



## wwPDB EM Validation Summary Report ⓘ

Dec 21, 2024 – 04:24 pm GMT

PDB ID : 8RGN  
EMDB ID : EMD-19135  
Title : BmrA E504-R6G-70uMATPMg  
Authors : Gobet, A.; Zarkadas, E.; Schoehn, G.; Falson, P.; Chaptal, V.  
Deposited on : 2023-12-14  
Resolution : 3.70 Å(reported)  
Based on initial model : 6r72

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.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

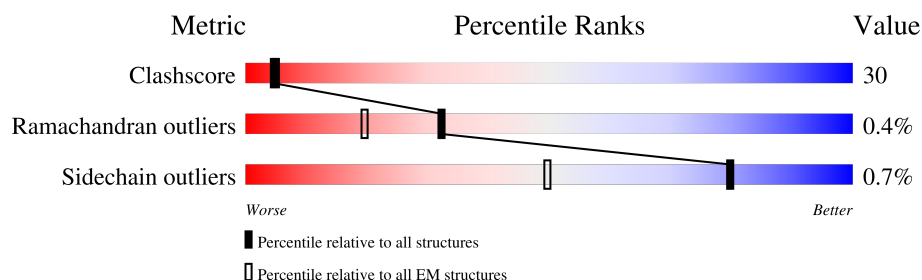
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.70 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  $\geq 3$ , 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	599	<div> <div>9%</div> <div>48%</div> <div>48%</div> <div>• •</div> </div>
1	B	599	<div> <div>9%</div> <div>47%</div> <div>47%</div> <div>• •</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9031 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.

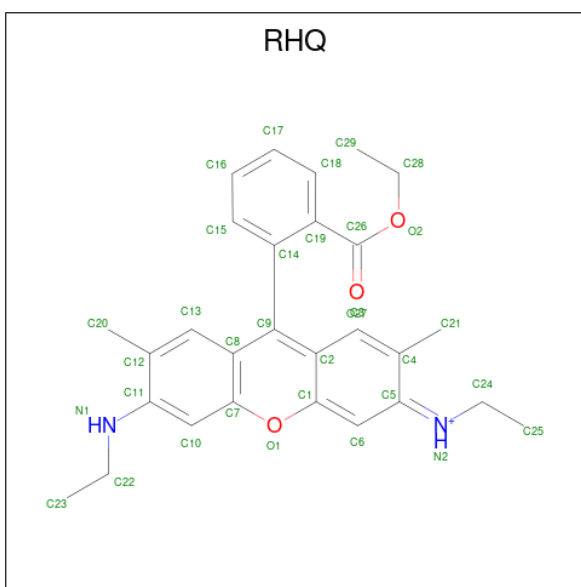
- Molecule 1 is a protein called Multidrug resistance ABC transporter ATP-binding/permease protein BmrA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	578	Total	C	N	O	S	0	0
			4448	2853	742	835	18		
1	B	578	Total	C	N	O	S	0	0
			4448	2853	742	835	18		

There are 22 discrepancies between the modelled and reference sequences:

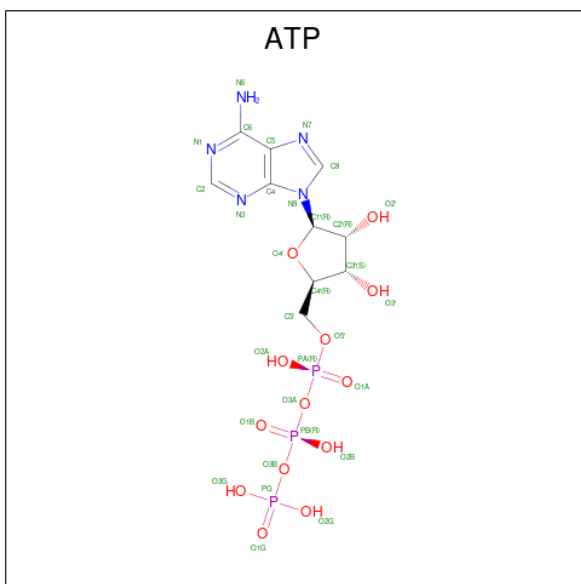
Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	initiating methionine	UNP O06967
A	-8	SER	-	expression tag	UNP O06967
A	-7	SER	-	expression tag	UNP O06967
A	-6	SER	-	expression tag	UNP O06967
A	-5	HIS	-	expression tag	UNP O06967
A	-4	HIS	-	expression tag	UNP O06967
A	-3	HIS	-	expression tag	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: C<sub>28</sub>H<sub>31</sub>N<sub>2</sub>O<sub>3</sub>).



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	

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

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Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	
4	B	1	Total	Mg	0
			1	1	

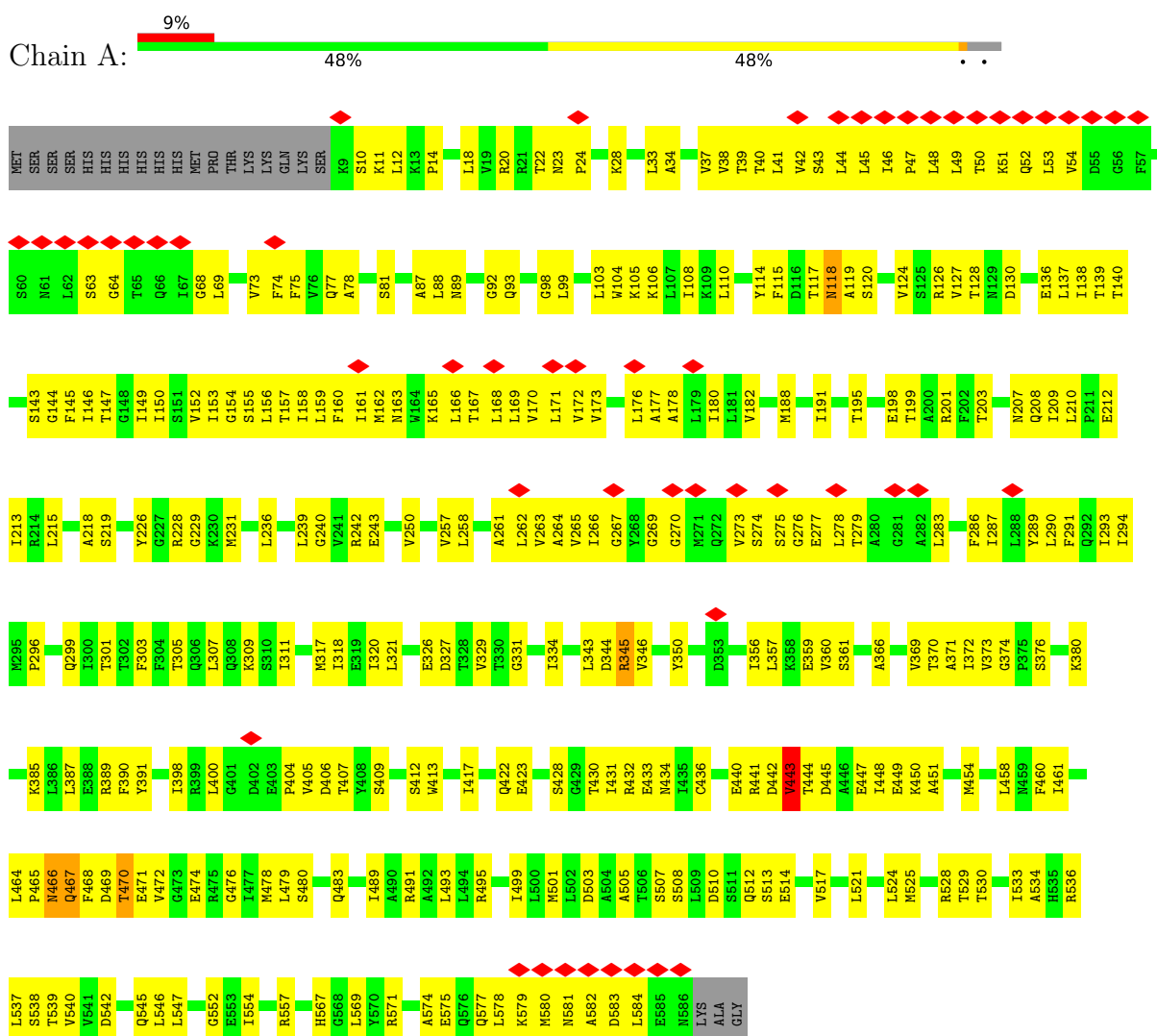
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		AltConf
5	A	3	Total	O	0
			3	3	
5	B	2	Total	O	0
			2	2	

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Multidrug resistance ABC transporter ATP-binding/permease protein BmrA



- Molecule 1: Multidrug resistance ABC transporter ATP-binding/permease protein BmrA



