



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 09:38 PM UTC

PDB ID : 8VIX / pdb_00008vix
EMDB ID : EMD-43270
Title : Hydrogen Peroxide-bound Vanadium-dependent Bromoperoxidase from *Coralina pilulifera*
Authors : Hessefort, L.Z.; Williams, D.R.; Biegasiewicz, K.F.
Deposited on : 2024-01-05
Resolution : 2.31 Å(reported)
Based on initial model : .

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

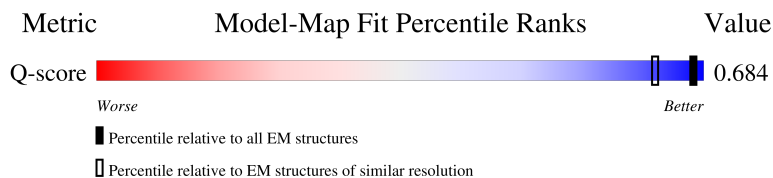
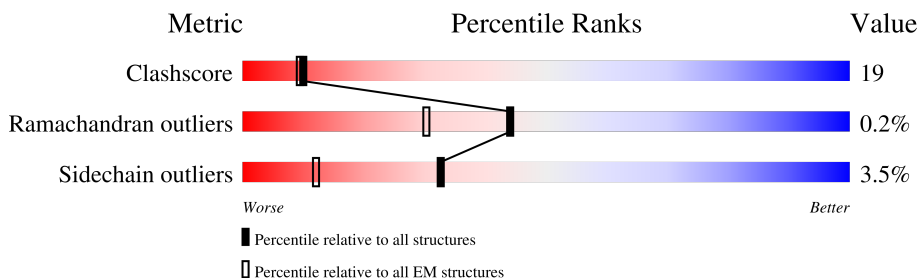
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.31 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	4306 (1.81 - 2.81)

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	634	
1	B	634	

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	VO4	A	601	-	-	X	-
2	VO4	B	602	-	-	X	-
3	PER	A	602	-	X	X	-
3	PER	B	601	-	X	-	-
3	PER	B	603	-	X	X	-
3	PER	B	604	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9146 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 Vanadium-dependent bromoperoxidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	590	Total	C	N	O	S	0	0
			4559	2898	761	893	7		
1	B	590	Total	C	N	O	S	0	0
			4559	2898	761	893	7		

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-35	MET	-	initiating methionine	UNP O81959
A	-34	GLY	-	expression tag	UNP O81959
A	-33	SER	-	expression tag	UNP O81959
A	-32	SER	-	expression tag	UNP O81959
A	-31	HIS	-	expression tag	UNP O81959
A	-30	HIS	-	expression tag	UNP O81959
A	-29	HIS	-	expression tag	UNP O81959
A	-28	HIS	-	expression tag	UNP O81959
A	-27	HIS	-	expression tag	UNP O81959
A	-26	HIS	-	expression tag	UNP O81959
A	-25	SER	-	expression tag	UNP O81959
A	-24	SER	-	expression tag	UNP O81959
A	-23	GLY	-	expression tag	UNP O81959
A	-22	LEU	-	expression tag	UNP O81959
A	-21	VAL	-	expression tag	UNP O81959
A	-20	PRO	-	expression tag	UNP O81959
A	-19	ARG	-	expression tag	UNP O81959
A	-18	GLY	-	expression tag	UNP O81959
A	-17	SER	-	expression tag	UNP O81959
A	-16	HIS	-	expression tag	UNP O81959
A	-15	MET	-	expression tag	UNP O81959
A	-14	ALA	-	expression tag	UNP O81959
A	-13	SER	-	expression tag	UNP O81959
A	-12	MET	-	expression tag	UNP O81959
A	-11	THR	-	expression tag	UNP O81959
A	-10	GLY	-	expression tag	UNP O81959

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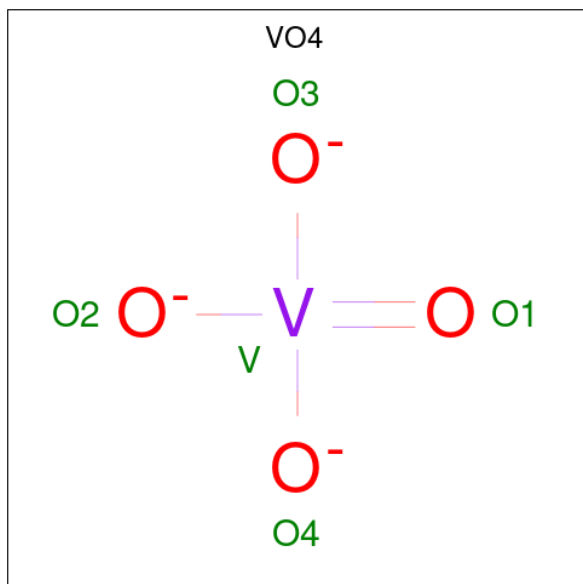
Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	GLY	-	expression tag	UNP O81959
A	-8	GLN	-	expression tag	UNP O81959
A	-7	GLN	-	expression tag	UNP O81959
A	-6	MET	-	expression tag	UNP O81959
A	-5	GLY	-	expression tag	UNP O81959
A	-4	ARG	-	expression tag	UNP O81959
A	-3	GLY	-	expression tag	UNP O81959
A	-2	SER	-	expression tag	UNP O81959
A	-1	GLU	-	expression tag	UNP O81959
A	0	PHE	-	expression tag	UNP O81959
B	-35	MET	-	initiating methionine	UNP O81959
B	-34	GLY	-	expression tag	UNP O81959
B	-33	SER	-	expression tag	UNP O81959
B	-32	SER	-	expression tag	UNP O81959
B	-31	HIS	-	expression tag	UNP O81959
B	-30	HIS	-	expression tag	UNP O81959
B	-29	HIS	-	expression tag	UNP O81959
B	-28	HIS	-	expression tag	UNP O81959
B	-27	HIS	-	expression tag	UNP O81959
B	-26	HIS	-	expression tag	UNP O81959
B	-25	SER	-	expression tag	UNP O81959
B	-24	SER	-	expression tag	UNP O81959
B	-23	GLY	-	expression tag	UNP O81959
B	-22	LEU	-	expression tag	UNP O81959
B	-21	VAL	-	expression tag	UNP O81959
B	-20	PRO	-	expression tag	UNP O81959
B	-19	ARG	-	expression tag	UNP O81959
B	-18	GLY	-	expression tag	UNP O81959
B	-17	SER	-	expression tag	UNP O81959
B	-16	HIS	-	expression tag	UNP O81959
B	-15	MET	-	expression tag	UNP O81959
B	-14	ALA	-	expression tag	UNP O81959
B	-13	SER	-	expression tag	UNP O81959
B	-12	MET	-	expression tag	UNP O81959
B	-11	THR	-	expression tag	UNP O81959
B	-10	GLY	-	expression tag	UNP O81959
B	-9	GLY	-	expression tag	UNP O81959
B	-8	GLN	-	expression tag	UNP O81959
B	-7	GLN	-	expression tag	UNP O81959
B	-6	MET	-	expression tag	UNP O81959
B	-5	GLY	-	expression tag	UNP O81959
B	-4	ARG	-	expression tag	UNP O81959

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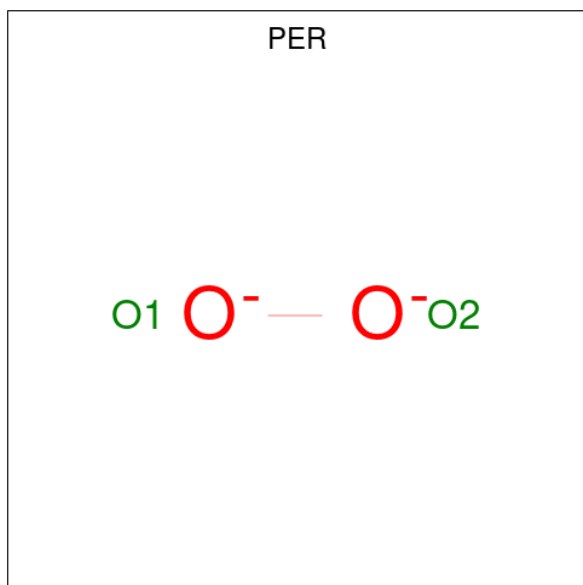
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP O81959
B	-2	SER	-	expression tag	UNP O81959
B	-1	GLU	-	expression tag	UNP O81959
B	0	PHE	-	expression tag	UNP O81959

- Molecule 2 is VANADATE ION (CCD ID: VO4) (formula: O_4V) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	O	V	0
			5	4	1	
2	B	1	Total	O	V	0
			5	4	1	

- Molecule 3 is PEROXIDE ION (CCD ID: PER) (formula: O_2).



Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total O 2 2	0
3	B	1	Total O 2 2	0
3	B	1	Total O 2 2	0
3	B	1	Total O 2 2	0

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

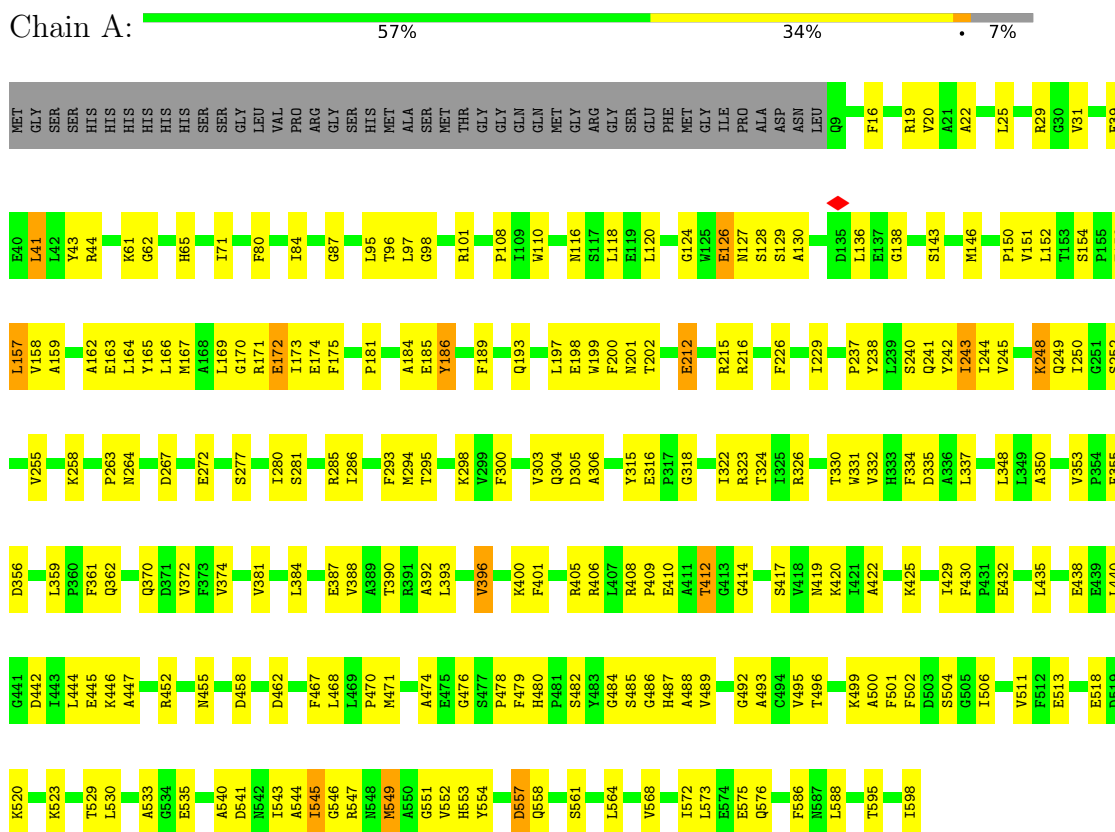
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	AltConf
5	A	4	Total O 4 4	0
5	B	4	Total O 4 4	0

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: Vanadium-dependent bromoperoxidase



- Molecule 1: Vanadium-dependent bromoperoxidase



L573	A493	T324	E410	S247	E160
E574	C494	I325	A411	K248	E163
E575	V495	T412	T412	Q249	L164
F586			N419	G251	Y165
	K499	K420	K420	S252	L166
L588	S503	V332	I421		
I598	F501	D335	A422	V255	L169
	D503	A336			G170
	S504	L337	K425	S262	R171
		Y338	I429	P263	E172
	V511	E339		N264	I173
	F512	A340	E432	D267	E174
	E513	Y341			F175
	V514		L435	D270	S176
	D515	A344	A436	E271	E177
	K516	L348	V437	E272	P181
		L349	E438		K182
	L521	F355	E439	G276	N183
	V522	D356	L440	S277	A184
	K523			I278	E185
	F526	L359	I443	T279	Y186
		P360	L444	I280	I187
	L530	F361			Q188
	A533	Q362	A447	R283	F189
	G534		R452	V284	
	E535	N369	K453	R285	Q193
	L536	Q370	Q454	I286	
		D371	N455	A287	L197
		F372	I456	T288	E198
	A540	V373	A457	P289	W199
	D541	F374	D458	G290	F200
		V374		R291	N201
	A544	N375	F467	D292	
	I545	F376	L468	F293	P210
	G546	G377	L469	M294	A211
	B547	S378	P470	T295	E212
	N548	V381	M471	D296	I213
	M549			L297	
	A550	T386	A474	K298	E219
	G551	E387	G475	V299	V220
	V552	V388	G476	F300	T221
	H553	A389	S477		V222
	Y554	T390	P478	V303	
	F555	R391	F479	Q304	F226
	S556	A392	H480	D305	
	D557	L393	P481	A306	
	Q558		S482		
		V396	Y483	F312	G236
	S561	G484	G484		P237
	L564	S485	K486	Y315	Y238
		H487	F401	E316	L239
	V568	A488		P317	S240
	A569	V489	R406	G318	Q241
	I570	V490	L407	A319	Y242
	G571	A491	R408	R320	I243
	I572	G492	P409	I322	I244
				R323	G246

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, T	Depositor
Number of particles used	349552	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	-800	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	16.650	Depositor
Minimum map value	-9.108	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.236	Depositor
Recommended contour level	0.8	Depositor
Map size ($\text{\AA}$)	527.36, 527.36, 527.36	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.03, 1.03, 1.03	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: VO4, CA, PER

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	0.26	2/4659 (0.0%)	0.38	3/6332 (0.0%)
1	B	0.60	13/4659 (0.3%)	0.58	20/6332 (0.3%)
All	All	0.46	15/9318 (0.2%)	0.49	23/12664 (0.2%)

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	1

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	412	THR	C-O	-15.98	1.05	1.24
1	B	165	TYR	C-O	-15.64	1.05	1.24
1	B	181	PRO	N-CD	-13.77	1.28	1.47
1	B	166	LEU	C-O	-10.79	1.11	1.24
1	B	238	TYR	C-O	-10.04	1.12	1.24

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	295	THR	CB-CA-C	8.98	123.58	109.03
1	B	164	LEU	CA-C-N	8.74	132.33	120.44
1	B	164	LEU	C-N-CA	8.74	132.33	120.44
1	B	295	THR	N-CA-C	-8.51	103.42	113.88
1	B	237	PRO	O-C-N	-7.82	113.45	122.91

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	238	TYR	Mainchain

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	4559	0	4444	188	0
1	B	4559	0	4444	190	0
2	A	5	0	0	3	0
2	B	5	0	0	3	0
3	A	2	0	0	3	0
3	B	6	0	0	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
All	All	9146	0	8888	350	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 19.

The worst 5 of 350 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:408:ARG:HD3	1:A:482:SER:HB3	1.57	0.85
1:B:408:ARG:HD3	1:B:482:SER:HB3	1.60	0.82
1:A:126:GLU:HG3	1:A:480:HIS:HD2	1.42	0.82
1:B:504:SER:HB2	1:B:533:ALA:HB2	1.62	0.81
1:B:294:MET:HE1	1:B:476:GLY:HA3	1.63	0.80

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	588/634 (93%)	576 (98%)	11 (2%)	1 (0%)	43	53
1	B	588/634 (93%)	572 (97%)	15 (3%)	1 (0%)	43	53
All	All	1176/1268 (93%)	1148 (98%)	26 (2%)	2 (0%)	44	53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	337	LEU
1	A	337	LEU

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	486/520 (94%)	465 (96%)	21 (4%)	26	38
1	B	486/520 (94%)	473 (97%)	13 (3%)	39	56
All	All	972/1040 (94%)	938 (96%)	34 (4%)	32	46

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	371	ASP
1	B	390	THR
1	B	513	GLU
1	A	396	VAL

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Mol	Chain	Res	Type
1	A	390	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	597	GLN
1	B	45	ASN
1	B	454	GLN
1	B	68	ASN
1	A	454	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](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	VO4	B	602	1	0,4,4	-	-	-		
2	VO4	A	601	1	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PER	A	602	-	1,1,1	2.03	1 (100%)	-		
3	PER	B	604	-	1,1,1	2.14	1 (100%)	-		
3	PER	B	601	-	1,1,1	2.17	1 (100%)	-		
3	PER	B	603	-	1,1,1	2.02	1 (100%)	-		

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	PER	O2-O1	-2.17	1.12	1.42
3	B	604	PER	O2-O1	-2.14	1.12	1.42
3	A	602	PER	O2-O1	-2.03	1.14	1.42
3	B	603	PER	O2-O1	-2.02	1.14	1.42

There are no bond angle outliers.

