



wwPDB EM Validation Summary Report ⓘ

Nov 14, 2022 – 09:34 AM EST

PDB ID : 7K36
EMDB ID : EMD-22650
Title : Cryo-EM structure of STRIPAK complex
Authors : Jeong, B.-C.; Bai, X.C.
Deposited on : 2020-09-10
Resolution : 3.30 Å(reported)
Based on initial models : 4N6J, 2NPP, 2YMU, 5YF4

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) : 2.31.2

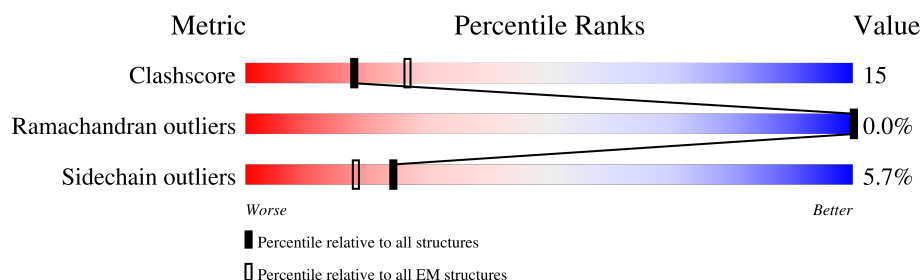
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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 ≥ 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	589	<div> <div>47%</div> <div>69%</div> <div>24%</div> <div>6%</div> </div>
2	B	713	<div> <div>9%</div> <div>22%</div> <div>19%</div> <div>58%</div> </div>
2	D	713	<div> <div>7%</div> <div>90%</div> </div>
2	E	713	<div> <div>6%</div> <div>91%</div> </div>
2	F	713	<div> <div>6%</div> <div>91%</div> </div>
2	G	713	<div> <div>6%</div> <div>92%</div> </div>
3	C	309	<div> <div>63%</div> <div>29%</div> <div>5%</div> </div>
4	H	225	<div> <div>10%</div> <div>45%</div> <div>32%</div> <div>21%</div> </div>

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Mol	Chain	Length	Quality of chain
5	I	837	 <div> <div>51%</div> <div>19%</div> <div>28%</div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 16613 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/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	554	Total	C	N	O	S	0	0
			3515	2209	625	671	10		

- Molecule 2 is a protein called Striatin-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	298	Total	C	N	O	S	0	0
			2296	1462	388	434	12		
2	D	74	Total	C	N	O	S	0	0
			621	394	118	107	2		
2	E	66	Total	C	N	O	S	0	0
			563	360	105	96	2		
2	F	62	Total	C	N	O	S	0	0
			510	327	94	87	2		
2	G	60	Total	C	N	O	S	0	0
			457	295	83	78	1		

- Molecule 3 is a protein called Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	293	Total	C	N	O	S	0	0
			2360	1494	402	449	15		

- Molecule 4 is a protein called MOB-like protein phocein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	177	Total	C	N	O	S	0	0
			1422	907	249	255	11		

- Molecule 5 is a protein called Striatin-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	599	Total	C	N	O	S	0	0
			4829	3107	831	859	32		

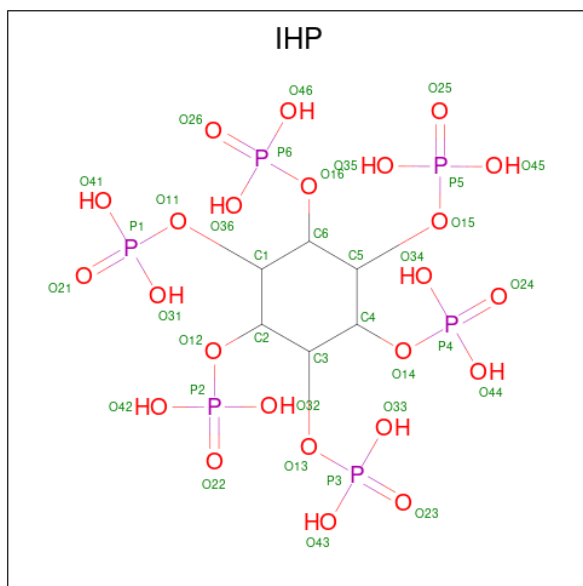
- Molecule 6 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		AltConf
6	C	2	Total	Mn	0
			2	2	

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
7	H	2	Total	Zn	0
			2	2	

- Molecule 8 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).