L533	F460	S376	F291	L209	L137	MET
A534	I461	K380	Q292	L210	I138	SER
R536	I461	K380	I293	P211	T139	SER
L537	L464	K385	I294	E212	T140	SER
S538	P465	L386	M295	R213	S143	HIS
T539	M466	L387	P296	L214	G144	HIS
V540	Q467	E388	Q299	L215	G145	HIS
V541	R389	F390	I300	A218	F146	HIS
D542	F468	Y391	T301	S219	T147	HIS
	T470	Y391	T302		G148	HIS
Q545	E471	S392	F303	Y226	I149	MET
L546	V472	P393	F504	G227	G68	PRO
L547	G473	T394	T305	R228	I150	THR
	E474	A395	Q306	G229	L69	LYS
L554	N478	I398	Q308	M231	V73	LYS
R557	L479	R399	K309	L236	F74	LYS
L563	S480	L400	S310	L239	F75	LYS
	Q483	G401	I311	G240	Q77	SER
H567	L489	E403	M317	V241	A78	K9
Q568	A490	P404	I318	R242	S81	S10
L569	R491	V405	E319	E243	A87	K11
V570	A492	D406	I320	M162	L88	L12
R571	L493	T407	L321	N163	N89	K13
	L494	Y408	E326	V164	L18	P14
A574	R495	S409	D327	K165	L18	L18
E575	L499	M413	T328	L166	V19	V19
Q576	L500	I417	V329	L167	R20	R20
L578	R501	Q422	T330	L168	R21	R21
K579	L502	Q423	G331	L169	T22	T22
M580	D503	S424	L343	L170	M23	M23
N581	A504	S424	L343	L171	P24	P24
A582	A505	S424	R345	V172	K28	K28
D583	T506	S428	V346	V173	L33	L33
L584	S507	G429	S347	L176	A34	A34
E585	S508	T430	Y350	A177	V37	V37
N586	L509	I431	D353	A178	V38	V38
LYS	D510	E432	I356	L179	T39	T39
ALA	S511	E433	L357	L180	T40	T40
GLY	Q512	M434	K358	L181	L41	L41
	S513	I435	E359	S113	V42	V42
	E514	C436	V360	Y114	S43	S43
	V517	E440	S361	F115	L44	L44
	Q518	R441	A366	D116	L45	L45
	Q519	D442	V369	T117	I46	I46
	A520	V443	T370	N118	P47	P47
	L521	T443	A371	A119	L48	L48
	L524	D445	I372	S120	L49	L49
	N525	A446	G374	G121	T50	T50
	E447	E448	F286	V124	K51	K51
	R528	A452	L288	S125	Q52	Q52
	T529	A457	L289	R126	V127	V127
	T530		L290	T202	T128	T128
				T203	N129	N129
				Q208	V54	V54
					D55	D55
					G56	G56
					F57	F57
					S58	S58

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	123402	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 ( $e^-/\text{\AA}^2$ )	37.95	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.798	Depositor
Minimum map value	-2.743	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.073	Depositor
Recommended contour level	0.381	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: MG, RHQ, ATP

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	0.37	0/4515	0.69	12/6110 (0.2%)
1	B	0.38	0/4515	0.74	13/6110 (0.2%)
All	All	0.37	0/9030	0.72	25/12220 (0.2%)

There are no bond length outliers.

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	119	ALA	N-CA-CB	-20.81	80.97	110.10
1	A	119	ALA	N-CA-CB	-19.44	82.88	110.10
1	B	470	THR	N-CA-C	-17.84	62.82	111.00
1	A	470	THR	N-CA-C	-12.25	77.93	111.00
1	B	118	ASN	CB-CA-C	12.16	134.72	110.40

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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	4448	0	4618	297	0
1	B	4448	0	4618	292	0
2	A	33	0	31	0	0
2	B	33	0	31	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	31	0	12	2	0
3	B	31	0	12	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	3	0	0	0	0
5	B	2	0	0	0	0
All	All	9031	0	9322	550	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 30.

The worst 5 of 550 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:466:ASN:HB3	1:A:468:PHE:CE2	1.55	1.40
1:A:466:ASN:CB	1:A:468:PHE:CE2	2.16	1.28
1:A:466:ASN:HB3	1:A:468:PHE:CD2	1.75	1.22
1:B:121:GLY:O	1:B:124:VAL:HG22	1.51	1.11
1:A:466:ASN:CB	1:A:468:PHE:CD2	2.41	0.99

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	576/599 (96%)	549 (95%)	25 (4%)	2 (0%)	37 67
1	B	576/599 (96%)	549 (95%)	24 (4%)	3 (0%)	25 57
All	All	1152/1198 (96%)	1098 (95%)	49 (4%)	5 (0%)	32 62

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	466	ASN
1	B	466	ASN
1	A	469	ASP
1	B	469	ASP
1	B	444	THR

### 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	487/506 (96%)	484 (99%)	3 (1%)	84	90
1	B	487/506 (96%)	483 (99%)	4 (1%)	79	85
All	All	974/1012 (96%)	967 (99%)	7 (1%)	80	88

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	344	ASP
1	B	448	ILE
1	B	542	ASP
1	B	467	GLN
1	A	542	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	434	ASN
1	A	512	GLN
1	A	581	ASN
1	B	434	ASN
1	B	581	ASN

### 5.3.3 RNA ⓘ

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](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	RHQ	A	601	-	34,36,36	1.68	6 (17%)	39,51,51	1.50	6 (15%)
3	ATP	B	602	4	26,33,33	0.95	1 (3%)	31,52,52	1.75	5 (16%)
2	RHQ	B	601	-	34,36,36	1.68	6 (17%)	39,51,51	1.50	6 (15%)
3	ATP	A	602	4	26,33,33	0.94	1 (3%)	31,52,52	1.76	5 (16%)

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	A	601	-	-	6/11/21/21	0/4/4/4
3	ATP	B	602	4	-	2/18/38/38	0/3/3/3
2	RHQ	B	601	-	-	6/11/21/21	0/4/4/4
3	ATP	A	602	4	-	2/18/38/38	0/3/3/3

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	RHQ	C11-N1	4.76	1.50	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	RHQ	C11-N1	4.76	1.50	1.37
2	B	601	RHQ	O2-C26	3.89	1.43	1.33
2	A	601	RHQ	O2-C26	3.86	1.43	1.33
2	A	601	RHQ	C21-C4	3.52	1.57	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	RHQ	O2-C26-C19	5.08	119.41	111.56
2	B	601	RHQ	O2-C26-C19	5.06	119.39	111.56
3	A	602	ATP	PB-O3B-PG	-4.87	116.11	132.83
3	B	602	ATP	PA-O3A-PB	-4.81	116.32	132.83
3	B	602	ATP	PB-O3B-PG	-4.77	116.45	132.83

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	RHQ	C19-C26-O2-C28
2	B	601	RHQ	C19-C26-O2-C28
2	A	601	RHQ	O27-C26-O2-C28
2	B	601	RHQ	O27-C26-O2-C28
2	A	601	RHQ	C10-C11-N1-C22

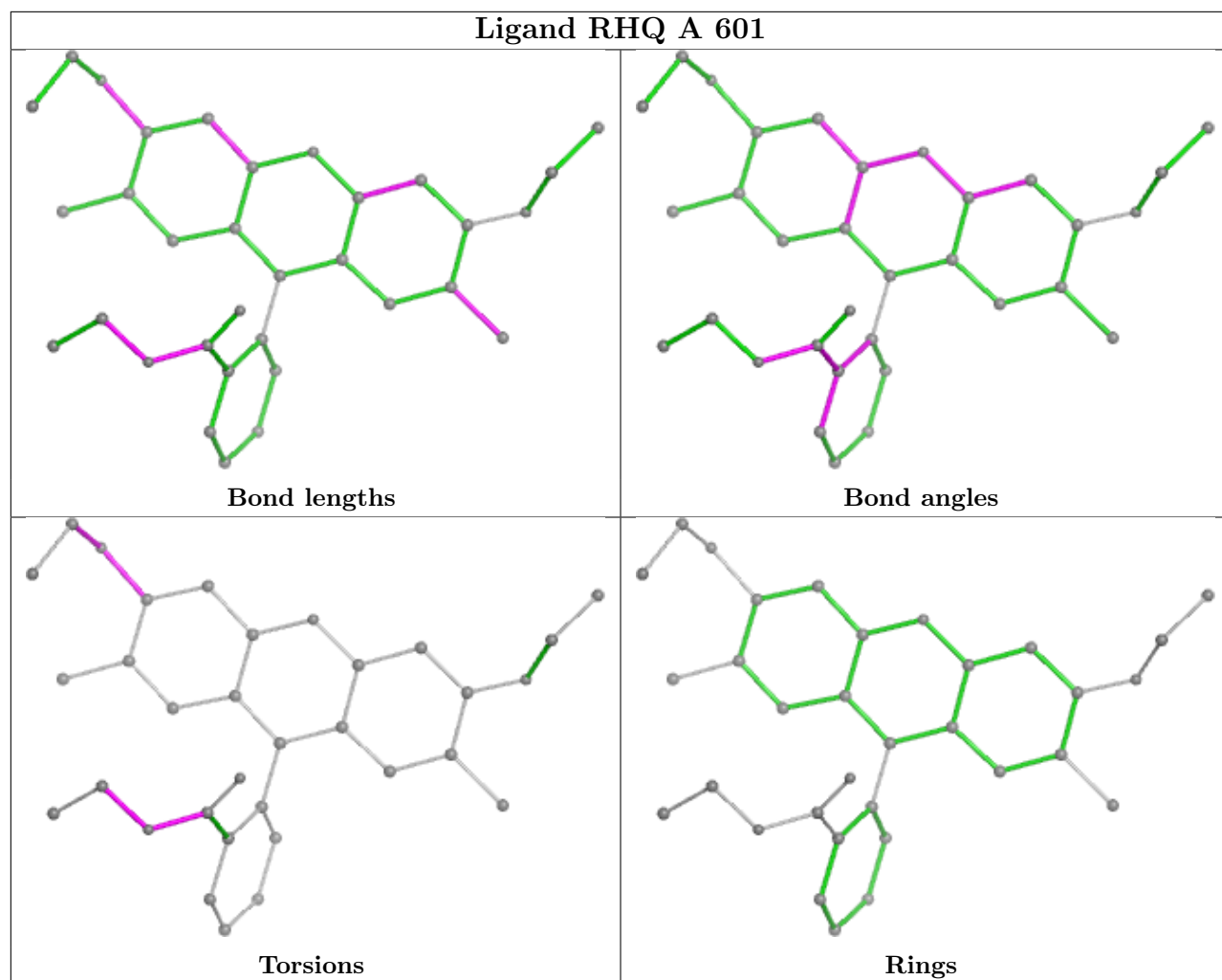
There are no ring outliers.

