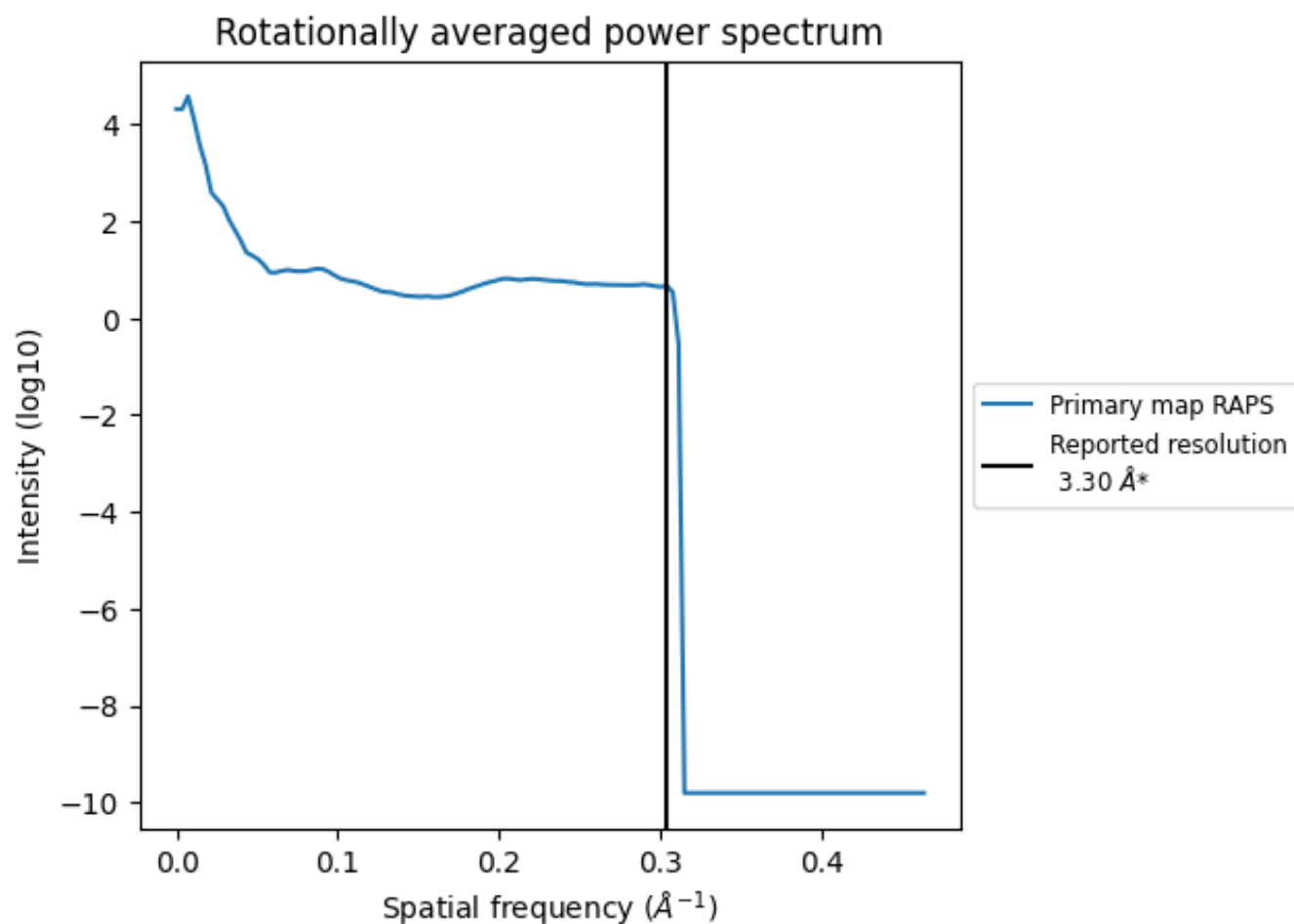
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 63 nm<sup>3</sup>; this corresponds to an approximate mass of 57 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 0.303  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation

