



wwPDB EM Validation Summary Report ⓘ

Dec 21, 2024 – 03:58 pm GMT

PDB ID : 8RG7
EMDB ID : EMD-19130
Title : BmrA E504-R6G-25uMATP-Mg
Authors : Gobet, A.; Zarkadas, E.; Schoehn, G.; Falson, P.; Chaptal, V.
Deposited on : 2023-12-13
Resolution : 3.90 Å(reported)
Based on initial model : 6r81

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.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

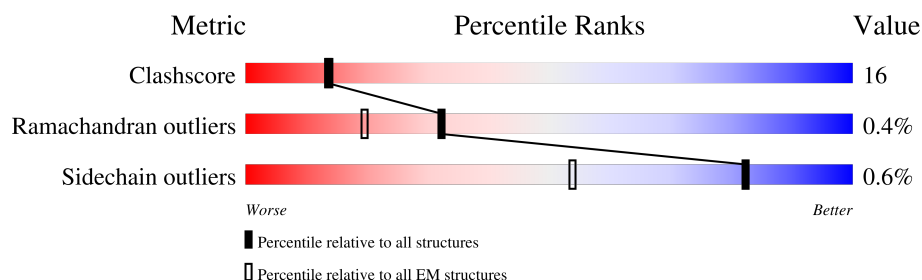
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	599	<div> <div>17%</div> <div>68%</div> <div>27%</div> <div>• 5%</div> </div>
1	B	599	<div> <div>18%</div> <div>60%</div> <div>34%</div> <div>• 5%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8868 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.

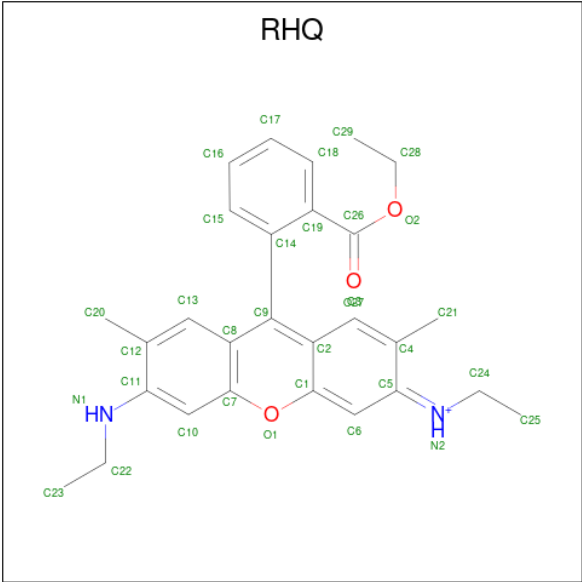
- Molecule 1 is a protein called Multidrug resistance ABC transporter ATP-binding/permease protein BmrA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	572	Total	C	N	O	S	0	0
			4401	2825	734	824	18		
1	B	572	Total	C	N	O	S	0	0
			4401	2825	734	824	18		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	initiating methionine	UNP O06967
A	-8	SER	-	expression tag	UNP O06967
A	-7	SER	-	expression tag	UNP O06967
A	-6	SER	-	expression tag	UNP O06967
A	-5	HIS	-	expression tag	UNP O06967
A	-4	HIS	-	expression tag	UNP O06967
A	-3	HIS	-	expression tag	UNP O06967
A	-2	HIS	-	expression tag	UNP O06967
A	-1	HIS	-	expression tag	UNP O06967
A	0	HIS	-	expression tag	UNP O06967
A	504	ALA	GLU	engineered mutation	UNP O06967
B	-9	MET	-	initiating methionine	UNP O06967
B	-8	SER	-	expression tag	UNP O06967
B	-7	SER	-	expression tag	UNP O06967
B	-6	SER	-	expression tag	UNP O06967
B	-5	HIS	-	expression tag	UNP O06967
B	-4	HIS	-	expression tag	UNP O06967
B	-3	HIS	-	expression tag	UNP O06967
B	-2	HIS	-	expression tag	UNP O06967
B	-1	HIS	-	expression tag	UNP O06967
B	0	HIS	-	expression tag	UNP O06967
B	504	ALA	GLU	engineered mutation	UNP O06967

- Molecule 2 is RHODAMINE 6G (three-letter code: RHQ) (formula: C₂₈H₃₁N₂O₃).

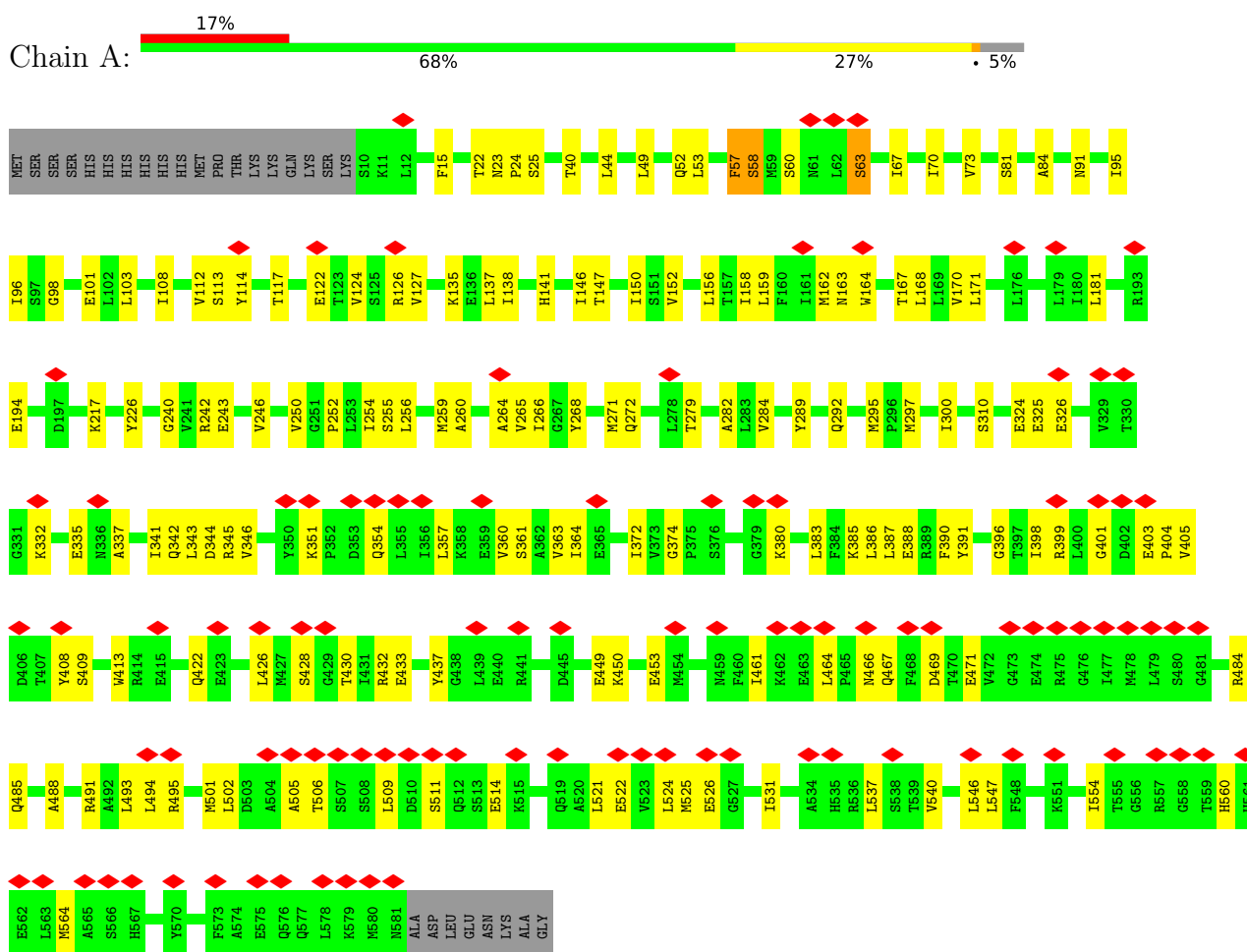


Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			33	28	2	3	
2	B	1	Total	C	N	O	0
			33	28	2	3	