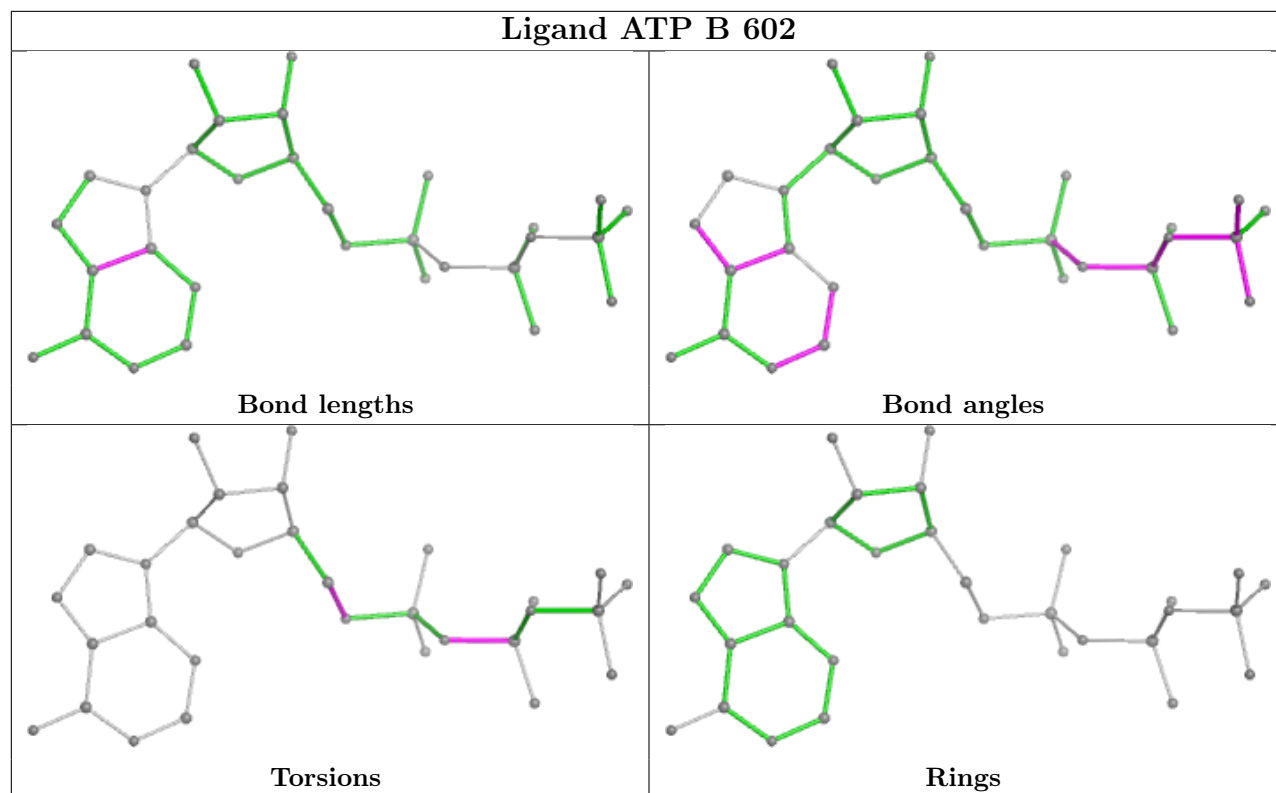
2 monomers are involved in 4 short contacts:

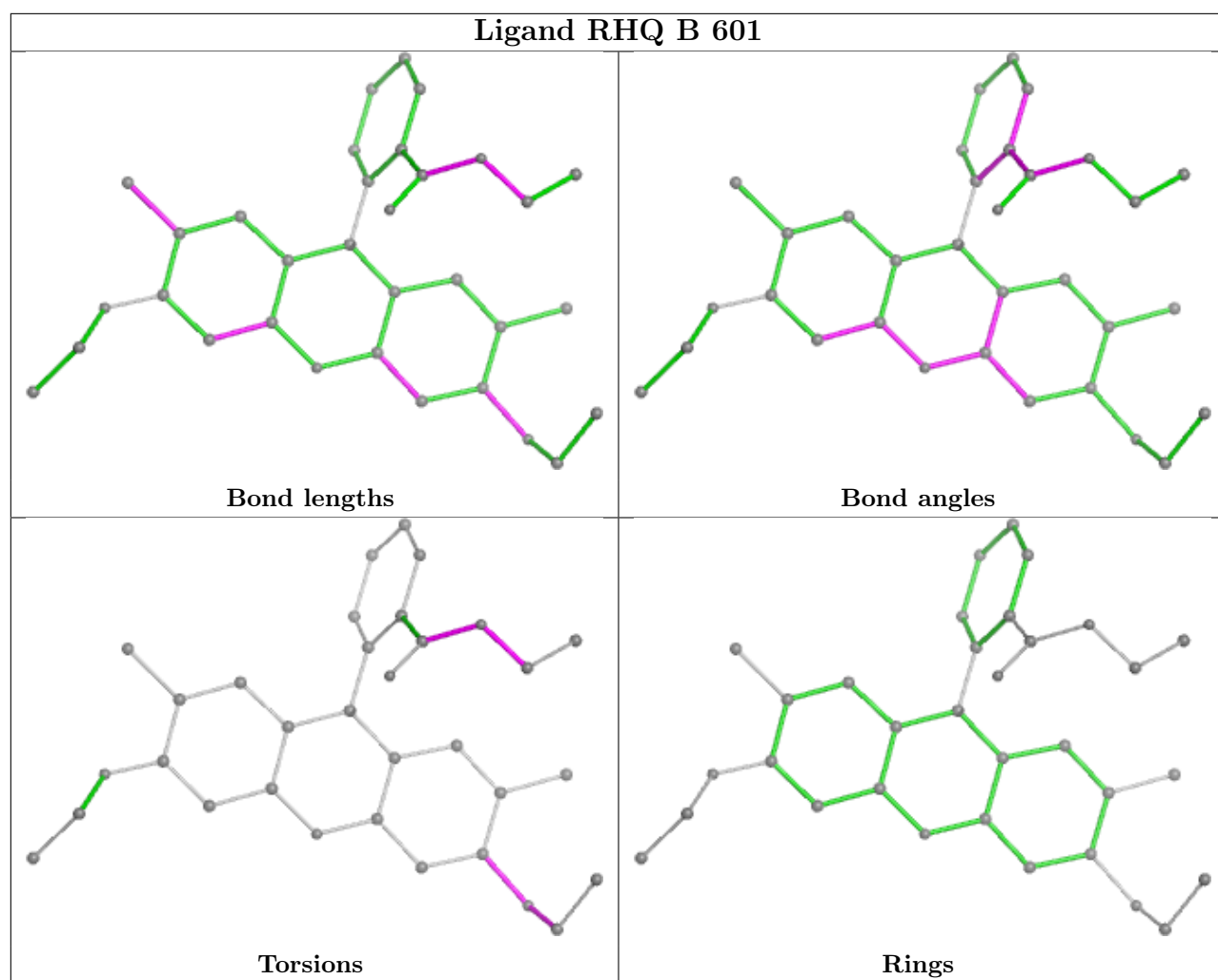
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	ATP	2	0
3	A	602	ATP	2	0

