



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 05:30 PM UTC

PDB ID : 8UPM / pdb_00008upm
EMDB ID : EMD-42452
Title : Pfr state of Stigmatella aurantiaca bacteriophytochrome 2
Authors : Malla, T.N.; Schmidt, M.; Stojkovic, E.A.
Deposited on : 2023-10-23
Resolution : 3.75 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:

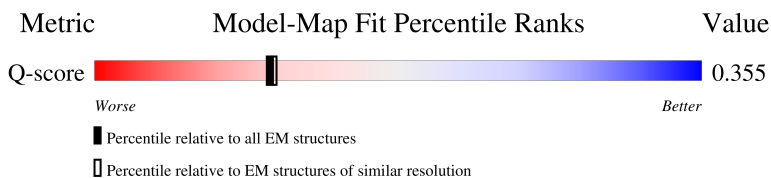
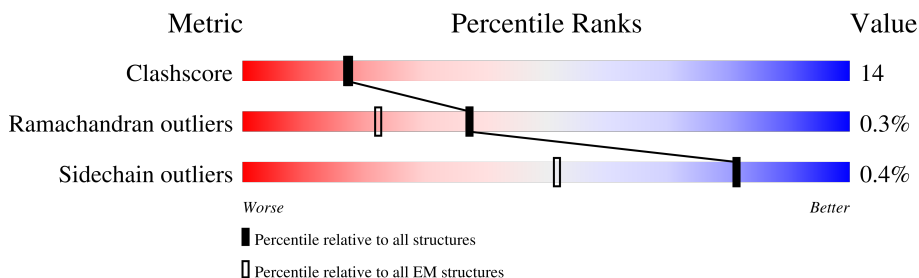
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.75 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	10301 (3.25 - 4.25)

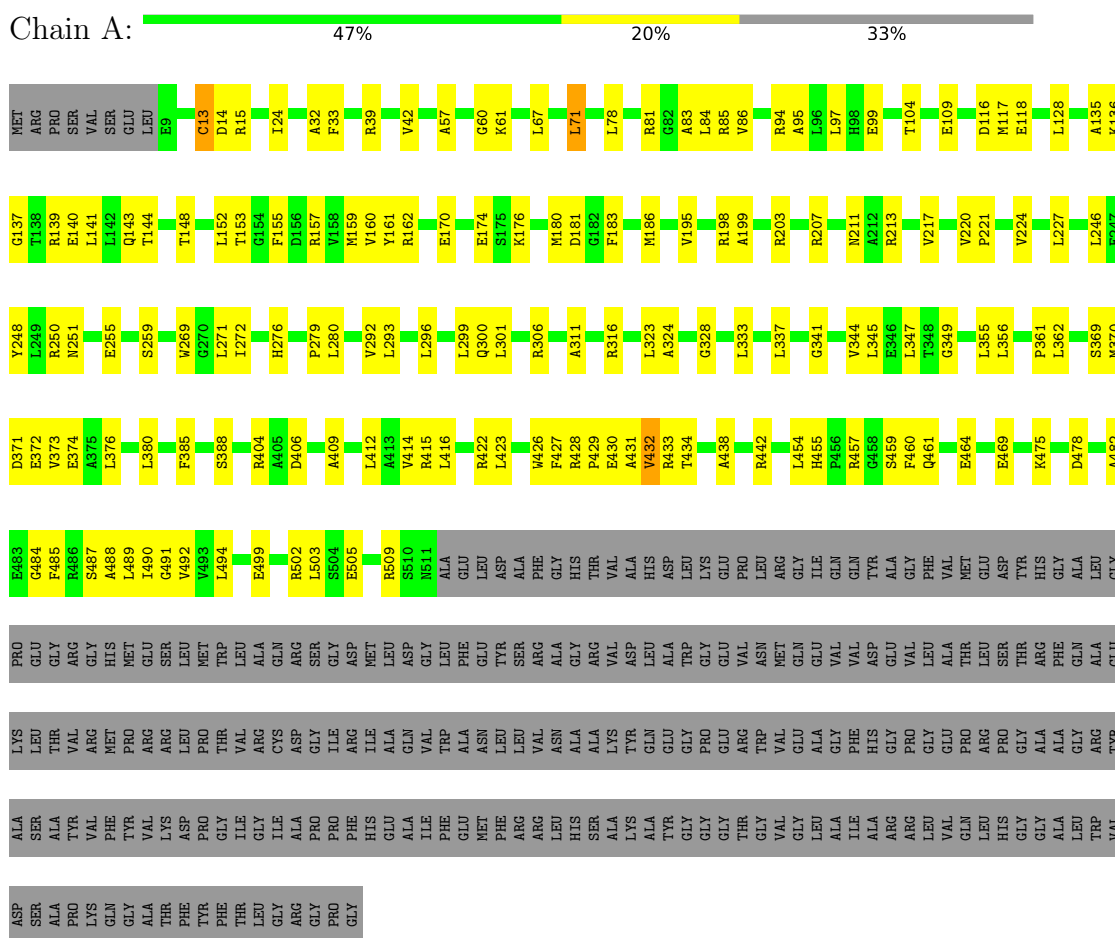
The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment 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	747	 47% 20% 33%
1	B	747	 46% 21% 33%

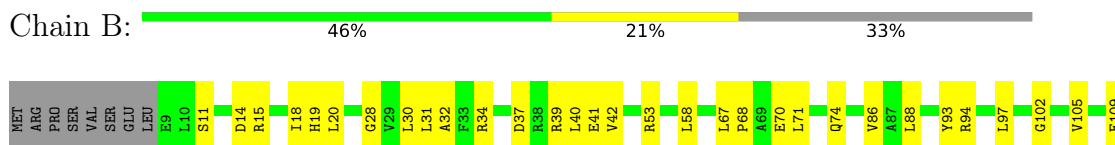
3 Residue-property plots [i](#)

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: Bacteriophytochrome (Light-regulated signal transduction histidine kinase)



