



wwPDB EM Validation Summary Report ⓘ

Mar 27, 2026 – 02:27 AM UTC

PDB ID : 7PW6 / pdb_00007pw6
EMDB ID : EMD-13676
Title : Human SMG1-8-9 kinase complex bound to a SMG1 inhibitor - SMG1 body
Authors : Langer, L.M.; Conti, E.
Deposited on : 2021-10-06
Resolution : 3.05 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

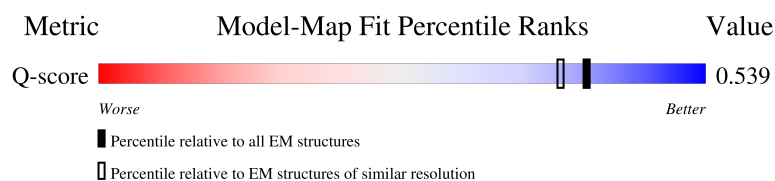
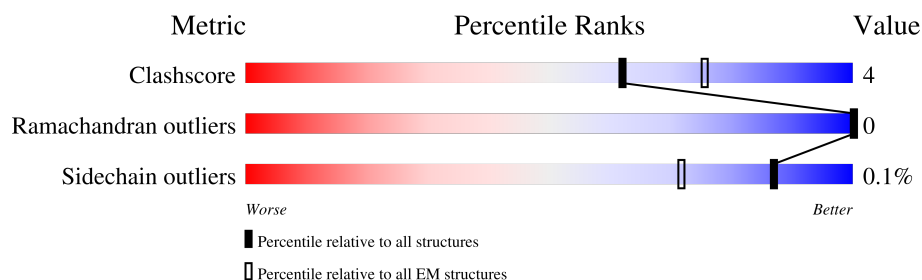
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.05 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13971 (2.55 - 3.55)

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	2896	44% 5% 51%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10393 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.

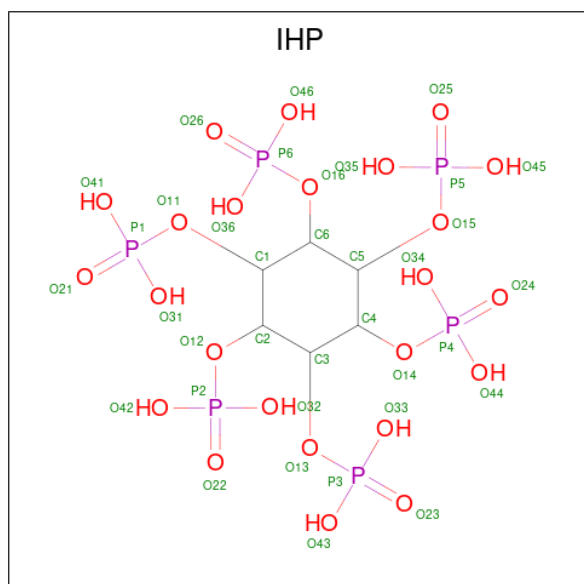
- Molecule 1 is a protein called Serine/threonine-protein kinase SMG1, Serine/threonine-protein kinase SMG1, Serine/threonine-protein kinase SMG1, Serine/threonine-protein kinase SMG1, Serine/threonine-protein kinase SMG1, Serine/threonine-protein kinase SMG1, Serine/threonine-protein kinase SMG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1416	Total	C	N	O	S	0	0
			10318	6612	1844	1810	52		

There are 2 discrepancies between the modelled and reference sequences:

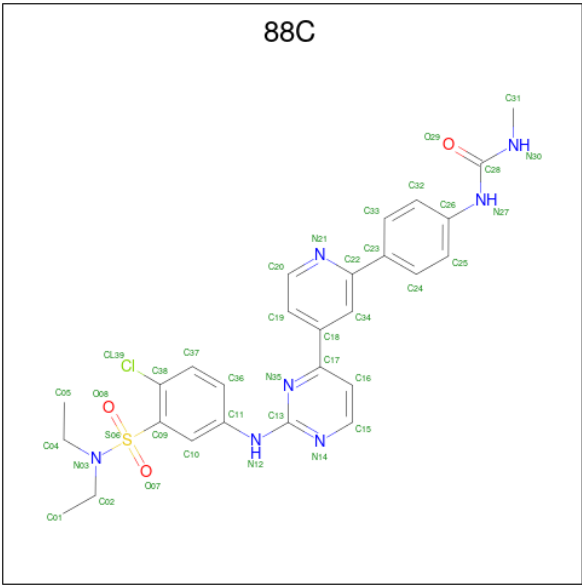
Chain	Residue	Modelled	Actual	Comment	Reference
A	1209	SER	ALA	conflict	UNP Q96Q15
A	1269	ASN	ASP	conflict	UNP Q96Q15

- Molecule 2 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 3 is 1-[4-[4-[2-[[4-chloranyl-3-(diethylsulfamoyl)phenyl]amino]pyrimidin-4-yl]pyrimidin-2-yl]phenyl]-3-methyl-urea (CCD ID: 88C) (formula: C₂₇H₂₈ClN₇O₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	Cl	N	O	S	
3	A	1	39	27	1	7	3	1	0