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

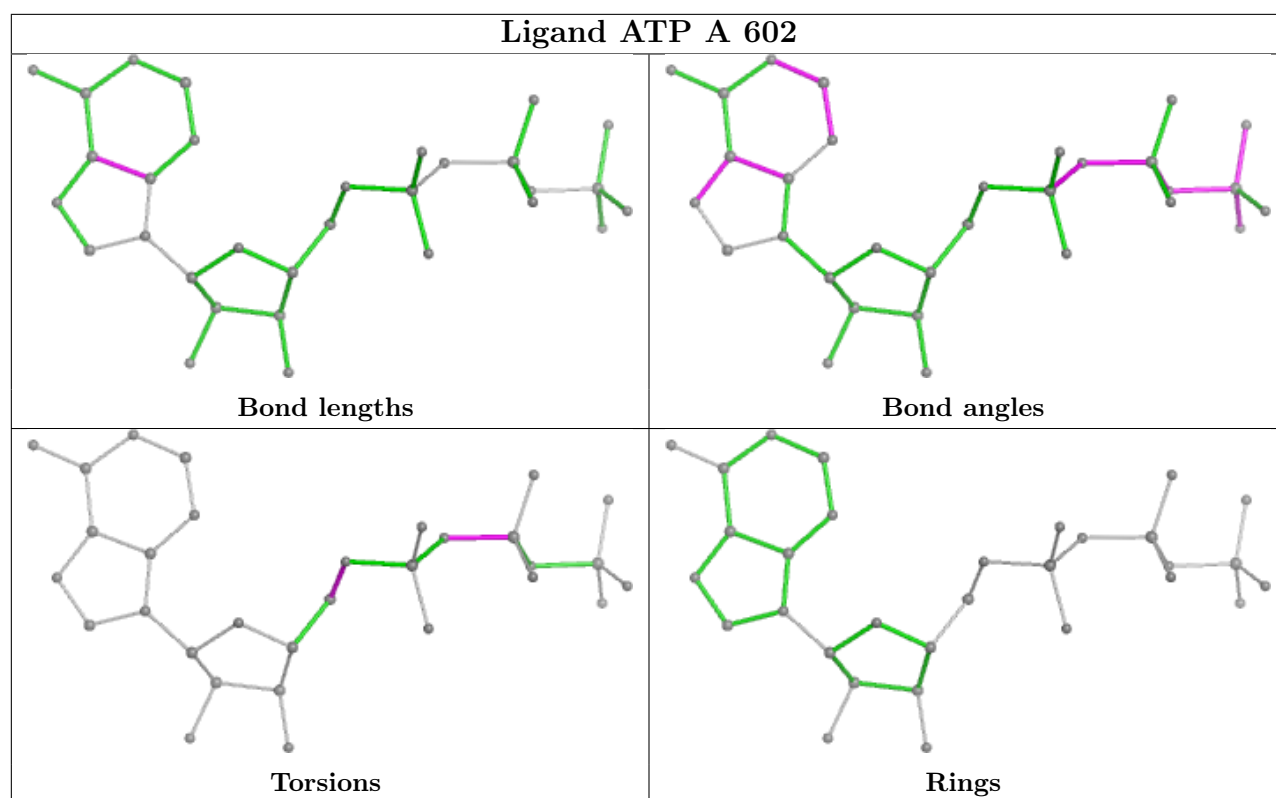
equivalents in the CSD to analyse the geometry.











## 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.

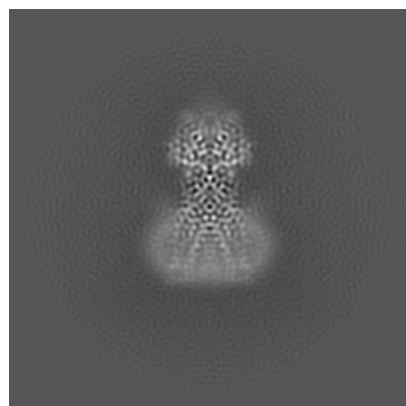
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19135. These allow visual inspection of the internal detail of the map and identification of artifacts.

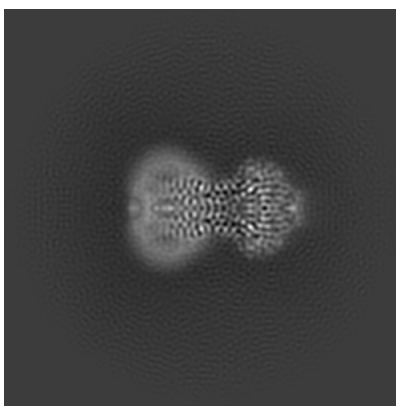
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

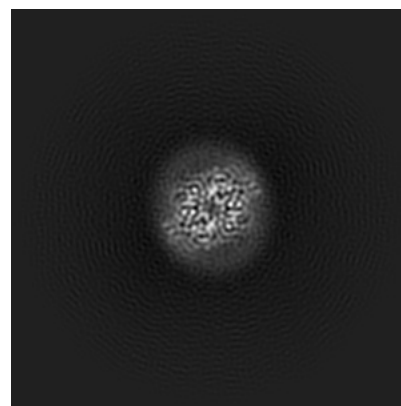
#### 6.1.1 Primary map



X

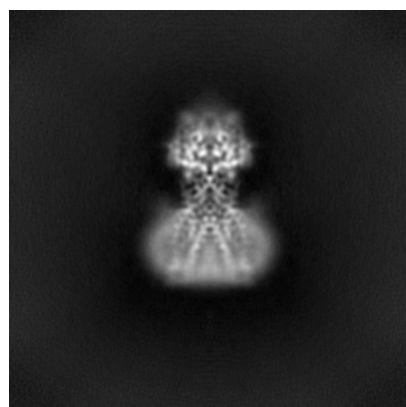


Y

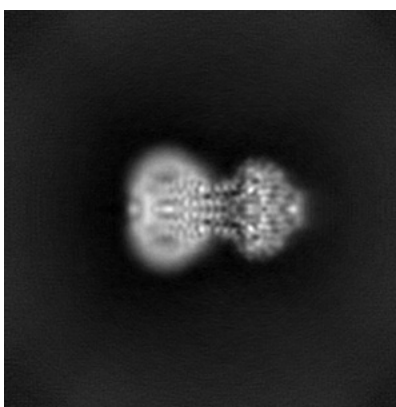


Z

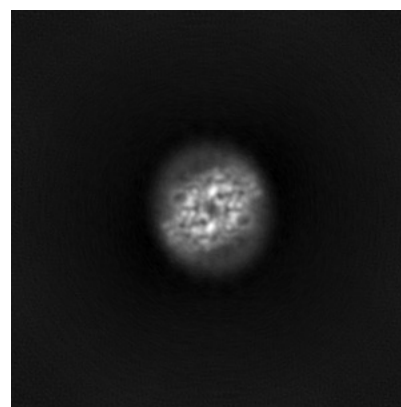
#### 6.1.2 Raw map



X



Y

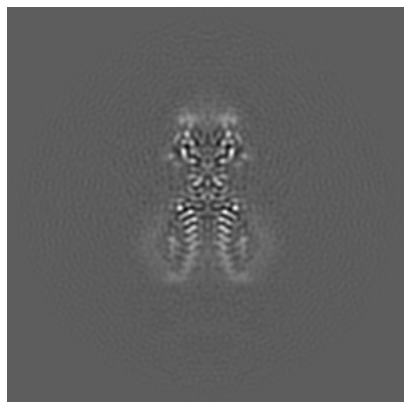


Z

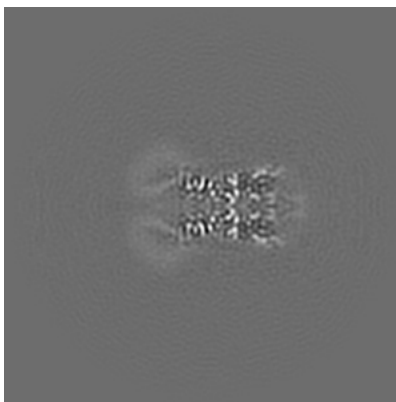
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