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LEU	VAL	GLY	LEU	PHE	E464	L337	T244	E12
GLN	THR	PRO	THR	VAL	E465	A388	H245	E118
HIS	LEU	ARG	GLU	MET	V466	K339	L246	L128
GLY	PRO	SER	THR	TYR	V467	L347	E247	A135
ALA	THR	ARG	THR	HIS	R468	T351	Y248	K136
ALA	PHE	ARG	ARG	GLY	D478	L479	R250	R139
LEU	GLN	ALA	ALA	ALA	A480	R386	M251	E140
TRP	ALA	ARG	LEU	LEU	L483	M370	G253	L141
VAL	TRP	ALA	GLU	GLY	E483	D371	V254	L142
ASP	VAL	ALA	PRO	PRO	R486	E372	S257	Q143
SER	LEU	THR	LEU	GLY	L489	L376	L263	L152
ALA	THR	THR	GLY	GLY	I490	A377	L263	F155
PRO	VAL	VAL	ARG	ARG	G491	M379	W269	Y161
LYS	GLN	PHE	MET	HIS	V492	L380	G270	R162
GLY	VAL	TYR	ARG	MET	V493	A381	L271	G169
ALA	ALA	VAL	ARG	SER	L494	P382	I272	E170
ASP	THR	ARG	ARG	LEU	R495	F385	H276	M190
PRO	PRO	PRO	LEU	LEU	Q496	T387	A278	H186
THR	THR	THR	THR	TRP	L500	Y398	Y284	H187
LEU	THR	VAL	VAL	TRP	F561	L401	C290	F188
GLY	ARG	ARG	ALA	LEU	R502	R404	T294	L200
ILE	CYS	ARG	ALA	ALA	L503	V407	Q295	Y201
ALA	ASP	ARG	GLN	GLY	S604	V414	L296	T202
ALA	GLY	LEU	ARG	GLY	E505	R415	L289	R207
PRO	PRO	ILE	SER	SER	A506	L416	Q300	I209
PRO	PHE	PRO	LEU	TYR	I567	R422	S302	L288
HIS	PHE	HIS	LEU	ASP	S608	N422	S303	A210
GLU	ARG	ALA	LEU	ALA	M511	R428	E304	N211
ALA	ARG	VAL	VAL	PHE	ALA	P429	F305	A212
ILE	LEU	VAL	TRP	GLU	LEU	R306	R306	R213
PHE	LEU	ALA	ALA	GLY	ASP	E430	E309	P221
ARG	LEU	LYS	TYR	ASP	ALA	A431	A310	R229
ARG	VAL	ALA	GLN	LEU	HIS	V432	A311	D232
LEU	VAL	GLN	ALA	LEU	ASP	N440	E312	L233
ASN	TRP	GLY	ALA	TRP	LEU	G450	H315	S234
ALA	GLY	PRO	ALA	GLY	LYS	H451	R316	G295
GLY	GLY	GLU	GLY	GLY	GLU	A452	L319	S236
GLY	THR	ARG	VAL	VAL	PRO	R453	P322	A237
GLY	GLY	ARG	VAL	ASN	LEU	L454	L327	R239
VAL	VAL	TRP	TRP	LEU	LEU	H455	E334	S240
VAL	VAL	VAL	VAL	GLY	GLY	P456	E335	S242
LEU	ALA	VAL	GLY	GLY	ILE	F460	Q461	V241
ALA	ALA	PHE	VAL	VAL	GLN	A461	A462	S243
ILE	ILE	HIS	VAL	VAL	GLN	E462	W463	
ALA	ALA	HIS	ASP	ASP	TYR			
ALA	ALA	GLY	GLY	GLY	ALA			
ARG	ARG	PRO	PRO	VAL	GLY			

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	155342	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	59.31	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.328	Depositor
Minimum map value	-0.157	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.032	Depositor
Map size (\AA)	337.6, 337.6, 337.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.84400004, 0.84400004, 0.84400004	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: BLA

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	0.13	0/3920	0.39	0/5339
1	B	0.14	0/3920	0.44	0/5339
All	All	0.14	0/7840	0.42	0/10678

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.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	220	VAL	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	3837	0	3880	104	0
1	B	3837	0	3880	123	0
2	A	43	0	31	2	0
2	B	43	0	31	3	0
All	All	7760	0	7822	214	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 14.

The worst 5 of 214 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:13:CYS:SG	1:A:14:ASP:N	2.62	0.72
1:B:370:MET:HE3	1:B:370:MET:H	1.55	0.71
1:A:355:LEU:HD23	1:A:362:LEU:HD21	1.73	0.71
1:A:136:LYS:HZ3	1:B:306:ARG:HD2	1.55	0.70
1:B:251:ASN:ND2	1:B:453:ARG:O	2.25	0.69

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	502/747 (67%)	480 (96%)	19 (4%)	3 (1%)	21	52
1	B	502/747 (67%)	468 (93%)	34 (7%)	0	100	100
All	All	1004/1494 (67%)	948 (94%)	53 (5%)	3 (0%)	37	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	CYS

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Mol	Chain	Res	Type
1	A	432	VAL
1	A	457	ARG

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	390/574 (68%)	389 (100%)	1 (0%)	86	84
1	B	390/574 (68%)	387 (99%)	3 (1%)	73	75
All	All	780/1148 (68%)	776 (100%)	4 (0%)	81	81

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	LEU
1	B	296	LEU
1	B	315[A]	HIS
1	B	315[B]	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	281	HIS
1	B	300	GLN
1	B	496	GLN
1	B	25	GLN
1	A	143	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 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
2	BLA	A	801	1	46,46,46	3.85	23 (50%)	66,67,67	1.76	11 (16%)
2	BLA	B	801	1	46,46,46	3.86	23 (50%)	66,67,67	1.85	12 (18%)

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
2	BLA	A	801	1	-	15/26/74/74	0/4/4/4
2	BLA	B	801	1	-	18/26/74/74	0/4/4/4

The worst 5 of 46 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	BLA	C4C-NC	9.53	1.54	1.37
2	A	801	BLA	C4C-NC	9.50	1.54	1.37
2	B	801	BLA	C1B-NB	9.48	1.54	1.37
2	A	801	BLA	C1B-NB	9.43	1.53	1.37
2	B	801	BLA	C3C-C2C	7.84	1.53	1.37

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	BLA	CMC-C2C-C3C	-7.92	109.26	128.43
2	B	801	BLA	CMC-C2C-C3C	-7.81	109.52	128.43
2	B	801	BLA	CMC-C2C-C1C	-6.03	108.60	121.21
2	A	801	BLA	CMC-C2C-C1C	-5.60	109.50	121.21
2	B	801	BLA	C1A-CHA-C4D	-4.01	119.47	128.22