GLU ARG ASN	33607	ASN	THR	HIS	GLU	VAL	ASP	HIS	PRO	SER
	33608	GLN	GLY	GLU	HIS	LYS	VAL	ILE	ILE	ASN
	33609	LYS	THR	LYS	LEU	LEU	LEU	GLY	SER	PHE
		THR	GLN	GLN	LYS	ALA	TRP	GLU	SER	GLU
	33623	PRO	PRO	ILE	MET	ALA	LEU	LEU	ARG	LEU
	33627	ASP	THR	THR	LYS	ALA	LEU	SER	THR	THR
	33640	MET	THR	THR	ASP	ASP	ALA	ASN	ALA	ARG
	33644	ASN	GLN	LYS	GLU	GLU	GLY	ASP	LYS	THR
	33658	ALA	ALA	LYS	LEU	ALA	LEU	LEU	GLN	ALA
	33661	ARG	LYS	THR	GLN	ASP	ASP	GLN	ASN	LEU
GLU ARG ASN	33667	ILE	ILE	SER	GLY	GLY	GLY	MET	MET	LEU
	33670	GLN	GLN	GLN	ASP	ASP	GLY	THR	THR	ALA
	33673	ASN	ALA	ILE	VAL	VAL	PRO	ARG	ARG	PHE
	33676	LEU	ALA	ASN	TYR	TYR	GLU	GLY	GLY	GLU
	33679	THR	THR	ASN	ASN	ASN	GLU	ILE	ILE	LEU
	33682	ALA	ALA	VAL	VAL	VAL	GLY	ILE	CYS	ARG
	33685	ASP	ASP	SER	SER	VAL	VAL	LYS	LYS	GLY
	33688	THR	THR	PHE	PHE	ARG	ARG	GLN	GLN	CYS
	33691	PRO	PRO	ALA	GLN	GLN	GLN	GLN	GLN	GLN
	33694	PRO	SER	SER	PHE	PHE	LEU	LEU	LEU	GLN

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	228291	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 ($e^-/\text{\AA}^2$)	89.32	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	5.024	Depositor
Minimum map value	-2.795	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.073	Depositor
Recommended contour level	0.586	Depositor
Map size ($\text{\AA}$)	326.86078, 326.86078, 326.86078	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.8511999, 0.8511999, 0.8511999	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: 88C, IHP

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	0.12	0/10141	0.34	0/13823

There are no bond length outliers.

There are no bond angle outliers.

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	10318	0	9648	87	0
2	A	36	0	6	4	0
3	A	39	0	0	0	0
All	All	10393	0	9654	87	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 4.

The worst 5 of 87 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:2293:PRO:HB3	1:A:2377:GLN:HG2	1.71	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1300:LEU:HD22	1:A:1364:VAL:HG22	1.77	0.67
1:A:2372:PRO:HD2	1:A:3644:ALA:HB2	1.77	0.66
1:A:963:GLN:O	1:A:979:ARG:NH2	2.28	0.65
1:A:2193:TYR:OH	1:A:2353:ILE:O	2.15	0.64

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	1298/2896 (45%)	1261 (97%)	37 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	964/2393 (40%)	963 (100%)	1 (0%)	88	89

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1831	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1542	GLN
1	A	1825	GLN
1	A	2315	GLN
1	A	2206	GLN
1	A	2278	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
3	88C	A	3702	-	42,42,42	1.39	6 (14%)	57,59,59	1.97	13 (22%)
2	IHP	A	3701	-	36,36,36	1.58	6 (16%)	60,60,60	0.94	3 (5%)

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	88C	A	3702	-	-	3/34/34/34	0/4/4/4
2	IHP	A	3701	-	-	5/30/54/54	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3701	IHP	P5-O15	3.60	1.65	1.59
2	A	3701	IHP	P3-O13	3.49	1.65	1.59
2	A	3701	IHP	P4-O14	3.41	1.65	1.59
3	A	3702	88C	C28-N27	3.32	1.44	1.37
2	A	3701	IHP	P2-O12	3.26	1.65	1.59

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3702	88C	C37-C38-C09	6.54	124.30	120.04
3	A	3702	88C	C10-C09-S06	5.45	124.28	117.53
3	A	3702	88C	C10-C09-C38	-5.27	112.81	118.33
3	A	3702	88C	N27-C28-N30	4.58	120.66	114.68
3	A	3702	88C	C32-C26-C25	-3.12	114.90	119.04

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	3701	IHP	C4-C3-O13-P3
2	A	3701	IHP	C6-C5-O15-P5
3	A	3702	88C	C04-N03-S06-O08
2	A	3701	IHP	C2-C3-O13-P3
3	A	3702	88C	C04-N03-S06-C09