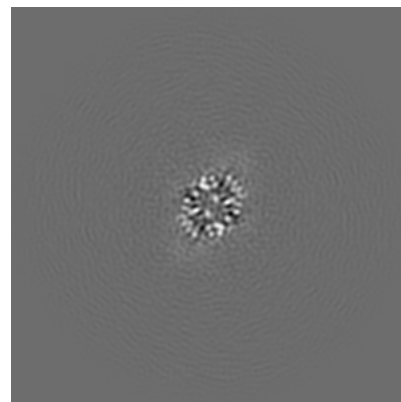
### 6.2.1 Primary map



X Index: 128

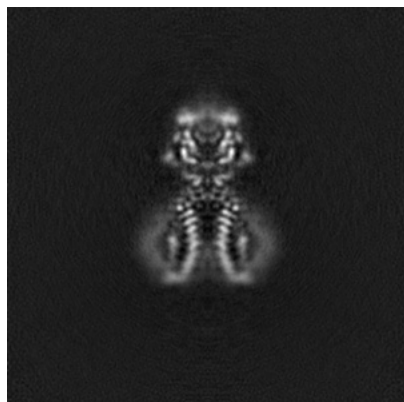


Y Index: 128

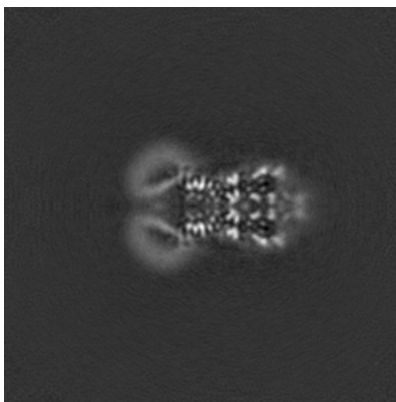


Z Index: 128

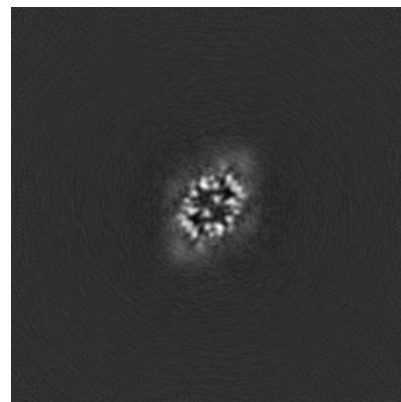
### 6.2.2 Raw map



X Index: 128



Y Index: 128

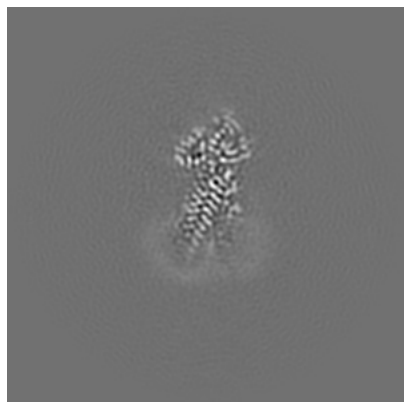


Z Index: 128

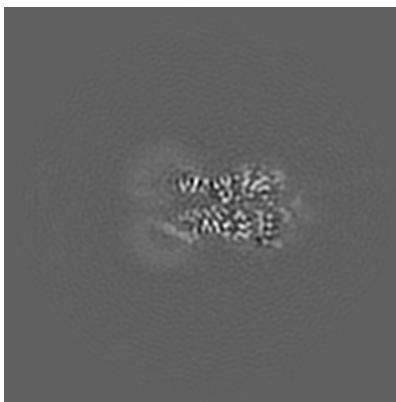
The images above show central slices of the map in three orthogonal directions.

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

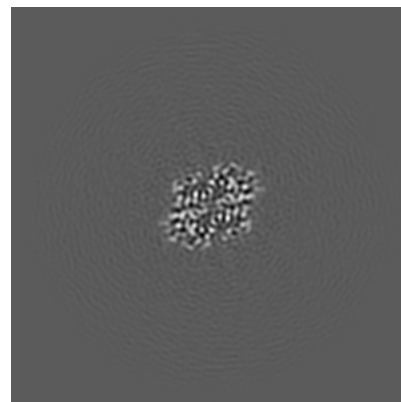
### 6.3.1 Primary map



X Index: 140

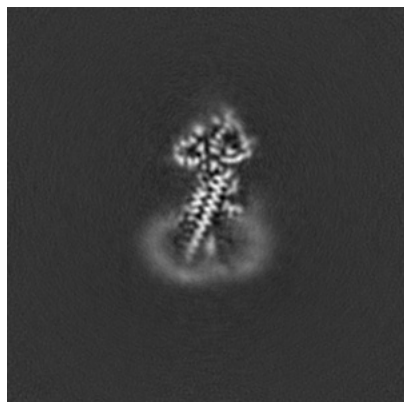


Y Index: 125

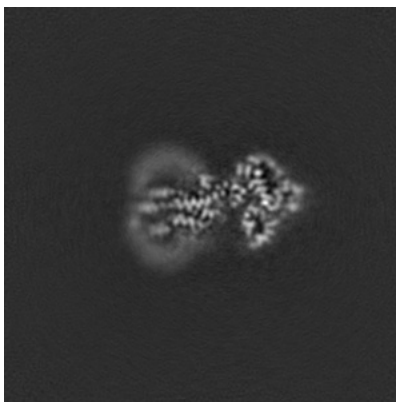


Z Index: 163

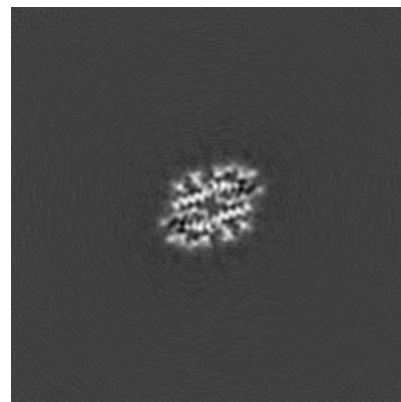
### 6.3.2 Raw map



X Index: 141



Y Index: 140

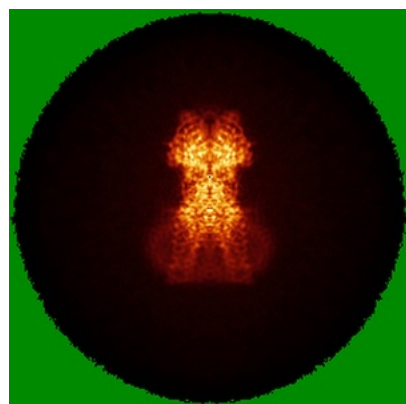


Z Index: 165

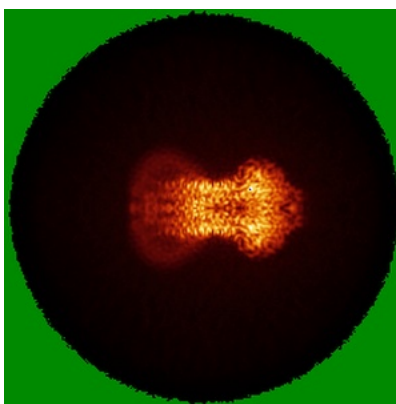
The images above show the largest variance slices of the map in three orthogonal directions.

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

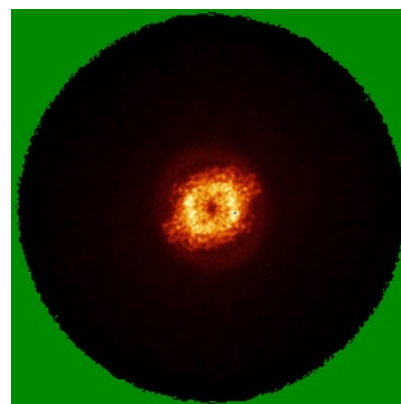
### 6.4.1 Primary map



X

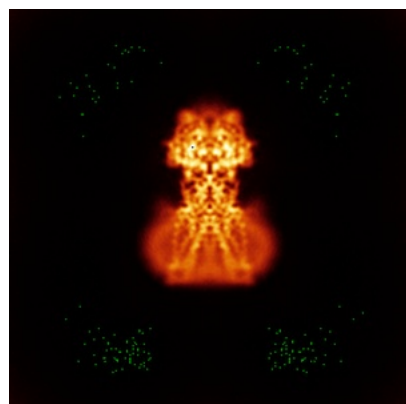


Y

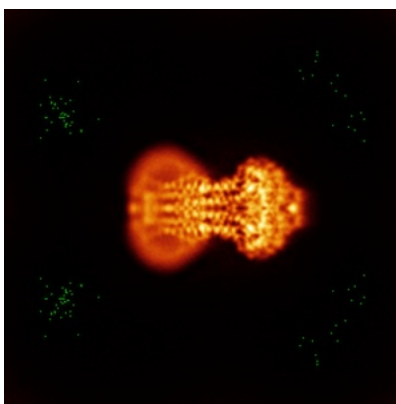


Z

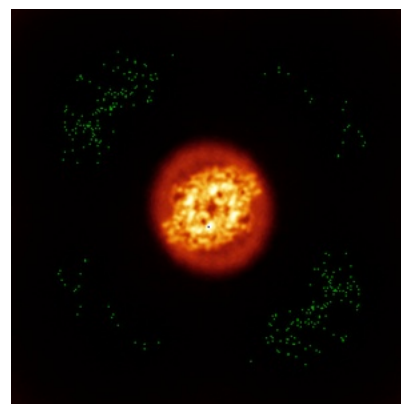
### 6.4.2 Raw map



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.

