



## wwPDB EM Validation Summary Report ⓘ

Jun 9, 2026 – 12:18 PM EDT

PDB ID : 9YXN / pdb\_00009yxn  
EMDB ID : EMD-73612  
Title : Pr-Pfr heterodimer state of Stigmatella aurantiaca bacteriophytochrome 2  
Authors : Karki, P.; Stojkovic, E.A.; Schmidt, M.  
Deposited on : 2025-10-27  
Resolution : 5.01 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.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

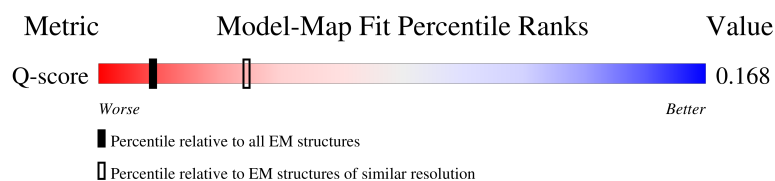
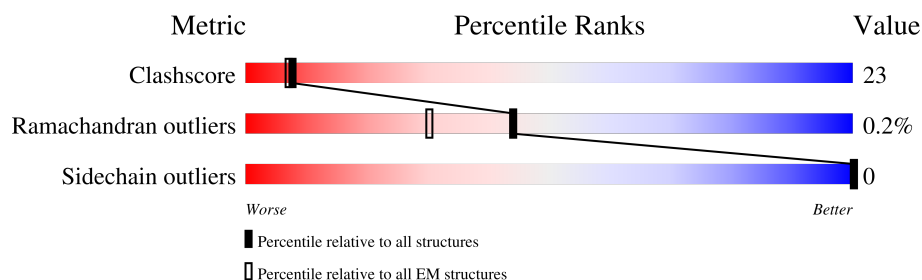
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 5.01 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	859 ( 4.51 - 5.51 )

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	739	 6% 66% 34%
1	B	739	 8% 67% 33%

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
2	BLA	B	801	-	-	X	-

## 2 Entry composition [i](#)

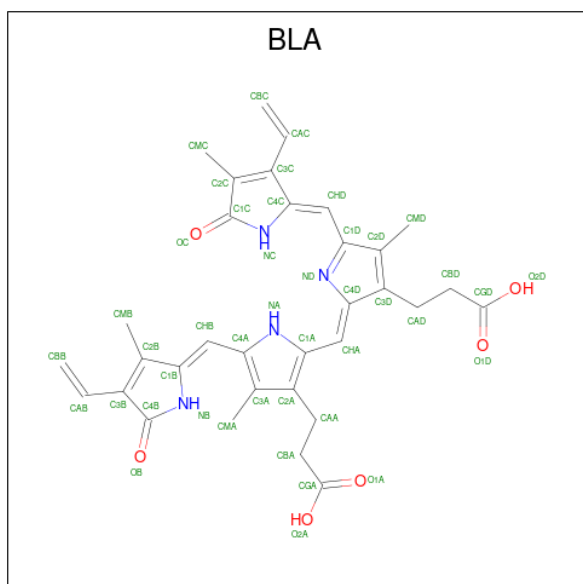
There are 2 unique types of molecules in this entry. The entry contains 10153 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Bacteriophytochrome.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	739	Total	C	N	O	S	0	0
			5035	3142	939	945	9		
1	B	739	Total	C	N	O	S	0	0
			5032	3141	939	943	9		

- Molecule 2 is BILIVERDINE IX ALPHA (CCD ID: BLA) (formula:  $C_{33}H_{34}N_4O_6$ ) (labeled as "Ligand of Interest" by depositor).

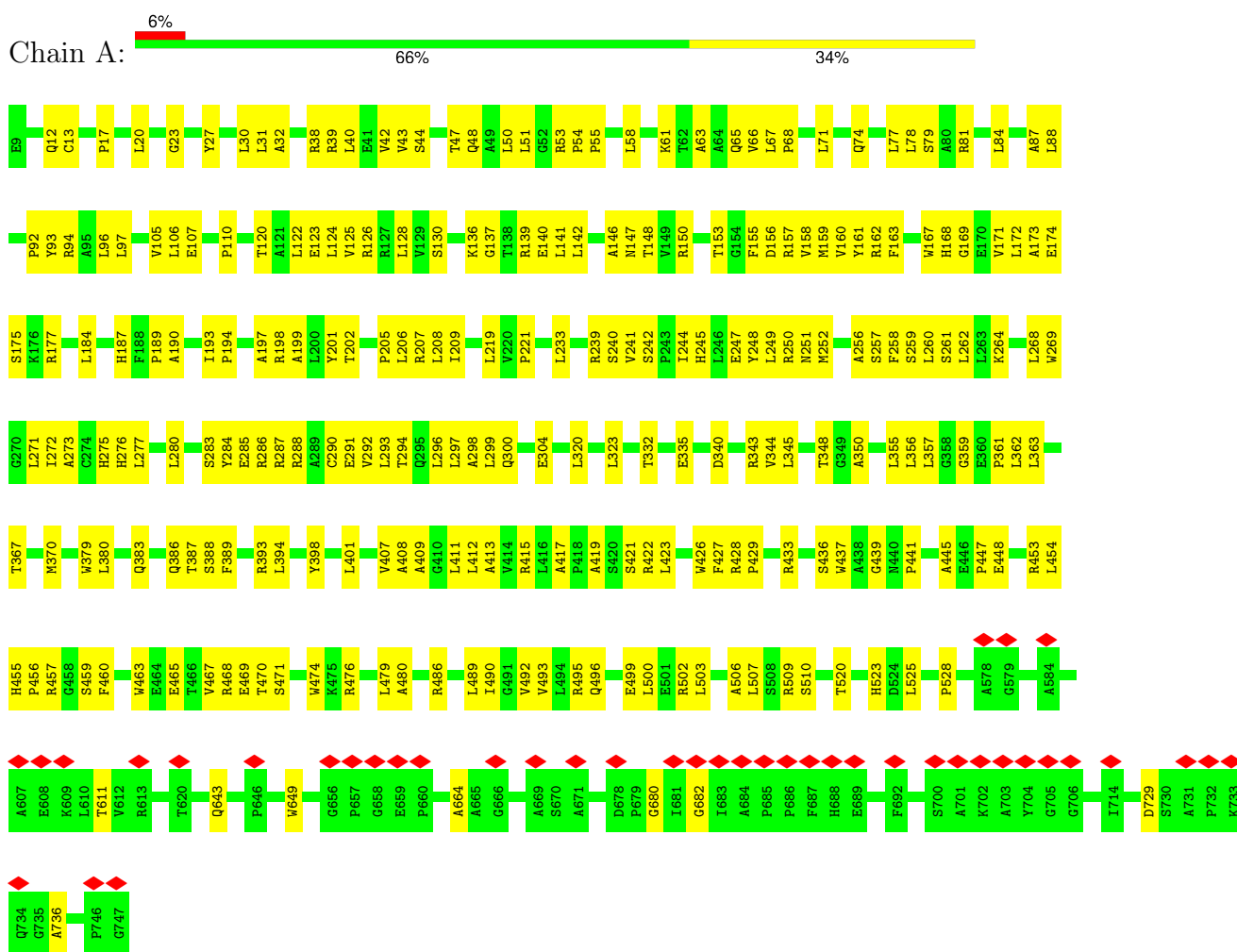


Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			43	33	4	6	
2	B	1	Total	C	N	O	0
			43	33	4	6	

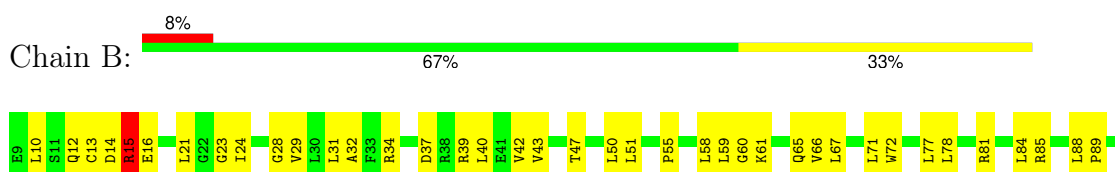
### 3 Residue-property plots [i](#)