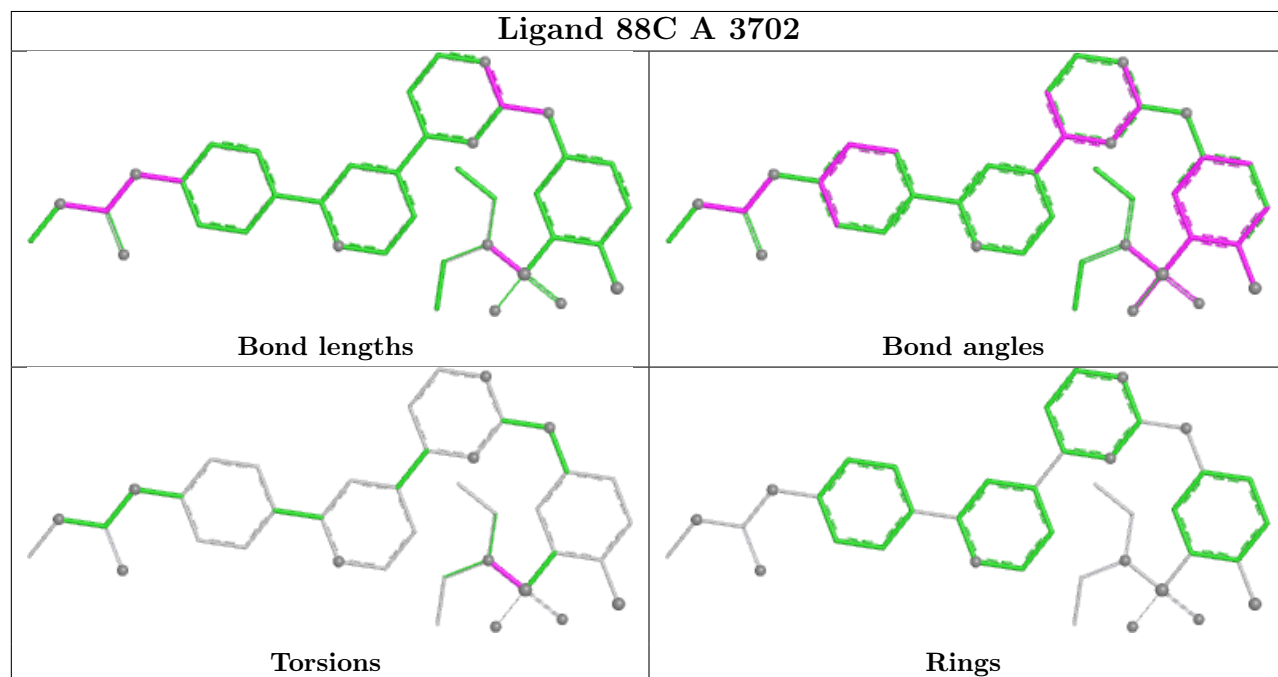
There are no ring outliers.

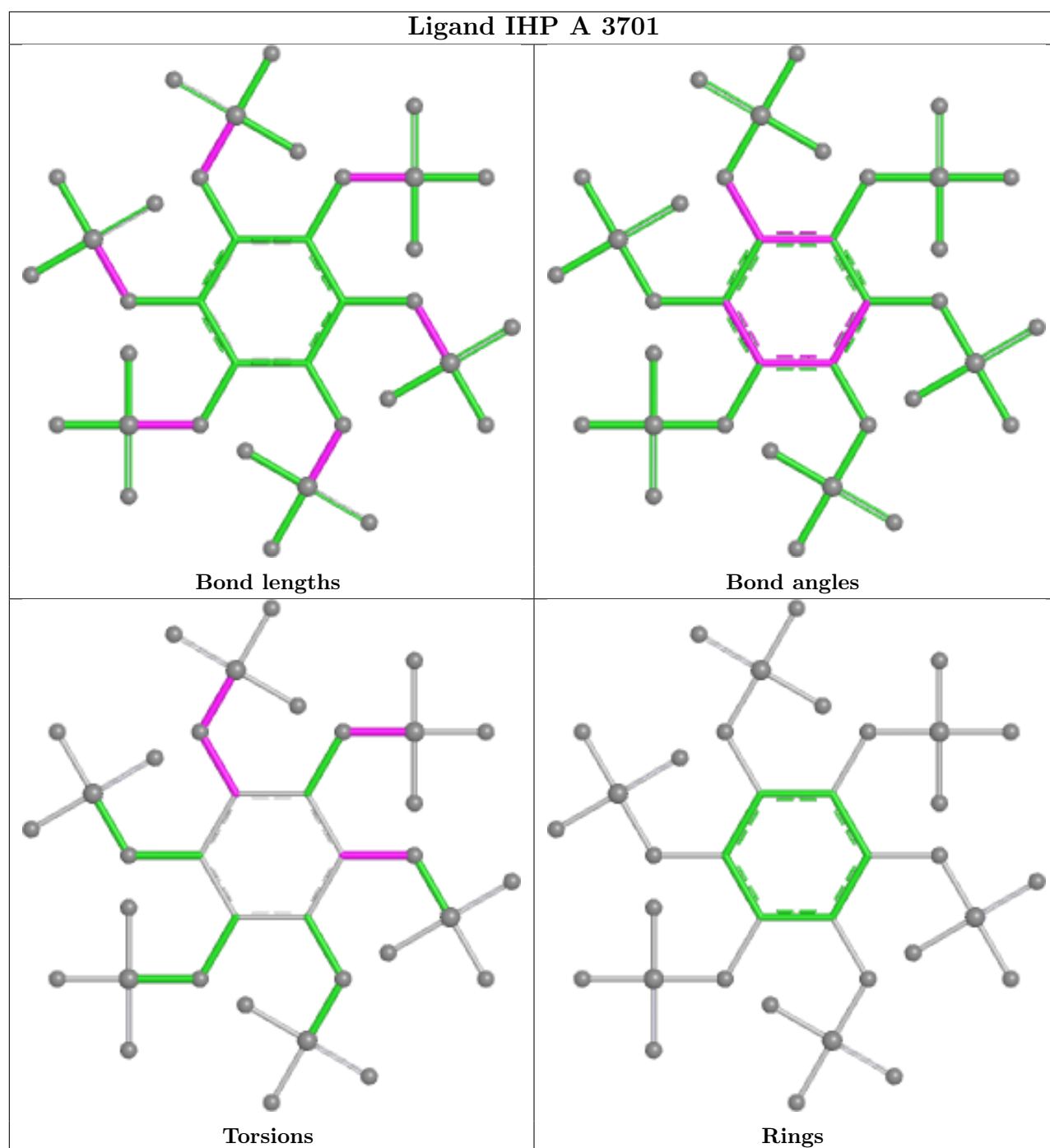
1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3701	IHP	4	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.