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

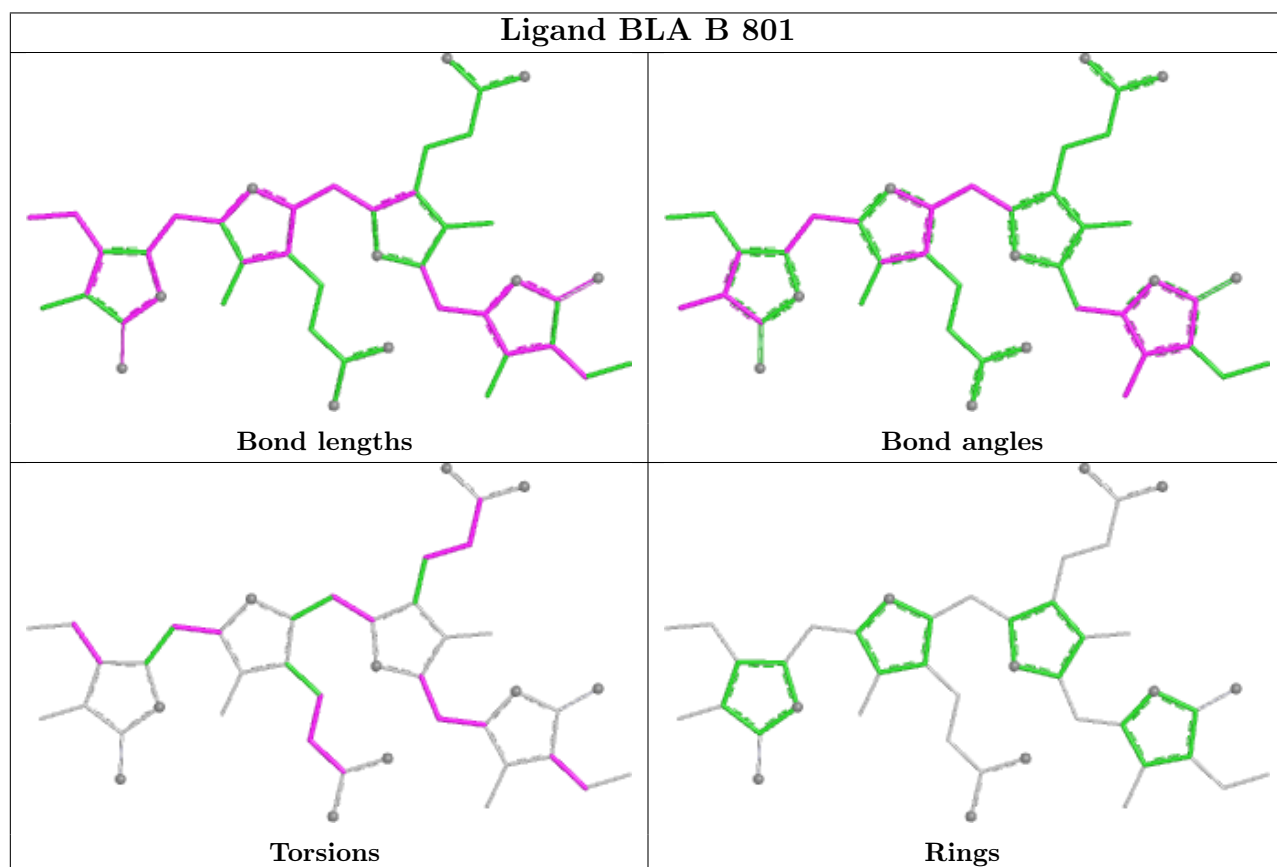
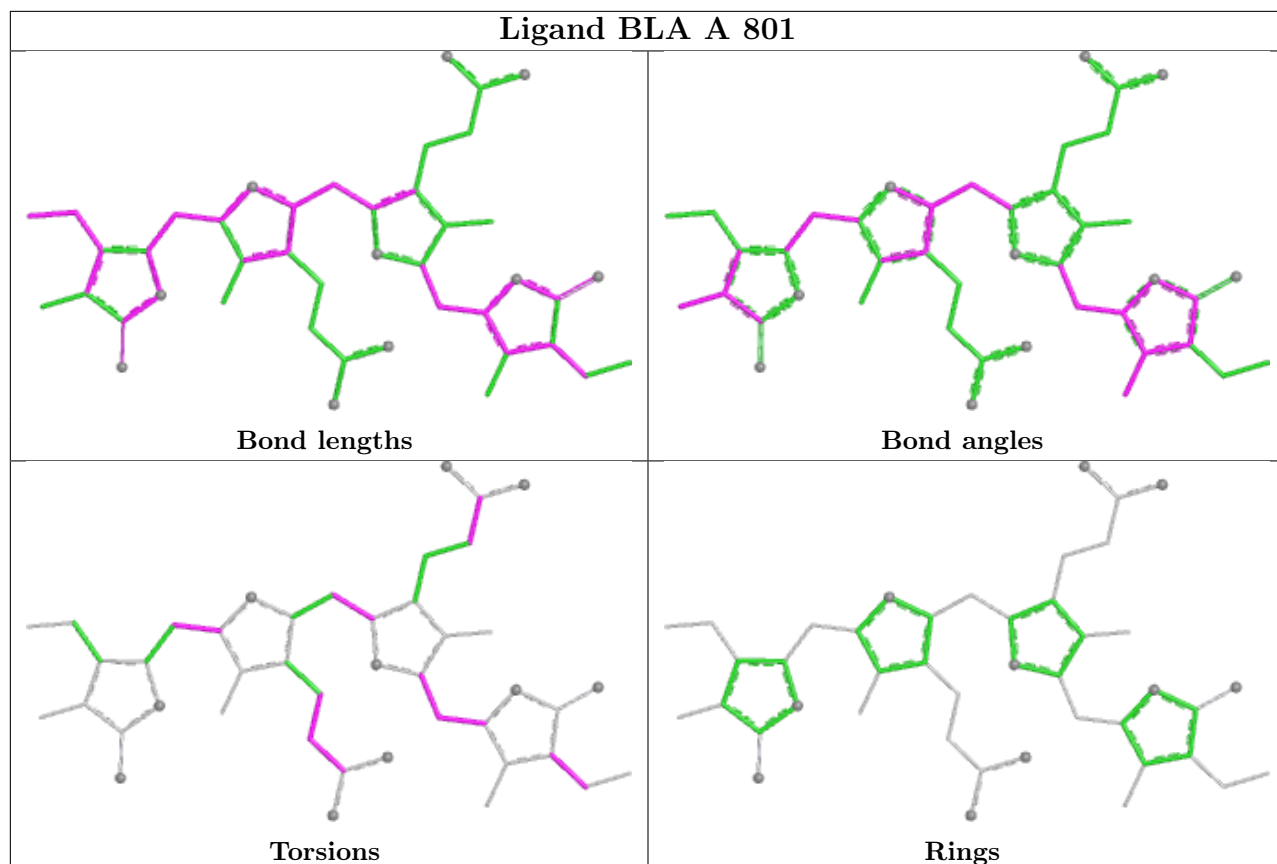
Mol	Chain	Res	Type	Atoms
2	A	801	BLA	NB-C1B-CHB-C4A
2	A	801	BLA	C2B-C1B-CHB-C4A
2	A	801	BLA	ND-C1D-CHD-C4C
2	B	801	BLA	NA-C4A-CHB-C1B
2	B	801	BLA	C3A-C4A-CHB-C1B

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	BLA	2	0
2	B	801	BLA	3	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.

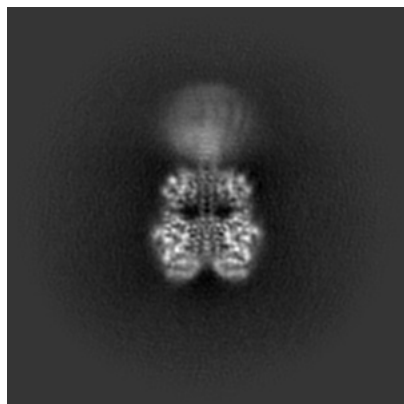
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42452. These allow visual inspection of the internal detail of the map and identification of artifacts.