There are no chirality outliers.

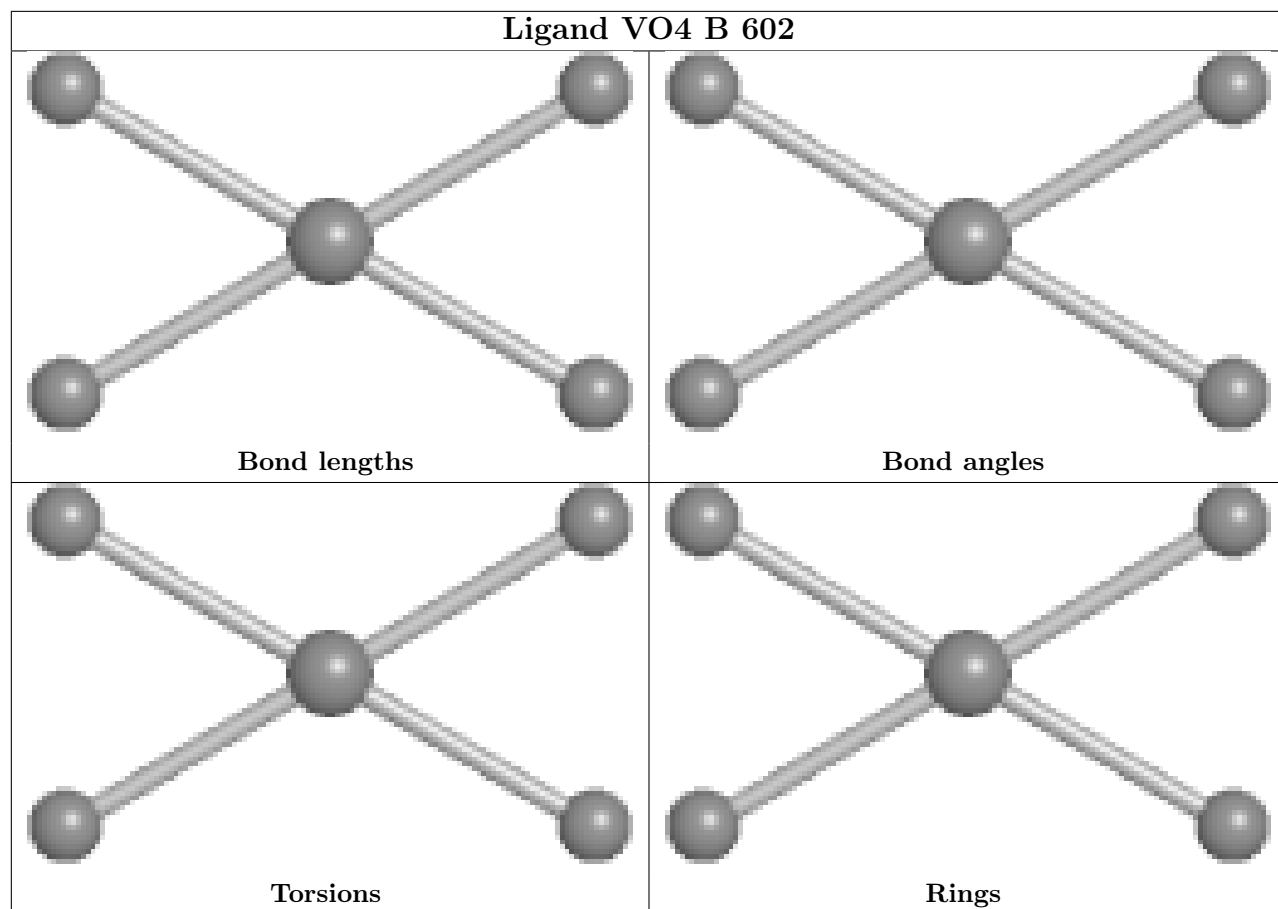
There are no torsion outliers.

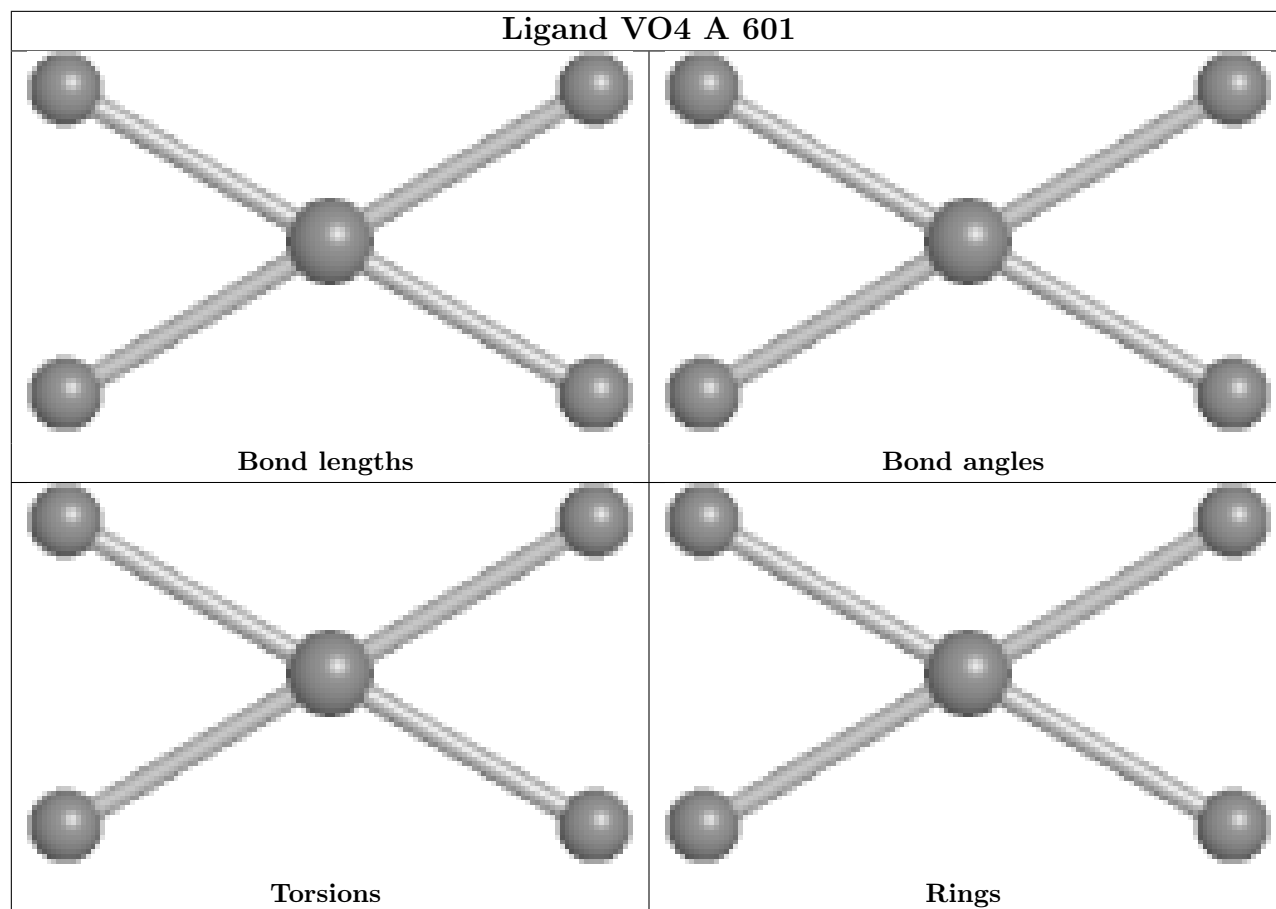
There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	602	VO4	3	0
2	A	601	VO4	3	0
3	A	602	PER	3	0
3	B	603	PER	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.

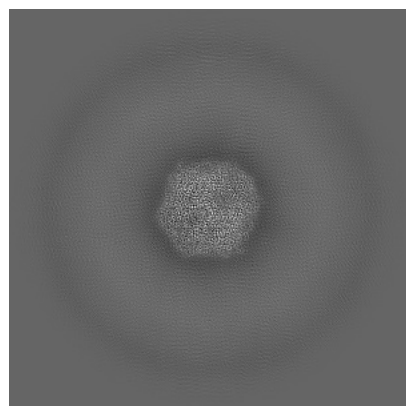
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43270. These allow visual inspection of the internal detail of the map and identification of artifacts.