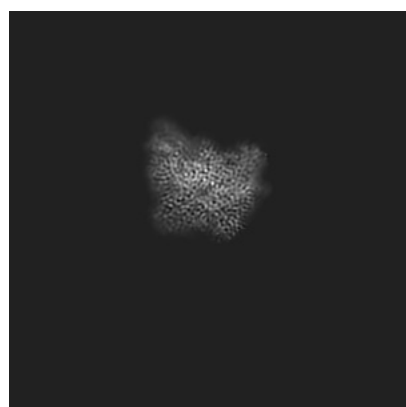
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13676. These allow visual inspection of the internal detail of the map and identification of artifacts.

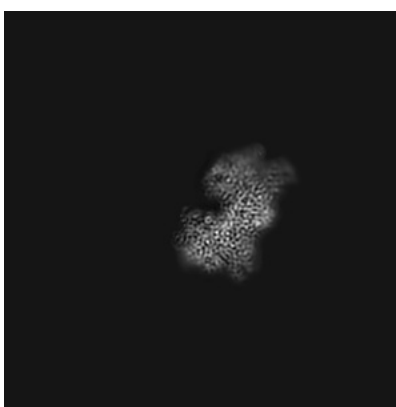
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

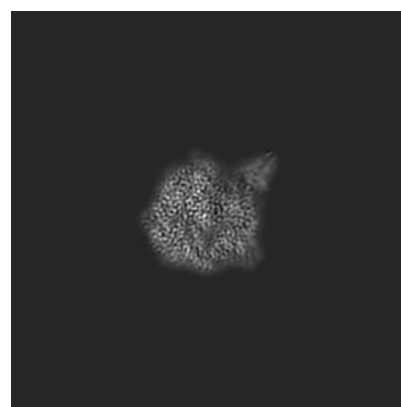
6.1.1 Primary map



X



Y

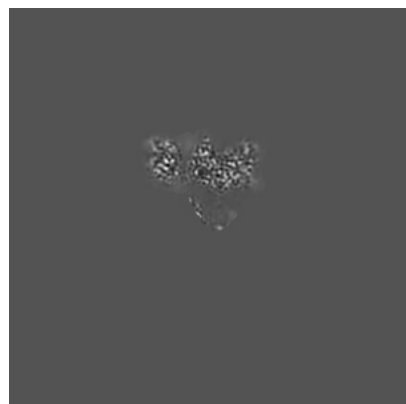


Z

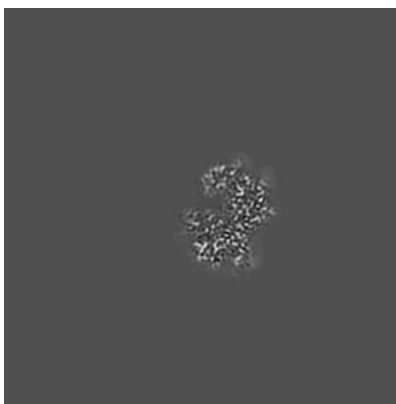
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

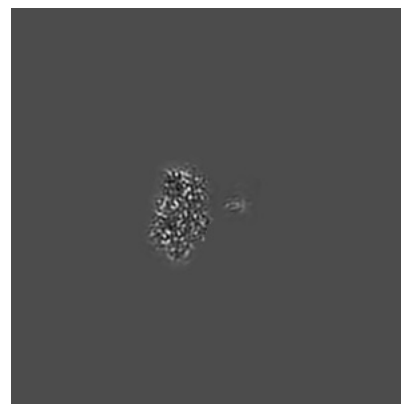
6.2.1 Primary map



X Index: 192



Y Index: 192



Z Index: 192

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

6.3 Largest variance slices [i](#)

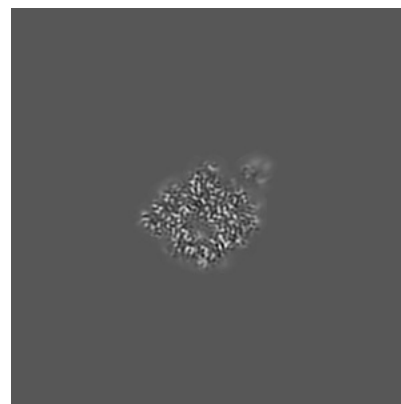
6.3.1 Primary map



X Index: 176



Y Index: 200

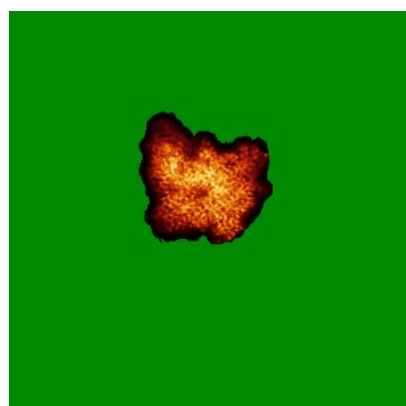


Z Index: 225

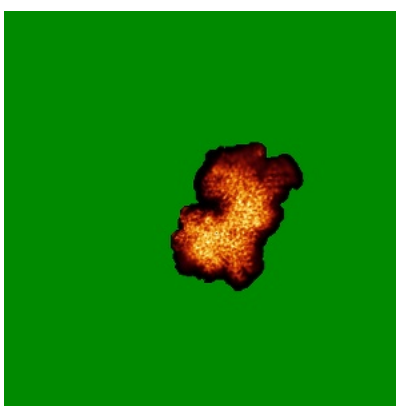
The images above show the largest variance slices of the map in three orthogonal directions.