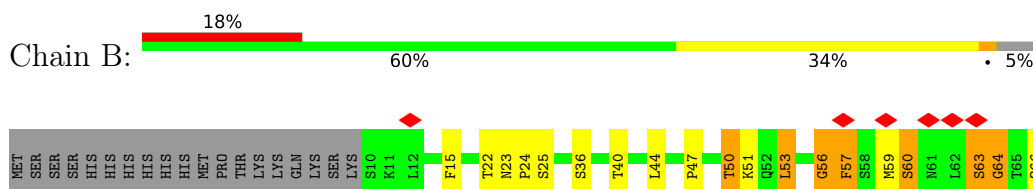
3 Residue-property plots [i](#)

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: Multidrug resistance ABC transporter ATP-binding/permease protein BmrA



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V73	R193	Y289	G379	T444	Q512	Q576
T85	E194	L290	K380	D445	S513	Q577
N89	D197	I293	T381	A446	E514	L578
Y90	N207	I294	L382	E447	K515	K579
N91	Q208	M295	L383	E453	S516	M580
I95	R214	M297	F384	M454	Q519	M581
G98	L215	I300	K385	A457	A520	ALA
E101	K217	Q308	L386	L458	L521	ASP
L102	Y226	K309	F390	N459	E522	LEU
L103	S310	I311	Y391	F460	V523	GLU
W104	E315	E325	A395	I461	L524	ASN
K105	T233	E326	T398	K462	M525	LYS
S113	S234	D327	R399	E463	E526	ALA
Y114	G240	T328	L400	L464	G527	GLY
T117	V241	Q333	G401	Q467	R528	
N118	R242	I334	D402	F468	T529	
A119	E243	E335	E403	D469	F530	
E122	A244	A337	P404	T470	F531	
T123	K245	Q342	V405	E471	V532	
V124	S248	L343	D406	V472	A534	
S125	P252	L344	T407	G473	H535	
R126	L253	D344	Y408	E474	L537	
V127	I254	R345	L410	R475	S538	
D130	S255	V346	E411	G476	T539	
E136	L256	S347	S412	I477	V540	
L137	V257	F348	W413	M478	V541	
I138	L258	G349	R414	L479	D542	
H141	M259	K351	E415	S480	A543	
T147	A260	D352	H416	R484	L547	
G148	A261	D353	I417	Q485	F548	
V152	Y268	Q354	G418	R486	V549	
L156	M271	L355	Y419	I487	E550	
T157	Q272	I356	Q422	A488	K551	
I158	V273	L357	E423	I489	Q552	
L159	S274	K358	S424	A490	E553	
F160	S275	E359	P425	R491	L554	
I161	G276	V360	L426	A492		
L168	E277	E365	M427	L493	R557	
L176	L278	A366	S428	L494	G558	
L179	T279	V369	G429	R495	T559	
I180	A282	T370	I431	N496	H560	
L181	L283	A371	R432	P497	H561	
	V284	I372	E433	S498	E562	
	I287	V373	N434	L499	A565	
	L288	G378	I435	L500	S566	
			C436	M501	H567	
			Y437	L502	G568	
			G438	D503	L569	
			L439	A504	R570	
			E440	A505	R571	
			R441	T506	F572	
			D442	S507	A574	
			V443	L508	E575	
				D510		
				S511		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	150715	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 ($e^-/\text{\AA}^2$)	38.79	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.972	Depositor
Minimum map value	-0.620	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.195	Depositor
Map size (Å)	269.312, 269.312, 269.312	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.052, 1.052, 1.052	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: RHQ

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	0.33	1/4468 (0.0%)	0.54	1/6047 (0.0%)
1	B	0.35	3/4468 (0.1%)	0.63	5/6047 (0.1%)
All	All	0.34	4/8936 (0.0%)	0.59	6/12094 (0.0%)

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	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	51	LYS	C-O	6.70	1.36	1.23
1	B	64	GLY	C-O	6.47	1.34	1.23
1	B	56	GLY	C-O	-5.54	1.14	1.23
1	A	52	GLN	C-O	5.46	1.33	1.23

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	404	PRO	CA-N-CD	-16.73	88.07	111.50
1	B	404	PRO	N-CD-CG	6.14	112.41	103.20
1	B	400	LEU	N-CA-C	-6.13	94.44	111.00
1	B	50	THR	O-C-N	-6.09	112.95	122.70
1	A	57	PHE	CB-CA-C	-5.41	99.59	110.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	402	ASP	Mainchain
1	B	50	THR	Mainchain
1	B	57	PHE	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	4401	0	4573	128	0
1	B	4401	0	4573	173	0
2	A	33	0	29	5	0
2	B	33	0	28	4	0
All	All	8868	0	9203	284	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 16.

The worst 5 of 284 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:449:GLU:OE2	1:A:450:LYS:HG3	1.56	1.04
1:A:181:LEU:HD11	1:A:254:ILE:HG13	1.57	0.87
1:A:342:GLN:HB3	1:A:399:ARG:HB3	1.54	0.86
1:B:502:LEU:HD22	1:B:532:VAL:HG13	1.63	0.80
1:A:271:MET:HG2	1:B:57:PHE:HB3	1.61	0.80

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	570/599 (95%)	527 (92%)	42 (7%)	1 (0%)	44	75
1	B	570/599 (95%)	510 (90%)	56 (10%)	4 (1%)	19	54
All	All	1140/1198 (95%)	1037 (91%)	98 (9%)	5 (0%)	32	65

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	SER
1	B	60	SER
1	B	404	PRO
1	B	69	LEU
1	B	68	GLY

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	482/506 (95%)	480 (100%)	2 (0%)	89	91
1	B	482/506 (95%)	478 (99%)	4 (1%)	79	84
All	All	964/1012 (95%)	958 (99%)	6 (1%)	82	88

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	63	SER
1	B	316	ARG
1	B	404	PRO
1	A	63	SER
1	A	58	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	560	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	$\# Z > 2$
2	RHQ	B	601	-	34,36,36	5.82	13 (38%)	39,51,51	4.17	14 (35%)
2	RHQ	A	601	-	34,36,36	5.73	13 (38%)	39,51,51	4.13	14 (35%)

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	RHQ	B	601	-	-	6/11/21/21	0/4/4/4
2	RHQ	A	601	-	-	5/11/21/21	0/4/4/4

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	RHQ	C6-C5	19.50	1.62	1.40
2	A	601	RHQ	C6-C5	18.49	1.61	1.40
2	B	601	RHQ	C2-C1	-15.44	1.19	1.41
2	A	601	RHQ	C2-C1	-15.44	1.19	1.41
2	A	601	RHQ	C4-C5	14.23	1.65	1.43

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	RHQ	C14-C19-C26	14.23	148.72	122.25
2	A	601	RHQ	C14-C19-C26	14.20	148.66	122.25
2	B	601	RHQ	C18-C19-C26	-12.20	90.84	116.95
2	A	601	RHQ	C4-C5-C6	-12.02	92.33	120.11
2	A	601	RHQ	C18-C19-C26	-11.99	91.30	116.95

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	RHQ	O27-C26-O2-C28
2	B	601	RHQ	C25-C24-N2-C5
2	B	601	RHQ	O27-C26-O2-C28
2	A	601	RHQ	C19-C26-O2-C28
2	B	601	RHQ	C19-C26-O2-C28