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



#### • Molecule 1: Bacteriophytochrome



P92	Y93	R94	A95	L96	L97	V105	L106	E107	L108	E109	P110	A111	Q114	M117	E118	A121	L122	E123	L124	V125	R126	R127	L128	P131	L132	A133	G134	R139	E140	L141	L142	N147	T148	V149	R150	A151	L152	T153	G154	F155	D156	R157	V158	M159	V160	Y161	R162	H168	G169	E170	V171																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
L172	A173	E174	S175	K176	R177	M186	H187	F188	P189	P194	V195	Q196	A199	L200	T201	T202	R203	N204	P205	L206	R207	L208	N211	A214	R215	P216	V217	P218	L219	V220	P221	S222	V223	V224	L227	L231	D232	L233	S234	L238	R239	S242	P243	I244	H245	L246	E247	Y248	L249	R250																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
N251	M252	E255	A256	S257	F258	S259	L260	S261	L262	L263	K264	L268	W269	A273	C274	H275	H276	L277	L282	S283	Y284	E285	R286	R287	R288	A289	C290	E291	V292	L293	T294	Q295	L296	L297	L301	E304	L319	L320	G321	P322	L323	A324	T325	L337	D340	G341	A342	R343	V344																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
A350	A354	L355	L356	P361	L362	L363	P368	S369	M370	D371	E372	V373	E374	W379	F385	Q386	T387	S388	F389	H390	T391	E392	R393	Y398	L401	R404	G410	L411	L412	V414	R415	L416	A417	P418	L423	A424	L425	W426	F427	E430	A431	V432	R433	P449	A452																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
R453	L454	H455	P456	S459	F460	Q461	A462	W463	E464	V467	W474	K475	R476	A477	D478	L479	A480	A481	A482	E483	L490	V493	L494	R495	Q496	E499	L500	E501	R502	L503	R509	A512	E513	L514	Y543	H544	G545	A546	Y575	S576	R577	A578	G579	R580	V581	D582	L583	A584	W585																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
G586	E587	V588	N589	T600	Q606	A607	E608	K609	R617	T620	K641	Y642	Q643	F654	H655	G656	P657	G658	E659	P660	R661	P662	A665	A671	F674	Y675	V676	K677	G680	I681	A684	P685	P686	F687	I691	F692	F695	R696	R697	L698	H699	S700	A701	K702	A703	Y704																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
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## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	87111	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	59.37	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.225	Depositor
Minimum map value	-0.062	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0226	Depositor
Map size (Å)	299.6, 299.6, 299.6	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.856, 0.856, 0.856	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	0/5133	0.37	2/7027 (0.0%)
1	B	0.14	0/5130	1.04	8/7023 (0.1%)
All	All	0.14	0/10263	0.78	10/14050 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	577	ARG	O-C-N	-67.39	39.98	122.87
1	B	15	ARG	O-C-N	-38.54	71.33	122.59
1	B	15	ARG	CA-C-N	-13.39	98.78	122.48
1	B	15	ARG	C-N-CA	-13.39	98.78	122.48
1	B	577	ARG	N-CA-C	11.95	127.55	110.23

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	15	ARG	Mainchain
1	B	577	ARG	Mainchain



## 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	5035	0	4572	203	0
1	B	5032	0	4570	248	0
2	A	43	0	30	4	0
2	B	43	0	31	37	0
All	All	10153	0	9203	440	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 23.

The worst 5 of 440 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:B:12:GLN:C	2:B:801:BLA:CBC	1.76	1.56
1:B:12:GLN:O	2:B:801:BLA:CBC	1.66	1.39
1:B:13:CYS:CB	2:B:801:BLA:CHD	2.08	1.30
1:B:13:CYS:SG	2:B:801:BLA:HBC1	1.72	1.29
1:B:13:CYS:SG	2:B:801:BLA:C4C	2.22	1.27

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	737/739 (100%)	698 (95%)	38 (5%)	1 (0%)	48	83
1	B	737/739 (100%)	684 (93%)	51 (7%)	2 (0%)	36	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1474/1478 (100%)	1382 (94%)	89 (6%)	3 (0%)	44 77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	578	ALA
1	B	15	ARG
1	A	130	SER

### 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	411/566 (73%)	411 (100%)	0	100 100
1	B	410/566 (72%)	410 (100%)	0	100 100
All	All	821/1132 (72%)	821 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	440	ASN
1	B	496	GLN
1	B	511	ASN
1	A	451	HIS
1	A	461	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	3.86	23 (50%)	66,67,67	1.86	10 (15%)
2	BLA	B	801	-	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	-	17/26/74/74	0/4/4/4
2	BLA	B	801	-	-	17/26/74/74	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	A	801	BLA	C4C-NC	9.59	1.54	1.37
2	B	801	BLA	C4C-NC	9.53	1.54	1.37
2	A	801	BLA	C1B-NB	9.45	1.53	1.37
2	B	801	BLA	C1B-NB	9.44	1.53	1.37
2	A	801	BLA	C3C-C2C	7.84	1.53	1.37

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	BLA	CMC-C2C-C3C	-7.54	110.19	128.43
2	A	801	BLA	CMC-C2C-C3C	-7.53	110.21	128.43
2	A	801	BLA	C1A-CHA-C4D	-6.77	113.43	128.22
2	B	801	BLA	CMC-C2C-C1C	-5.32	110.09	121.21
2	A	801	BLA	CMC-C2C-C1C	-5.25	110.23	121.21