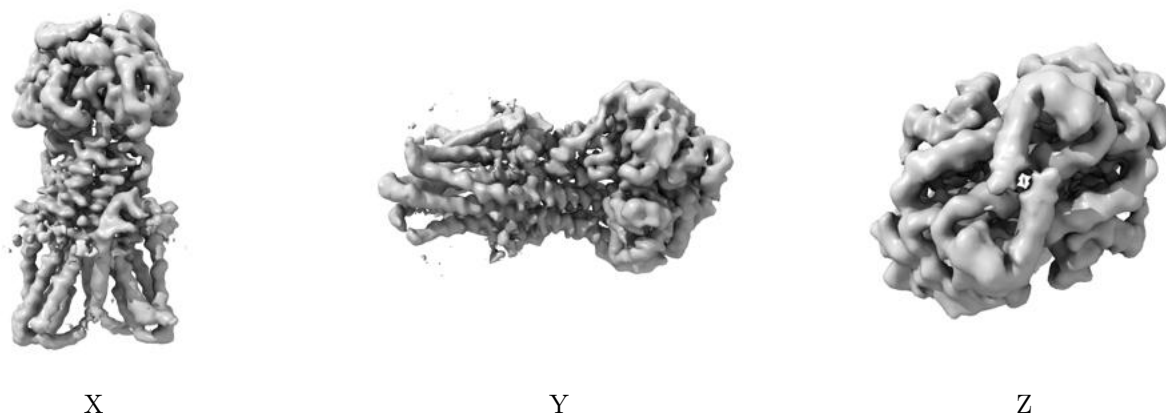
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.381. 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.

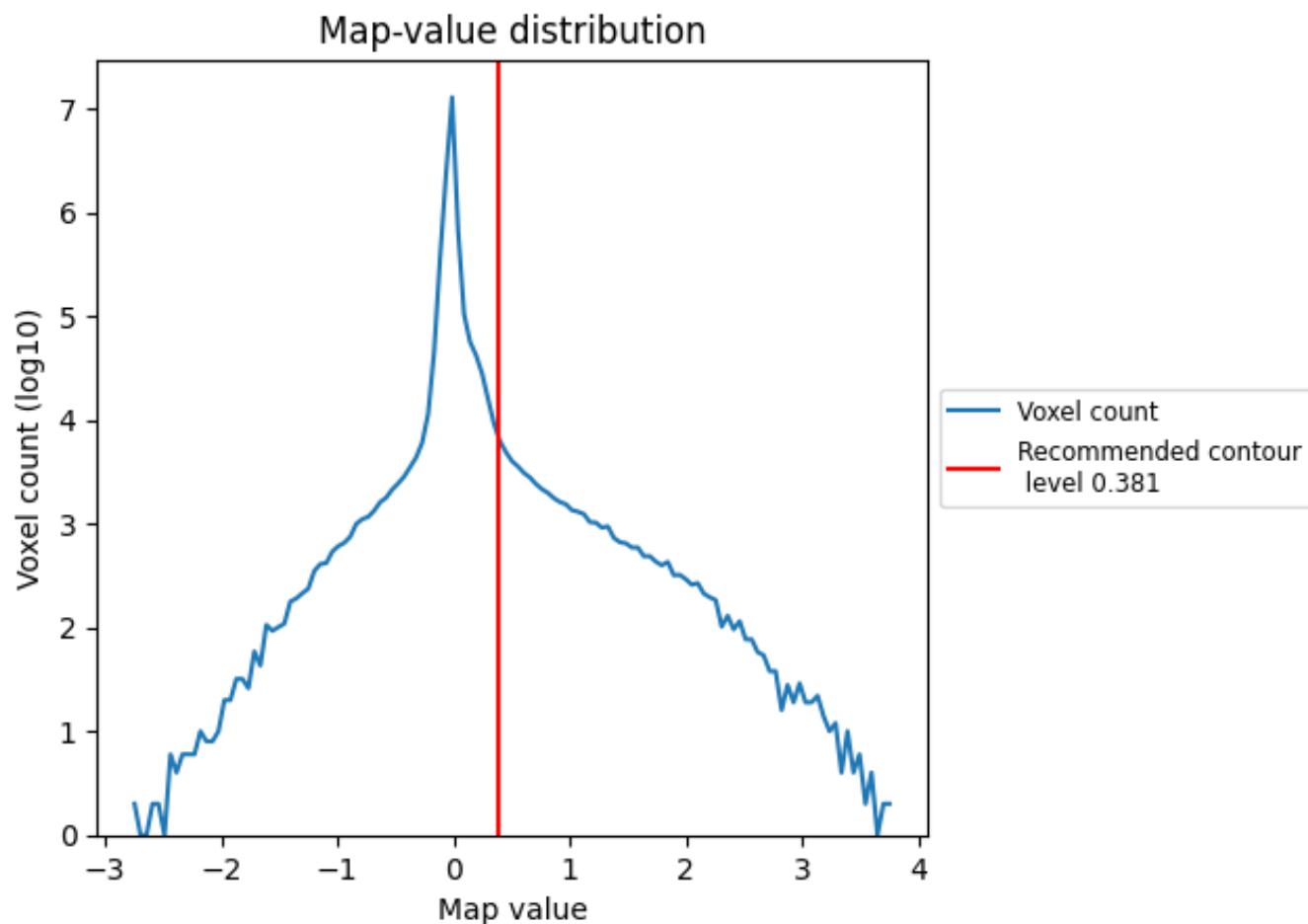
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

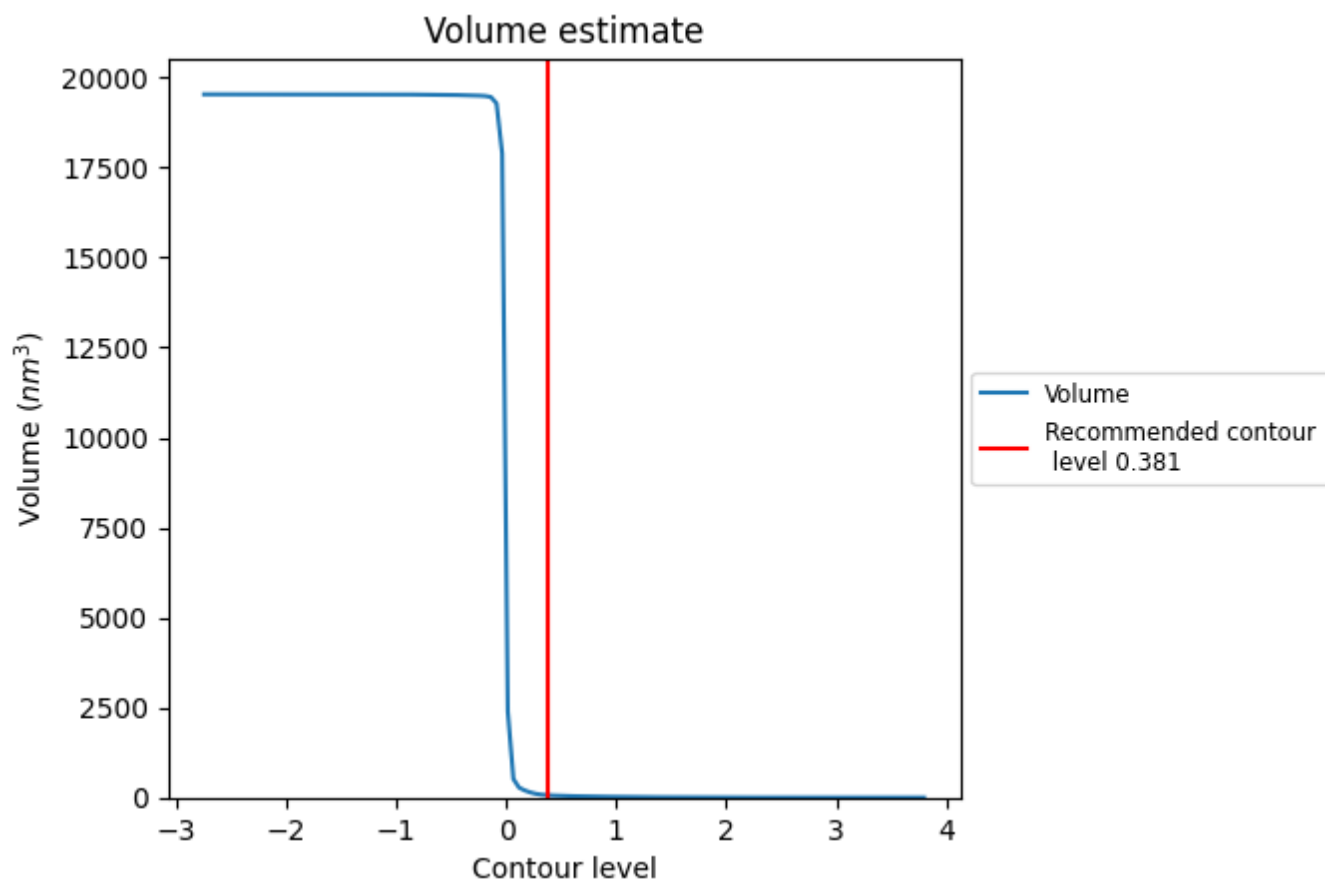
This section contains the results of statistical analysis of the map.