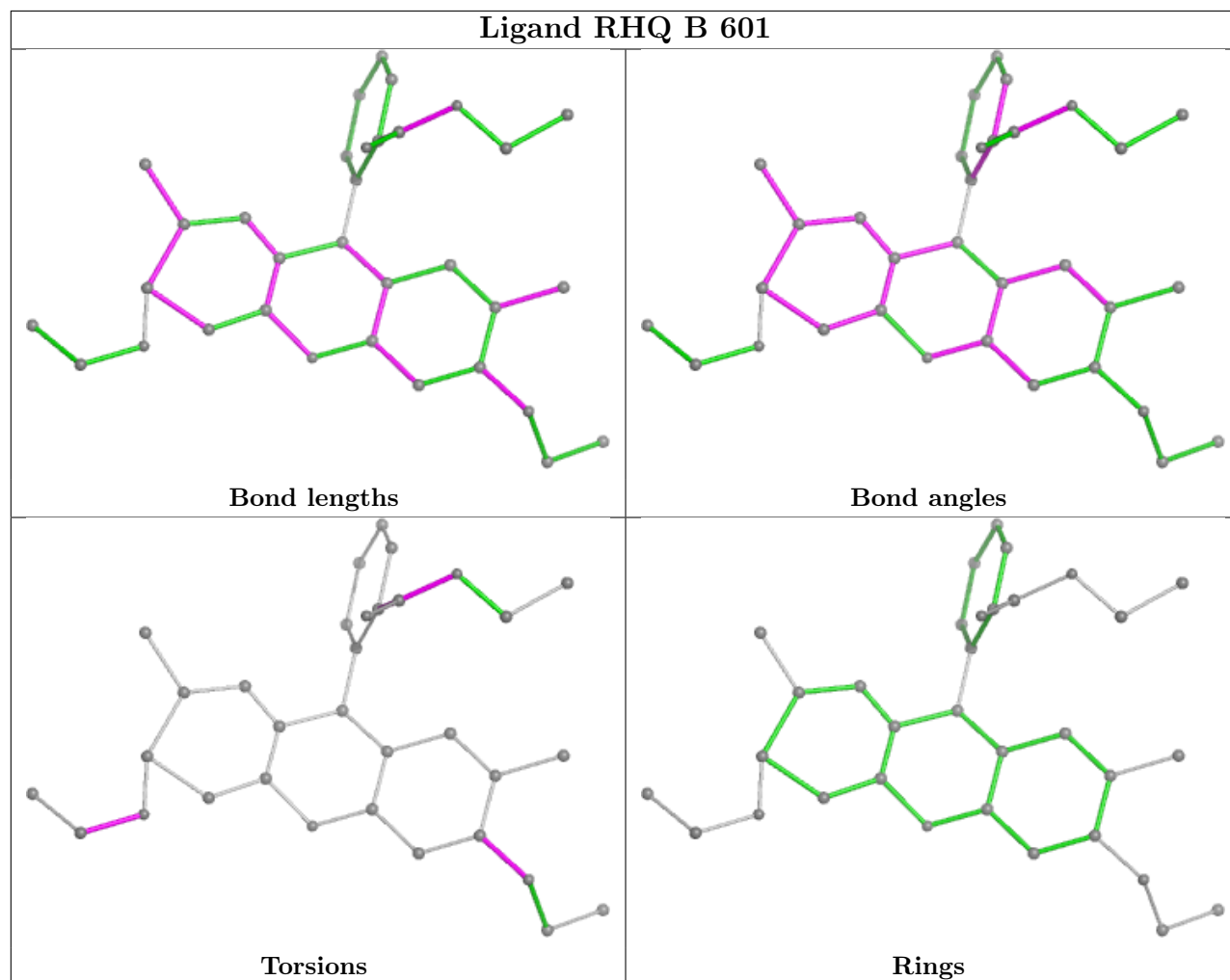
There are no ring outliers.

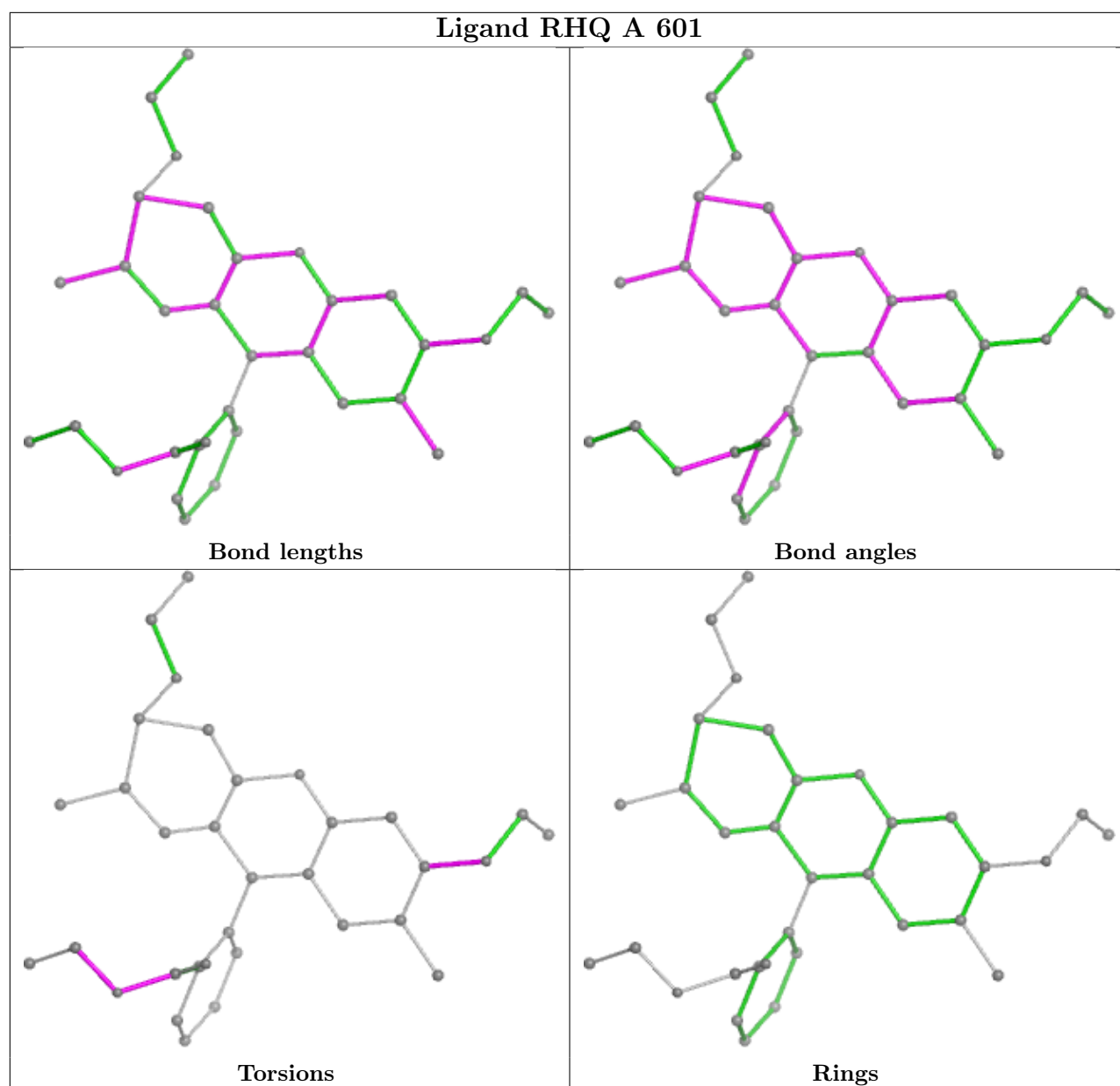
2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	RHQ	4	0
2	A	601	RHQ	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.

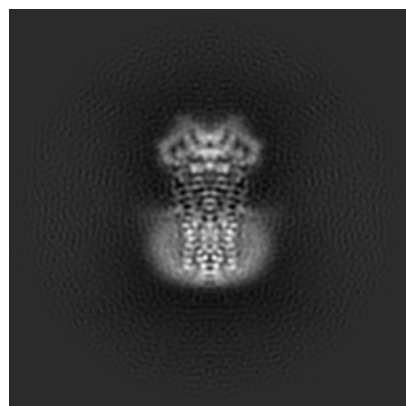
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19130. These allow visual inspection of the internal detail of the map and identification of artifacts.