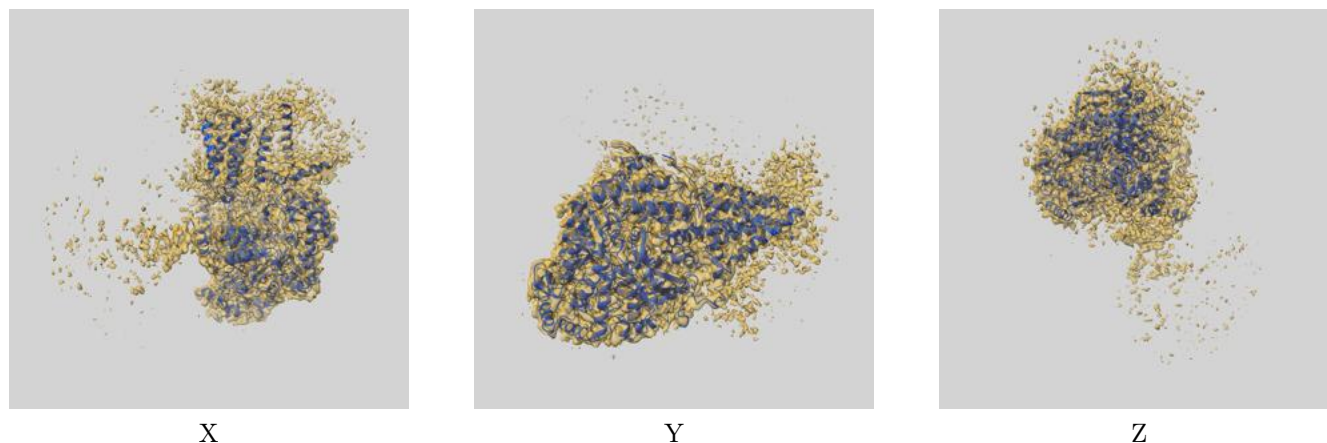
This section was not generated. No FSC curve or half-maps provided.



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

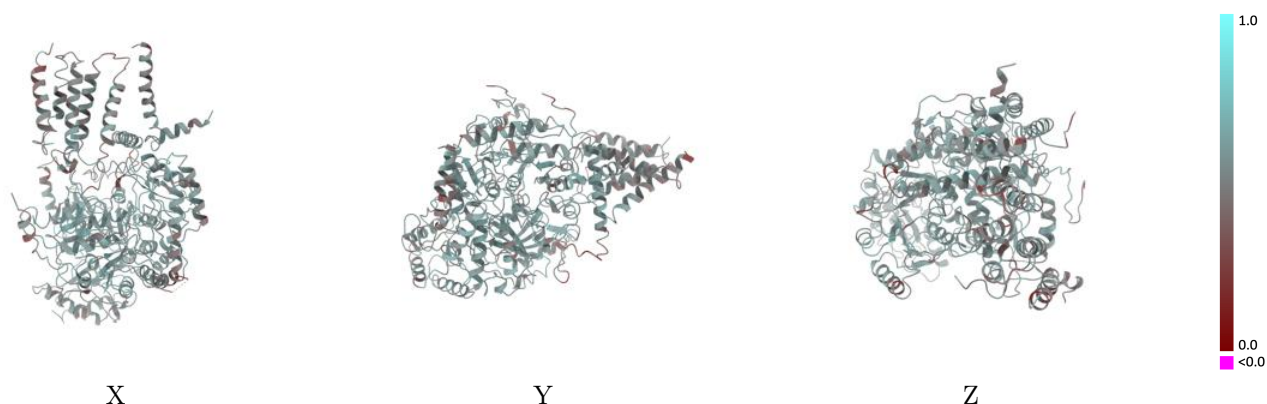
This section contains information regarding the fit between EMDB map EMD-30442 and PDB model 7CQK. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

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



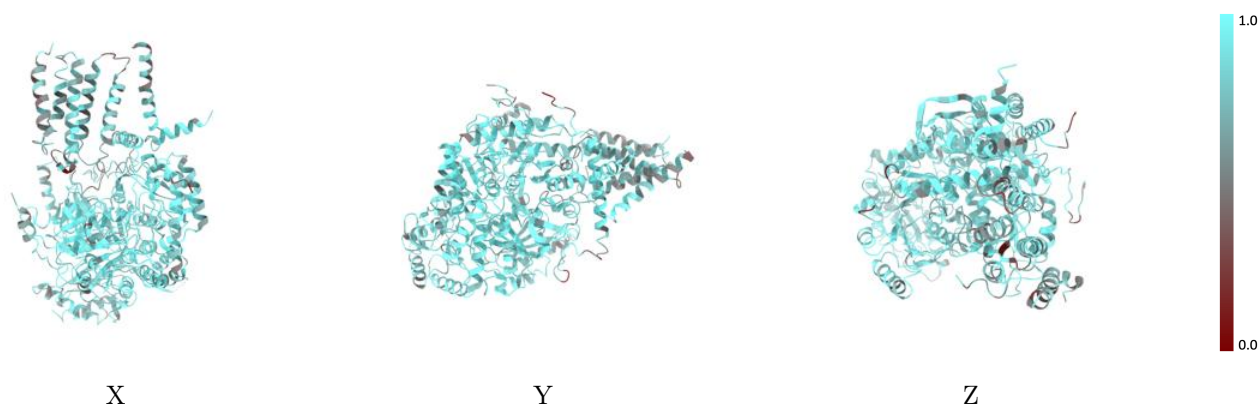
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