### 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](#)

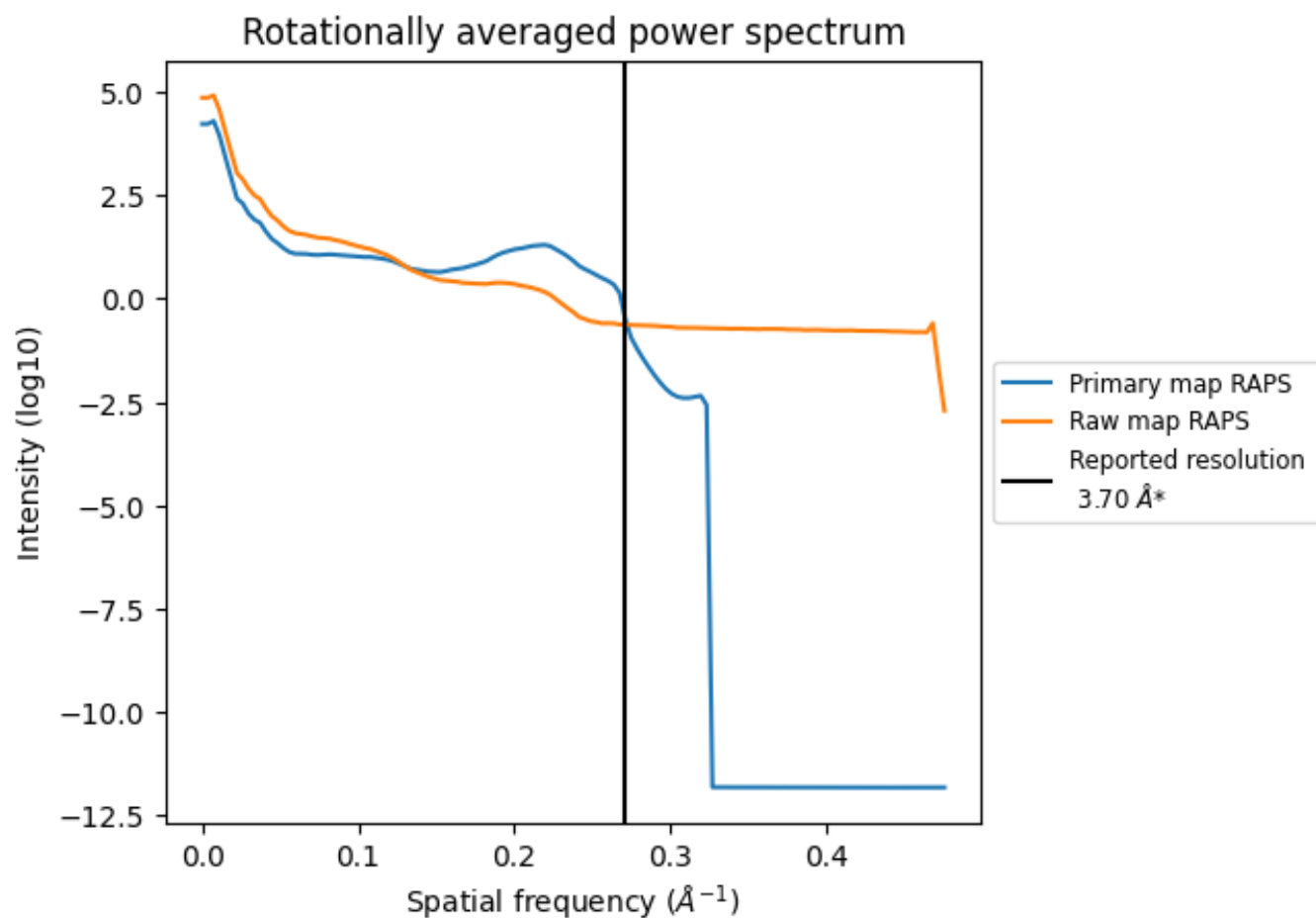


The volume at the recommended contour level is 64 nm<sup>3</sup>; this corresponds to an approximate mass of 58 kDa.

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 ⓘ

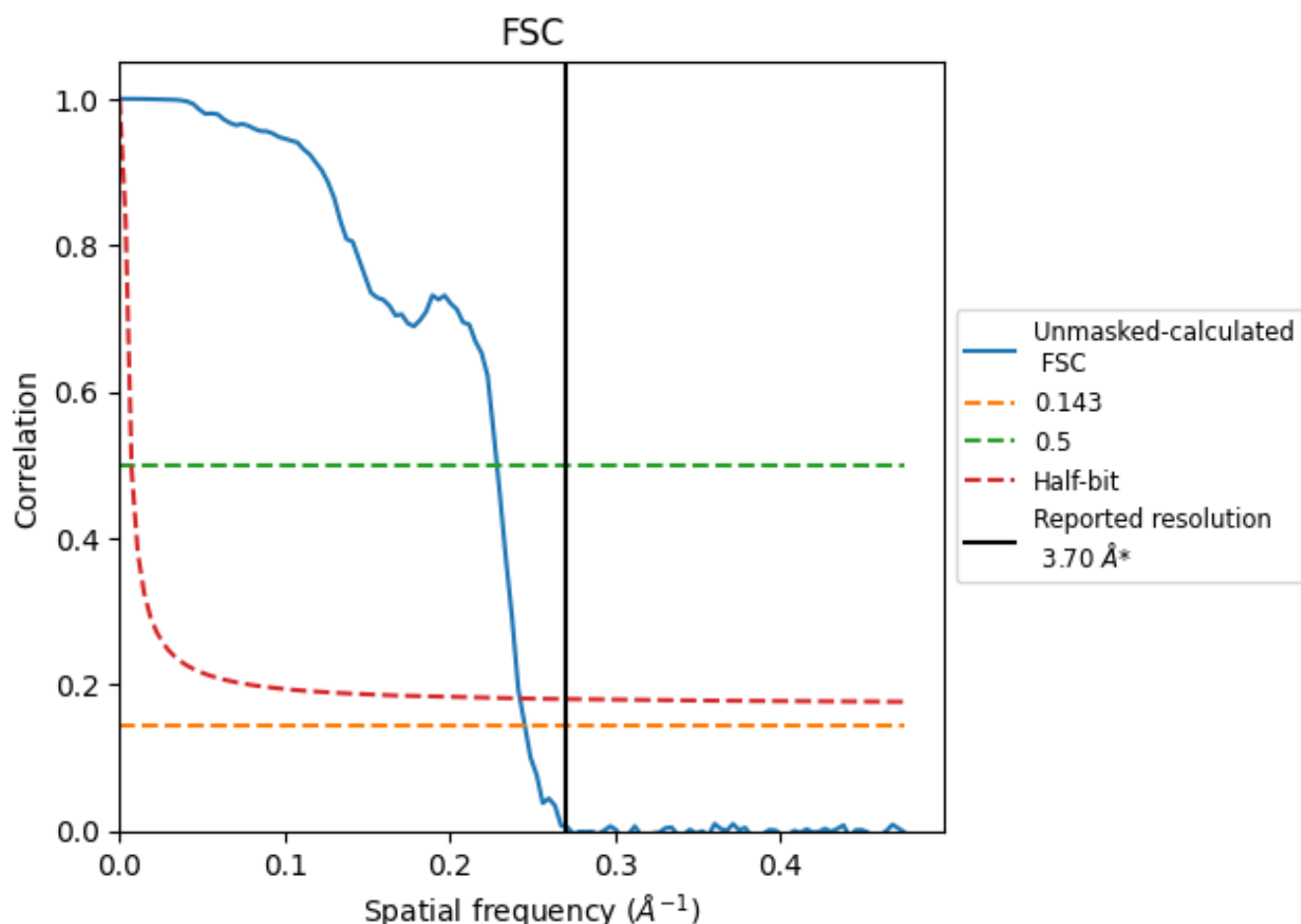


\*Reported resolution corresponds to spatial frequency of 0.270 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

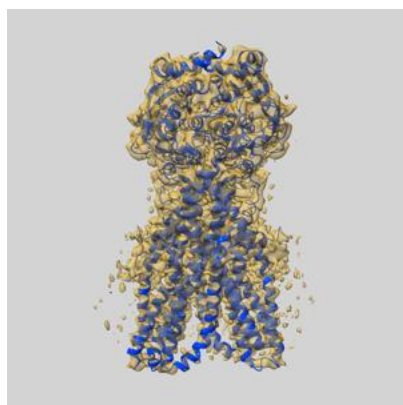
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.08	4.38	4.13