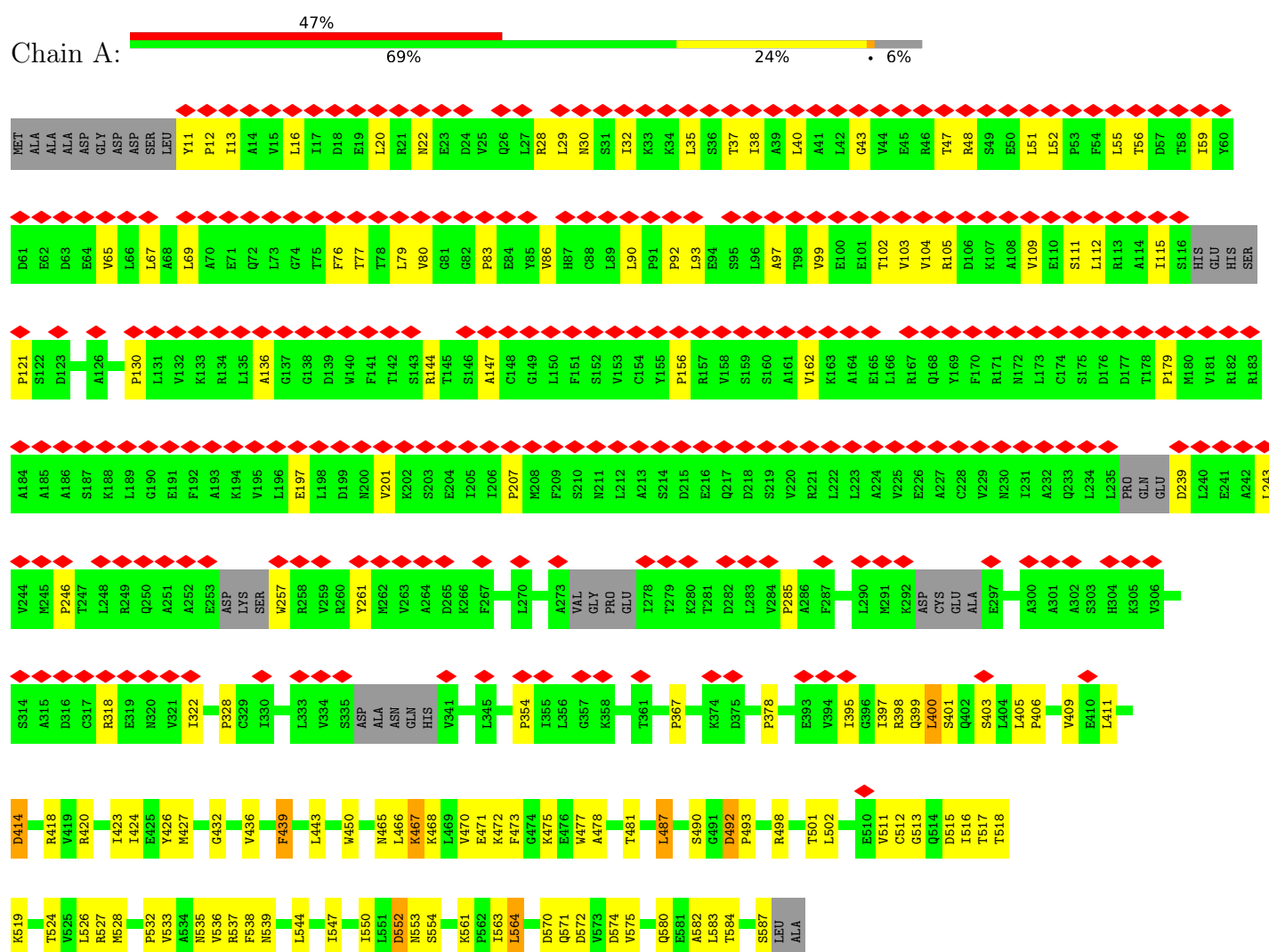


Mol	Chain	Residues	Atoms				AltConf
8	I	1	Total	C	O	P	0
			36	6	24	6	

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: Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform



- Molecule 2: Striatin-3



[illegible]

- Molecule 2: Striatin-3

Chain E: 6% 91%

[illegible]

[illegible]

- Molecule 2: Striatin-3

[illegible]

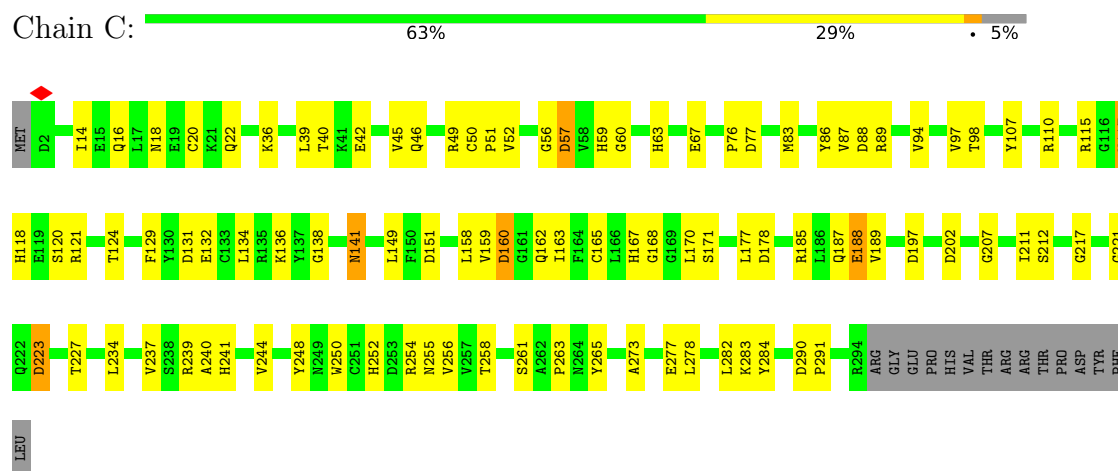
- Molecule 2: Striatin-3



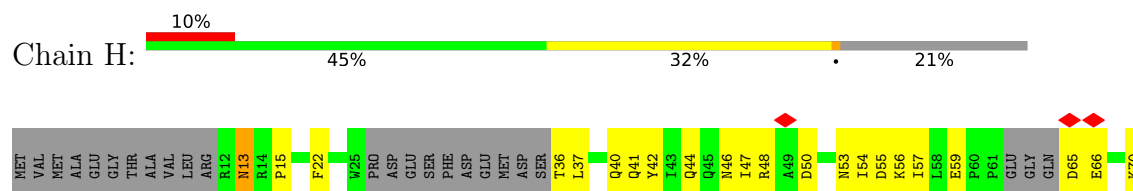
GLN	Q62	ASP	MET
	Y63	GLU	
	T64	LEU	
	I65	ALA	
	P66	GLY	
	G67	GLY	
	I68	GLY	
	L69	GLY	
	H70	GLY	
	Y71	GLY	
	I72	GLY	
	E75	GLY	
		MET	
	E82	ALA	
		ALA	
	W86	PRO	
		PRO	
		ARG	
	R90	GLN	
	A91	GLN	
	E92	GLN	
	L93	GLY	
	Q94	PRO	
	A95	GLY	
	I96	ASN	
	I97	LEU	
	A98	GLY	
	F99	LEU	
	L100	SER	
	Q101	PRO	
	G102	GLY	
	E103	ASN	
	R104	GLY	
	K105	ALA	
	G106	ALA	
	Q107	GLY	
	E108	GLY	
	N109	PRO	
	L110	PRO	
	K111	ALA	
	K112	SER	
	D113	GLY	
	L114	ALA	
	V115	GLY	
	R116	PRO	
	R117	ALA	
	I118	GLY	
	K119	PRO	
	M120	GLU	
	L121	LEU	
		SER	
		ARG	
		PRO	
GLU	TYR		
ALA	ALA		
LEU	LEU		
LYS	LYS		
GLN	GLN		
ARG	ARG		