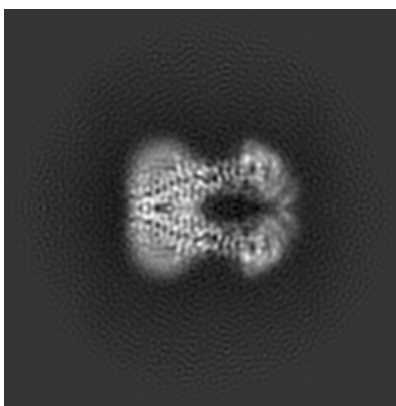
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

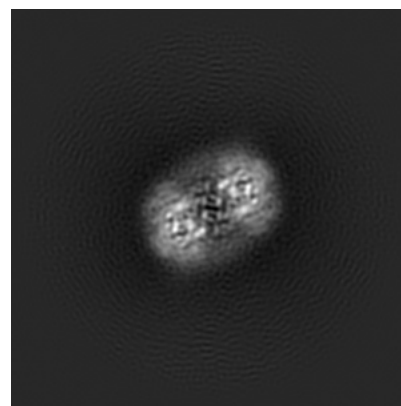
6.1.1 Primary map



X

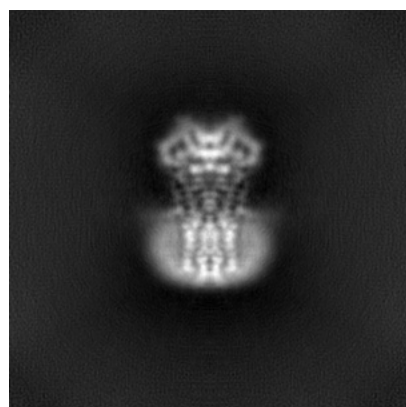


Y

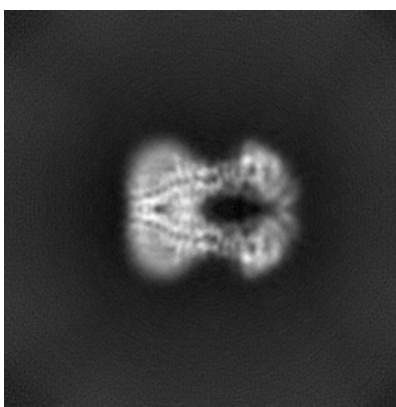


Z

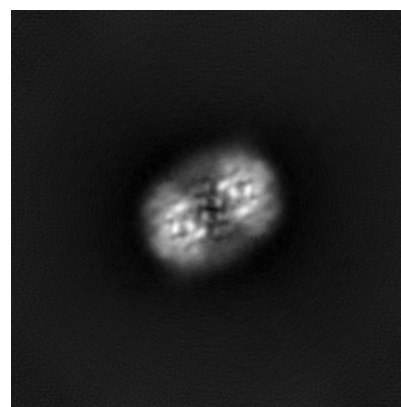
6.1.2 Raw map



X



Y

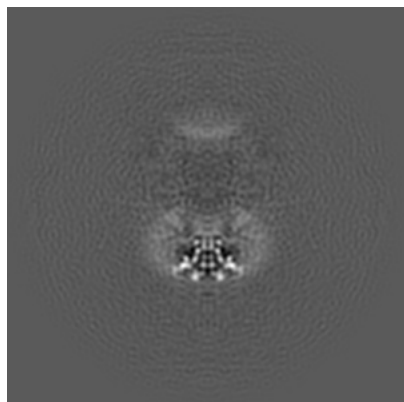


Z

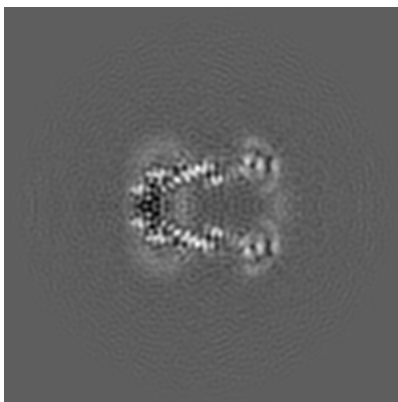
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

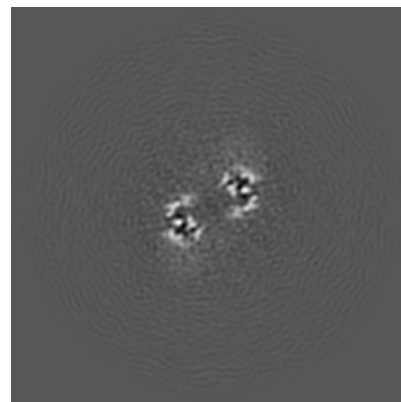
6.2.1 Primary map



X Index: 128

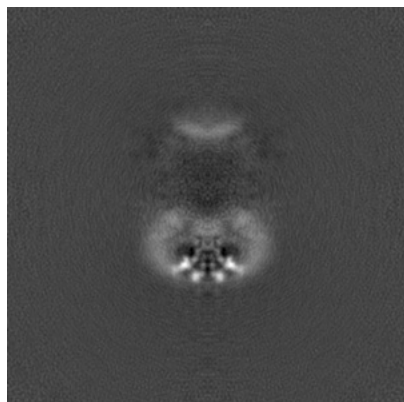


Y Index: 128

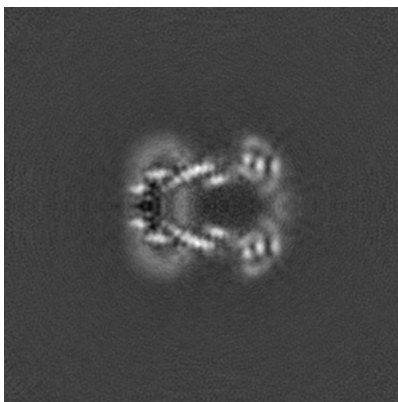


Z Index: 128

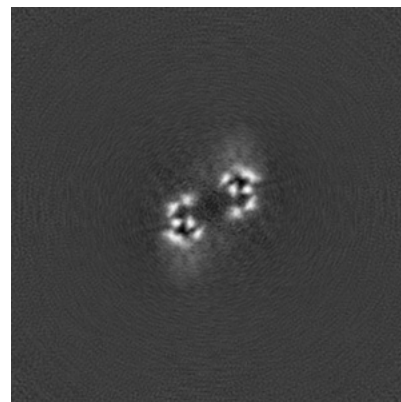
6.2.2 Raw map



X Index: 128



Y Index: 128

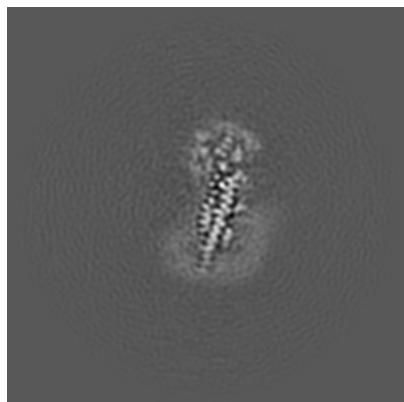


Z Index: 128

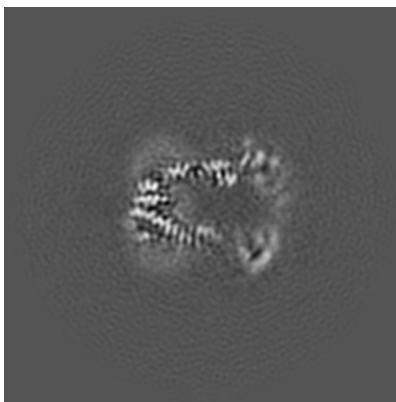
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