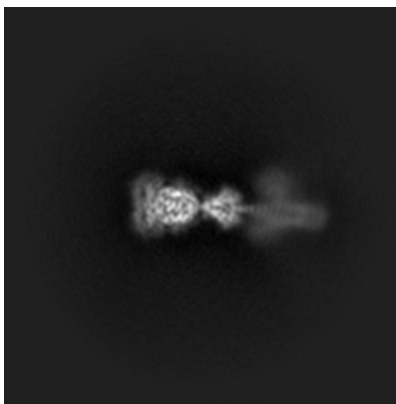
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

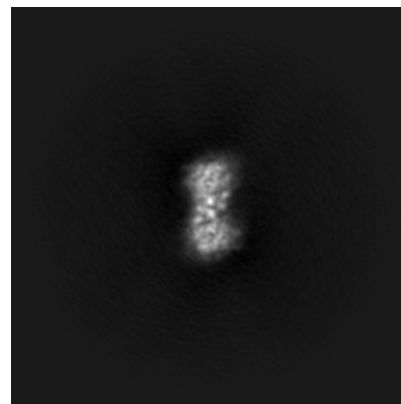
6.1.1 Primary map



X

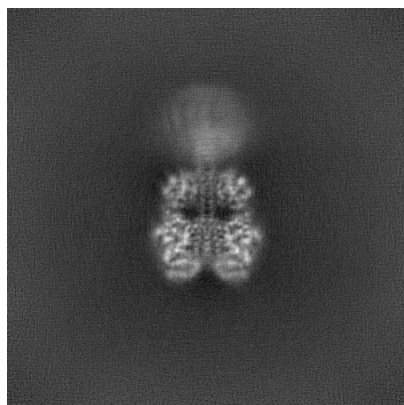


Y

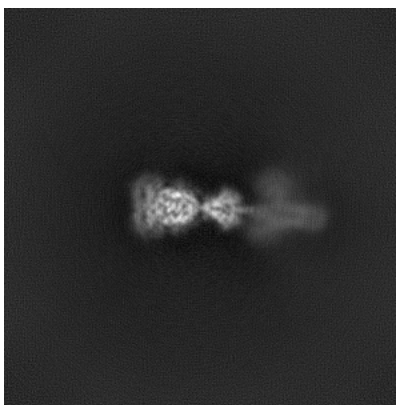


Z

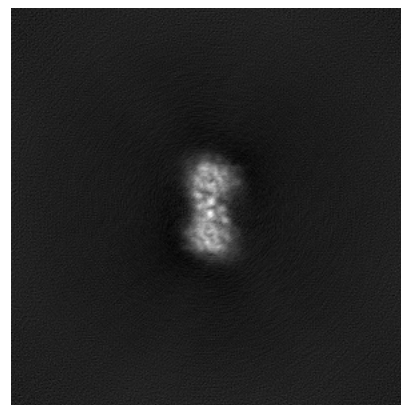
6.1.2 Raw map



X



Y

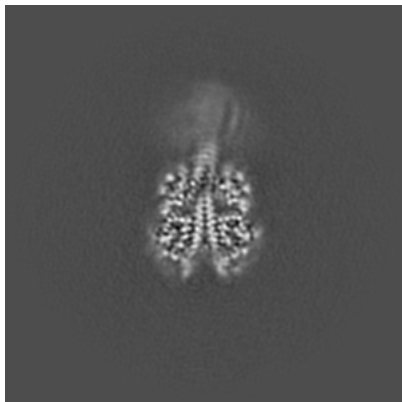


Z

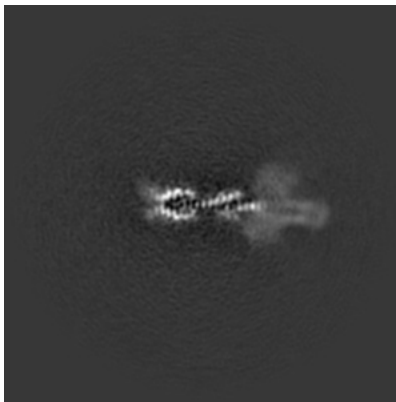
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

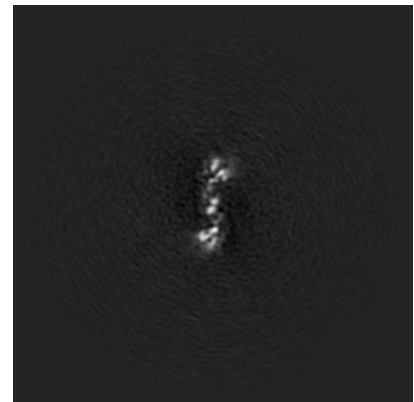
6.2.1 Primary map



X Index: 200

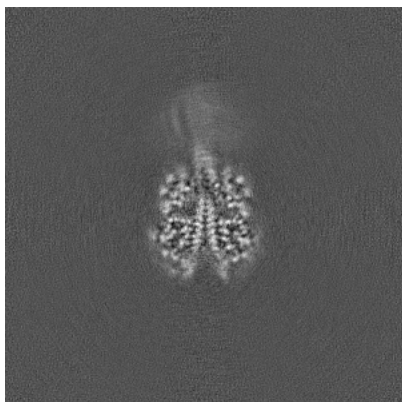


Y Index: 200

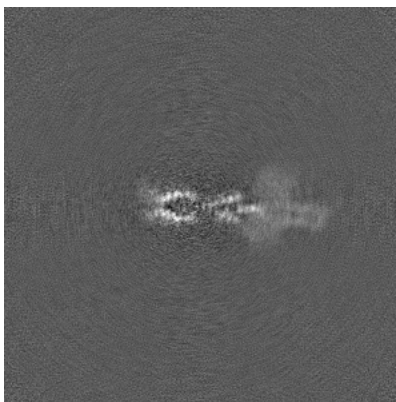


Z Index: 200

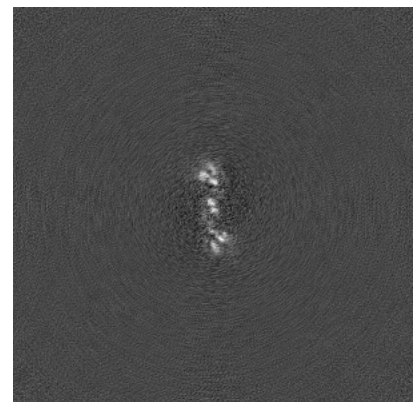
6.2.2 Raw map



X Index: 200



Y Index: 200

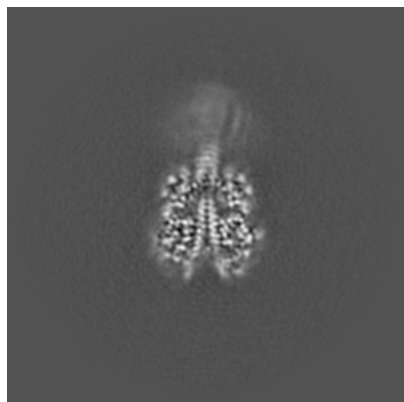


Z Index: 200

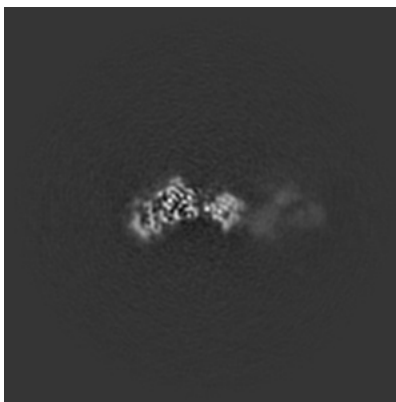
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