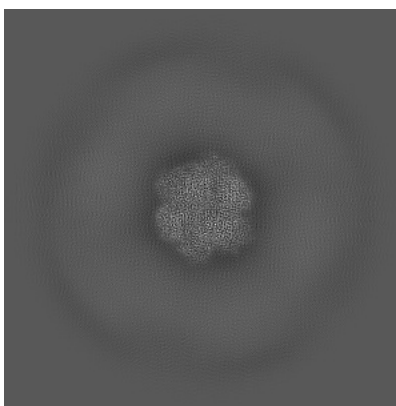
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

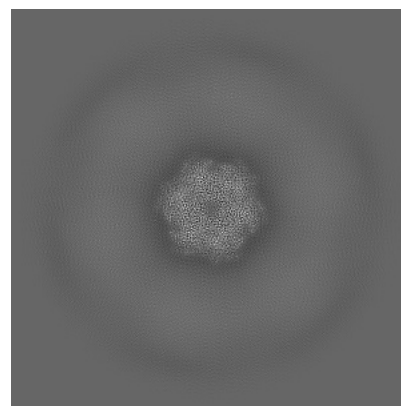
6.1.1 Primary map



X

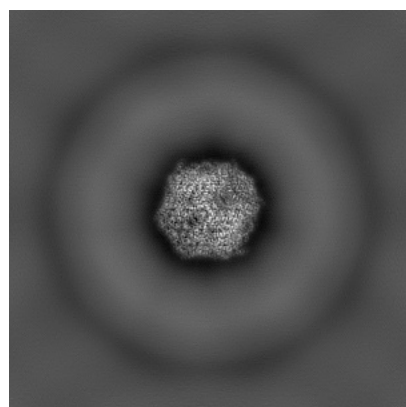


Y

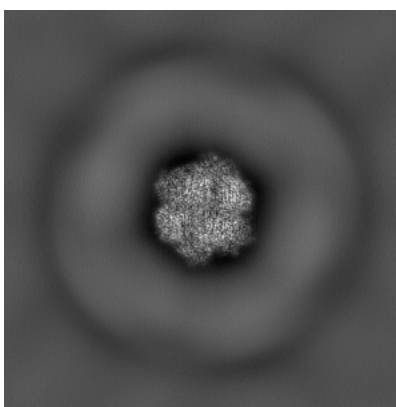


Z

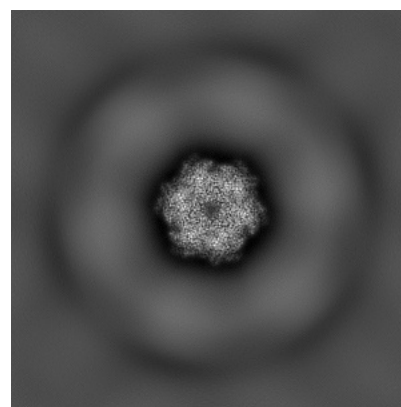
6.1.2 Raw map



X



Y

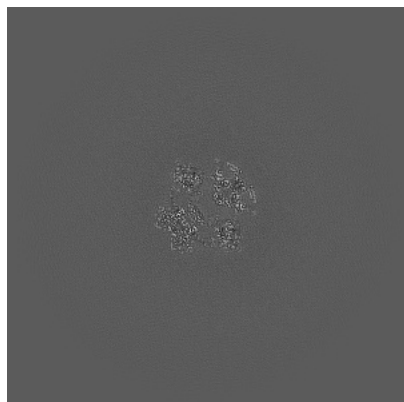


Z

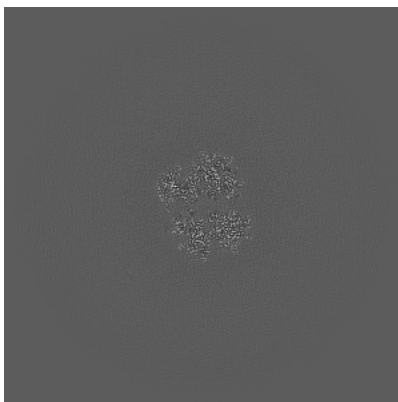
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

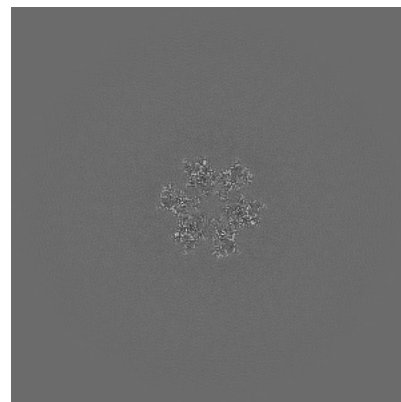
6.2.1 Primary map



X Index: 256

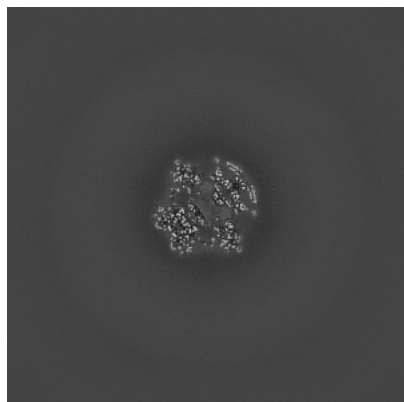


Y Index: 256

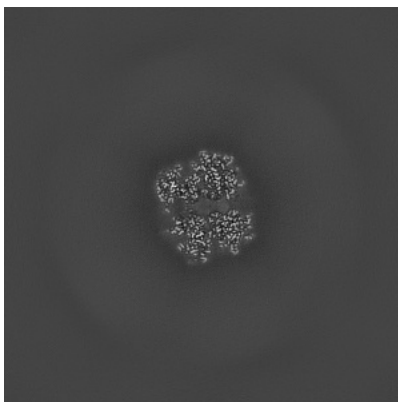


Z Index: 256

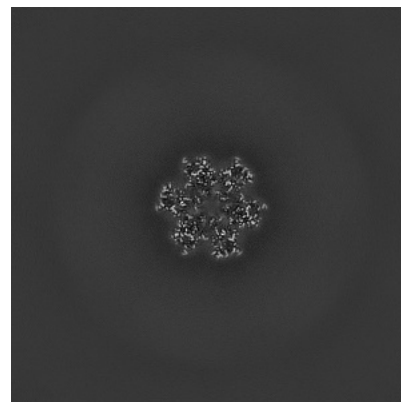
6.2.2 Raw map



X Index: 256



Y Index: 256



Z Index: 256

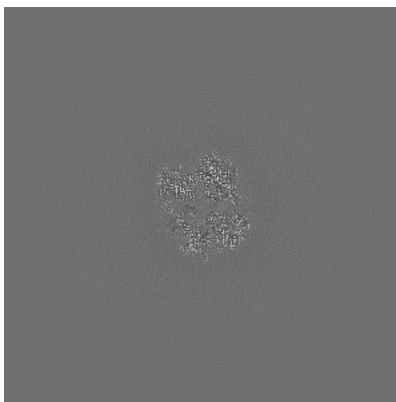
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