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

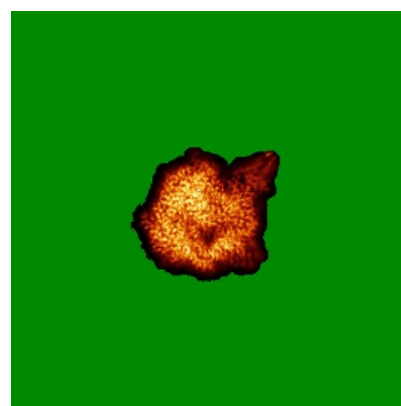
6.4.1 Primary map



X



Y

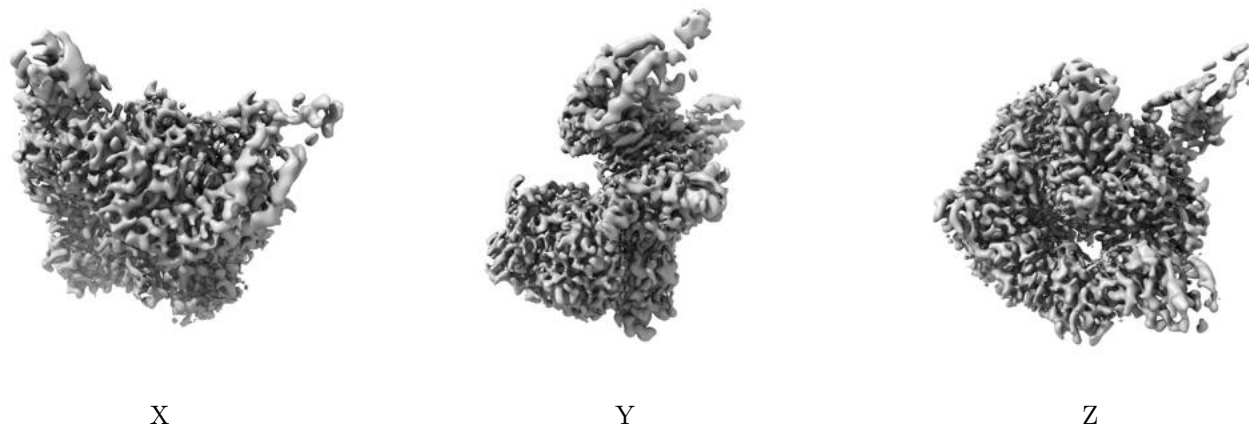


Z

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

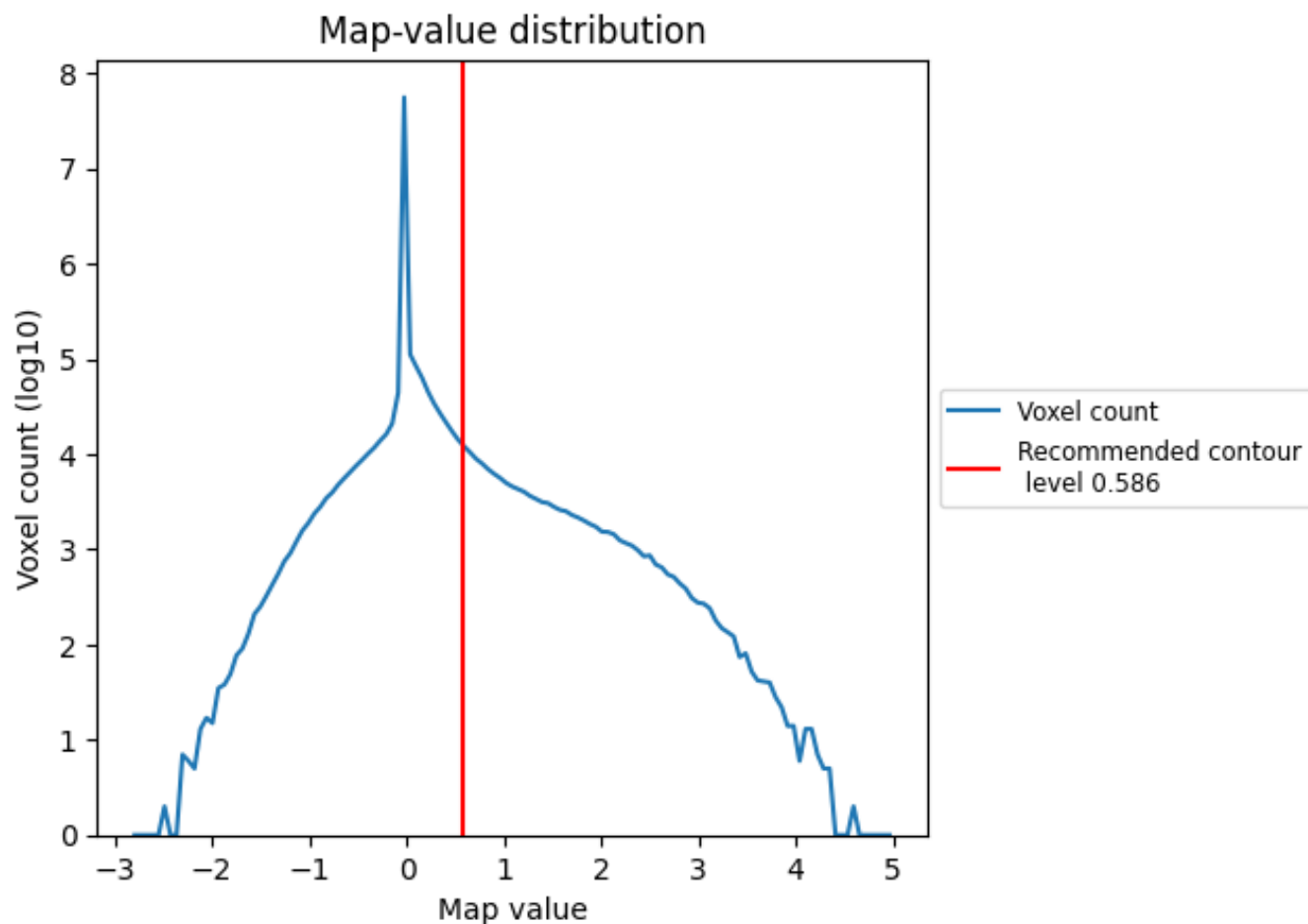
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