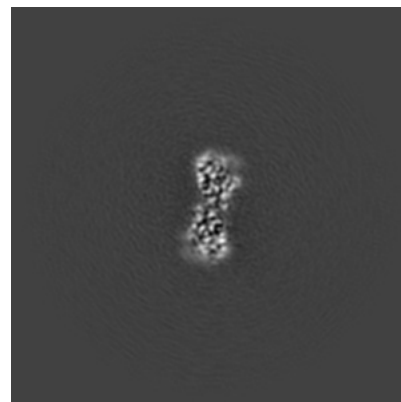
6.3.1 Primary map



X Index: 199

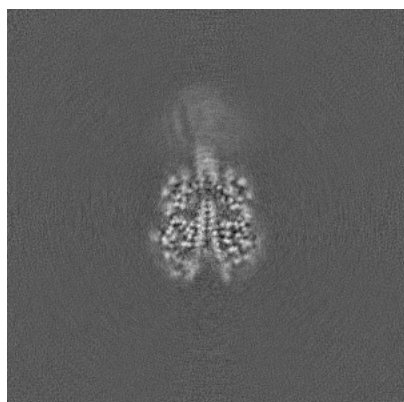


Y Index: 223

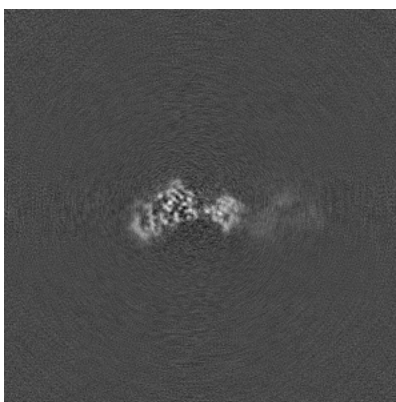


Z Index: 175

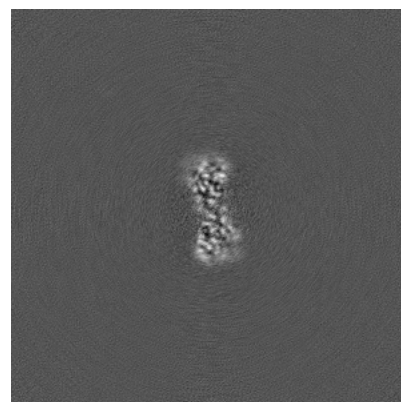
6.3.2 Raw map



X Index: 199



Y Index: 176

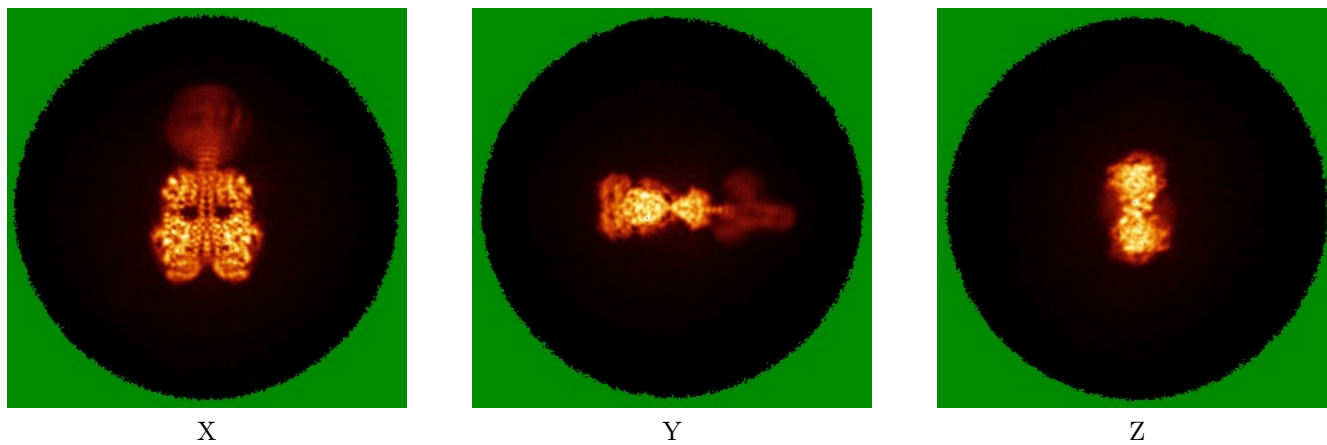


Z Index: 176

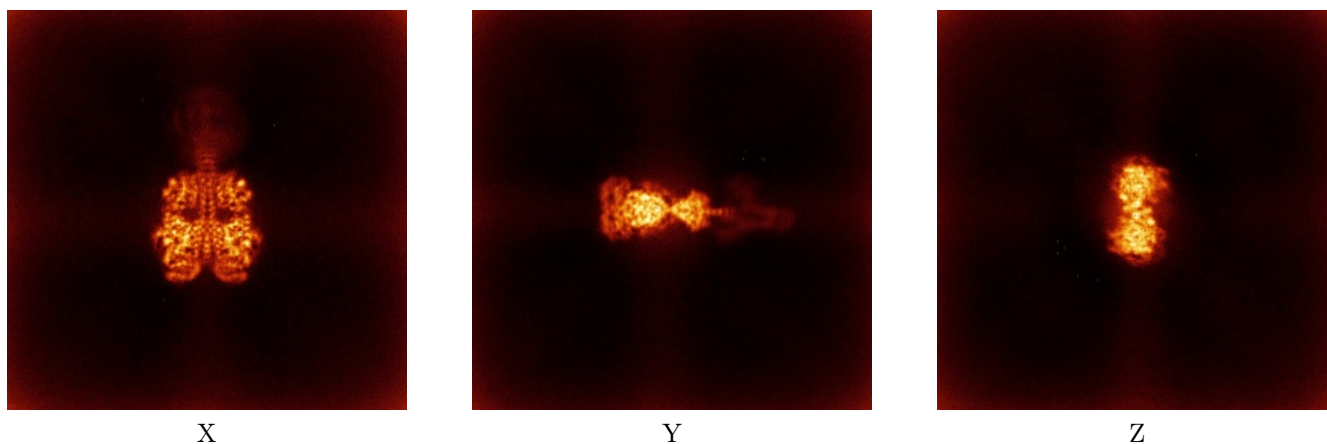
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