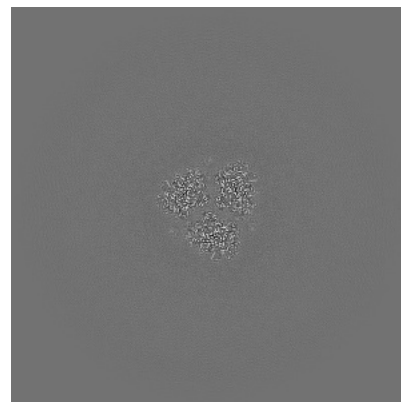
6.3.1 Primary map



X Index: 242

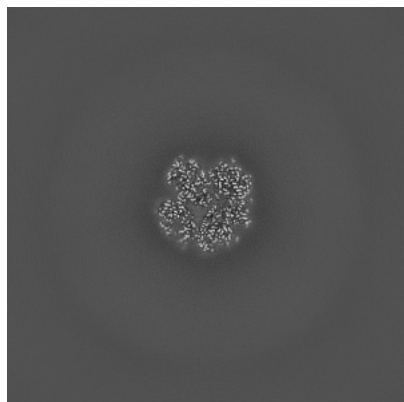


Y Index: 252

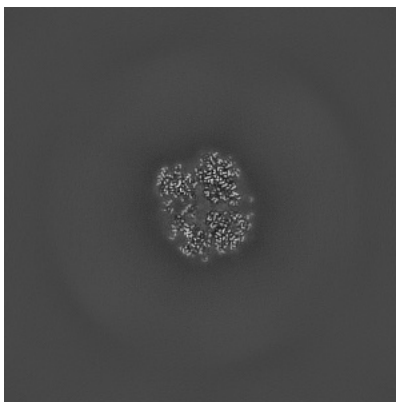


Z Index: 245

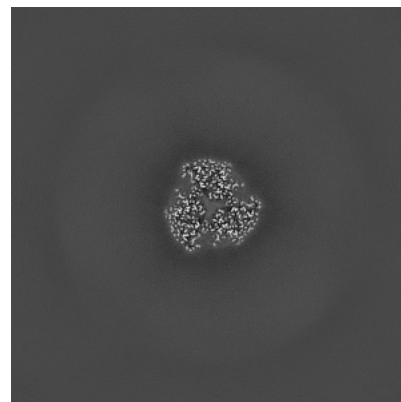
6.3.2 Raw map



X Index: 272



Y Index: 251

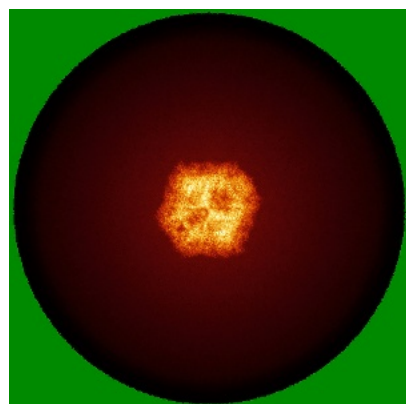


Z Index: 281

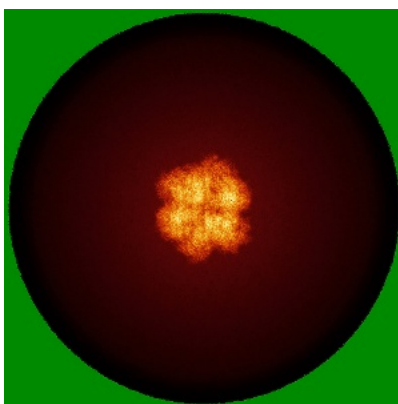
The images above show the largest variance slices of the map in three orthogonal directions.

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

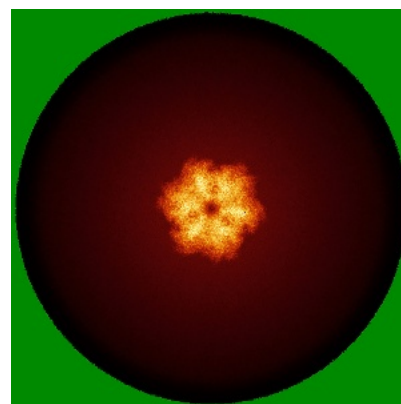
6.4.1 Primary map



X

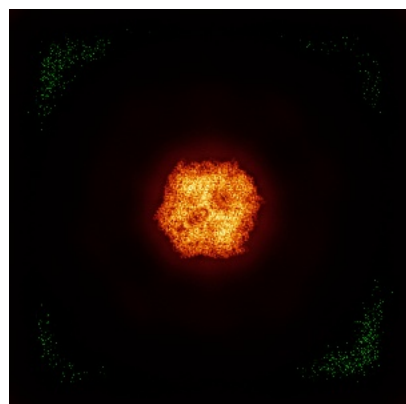


Y

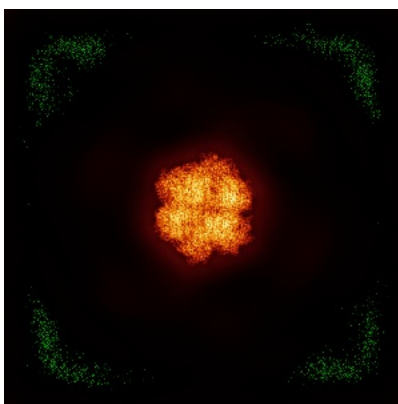


Z

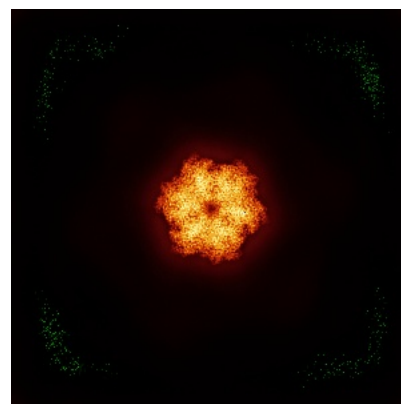
6.4.2 Raw map



X



Y

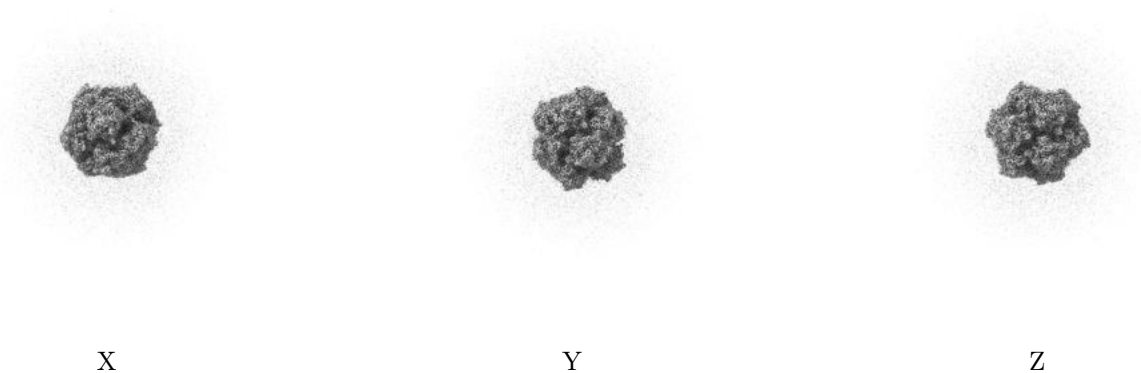


Z

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.

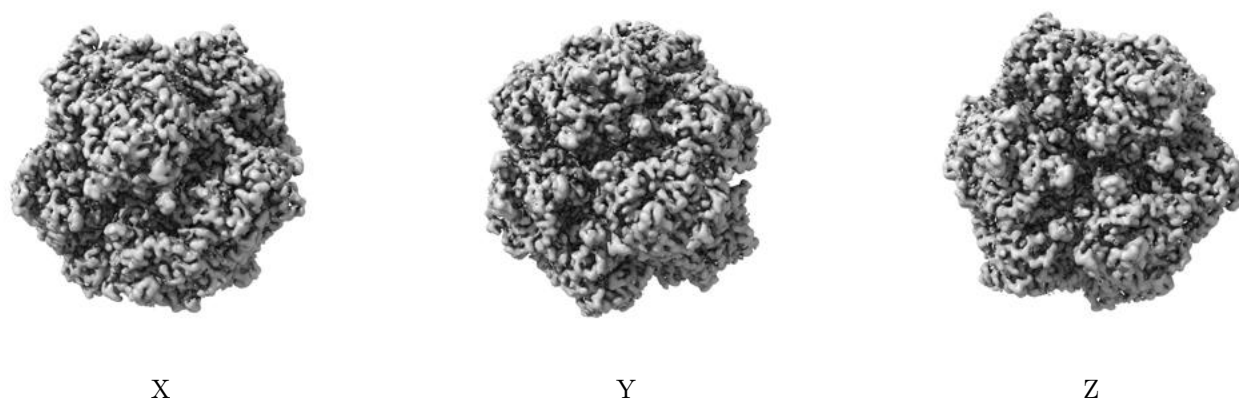
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.8. 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.