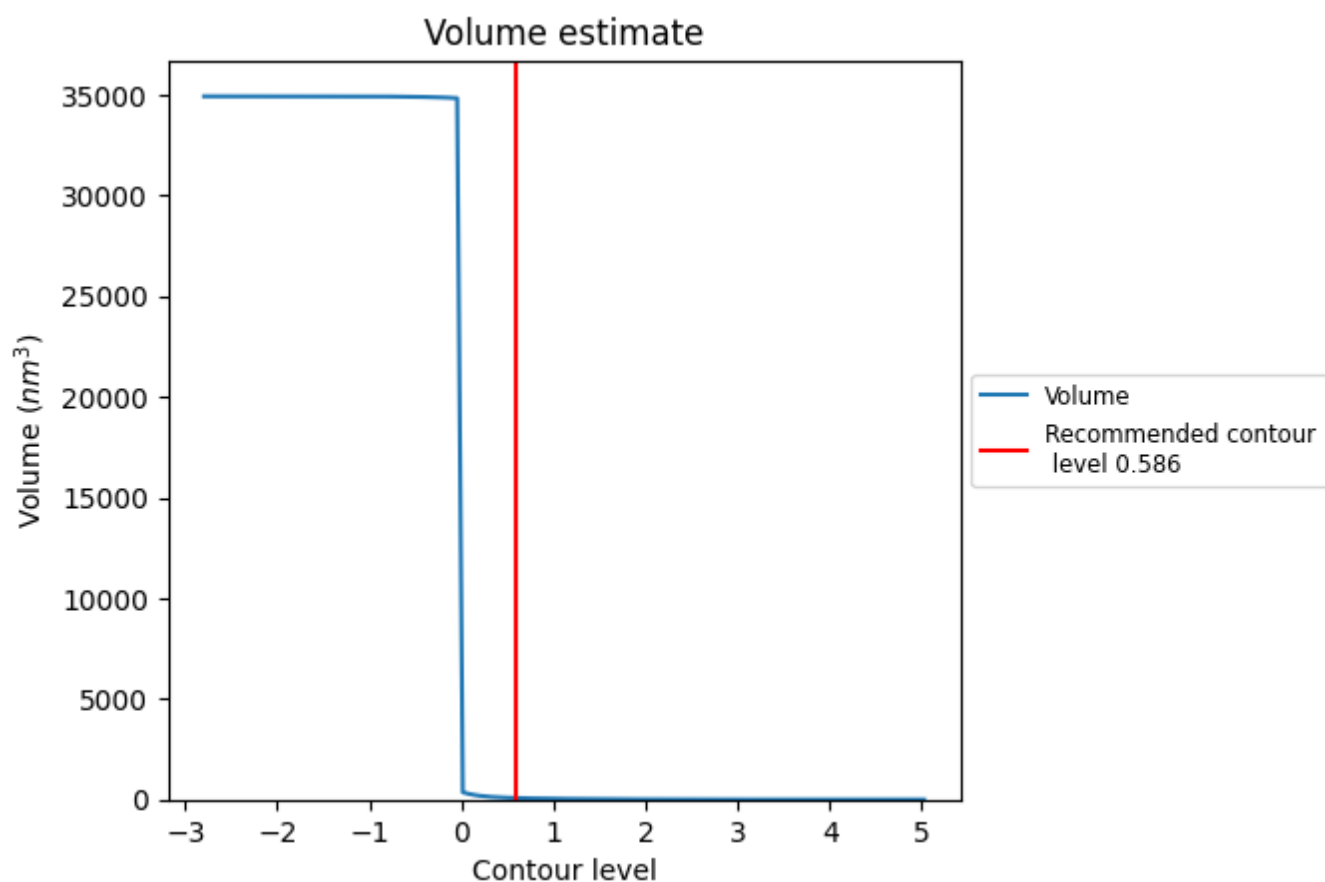
This section contains the results of statistical analysis of the map.

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.