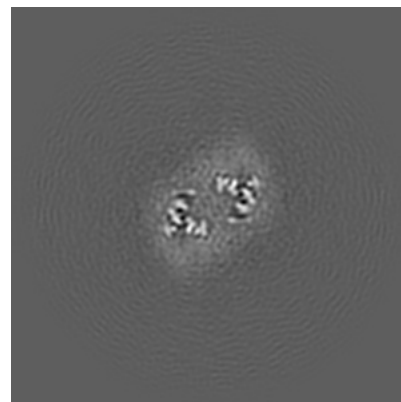
6.3.1 Primary map



X Index: 150

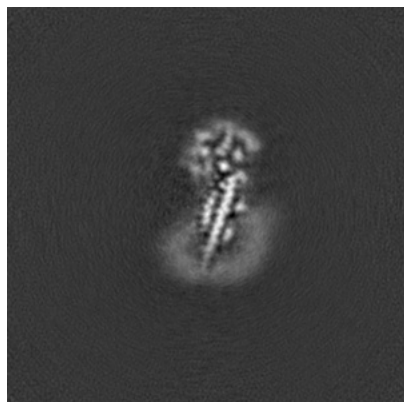


Y Index: 132

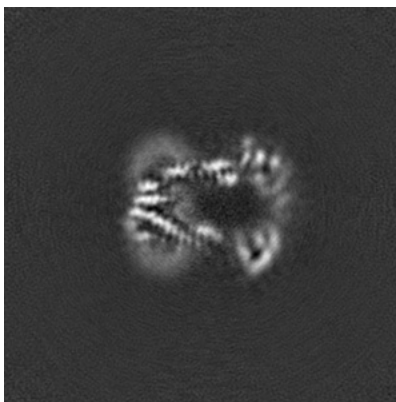


Z Index: 117

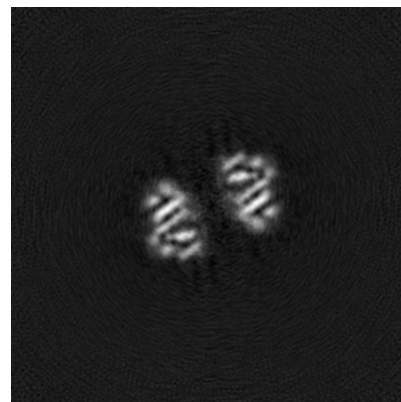
6.3.2 Raw map



X Index: 151



Y Index: 132

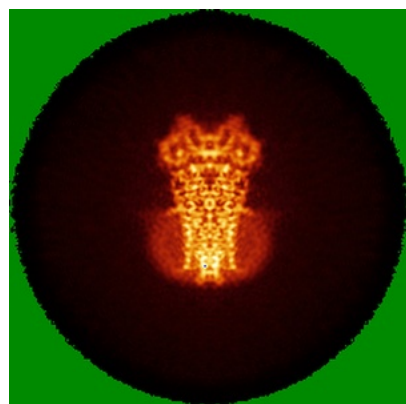


Z Index: 163

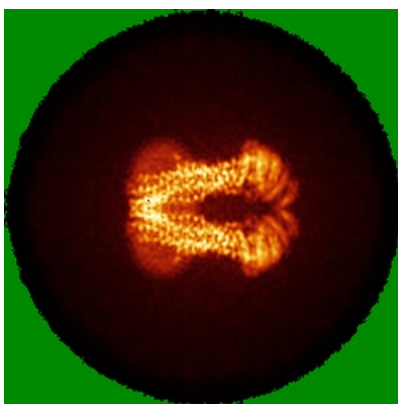
The images above show the largest variance slices of the map in three orthogonal directions.

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

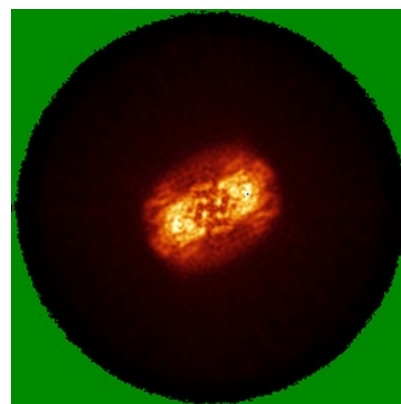
6.4.1 Primary map



X

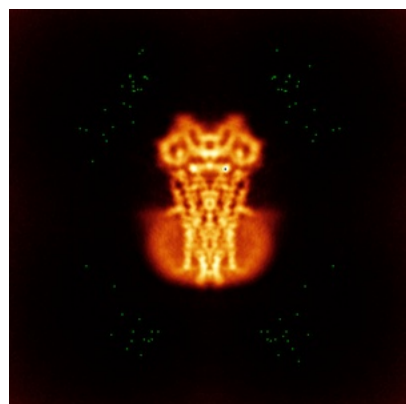


Y

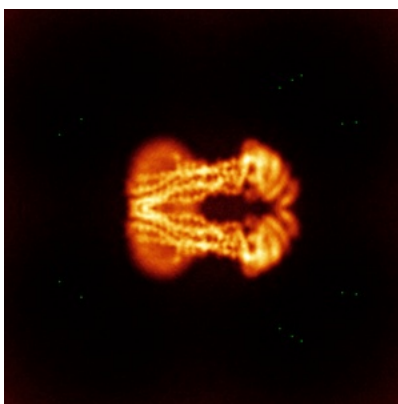


Z

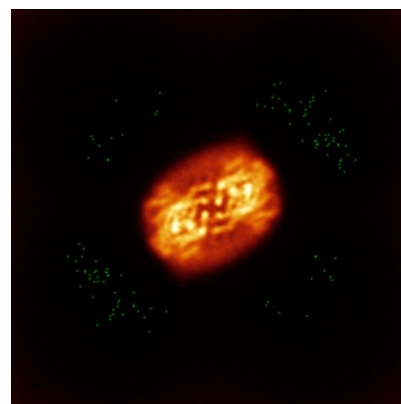
6.4.2 Raw map



X



Y

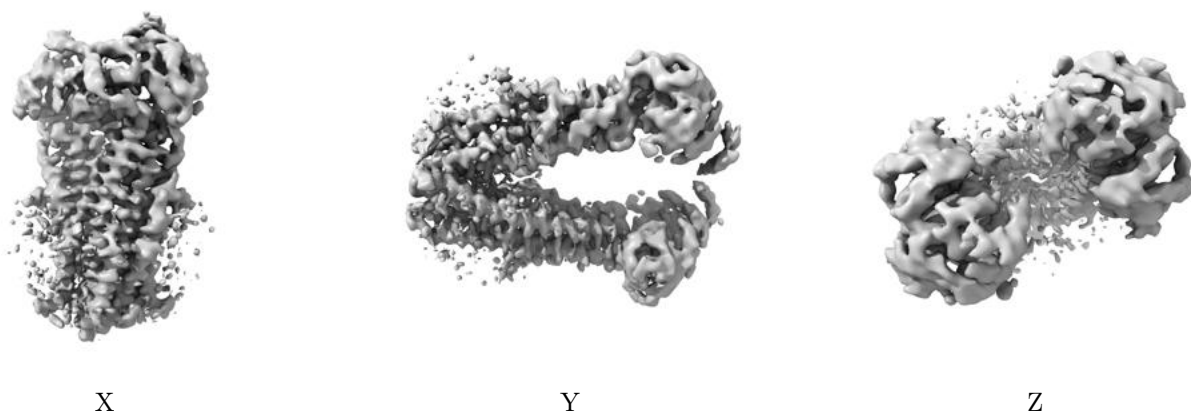


Z

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.

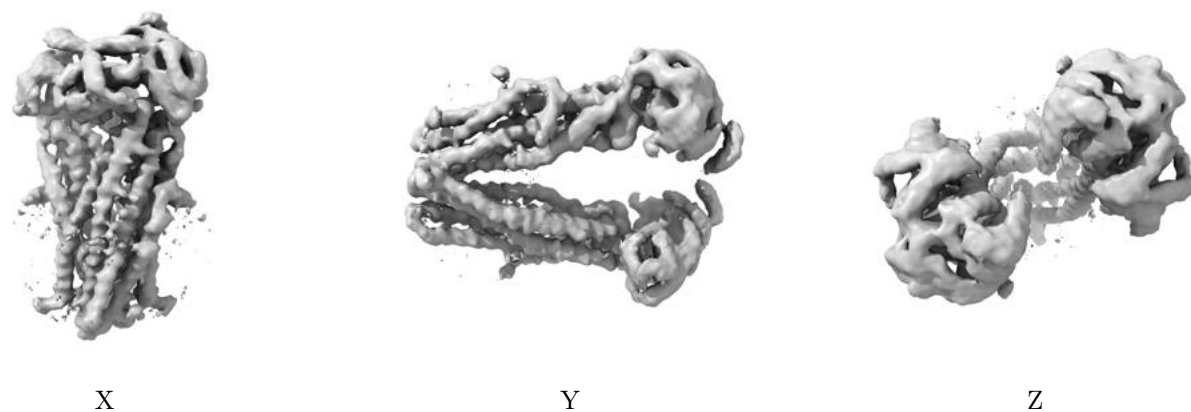
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.195. 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.