\*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 4.08 differs from the reported value 3.7 by more than 10 %

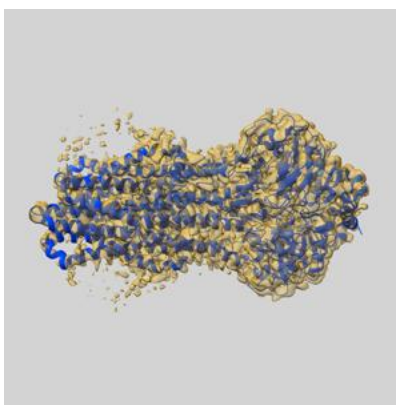
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-19135 and PDB model 8RGN. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

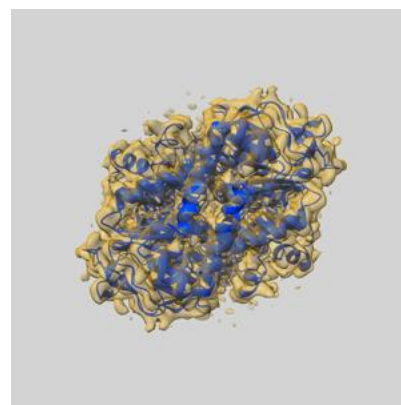
### 9.1 Map-model overlay [i](#)



X



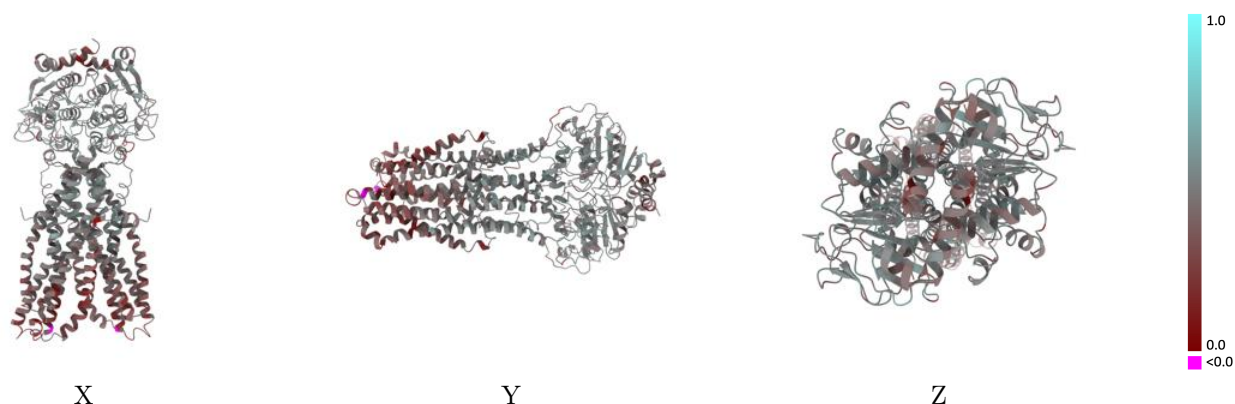
Y



Z

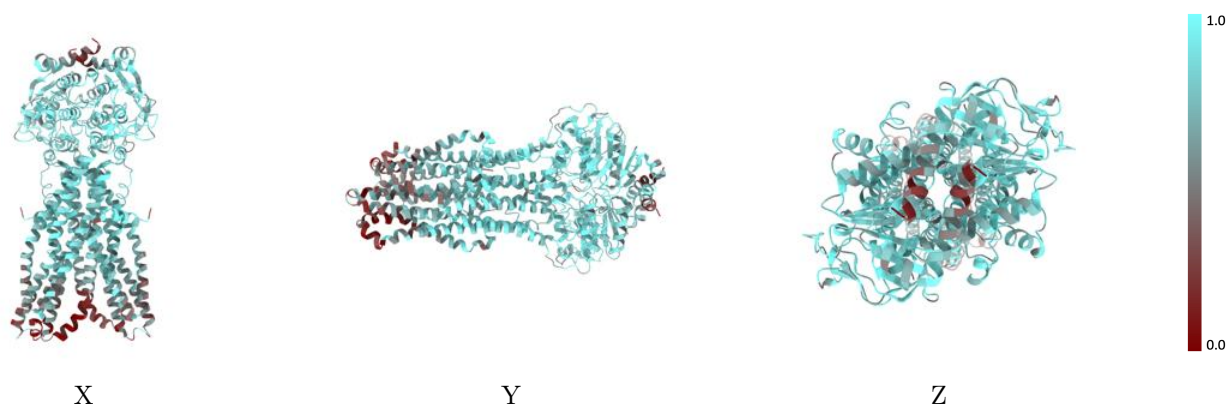
The images above show the 3D surface view of the map at the recommended contour level 0.381 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



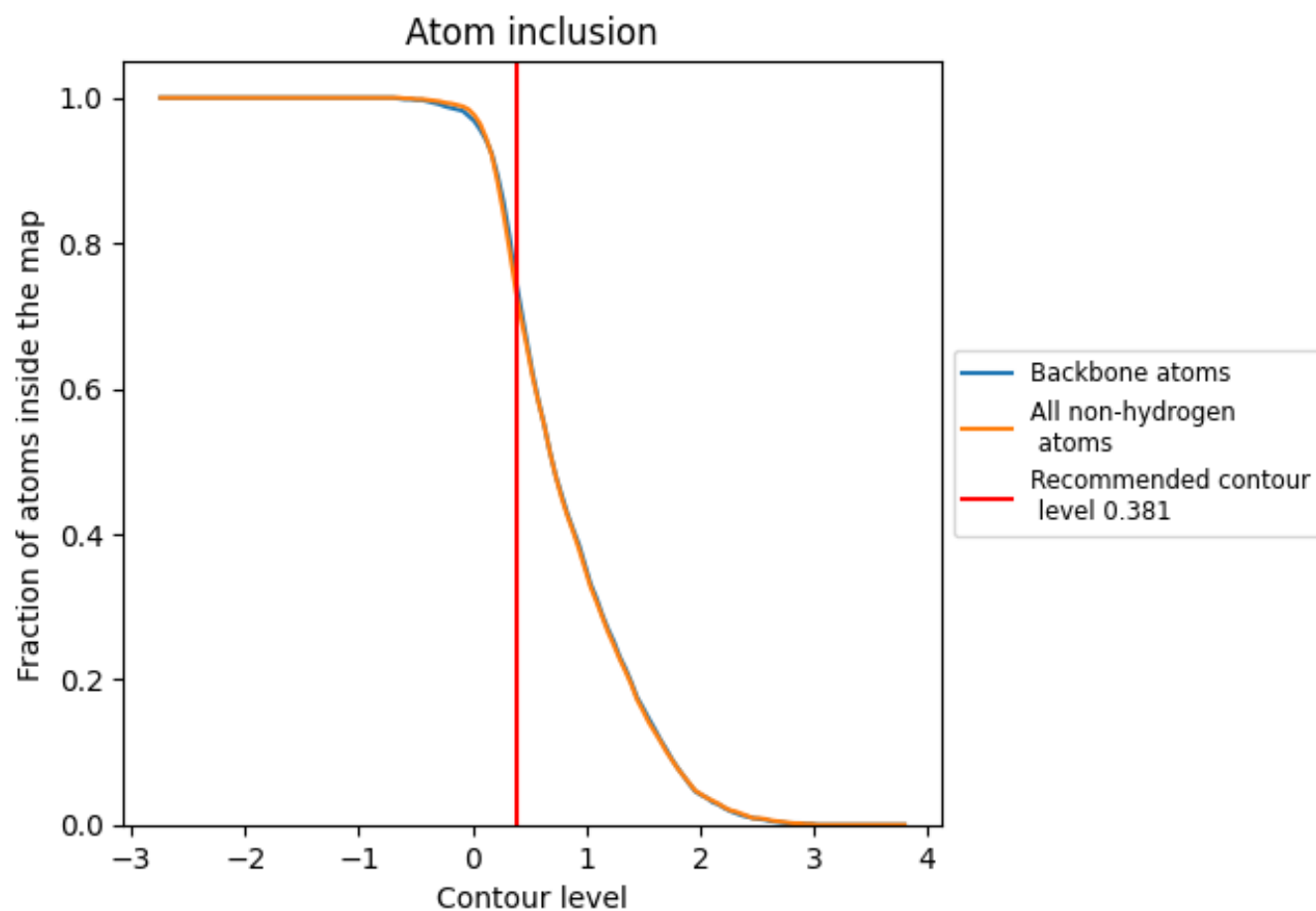
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.381).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 73% 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 (0.381) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7340	<div></div> 0.4380
A	<div></div> 0.7350	<div></div> 0.4380
B	<div></div> 0.7380	<div></div> 0.4380