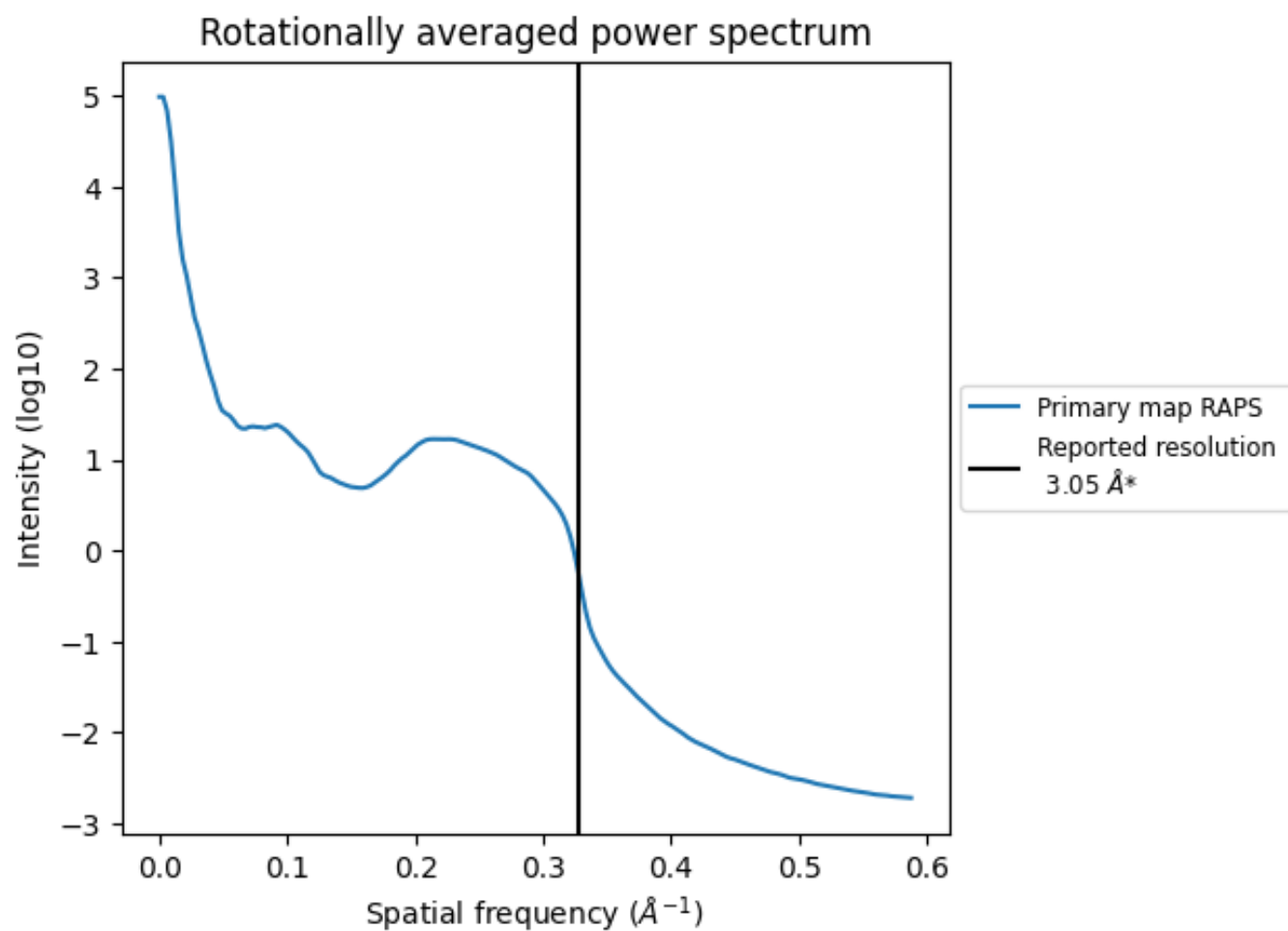
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 77 nm^3 ; this corresponds to an approximate mass of 69 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 0.328 Å⁻¹

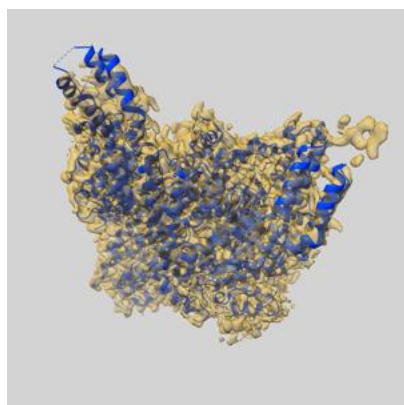
8 Fourier-Shell correlation

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

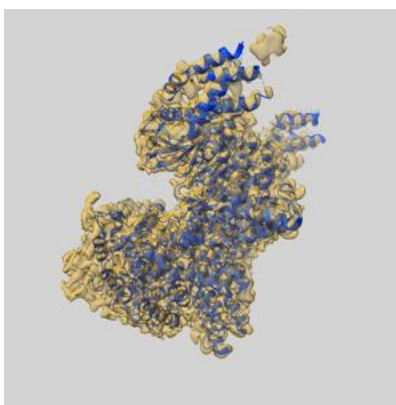
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13676 and PDB model 7PW6. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

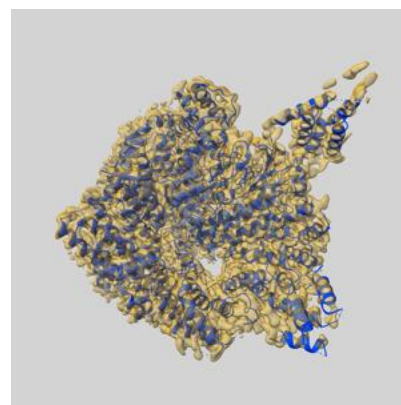
9.1 Map-model overlay [i](#)