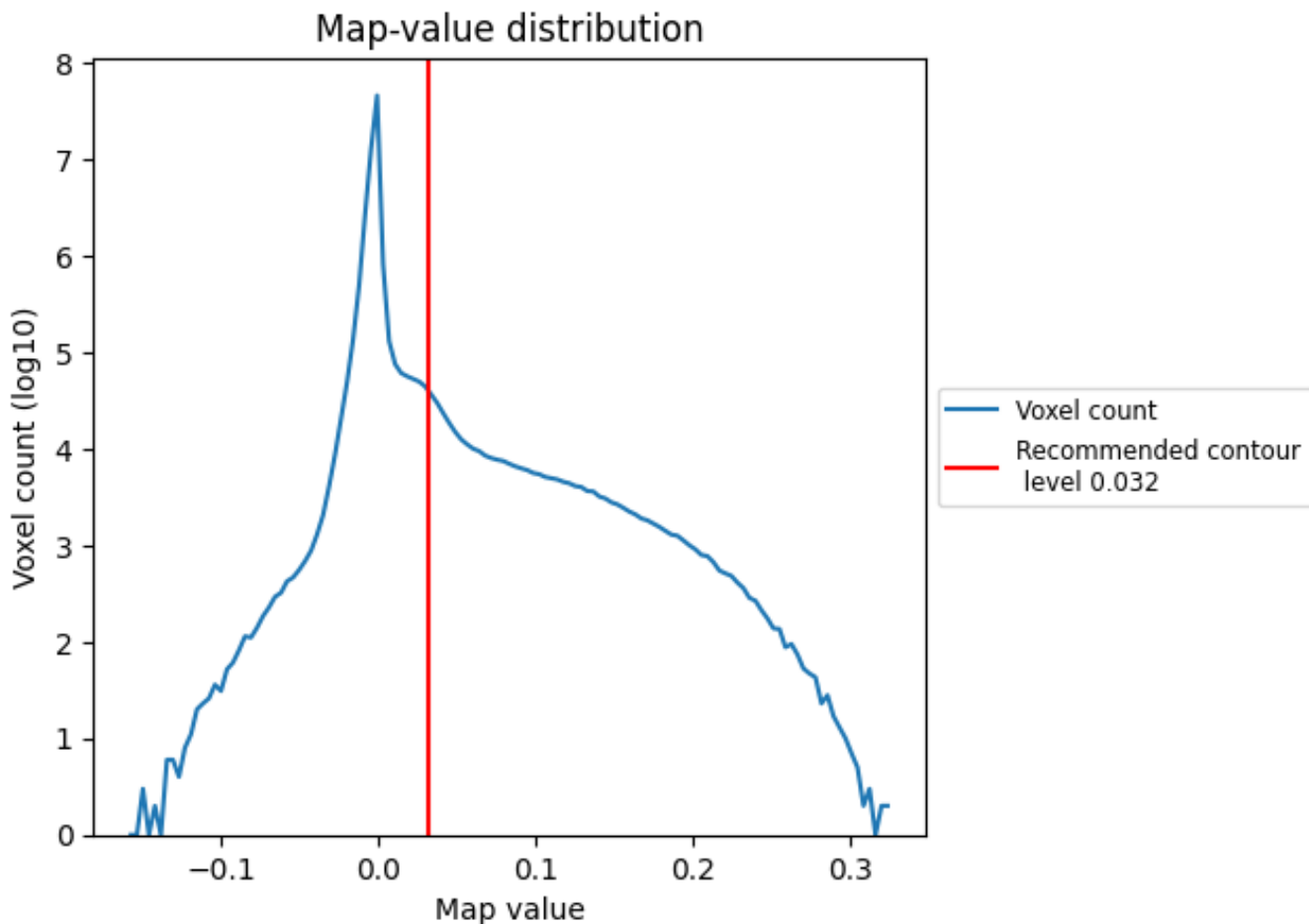
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

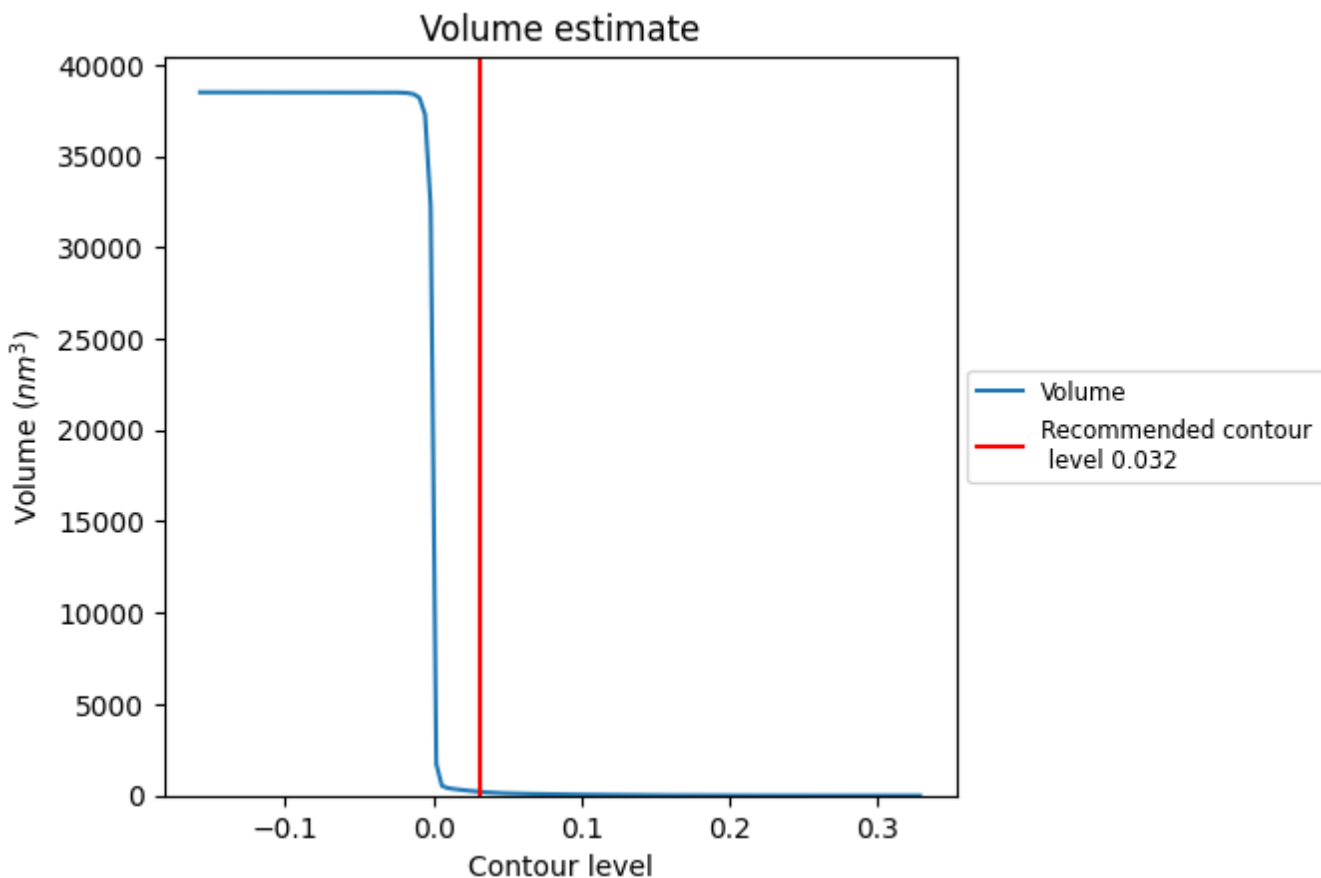
This section contains the results of statistical analysis of the map.

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.