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

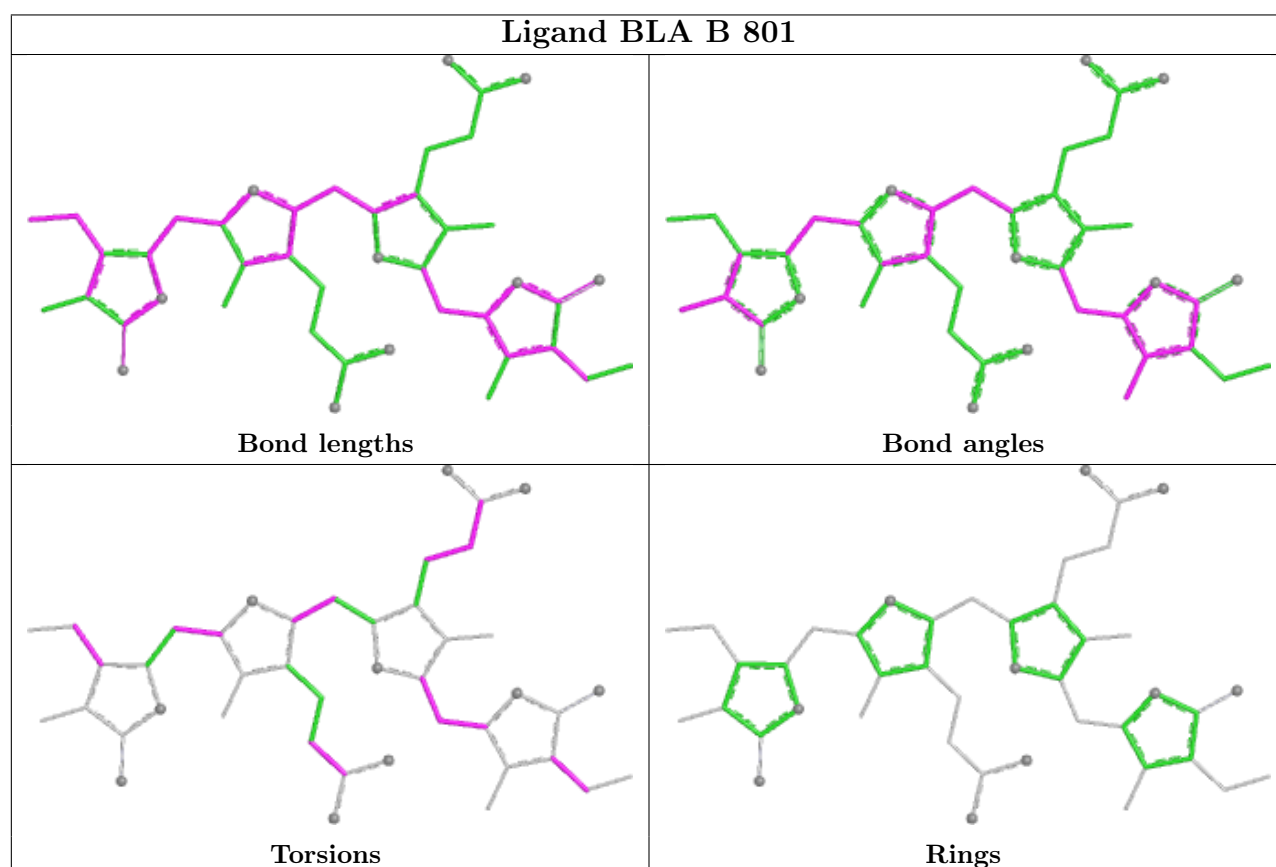
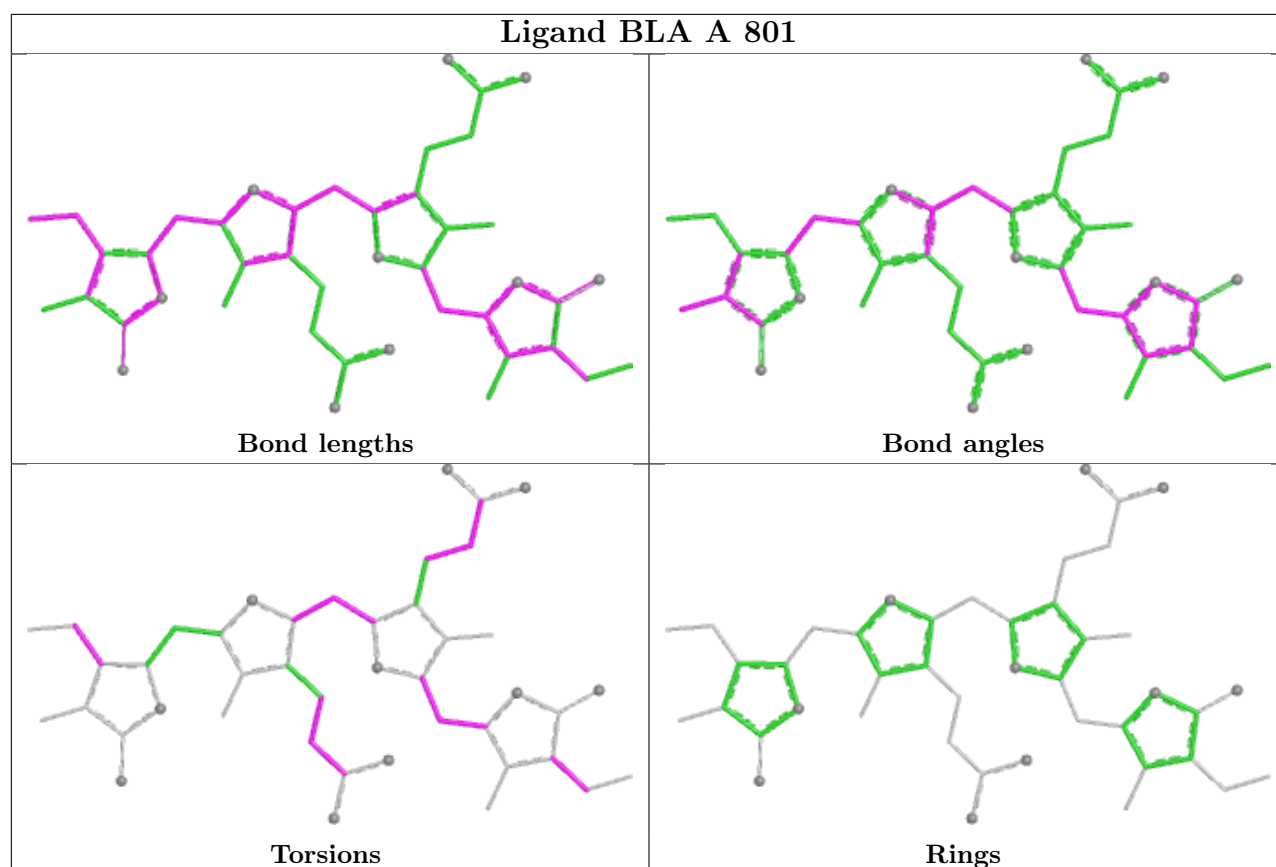
Mol	Chain	Res	Type	Atoms
2	A	801	BLA	NA-C1A-CHA-C4D
2	A	801	BLA	C2A-C1A-CHA-C4D
2	A	801	BLA	C2B-C3B-CAB-CBB
2	A	801	BLA	C4B-C3B-CAB-CBB
2	A	801	BLA	C2C-C3C-CAC-CBC

There are no ring outliers.

2 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	BLA	4	0
2	B	801	BLA	37	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.

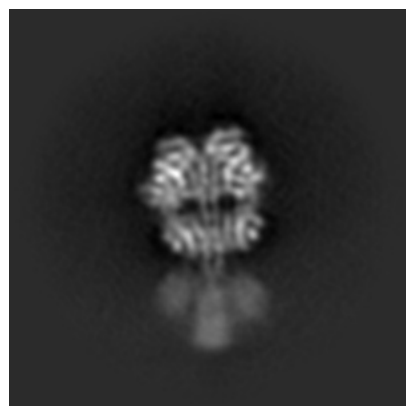
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-73612. These allow visual inspection of the internal detail of the map and identification of artifacts.

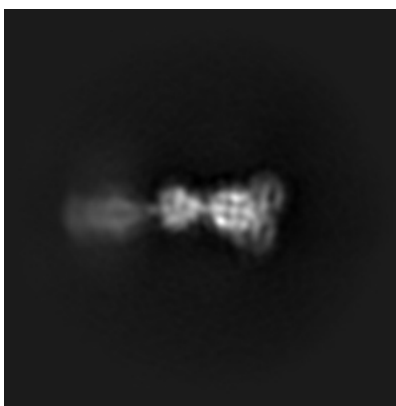
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