X



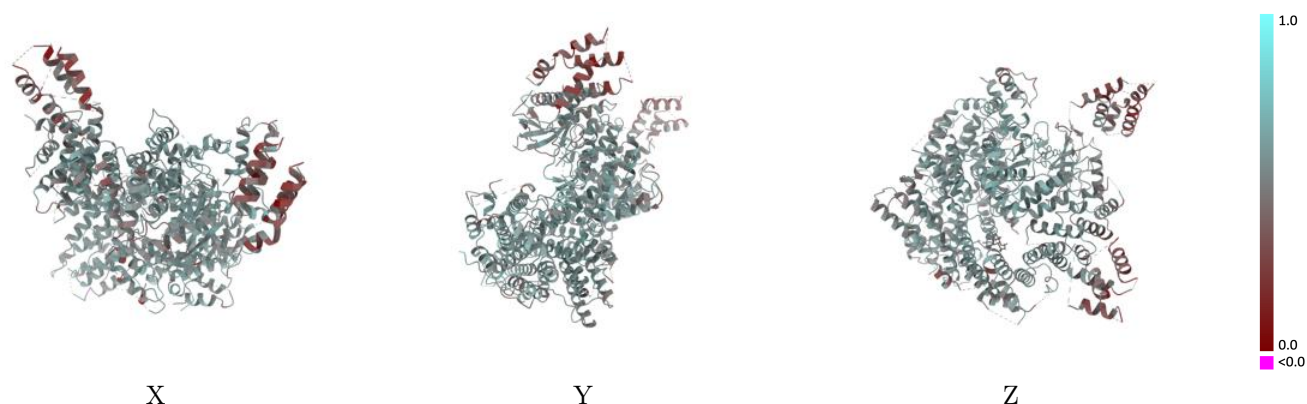
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.586 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](#)



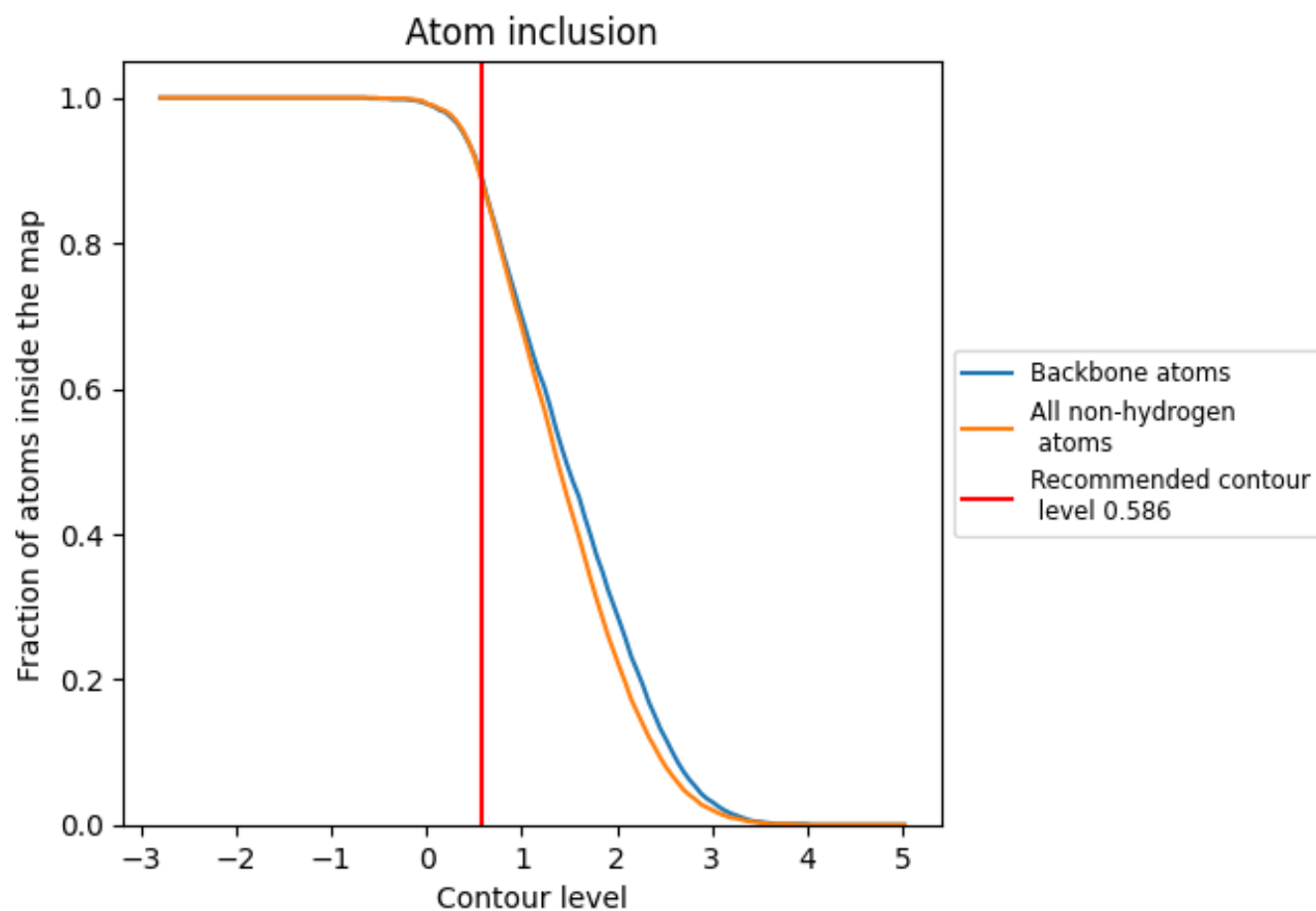
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.586).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 88% 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 (0.586) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8840	0.5390
A	0.8840	0.5390