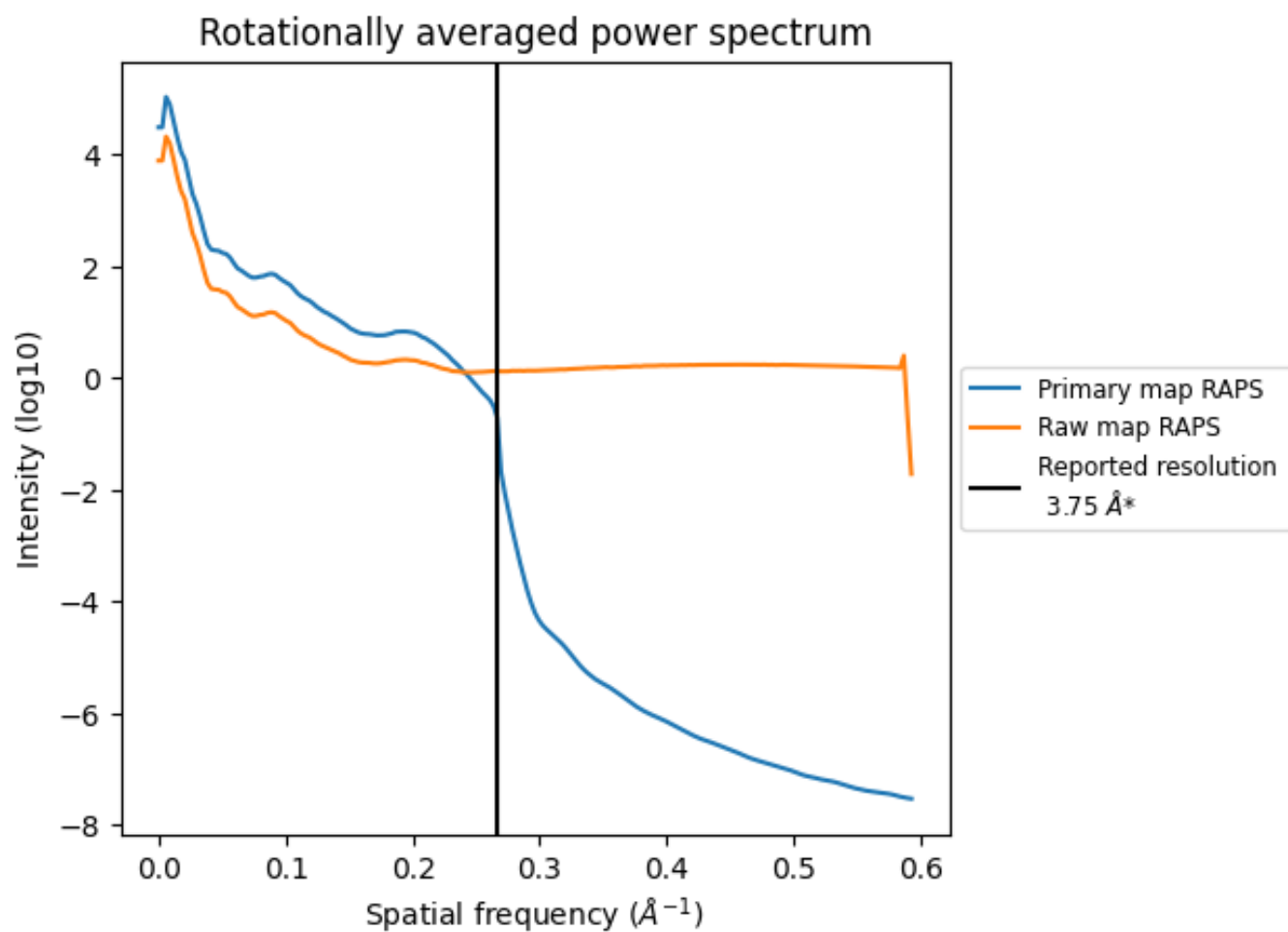
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 201 nm³; this corresponds to an approximate mass of 182 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](#)

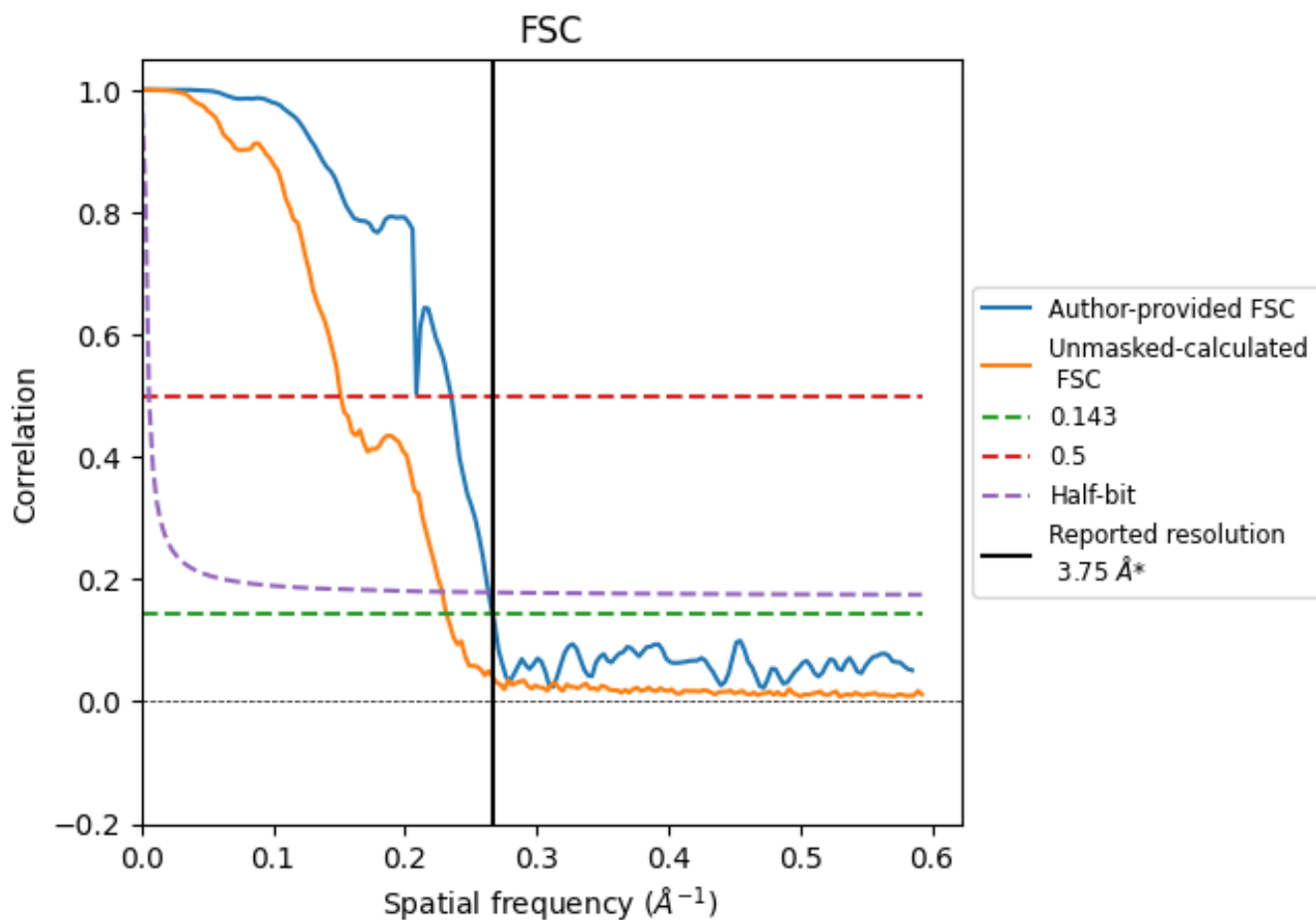


*Reported resolution corresponds to spatial frequency of 0.267 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.267 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.75	-	-
Author-provided FSC curve	3.75	4.25	3.79
Unmasked-calculated*	4.32	6.62	4.38

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.32 differs from the reported value 3.75 by more than 10 %