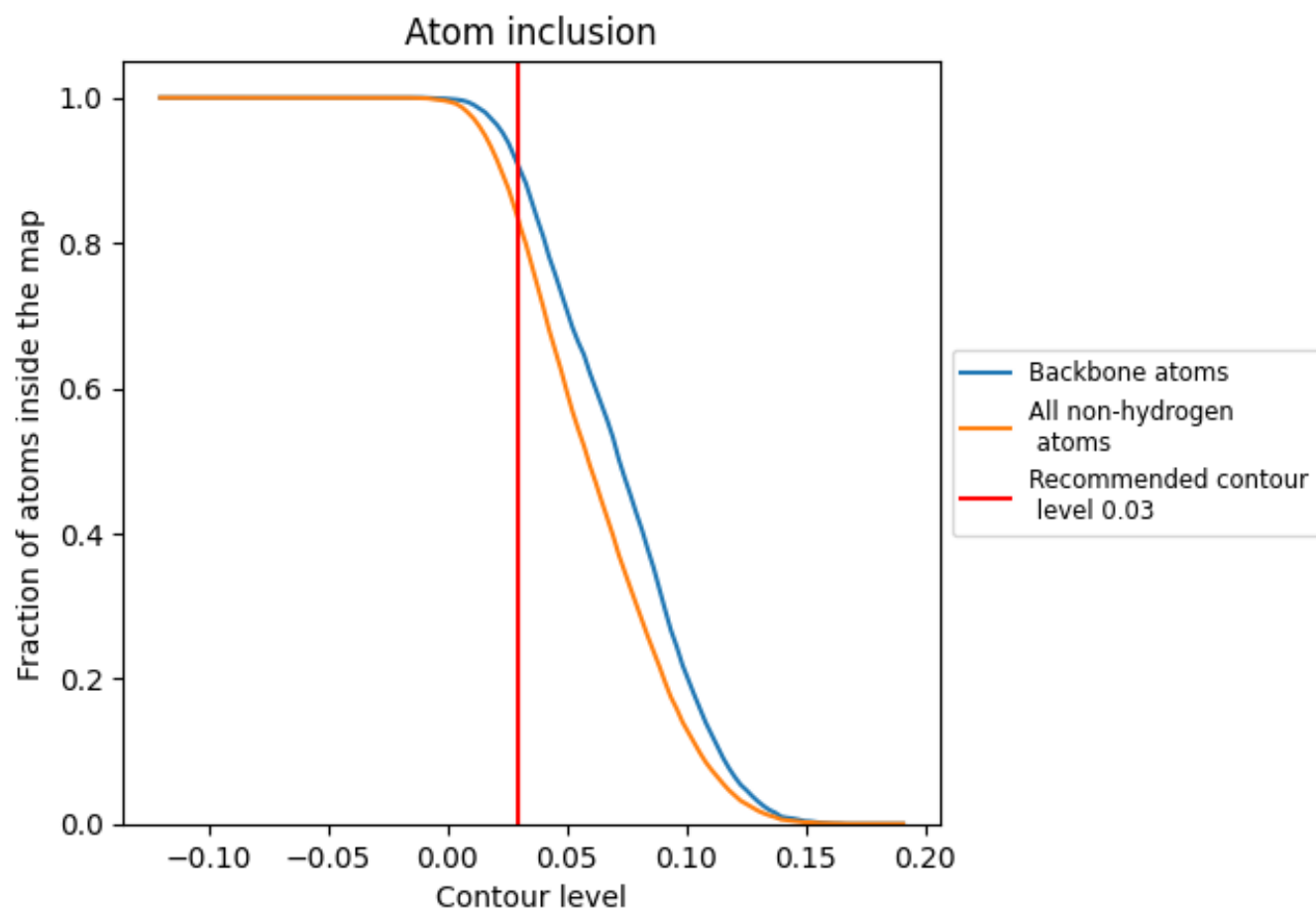
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 83% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8298	<div></div> 0.5390
A	<div></div> 0.6728	<div></div> 0.4960
C	<div></div> 0.5665	<div></div> 0.4510
E	<div></div> 0.7889	<div></div> 0.5060
S	<div></div> 0.8653	<div></div> 0.5540
T	<div></div> 0.8602	<div></div> 0.5470