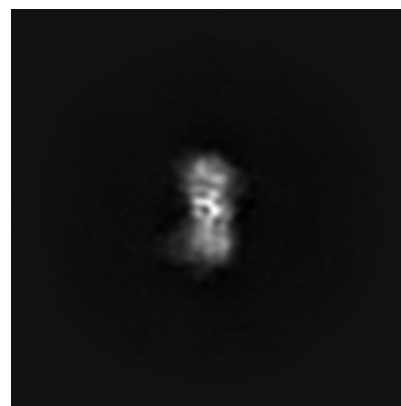
#### 6.1.1 Primary map



X

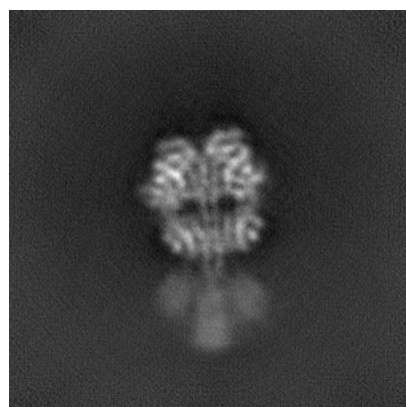


Y

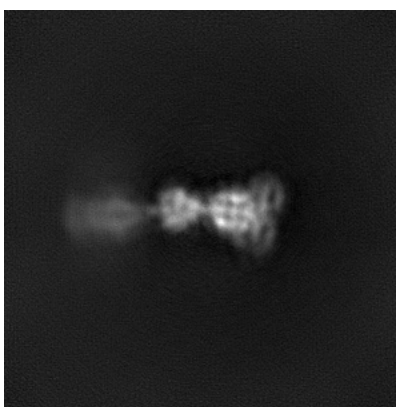


Z

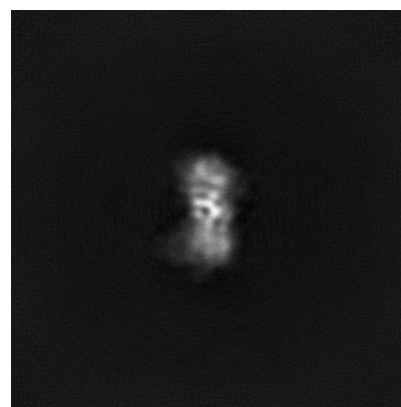
#### 6.1.2 Raw map



X



Y

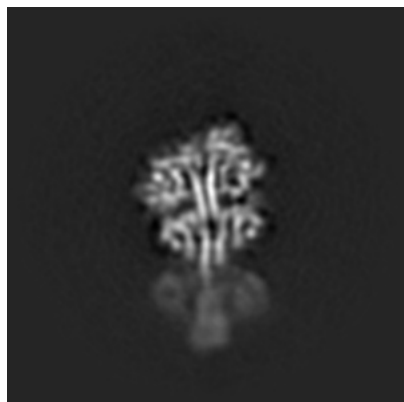


Z

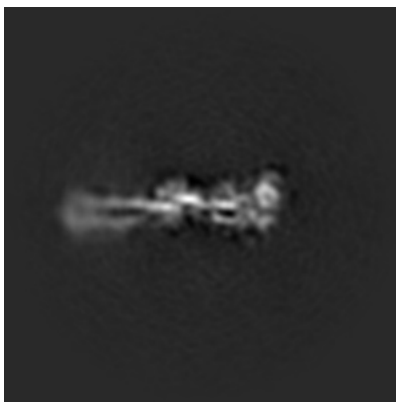
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

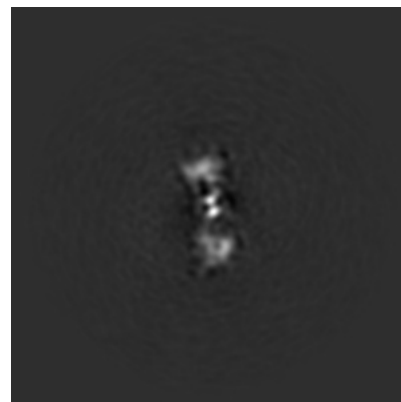
### 6.2.1 Primary map



X Index: 175

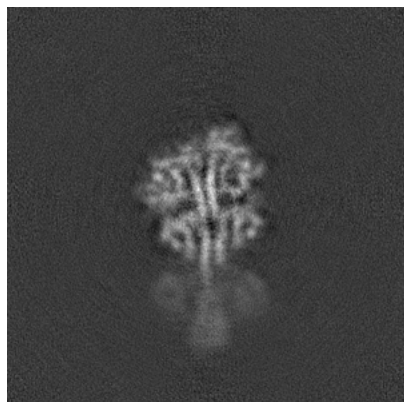


Y Index: 175

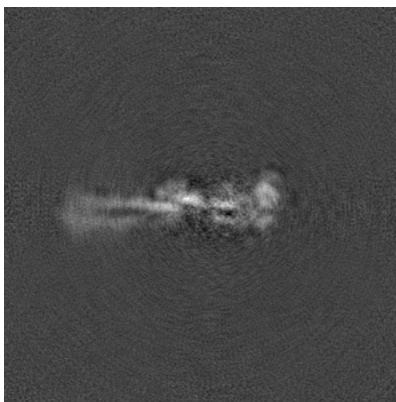


Z Index: 175

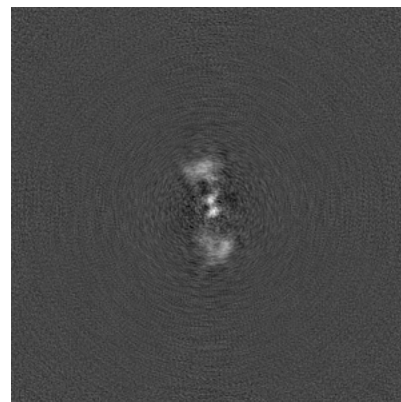
### 6.2.2 Raw map



X Index: 175



Y Index: 175



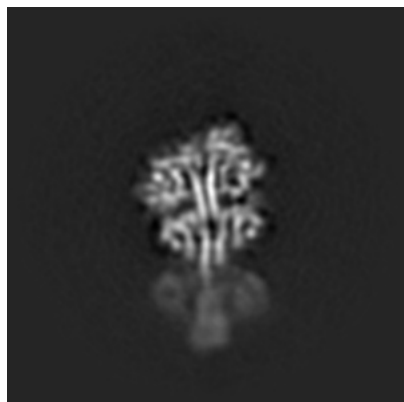
Z Index: 175

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

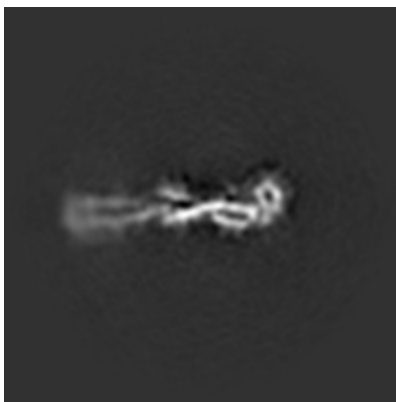


## 6.3 Largest variance slices [i](#)

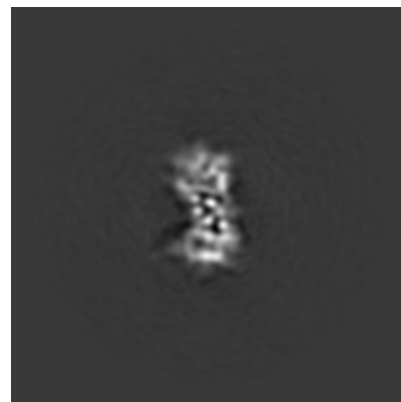
### 6.3.1 Primary map



X Index: 175

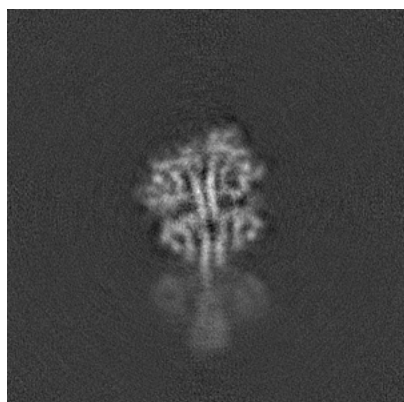


Y Index: 180

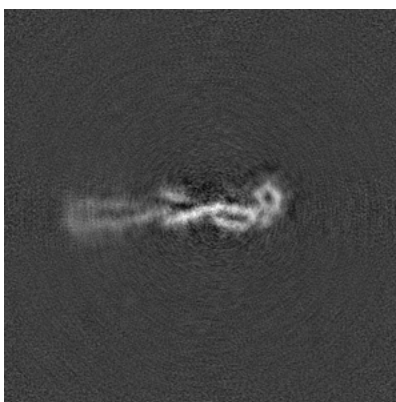


Z Index: 201

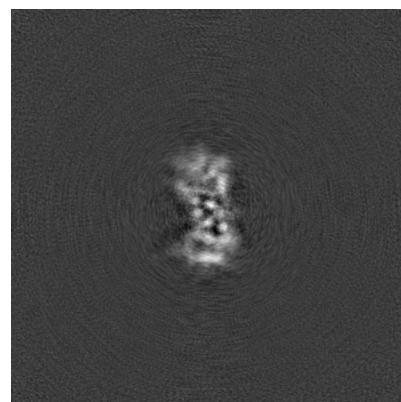
### 6.3.2 Raw map



X Index: 175



Y Index: 180



Z Index: 201

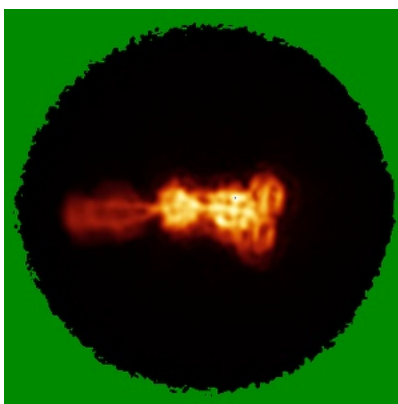
The images above show the largest variance slices of the map in three orthogonal directions.