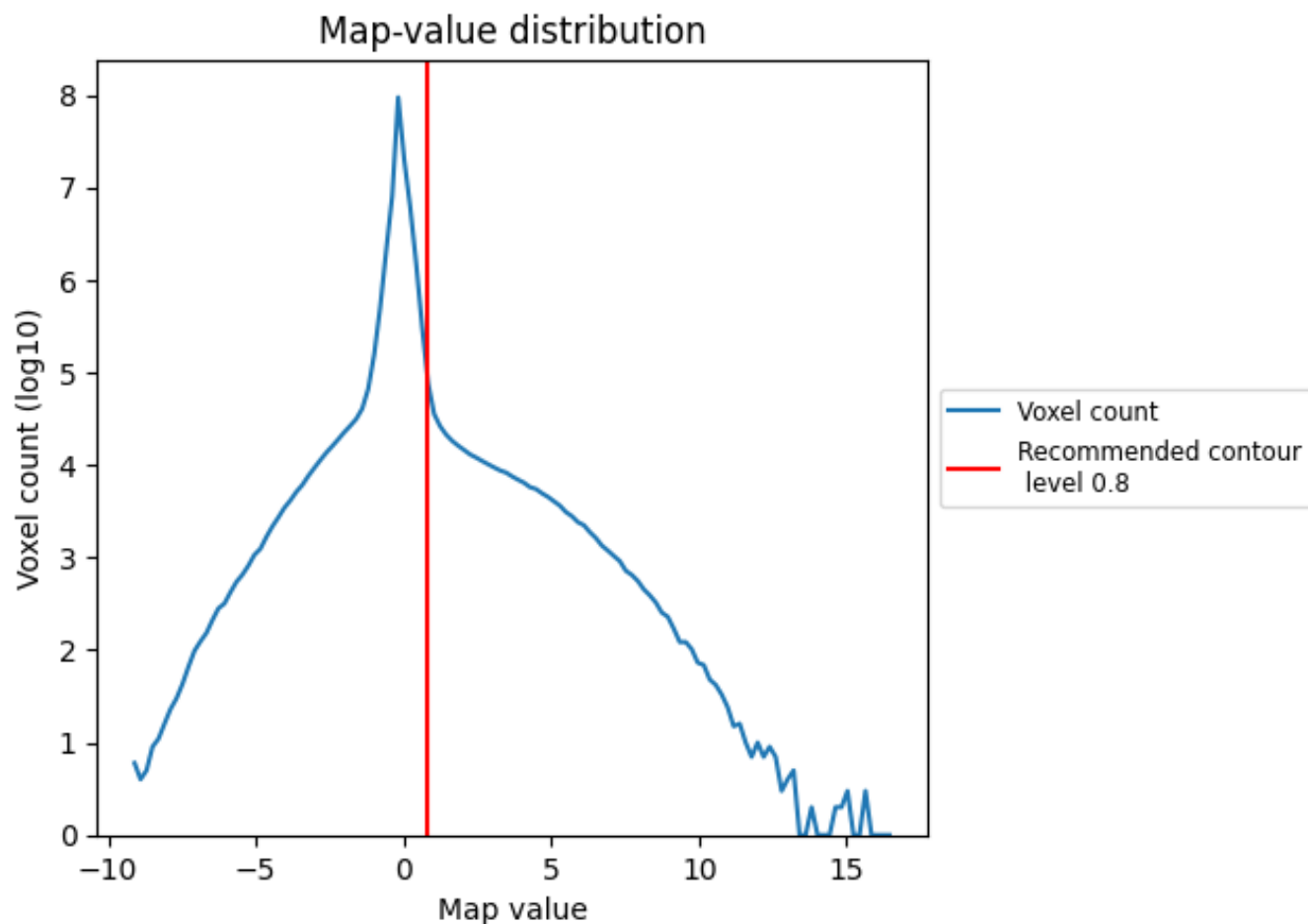
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

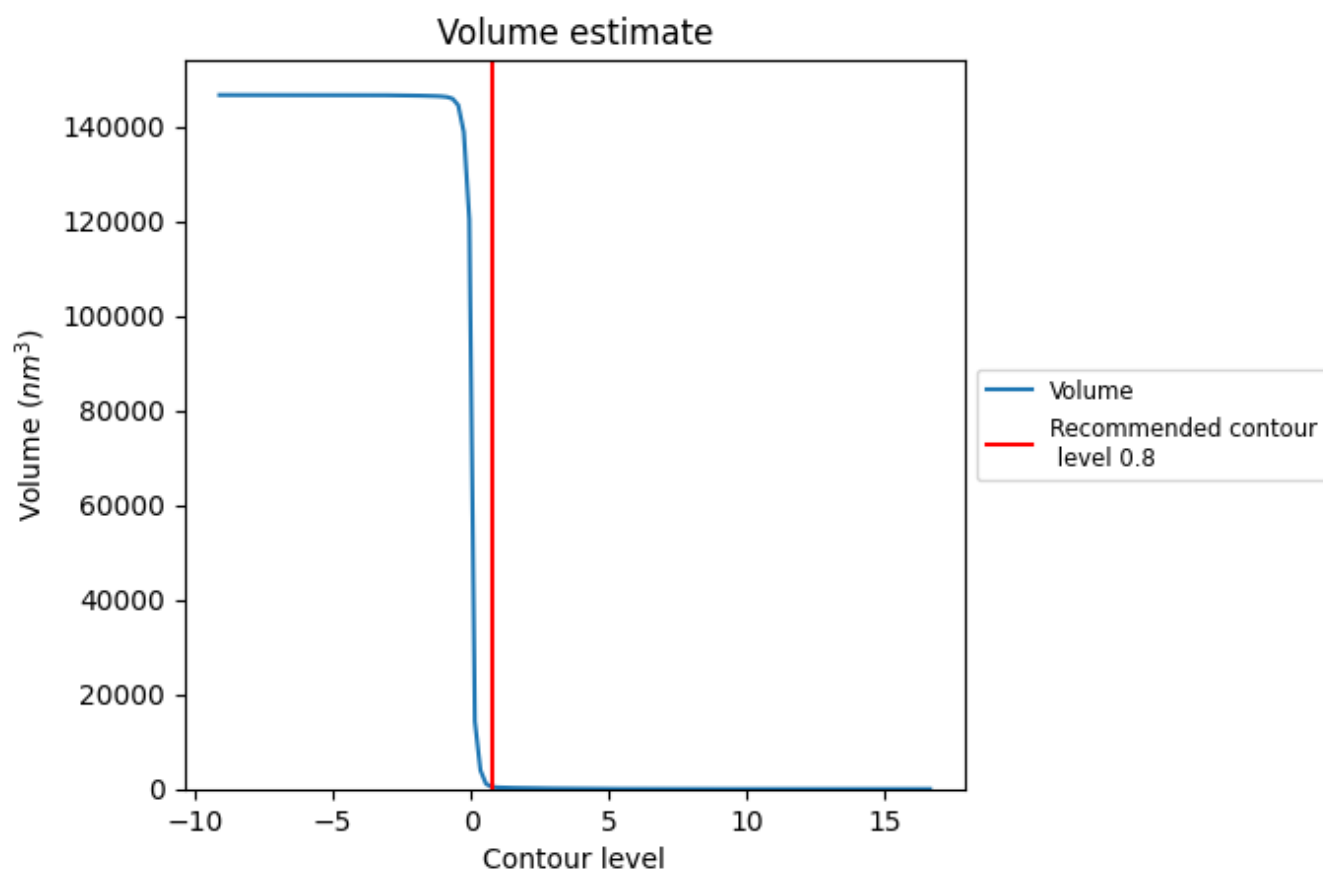
This section contains the results of statistical analysis of the map.

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.

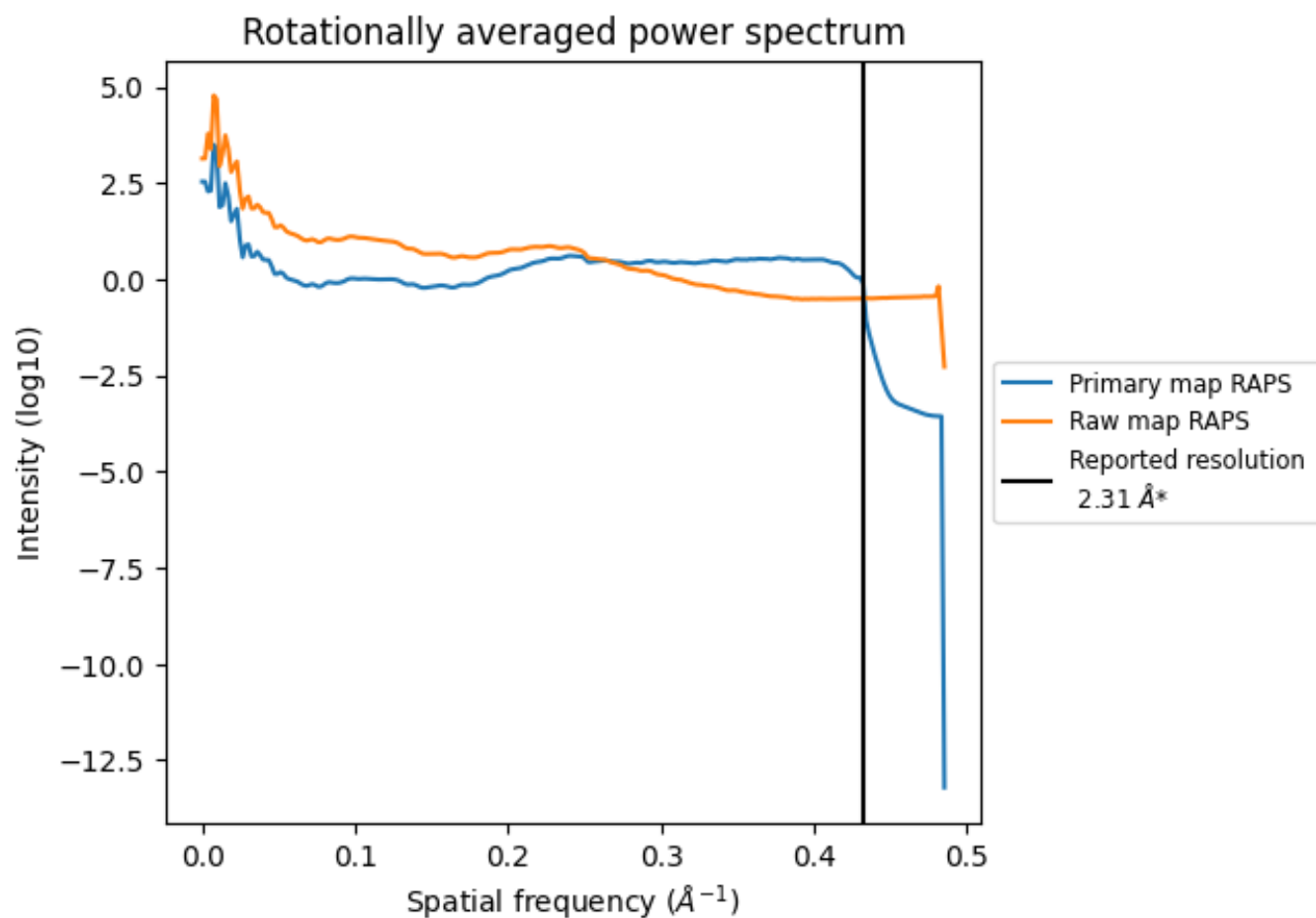
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 429 nm^3 ; this corresponds to an approximate mass of 388 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 ⓘ