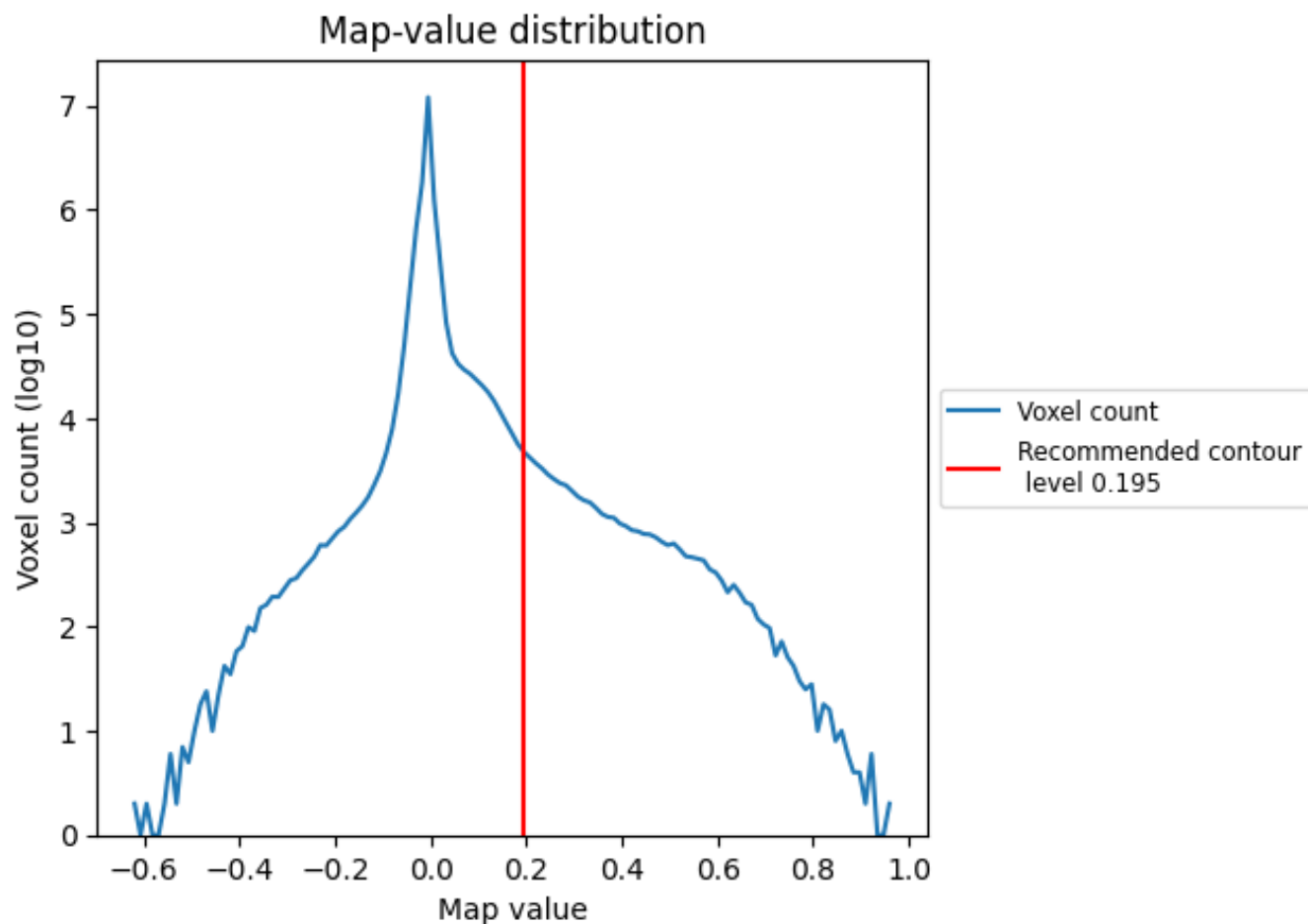
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

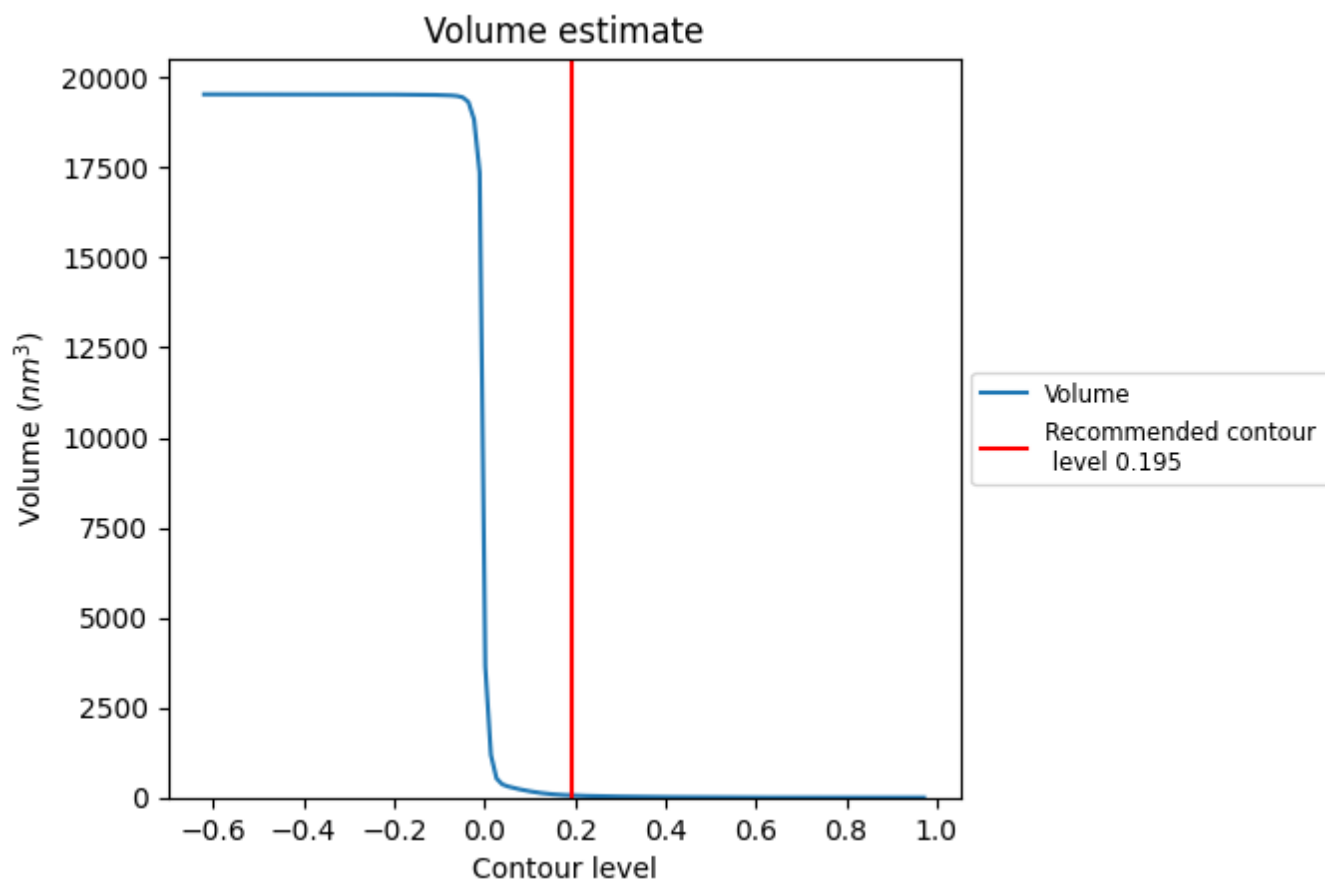
This section contains the results of statistical analysis of the map.

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.