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

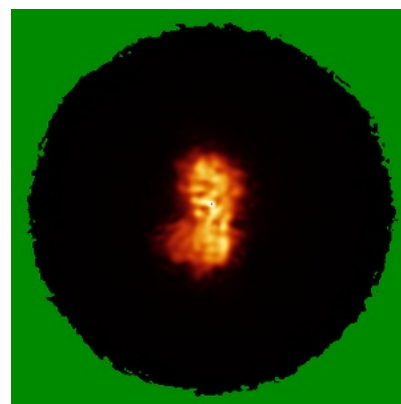
### 6.4.1 Primary map



X

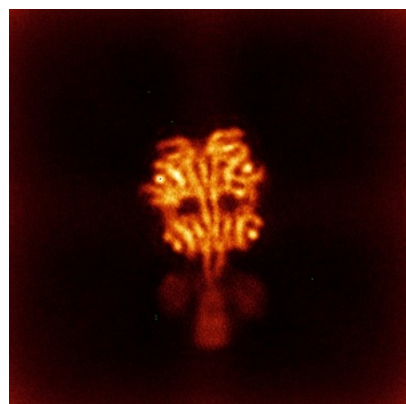


Y

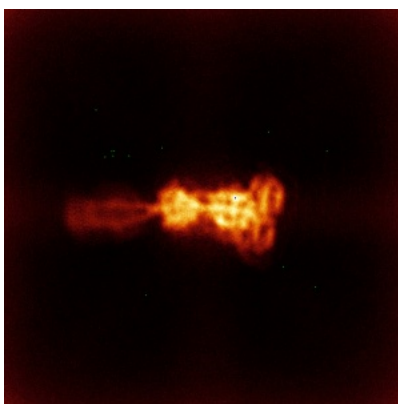


Z

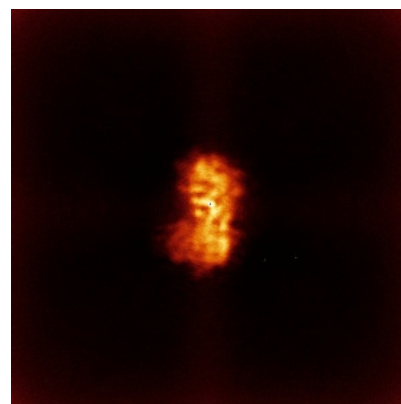
### 6.4.2 Raw map



X



Y

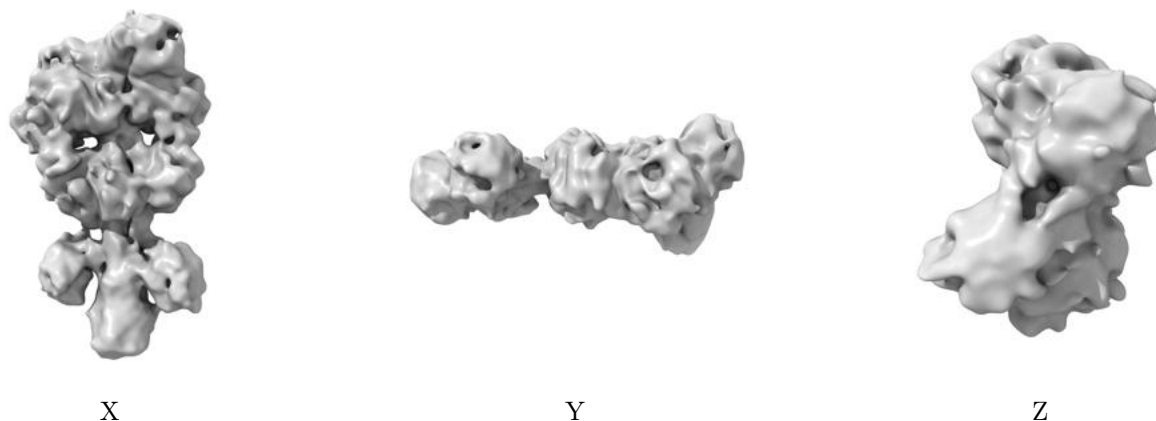


Z

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.

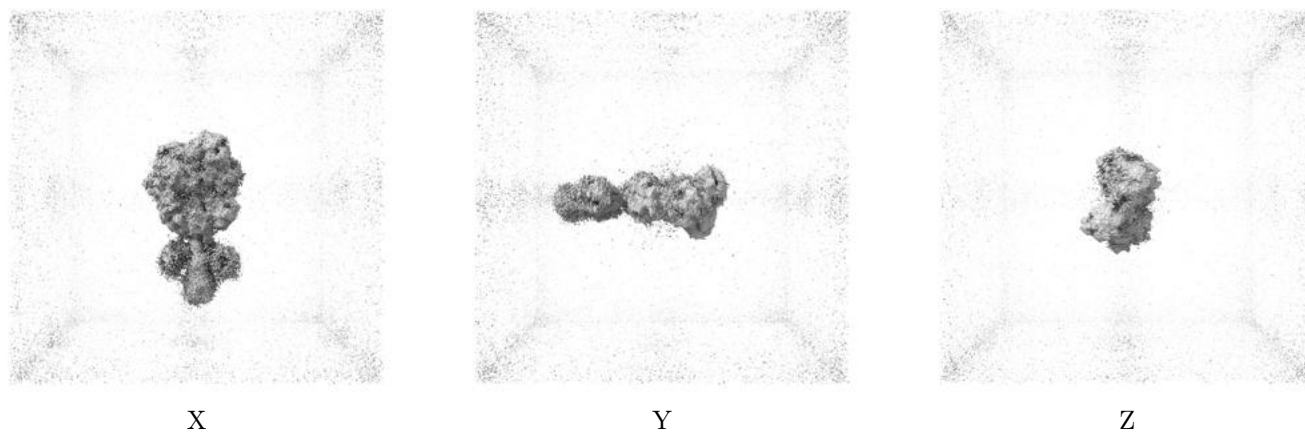
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0226. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

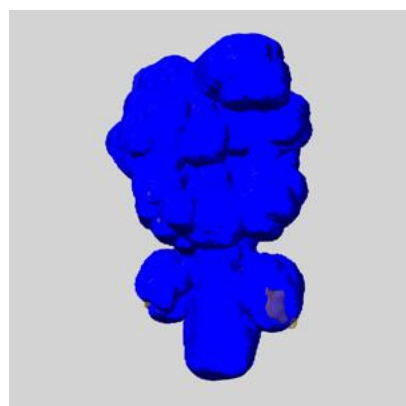
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

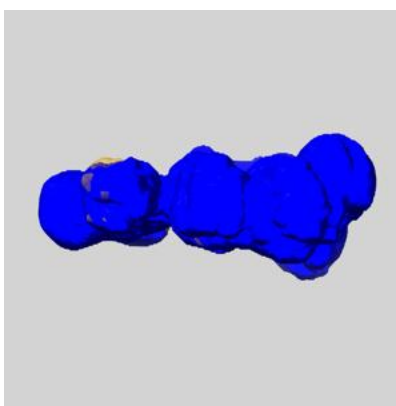
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

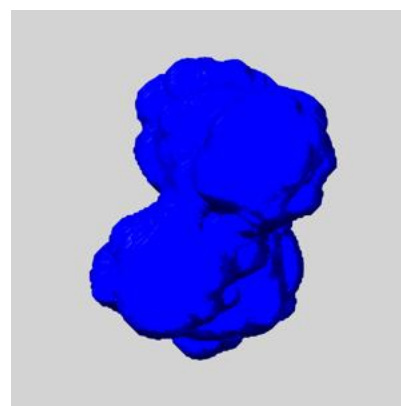
### 6.6.1 emd\_73612\_msk\_1.map [i](#)