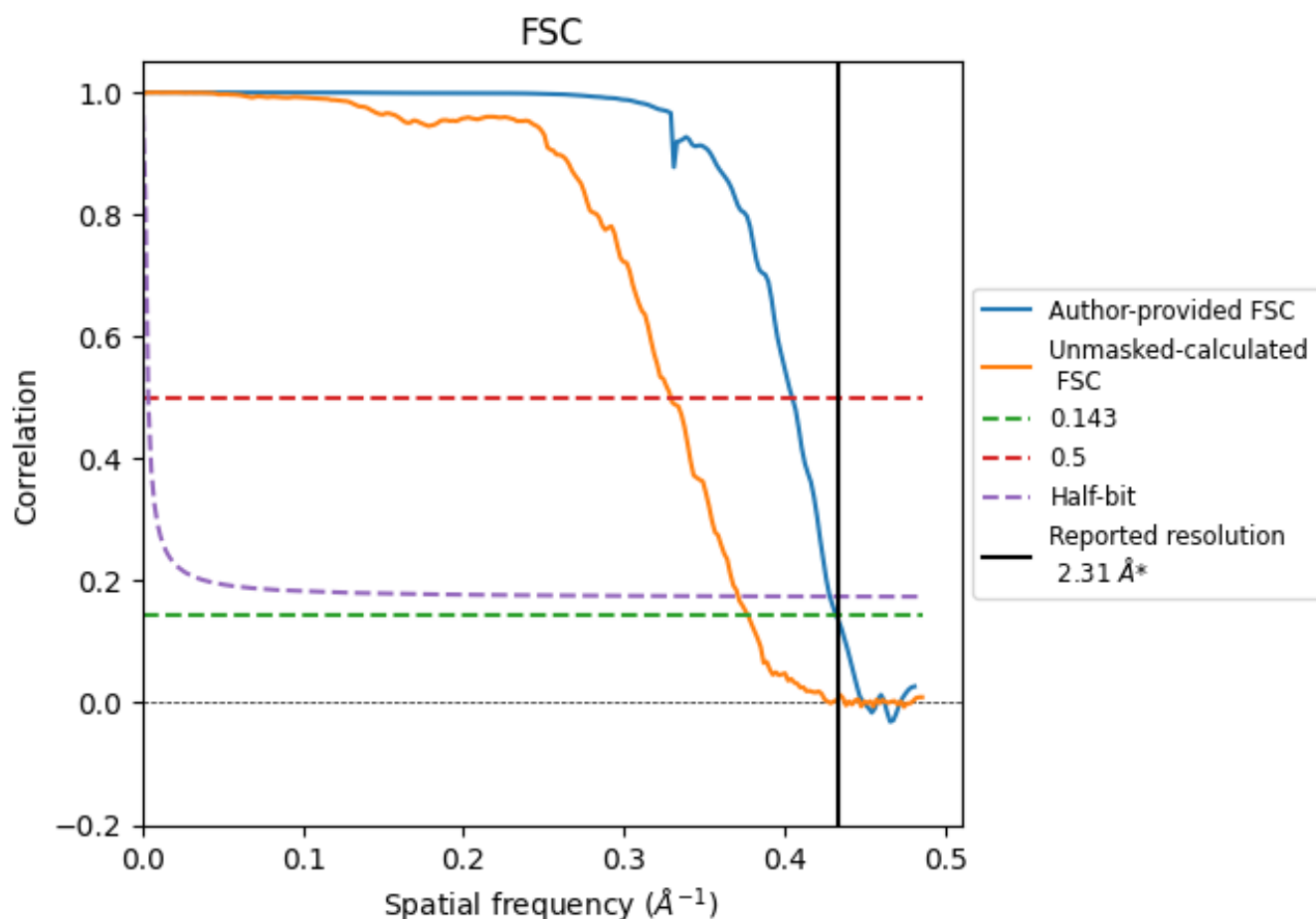


*Reported resolution corresponds to spatial frequency of 0.433 Å⁻¹

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 0.433 $\text{\AA}^{-1}$

8.2 Resolution estimates

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.31	-	-
Author-provided FSC curve	2.31	2.47	2.34
Unmasked-calculated*	2.65	3.04	2.70

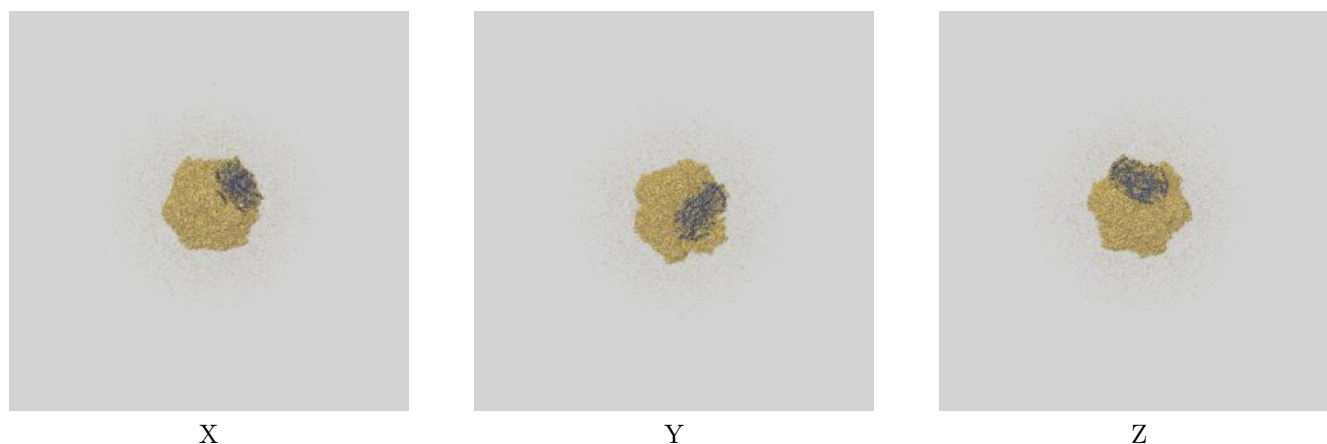
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.65 differs from the reported value 2.31 by more than 10 %