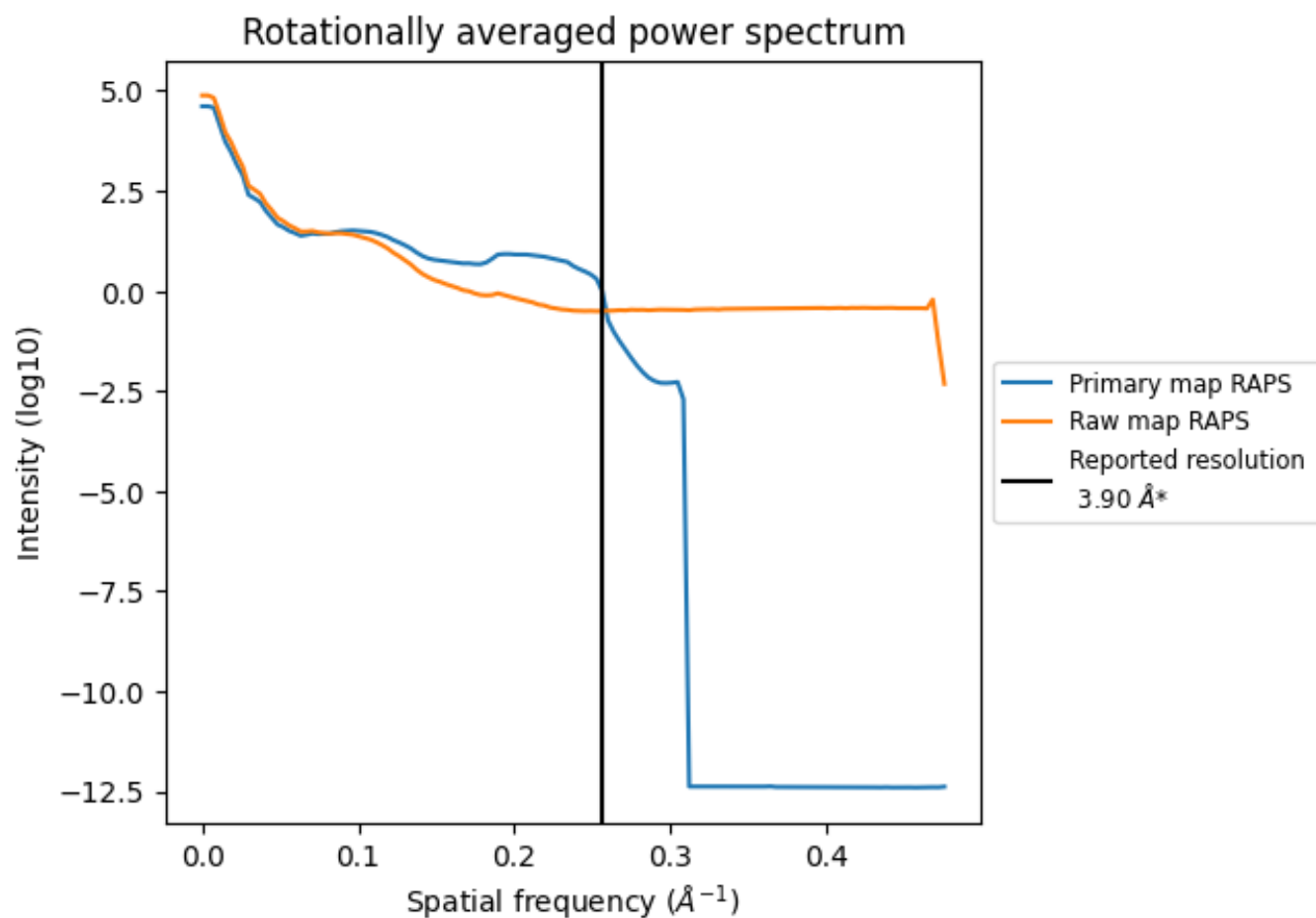
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 59 nm^3 ; this corresponds to an approximate mass of 53 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 ⓘ

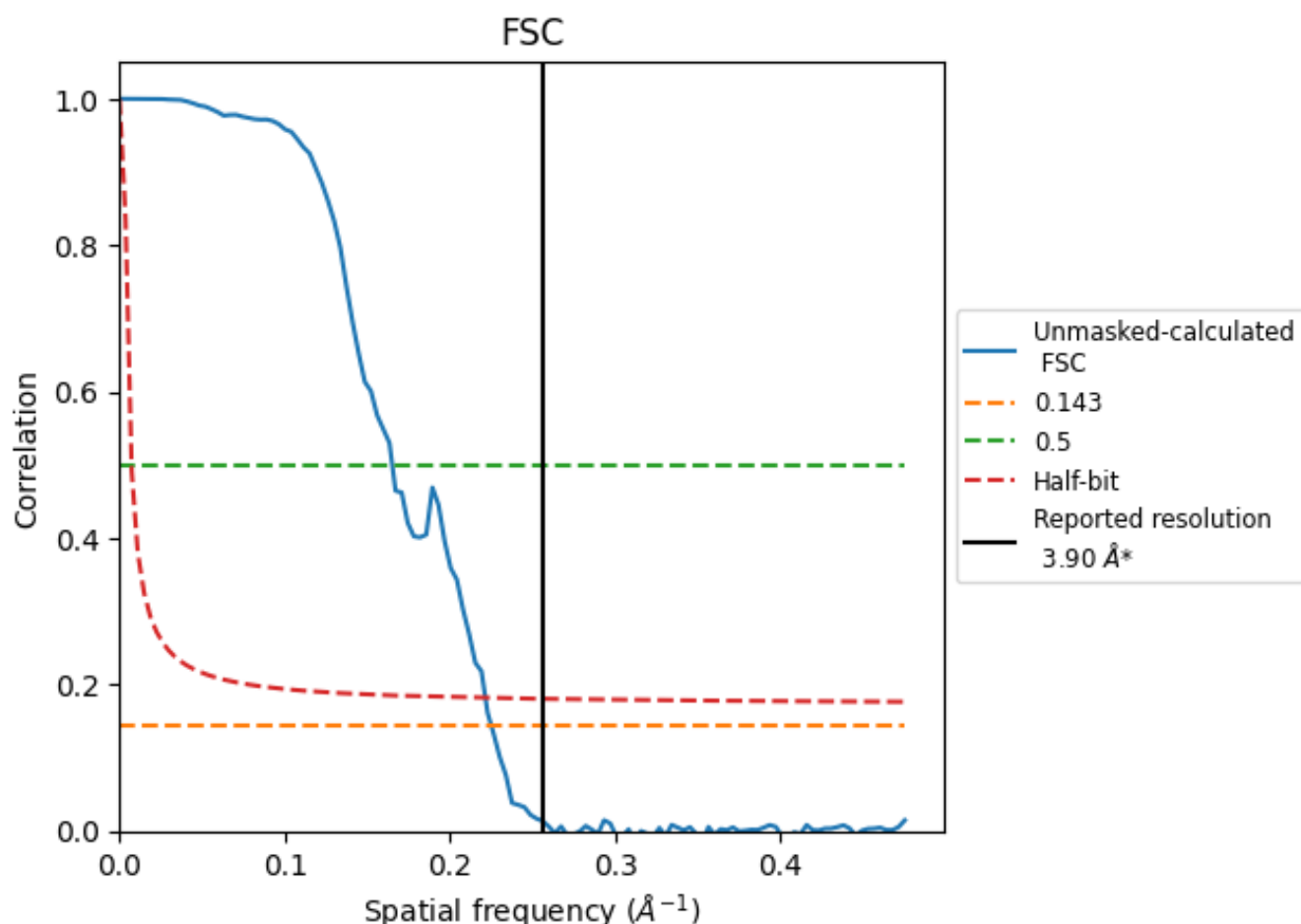


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

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 0.256 Å⁻¹

8.2 Resolution estimates [i](#)

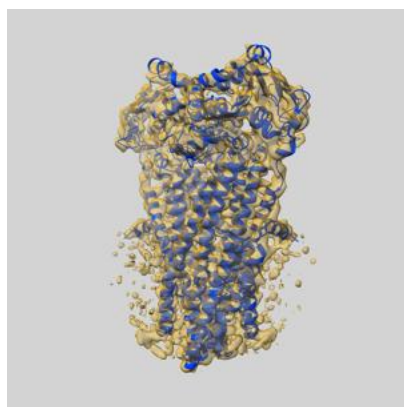
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.44	6.06	4.51

*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 4.44 differs from the reported value 3.9 by more than 10 %

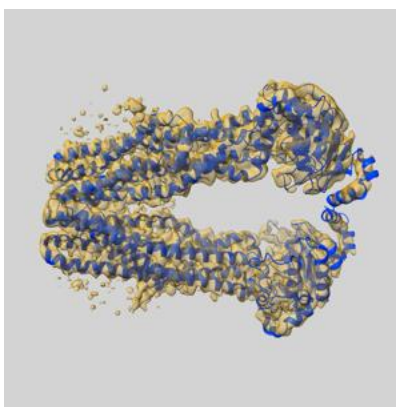
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-19130 and PDB model 8RG7. Per-residue inclusion information can be found in section [3](#) on page [5](#).