[illegible]

- Molecule 3: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform



- Molecule 4: MOB-like protein phocein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	87779	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	59524	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.042	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	298.8, 298.8, 298.8	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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: IHP, ZN, MN

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	0.30	0/3546	0.49	11/4874 (0.2%)
2	B	0.30	0/2356	0.49	1/3218 (0.0%)
2	D	0.35	0/633	0.40	0/848
2	E	0.38	0/575	0.41	0/771
2	F	0.31	0/522	0.39	0/705
2	G	0.35	0/468	0.37	0/637
3	C	0.49	0/2417	0.49	0/3278
4	H	0.31	0/1456	0.42	0/1968
5	I	0.44	0/4923	0.45	0/6645
All	All	0.38	0/16896	0.46	12/22944 (0.1%)

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	PRO	N-CA-CB	5.96	110.45	103.30
1	A	354	PRO	N-CA-CB	5.94	110.43	103.30
1	A	130	PRO	N-CA-CB	5.85	110.32	103.30
1	A	179	PRO	N-CA-CB	5.79	110.25	103.30
1	A	367	PRO	N-CA-CB	5.74	110.19	103.30

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	A	3515	0	2859	93	0
2	B	2296	0	2217	102	0
2	D	621	0	608	16	0
2	E	563	0	557	20	0
2	F	510	0	479	17	0
2	G	457	0	403	16	0
3	C	2360	0	2258	71	0
4	H	1422	0	1361	59	0
5	I	4829	0	4877	126	0
6	C	2	0	0	0	0
7	H	2	0	0	0	0
8	I	36	0	6	5	0
All	All	16613	0	15625	480	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 15.

The worst 5 of 480 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)
4:H:110:CYS:HB3	4:H:119:CYS:SG	2.04	0.98
5:I:452:ASP:OD2	5:I:455:THR:HG22	1.66	0.95
4:H:13:ASN:N	4:H:13:ASN:HD22	1.65	0.93
5:I:452:ASP:OD2	5:I:455:THR:CG2	2.17	0.92
4:H:13:ASN:HD22	4:H:13:ASN:H	1.18	0.89

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	540/589 (92%)	515 (95%)	24 (4%)	1 (0%)	47	77
2	B	288/713 (40%)	258 (90%)	30 (10%)	0	100	100
2	D	72/713 (10%)	72 (100%)	0	0	100	100
2	E	64/713 (9%)	64 (100%)	0	0	100	100
2	F	60/713 (8%)	60 (100%)	0	0	100	100
2	G	58/713 (8%)	58 (100%)	0	0	100	100
3	C	291/309 (94%)	263 (90%)	28 (10%)	0	100	100
4	H	169/225 (75%)	159 (94%)	10 (6%)	0	100	100
5	I	579/837 (69%)	544 (94%)	35 (6%)	0	100	100
All	All	2121/5525 (38%)	1993 (94%)	127 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	VAL

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	240/512 (47%)	224 (93%)	16 (7%)	16	45
2	B	255/589 (43%)	238 (93%)	17 (7%)	16	45
2	D	59/589 (10%)	52 (88%)	7 (12%)	5	21
2	E	55/589 (9%)	50 (91%)	5 (9%)	9	31
2	F	47/589 (8%)	40 (85%)	7 (15%)	3	13
2	G	37/589 (6%)	35 (95%)	2 (5%)	22	53
3	C	258/274 (94%)	245 (95%)	13 (5%)	24	55
4	H	153/202 (76%)	147 (96%)	6 (4%)	32	62
5	I	522/739 (71%)	503 (96%)	19 (4%)	35	63
All	All	1626/4672 (35%)	1534 (94%)	92 (6%)	24	51

5 of 92 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	112	LYS
4	H	185	THR
2	F	65	ILE
2	G	70	HIS
5	I	113	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	101	GLN
4	H	82	ASN
5	I	664	ASN
4	H	13	ASN
4	H	89	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](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

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
8	IHP	I	901	-	36,36,36	1.38	6 (16%)	54,60,60	1.20	5 (9%)

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
8	IHP	I	901	-	-	5/30/54/54	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	901	IHP	P3-O13	3.30	1.65	1.59
8	I	901	IHP	P1-O11	2.93	1.64	1.59
8	I	901	IHP	P6-O16	2.61	1.64	1.59
8	I	901	IHP	P5-O15	2.47	1.64	1.59
8	I	901	IHP	P4-O14	2.37	1.63	1.59

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	901	IHP	C6-C5-C4	4.11	119.41	110.41
8	I	901	IHP	C5-C6-C1	3.63	118.36	110.41
8	I	901	IHP	C5-C4-C3	3.40	117.85	110.41
8	I	901	IHP	C3-C2-C1	2.52	115.92	110.41
8	I	901	IHP	O13-C3-C4	2.29	114.08	108.69

There are no chirality outliers.

All (5) torsion outliers are listed below:

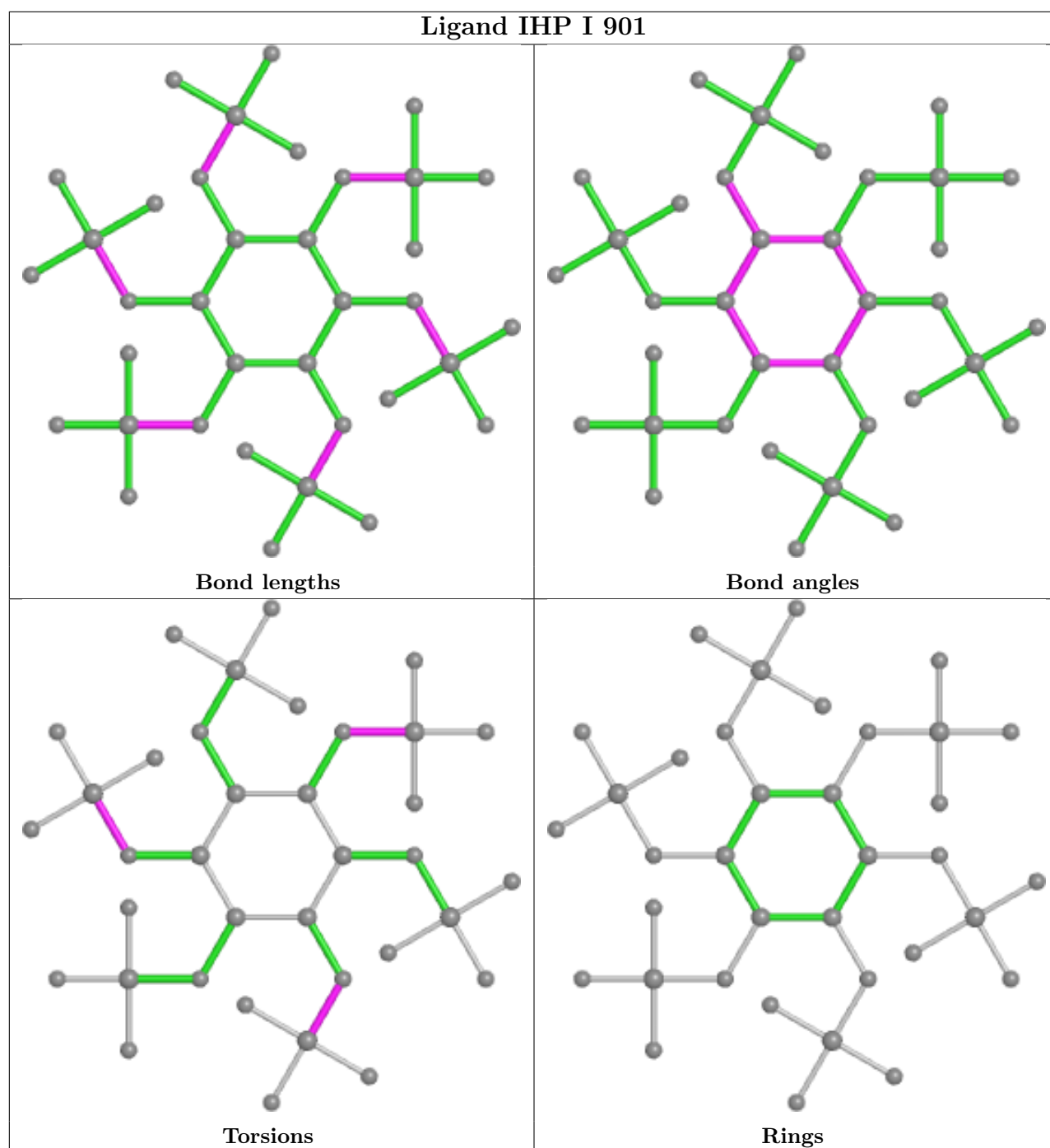
Mol	Chain	Res	Type	Atoms
8	I	901	IHP	C2-O12-P2-O42
8	I	901	IHP	C6-O16-P6-O36
8	I	901	IHP	C4-O14-P4-O44
8	I	901	IHP	C4-O14-P4-O34
8	I	901	IHP	C6-O16-P6-O46

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	I	901	IHP	5	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.

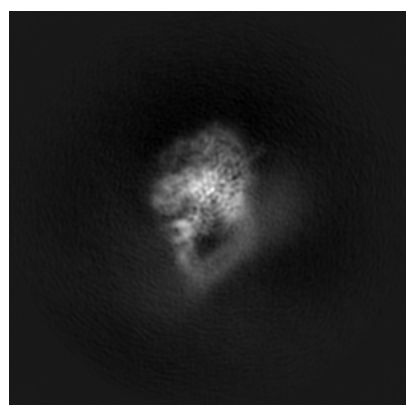
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22650. These allow visual inspection of the internal detail of the map and identification of artifacts.

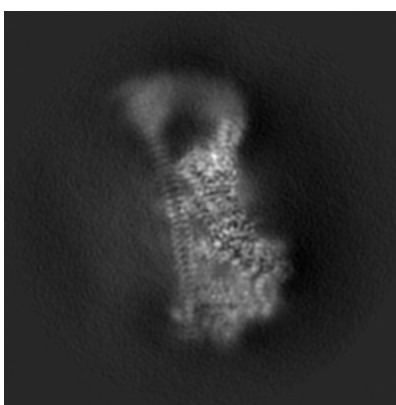
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

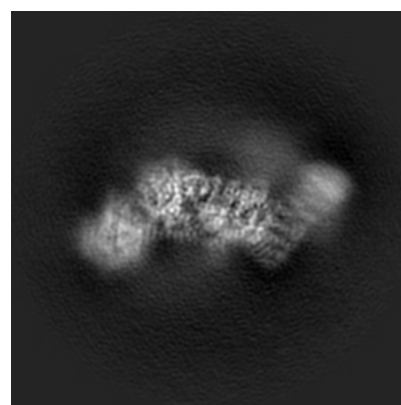
6.1.1 Primary map



X



Y

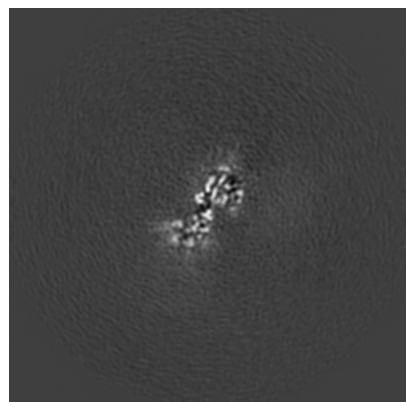


Z

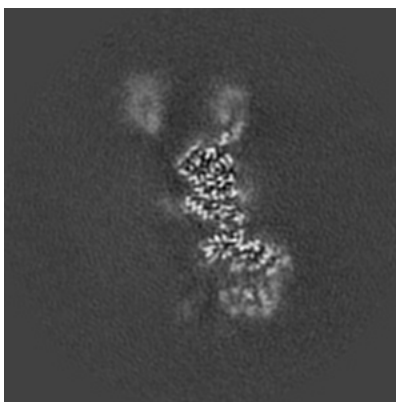
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