X



Y

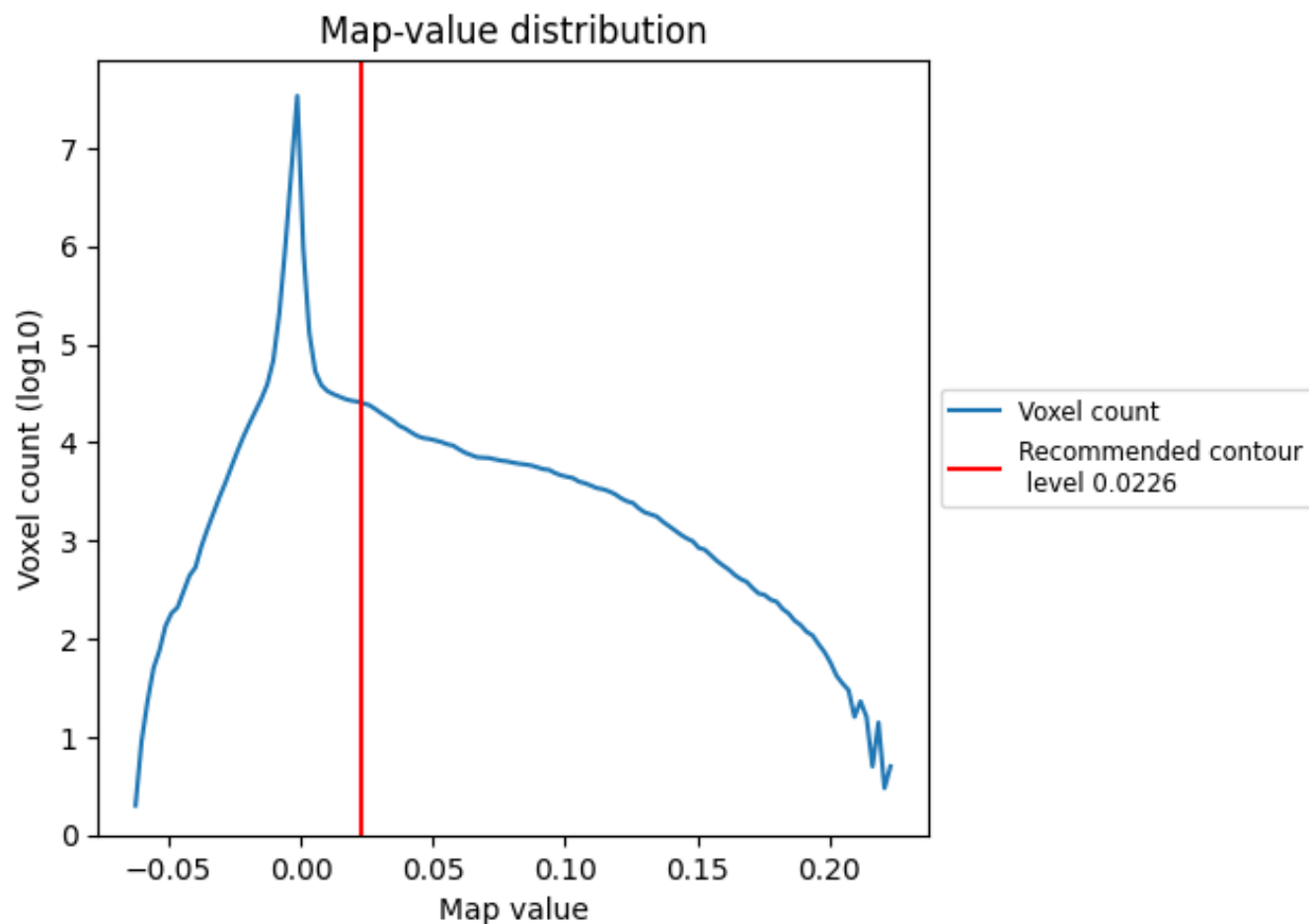


Z

## 7 Map analysis [i](#)

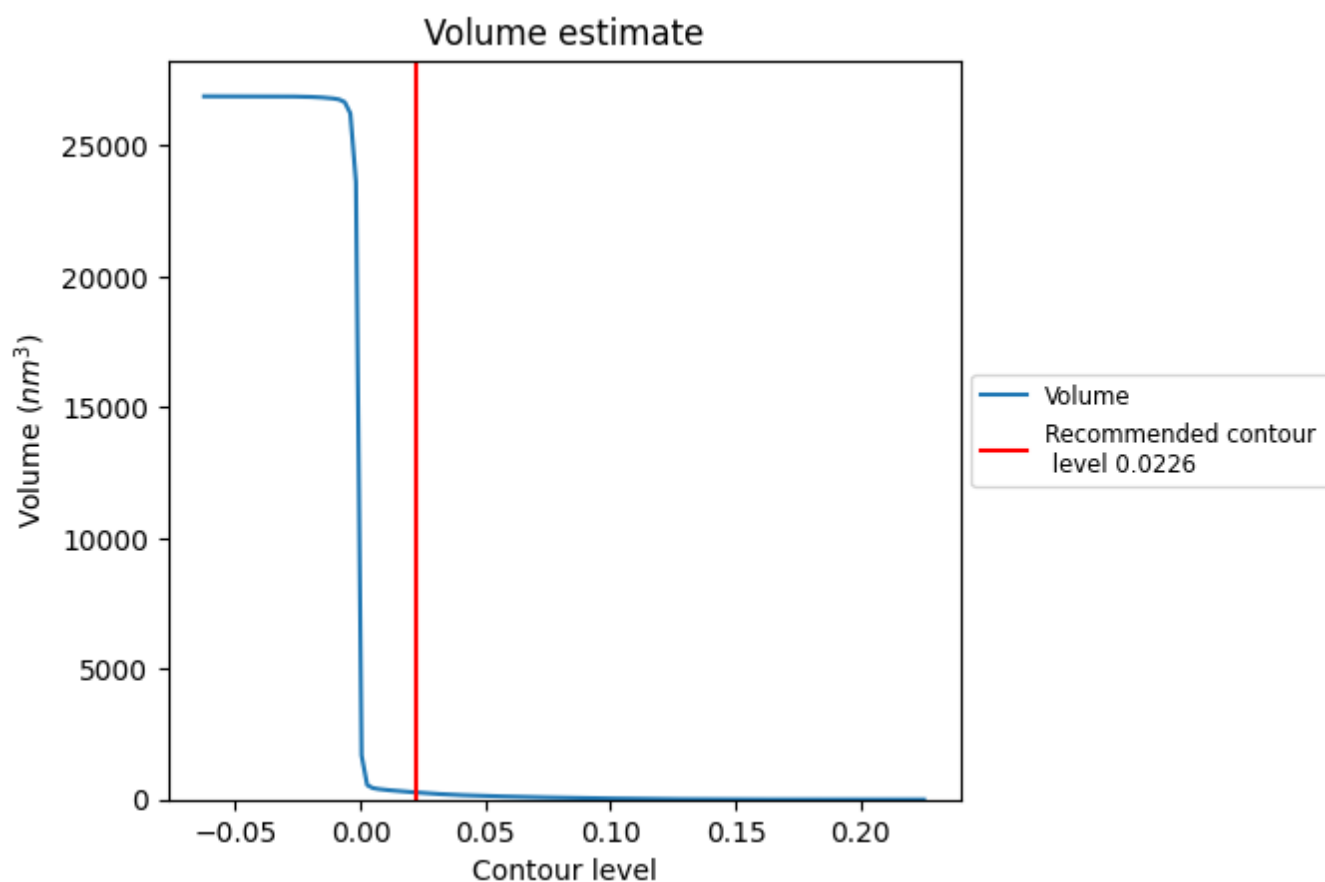
This section contains the results of statistical analysis of the map.