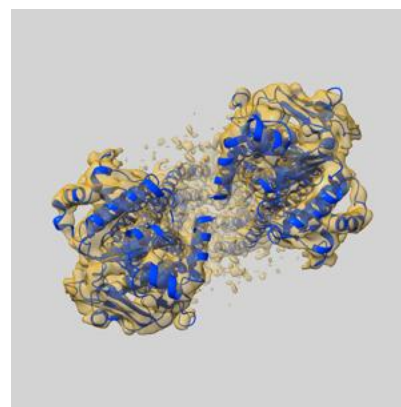
9.1 Map-model overlay [i](#)



X



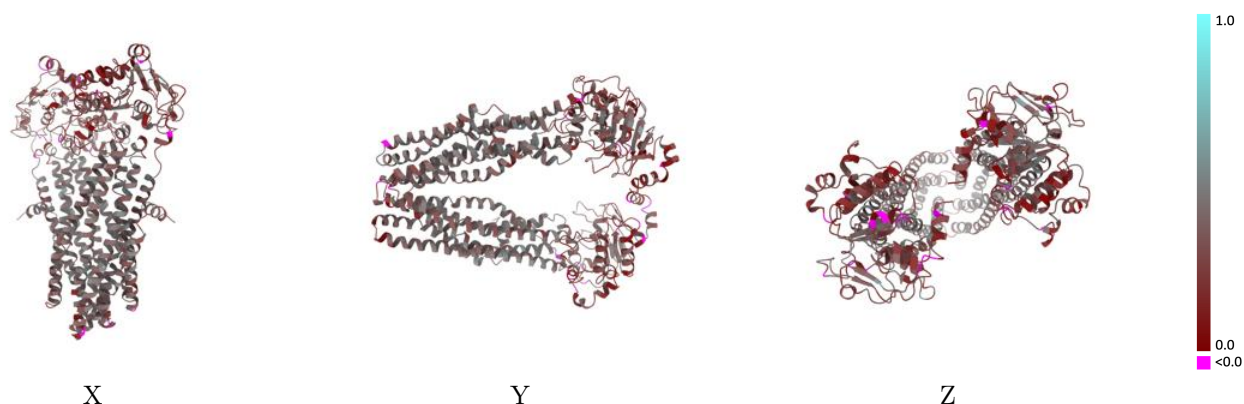
Y



Z

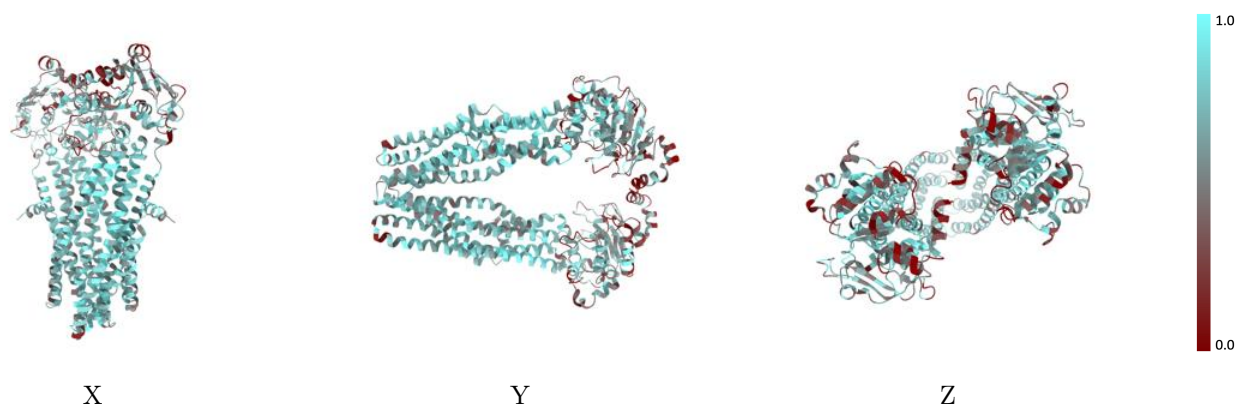
The images above show the 3D surface view of the map at the recommended contour level 0.195 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



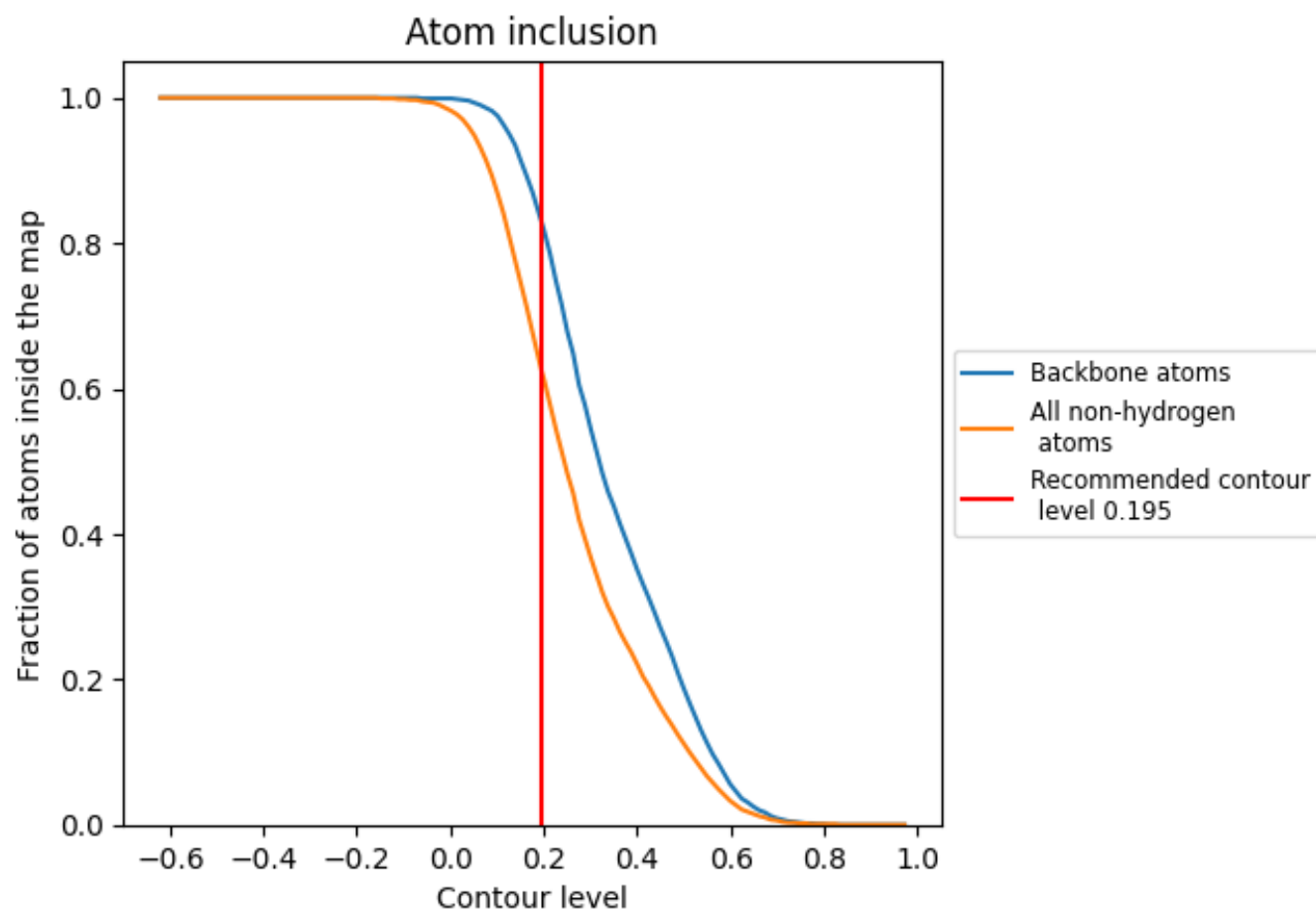
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.195).

9.4 Atom inclusion ⓘ



At the recommended contour level, 83% of all backbone atoms, 62% 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 (0.195) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6250	<div></div> 0.3290
A	<div></div> 0.6290	<div></div> 0.3330
B	<div></div> 0.6220	<div></div> 0.3250