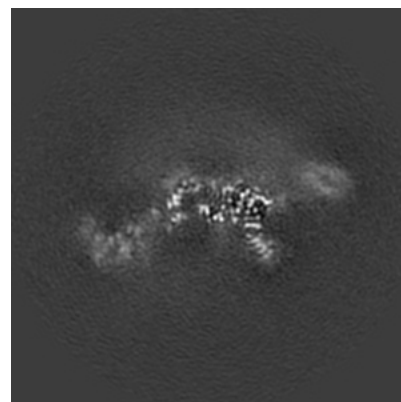
6.2.1 Primary map



X Index: 180



Y Index: 180

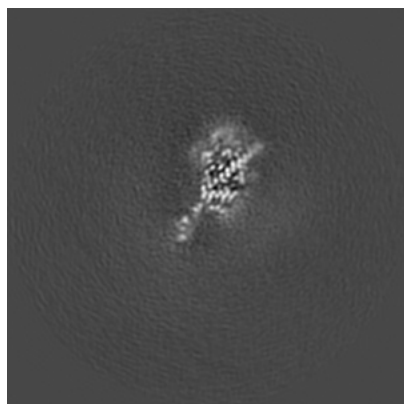


Z Index: 180

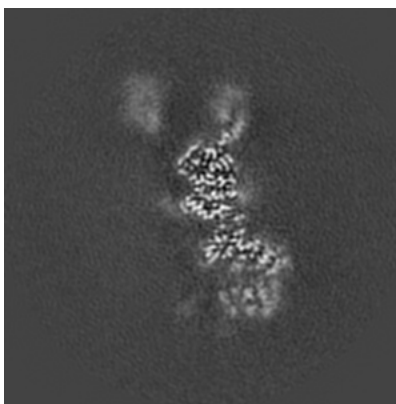
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