### 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.

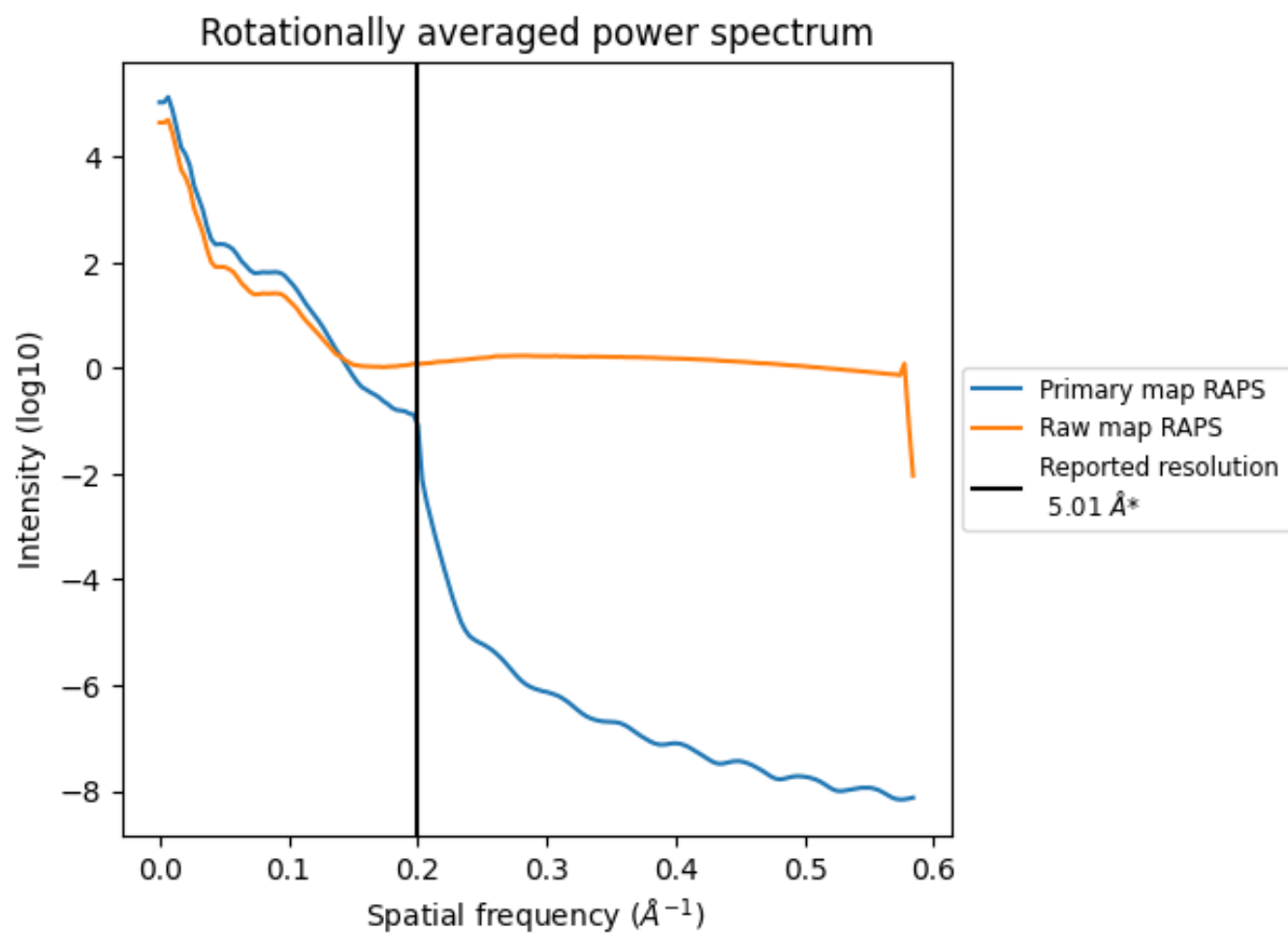
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 270 nm<sup>3</sup>; this corresponds to an approximate mass of 244 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 ⓘ

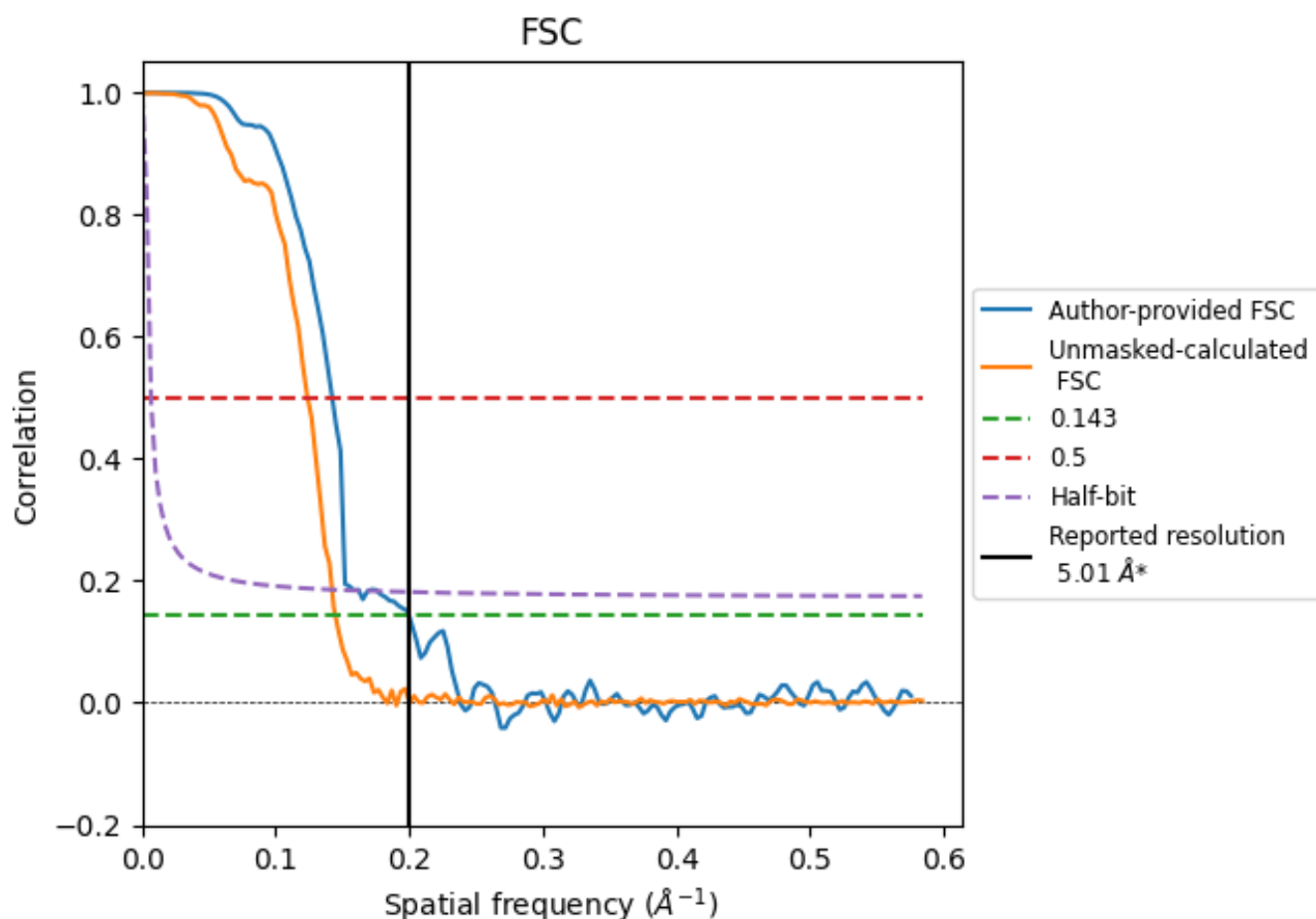


\*Reported resolution corresponds to spatial frequency of 0.200  $\text{\AA}^{-1}$

## 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 0.200  $\text{\AA}^{-1}$



## 8.2 Resolution estimates [i](#)

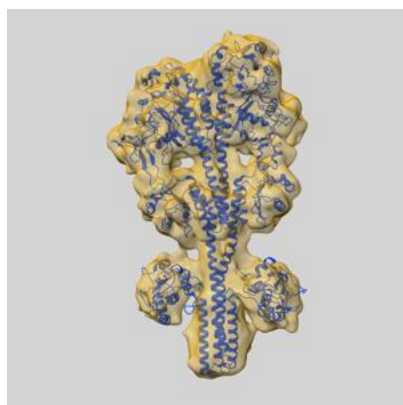
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.01	-	-
Author-provided FSC curve	5.01	7.03	6.16
Unmasked-calculated*	6.91	8.08	7.03

\*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 6.91 differs from the reported value 5.01 by more than 10 %

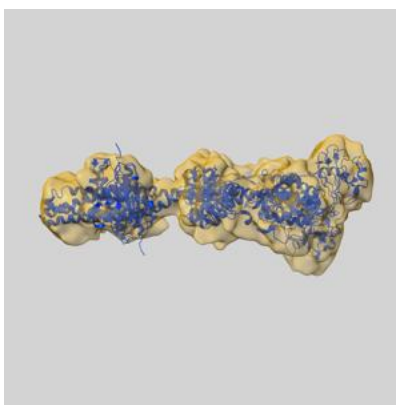
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-73612 and PDB model 9YXN. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