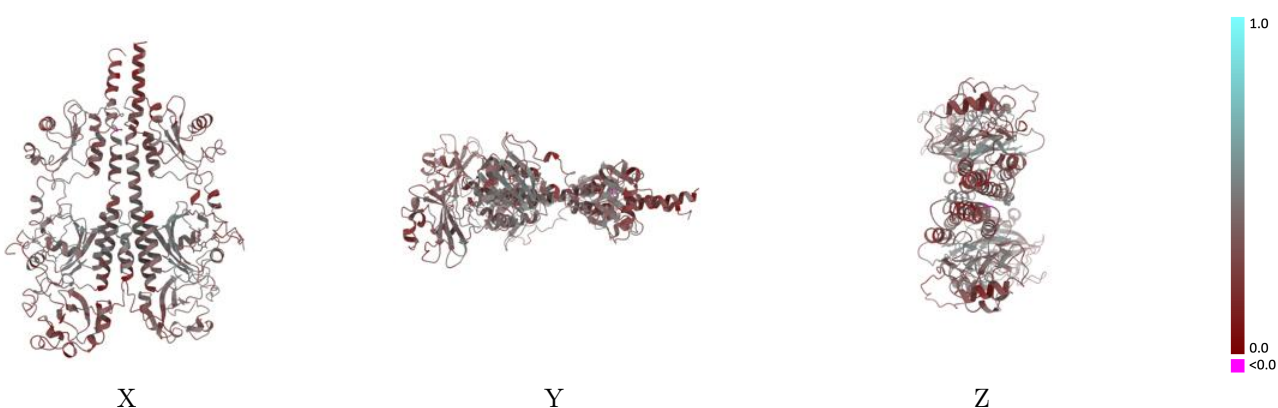
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42452 and PDB model 8UPM. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay [i](#)

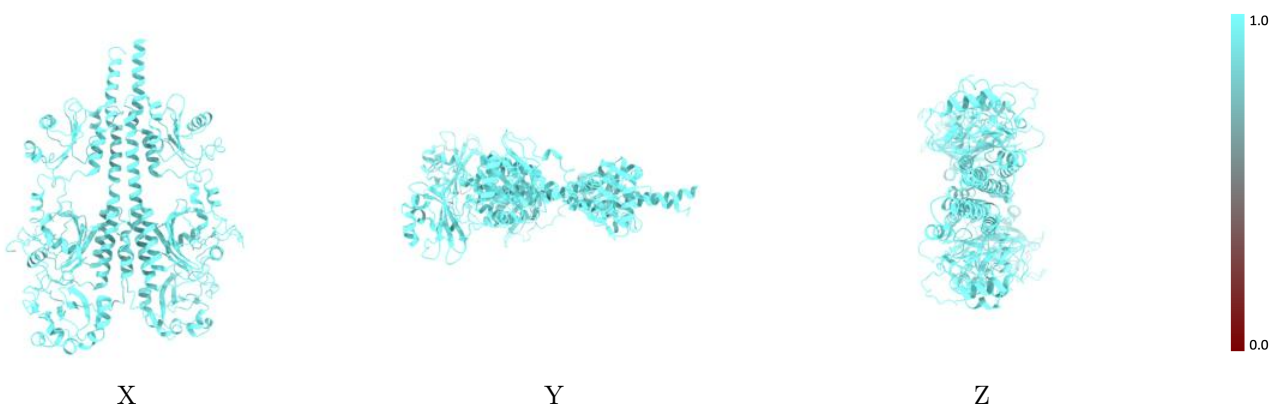
This section was not generated.

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



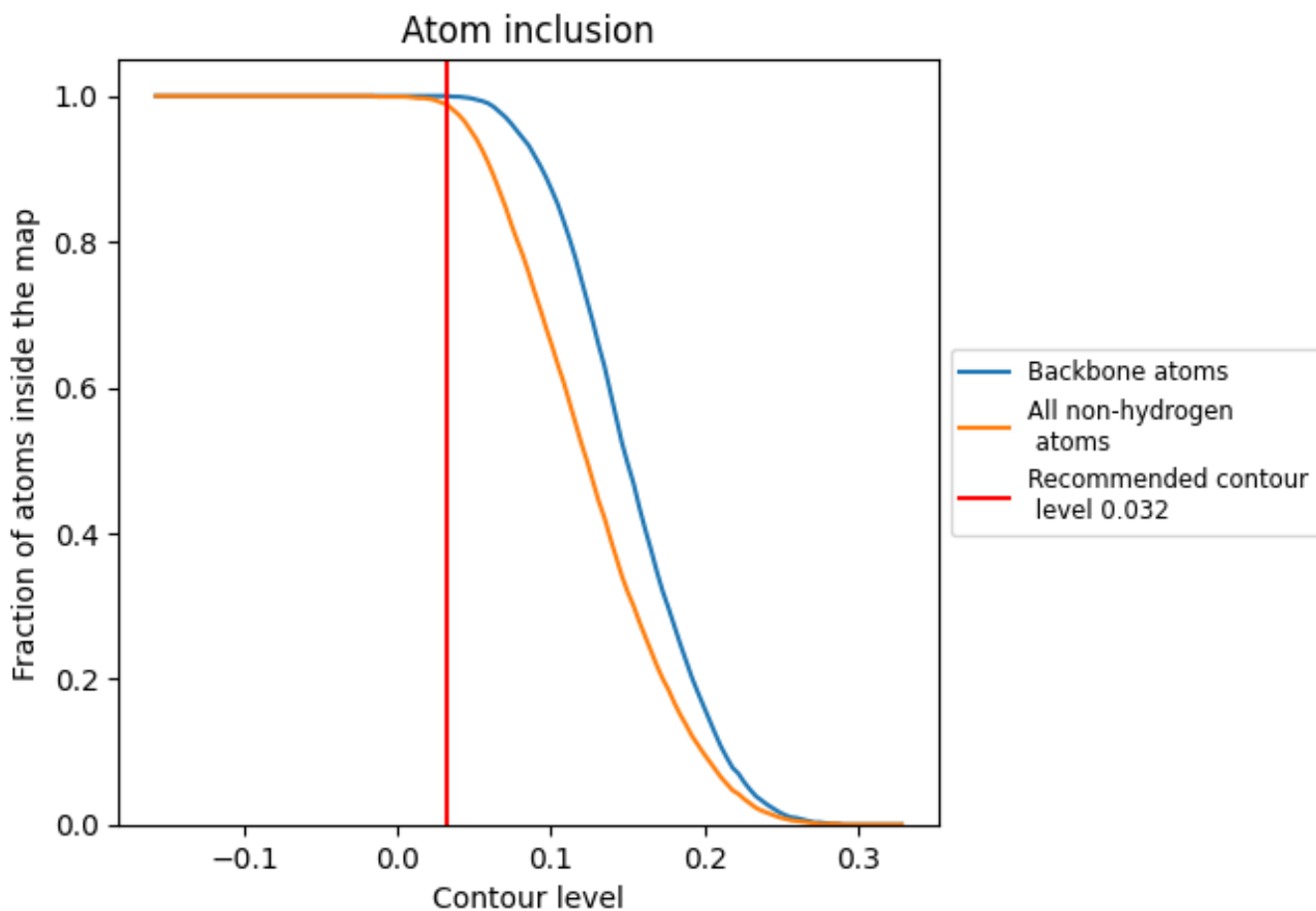
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.032).







9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 99% 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 (0.032) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9880	 0.3550
A	 0.9900	 0.3580
B	 0.9860	 0.3520