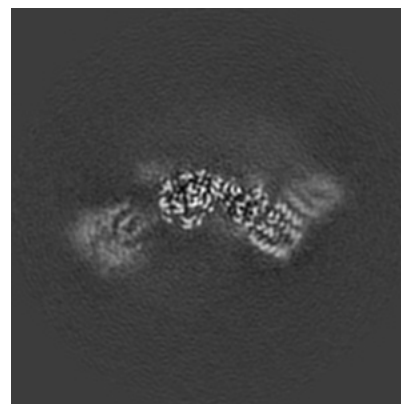
6.3.1 Primary map



X Index: 149



Y Index: 179

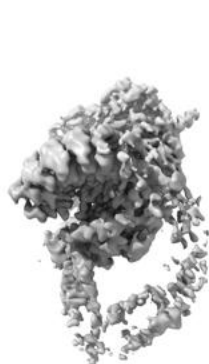


Z Index: 199

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

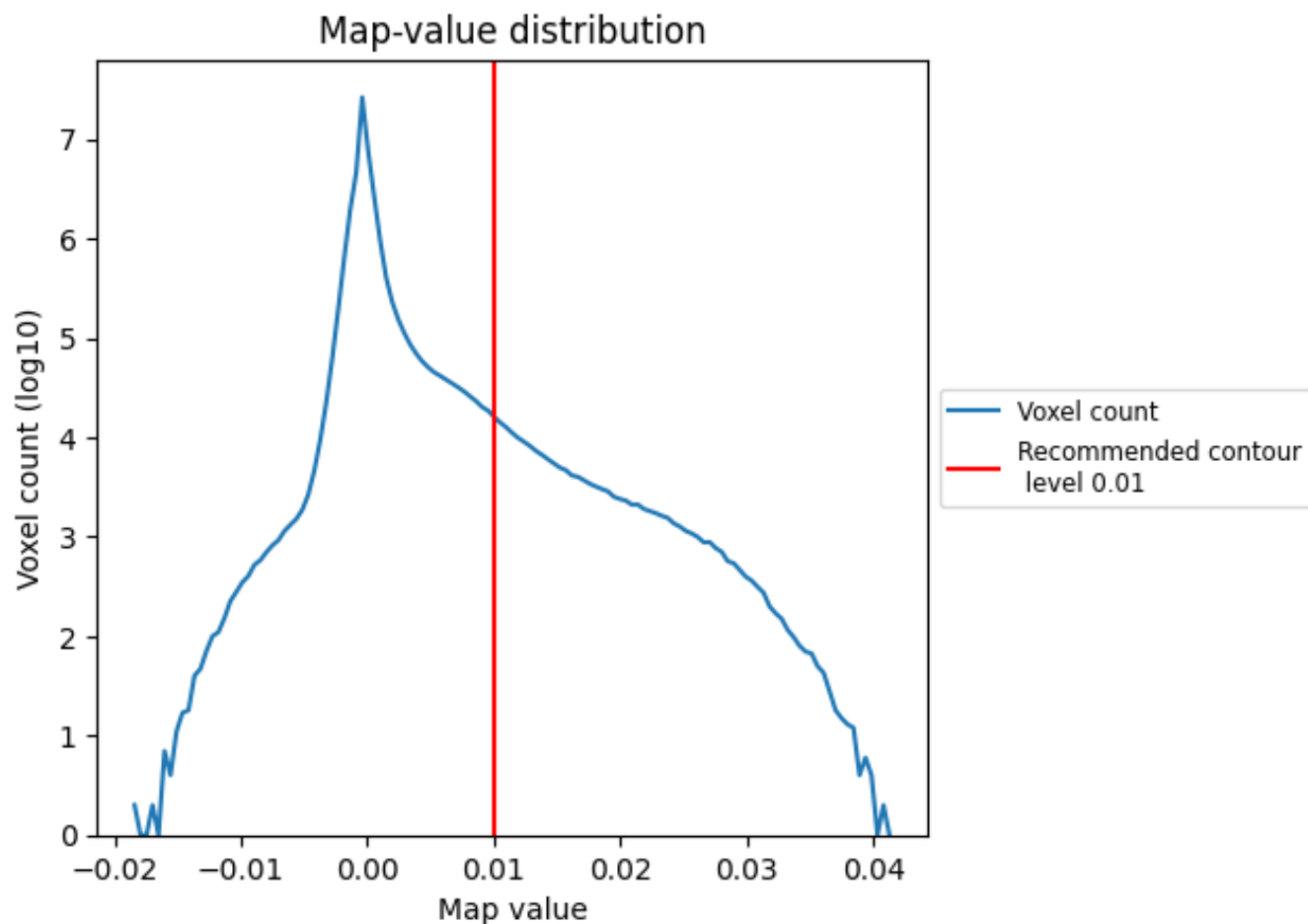
6.5 Mask visualisation

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

7 Map analysis [i](#)

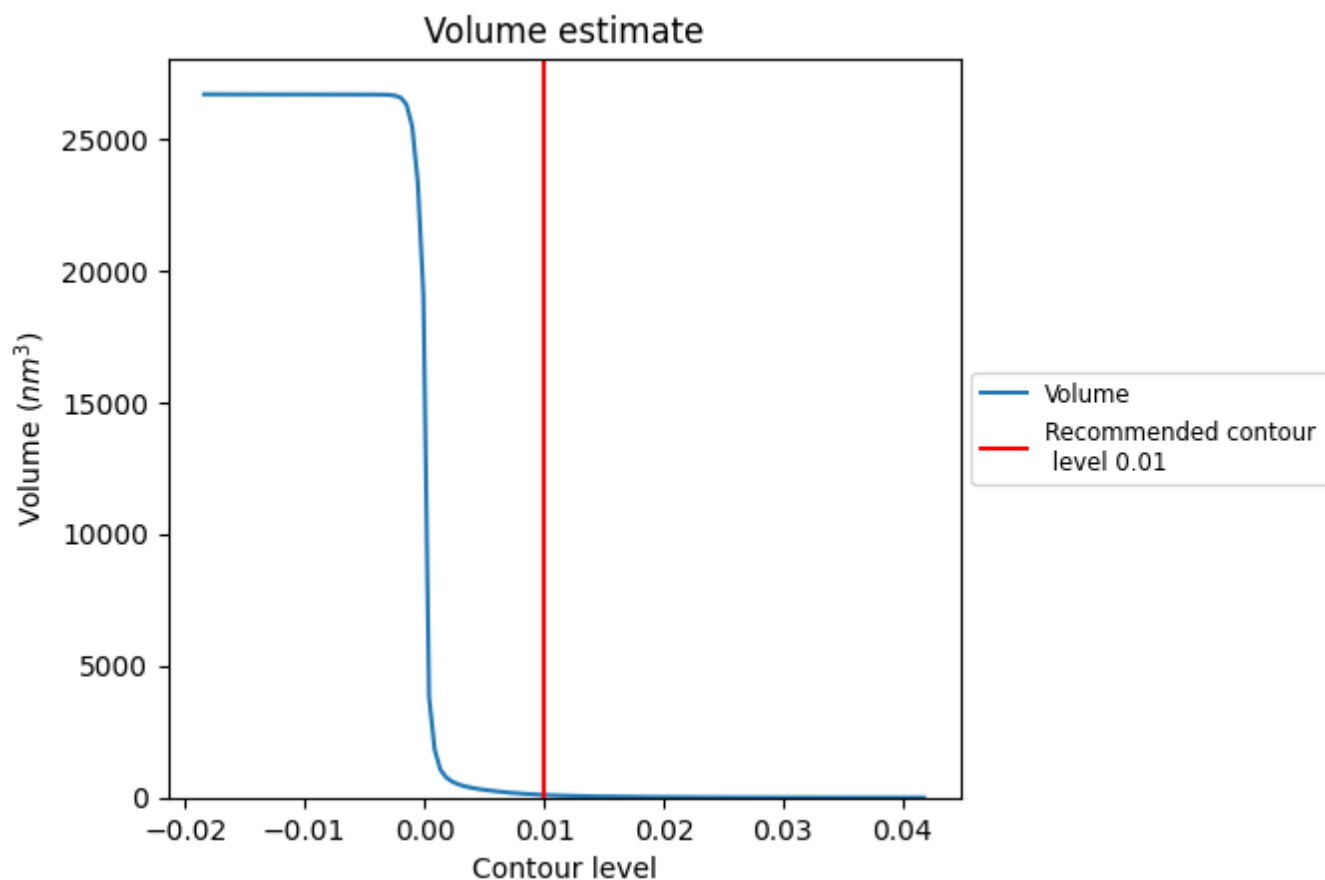
This section contains the results of statistical analysis of the map.

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.