9 Map-model fit [i](#)

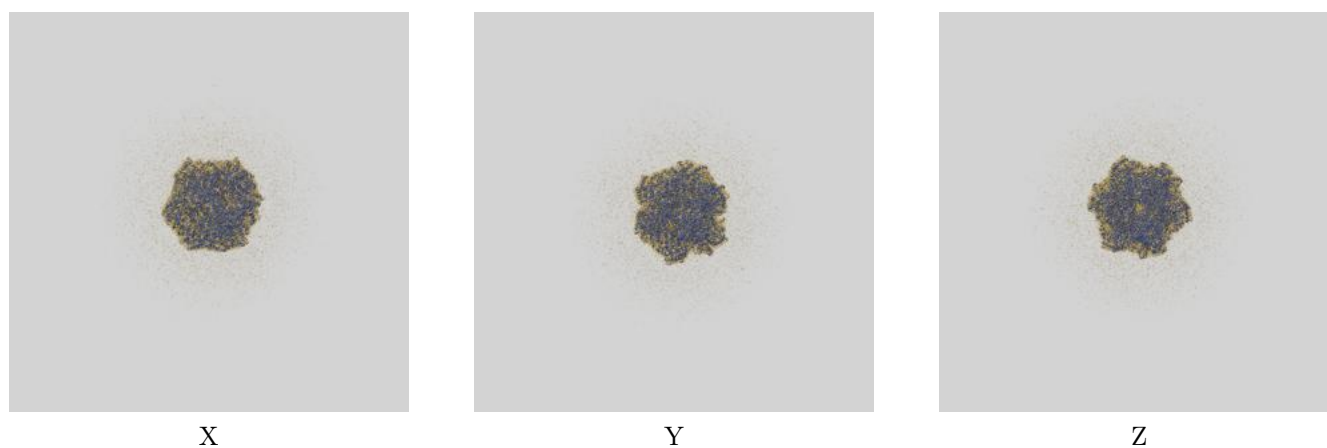
This section contains information regarding the fit between EMDB map EMD-43270 and PDB model 8VIX. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

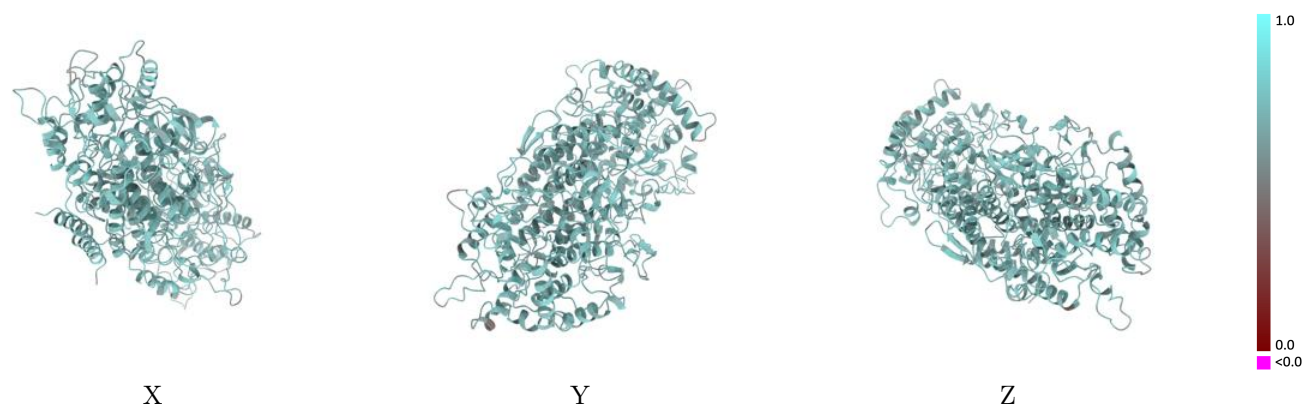


9.1.2 Map-model assembly overlay [i](#)



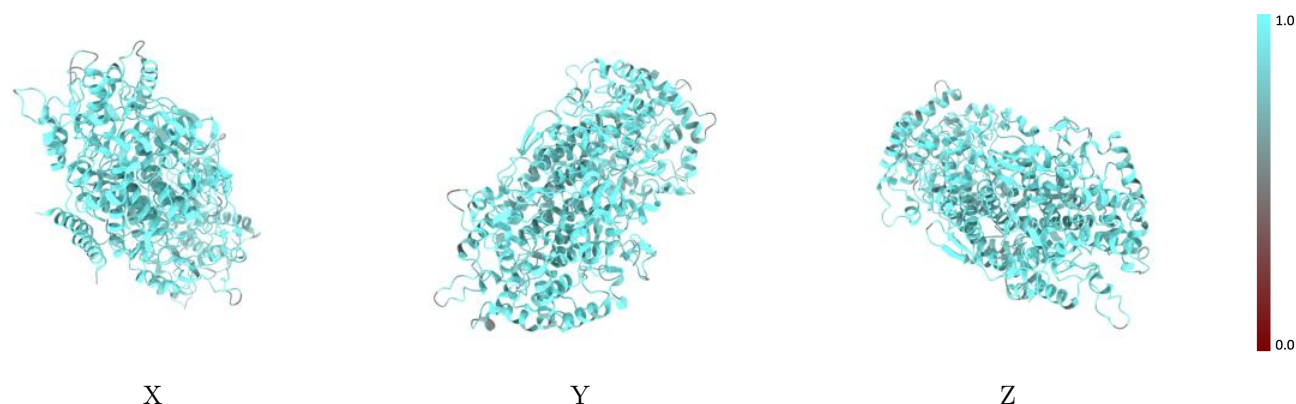
The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



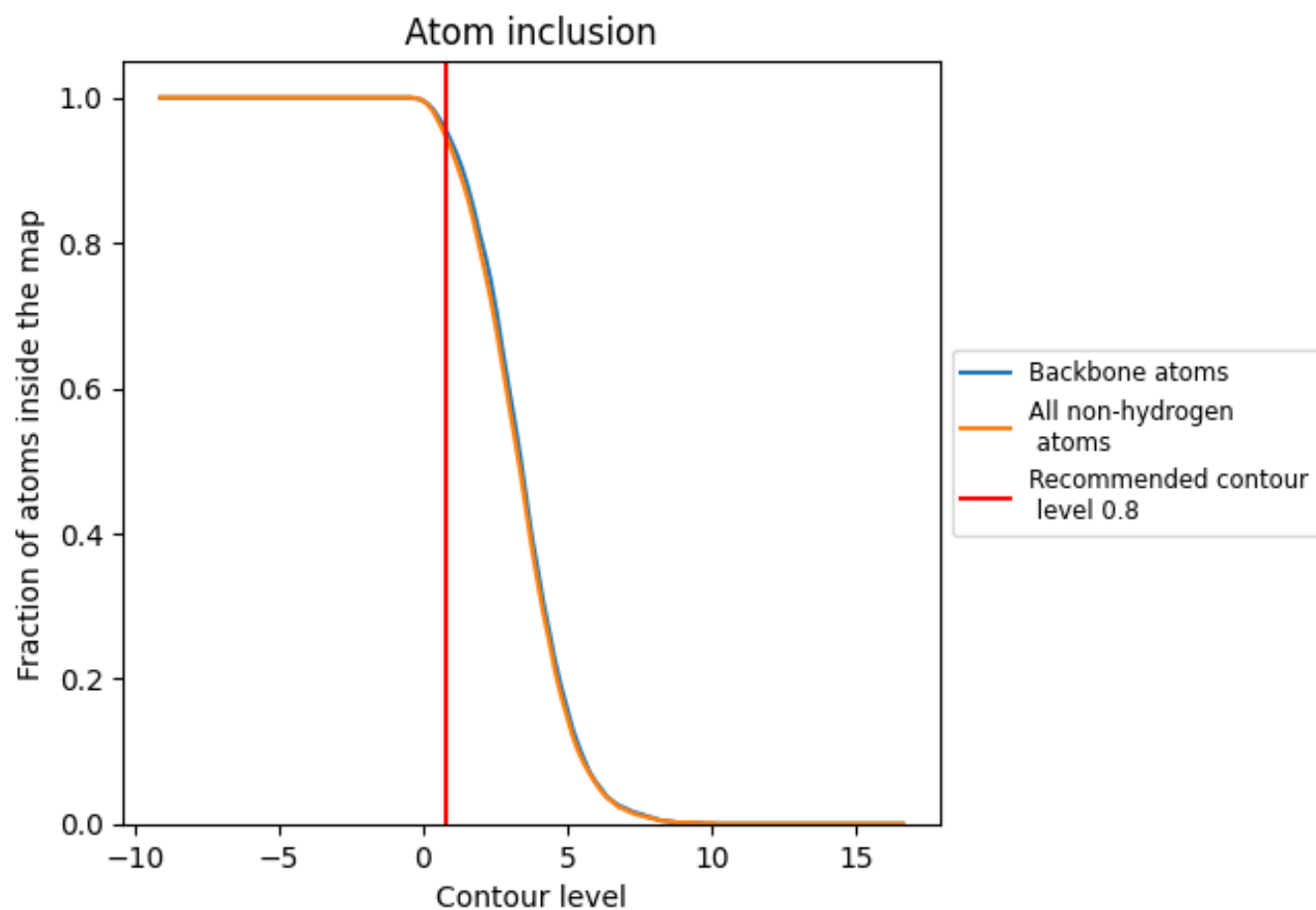
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 95% 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 (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9460	0.6840
A	0.9470	0.6830
B	0.9450	0.6840