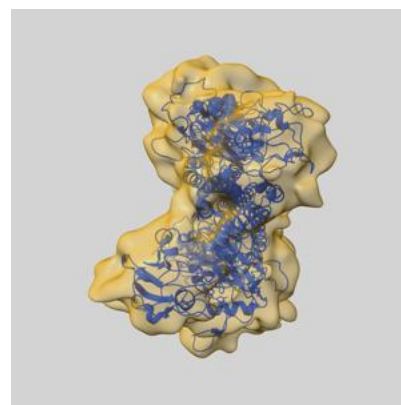
### 9.1 Map-model overlay [i](#)



X



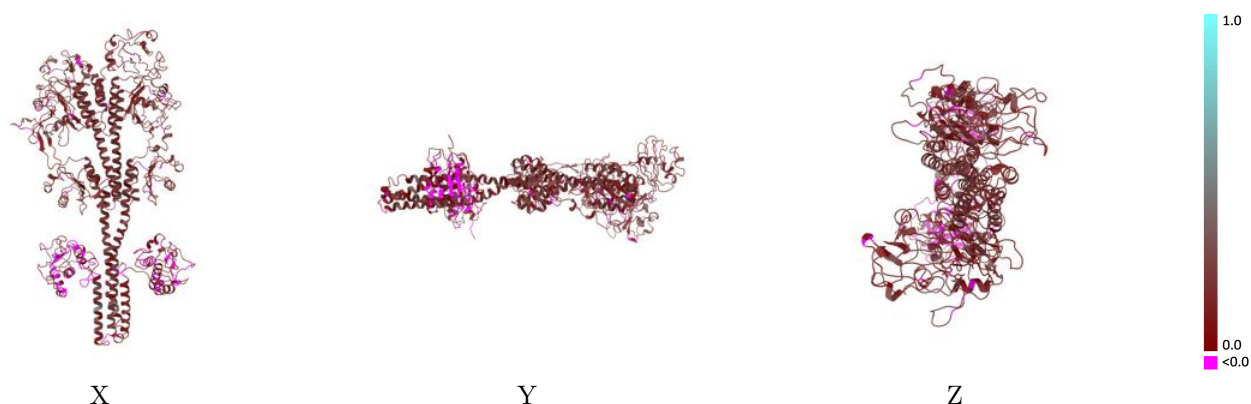
Y



Z

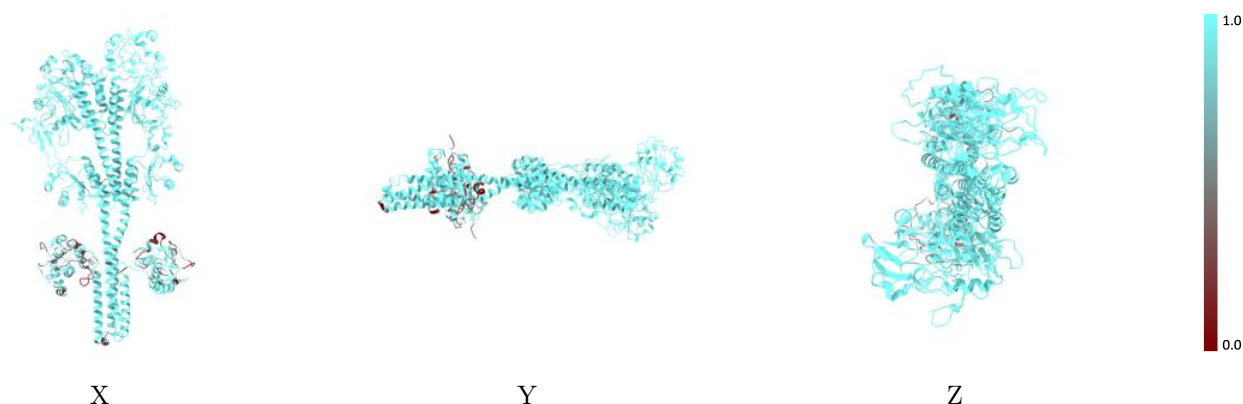
The images above show the 3D surface view of the map at the recommended contour level 0.0226 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



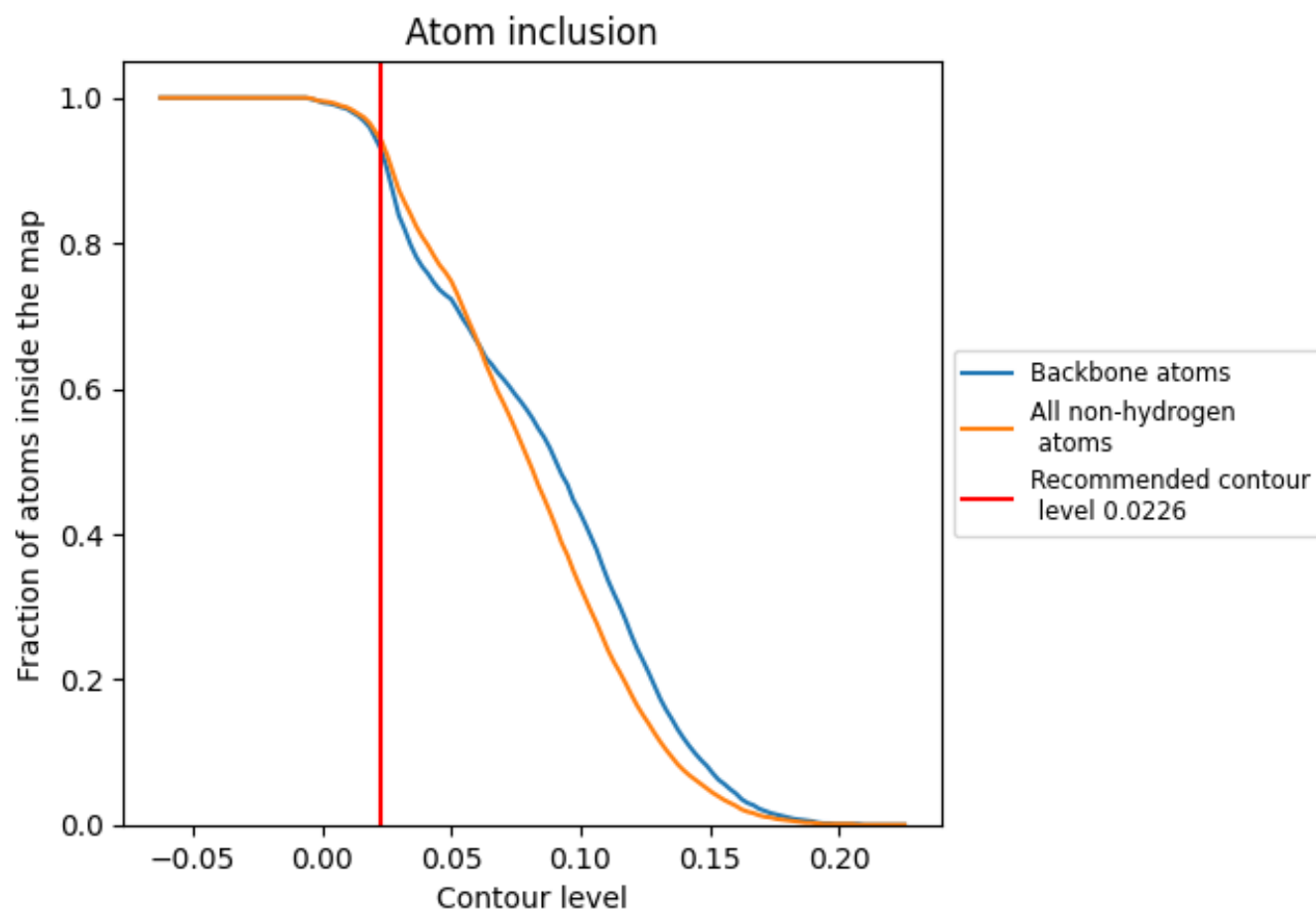
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0226).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 94% 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 (0.0226) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9430	<div></div> 0.1680
A	<div></div> 0.9490	<div></div> 0.1680
B	<div></div> 0.9370	<div></div> 0.1680