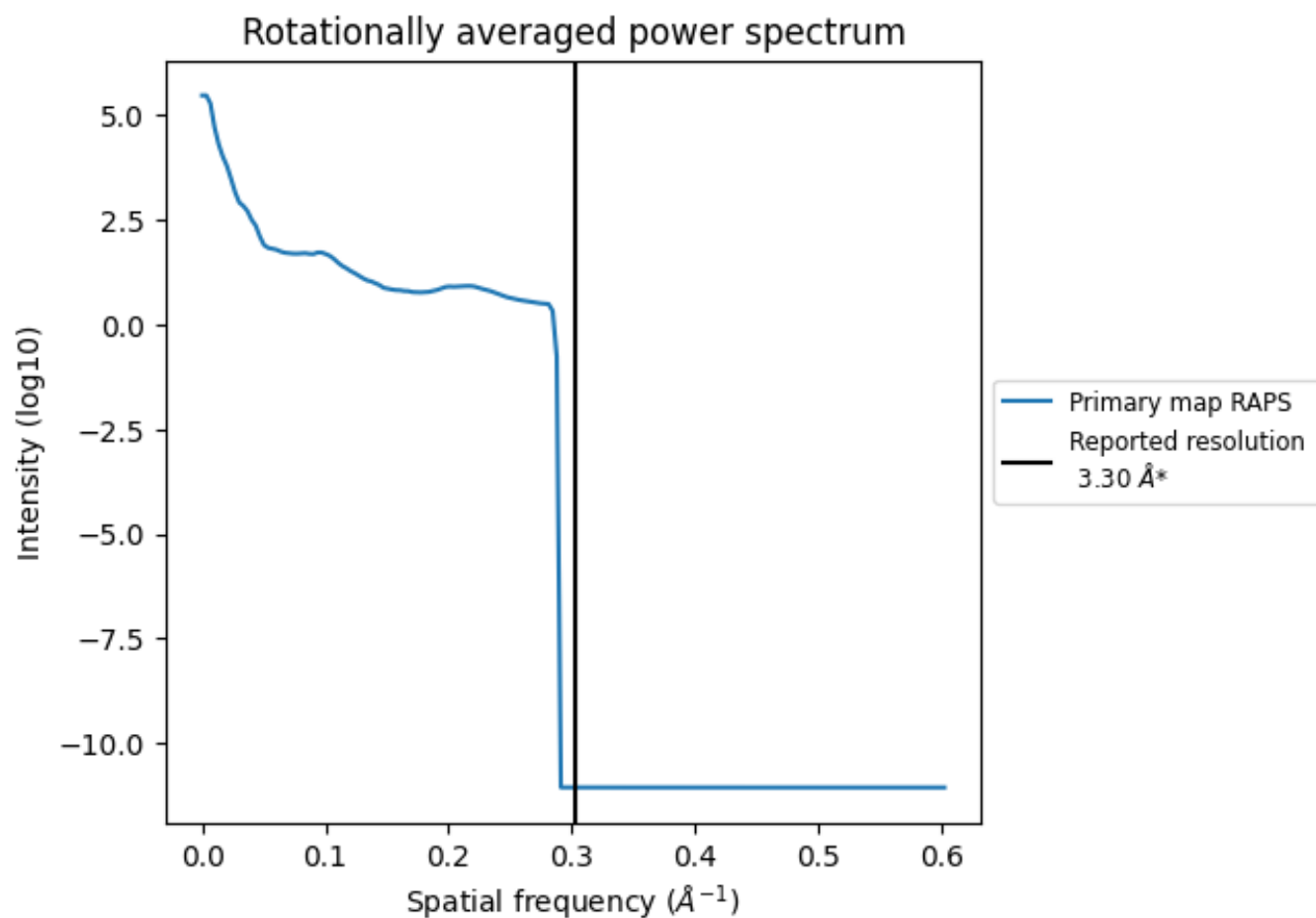
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 100 nm³; this corresponds to an approximate mass of 90 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 Å⁻¹

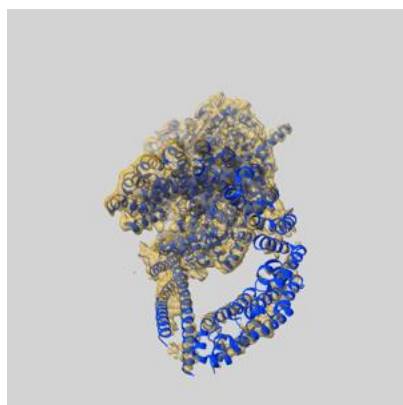
8 Fourier-Shell correlation

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

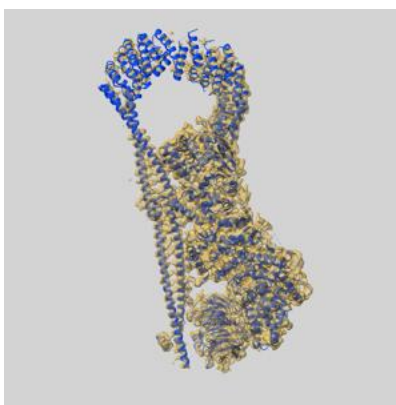
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22650 and PDB model 7K36. Per-residue inclusion information can be found in section [3](#) on page [6](#).

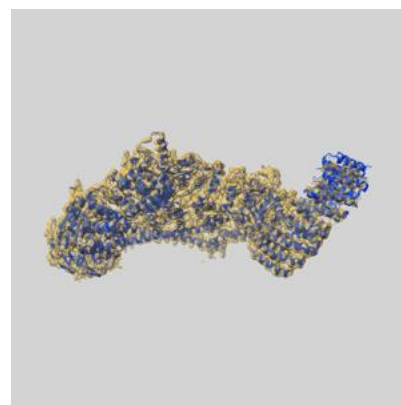
9.1 Map-model overlay [i](#)



X



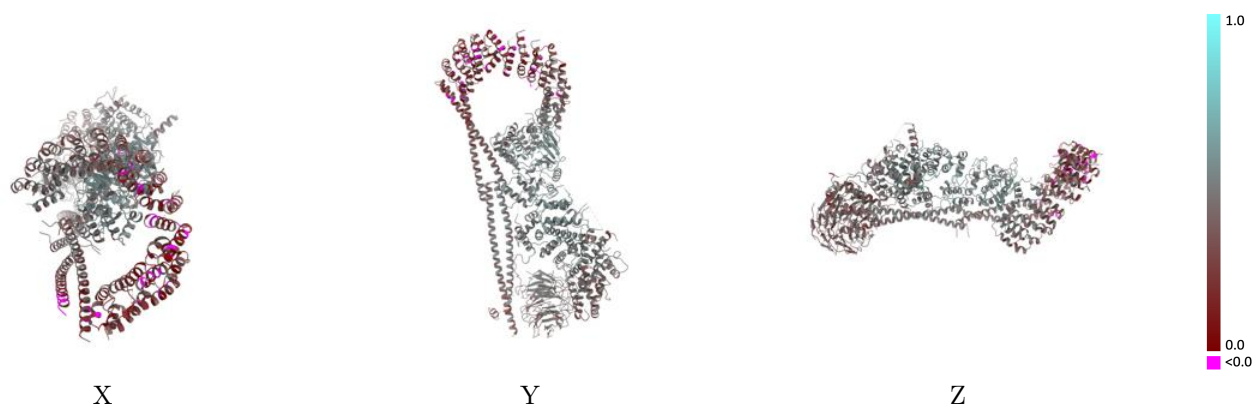
Y



Z

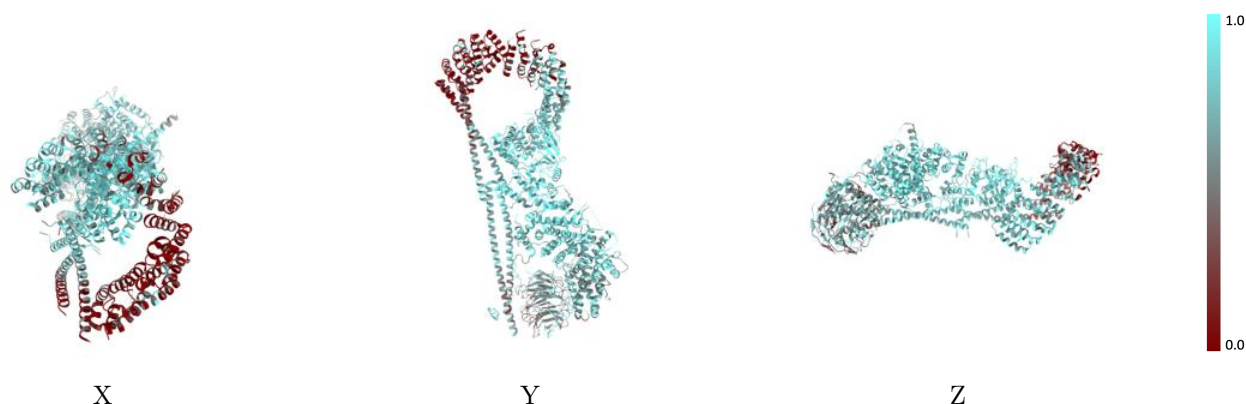
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



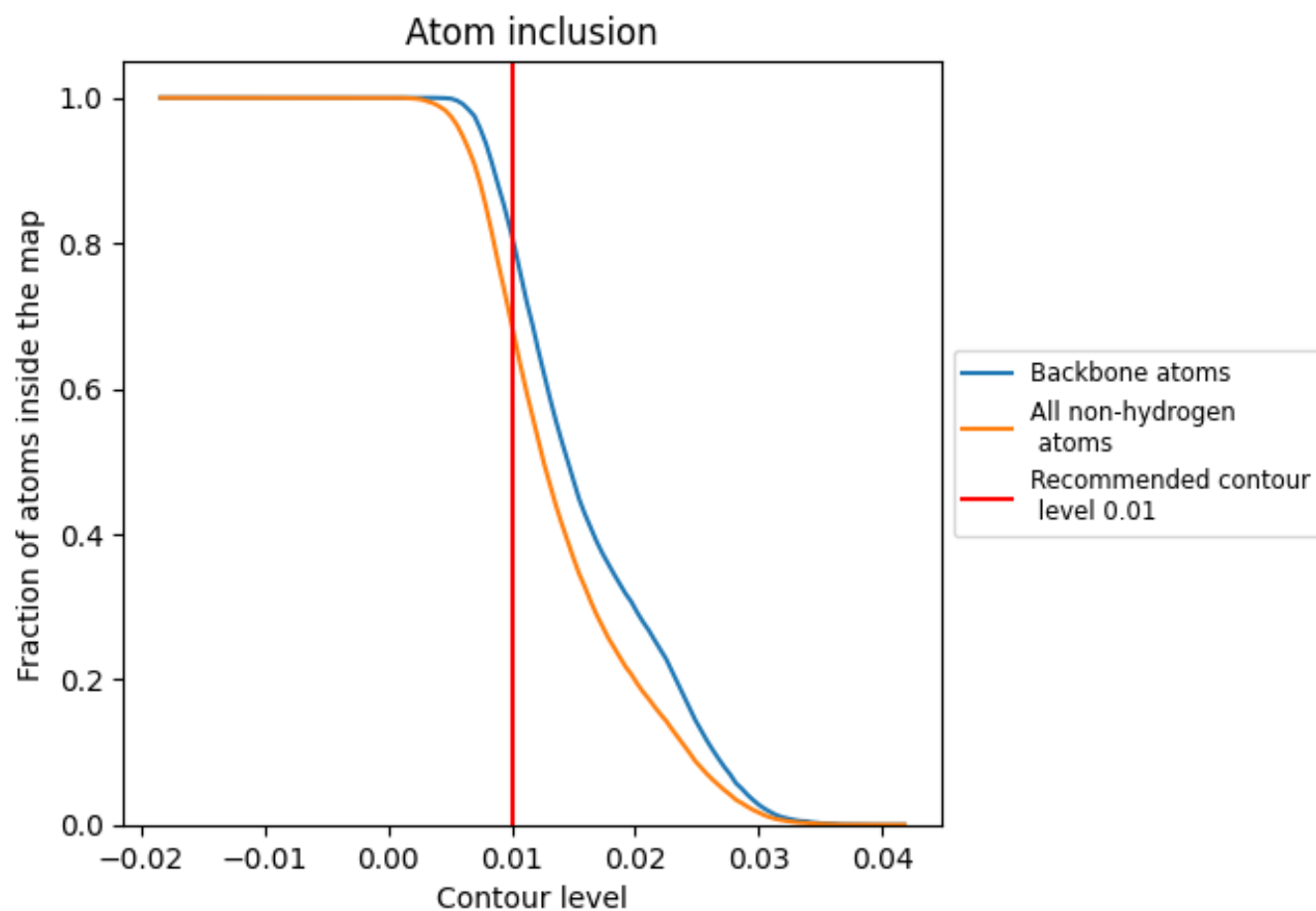
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 69% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6878	<div></div> 0.4300
A	<div></div> 0.4694	<div></div> 0.3250
B	<div></div> 0.5882	<div></div> 0.4170
C	<div></div> 0.8727	<div></div> 0.5170
D	<div></div> 0.6883	<div></div> 0.4200
E	<div></div> 0.7188	<div></div> 0.4350
F	<div></div> 0.5598	<div></div> 0.3450
G	<div></div> 0.5438	<div></div> 0.3310
H	<div></div> 0.6562	<div></div> 0.3900
I	<div></div> 0.8375	<div></div> 0.4990

1.0

0.0

<0.0