



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 01:32 PM UTC

PDB ID : 8Q7Y / pdb_00008q7y
EMDB ID : EMD-18244
Title : ESIBD structure of beta-galactosidase
Authors : Esser, T.; Boehning, J.; Bharat, T.A.M.; Rauschenbach, S.
Deposited on : 2023-08-17
Resolution : 2.60 Å (reported)
Based on initial model : 6DRV

This is a Full wwPDB EM Validation 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
MolProbity : 4-5-2 with Phenix2.0
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

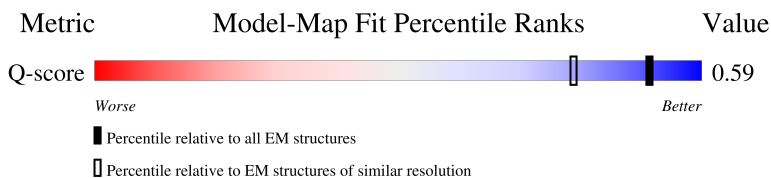
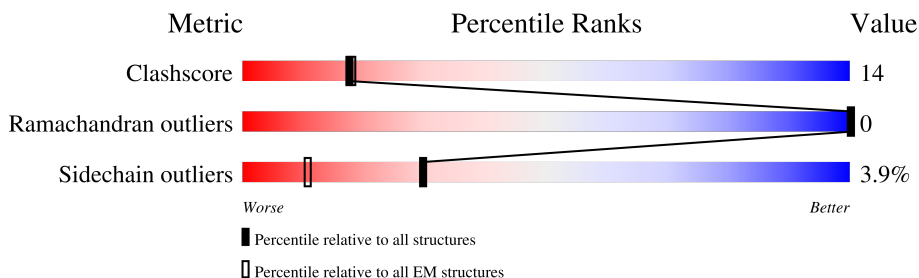
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 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	8728 (2.10 - 3.10)

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	1024	 22% 8% 70%
1	B	1024	 22% 8% 70%
1	C	1024	 21% 8% 70%
1	D	1024	 21% 8% . 70%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 10032 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 Beta-galactosidase.

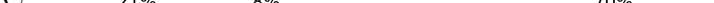
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	303	Total	C	N	O	S	0	0
			2508	1603	456	434	15		
1	B	303	Total	C	N	O	S	0	0
			2508	1603	456	434	15		
1	C	303	Total	C	N	O	S	0	0
			2508	1603	456	434	15		
1	D	303	Total	C	N	O	S	0	0
			2508	1603	456	434	15		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	334	VAL	GLU	conflict	UNP P00722
B	334	VAL	GLU	conflict	UNP P00722
C	334	VAL	GLU	conflict	UNP P00722
D	334	VAL	GLU	conflict	UNP P00722

ALA	GLU	GLU	GLY	THR	TRP	LEU	ASN	ILE	ASP	GLY	PHE	HIS	MET	GLY	ILE	GLY	GLY	ASP	ASP	SER	TRP	SER	PRO	SER	SER	VAL	SER	ALA	GLU	PHE	GLN	LEU	SER	ALA	GLY	ARG	TYR	HIS	TYR	GLN	LEU	VAL	TRP	CYS	GLN	LYS
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- Molecule 1: Beta-galactosidase

Chain C:  21% 8% 70%

TRP	LEU	LEU	CYS	ASP	LEU	PRO	GLU	GLU	ALA	ASP	THR	VAL	VAL	P87	S88	N89	Y100	THR	ASN	VAL	VAL	THR	THR	PRO	ILE	THR	VAL	VAL	ASN	PRO	PRO	THR	THR	CYS	THR	LEU	GLN	GLY	THR	E140
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H147	H151	LEU	TRP	CYS	ASN	GLY	ARG	TRP	V159	Q163	D164	S165	R166	L167	PRO	GLU	SER	GLY	PHE	ASP	LEU	ALA	SER	ALA	PHE	LEU	LEU	ARG	ALA	GLY	GLU	Q200	D201	D202	M203	R204	M205	F209	R210	D211	VAL	SER	LEU	LEU	HIS	LYS	PRO
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THR THR GLN THR ILE SER ASP PHE HTS VAL VAL THR ARG ARG PHE ASN ASP ASP PHE SER ARG ALA VAL LEU GLU ALA GLU VAL GLN VAL MET CYS GLY GLU LEU LEU ARG ASP TYR LEU ARG VAL VAL VAL SER SER TRP GLN THR THR THR VAL ALA ALA SER SER GLY GLY THR ALA PRO PHE GLY GLY GLU THR

ILE	GLU	ASP	GLY	ARG	GLY	TYR	ALA	ALA	ASP	VAL	THR	LEU	ARG	LEU	ASN	VAL	GLU	ASN	PRO	PRO	LEU	TYR	ARG	SER	TRP	LEU	LYS	LEU	GLU	ALA	ALA	ILE	ILE	ASN	ASN	PRO	PRO	VAL	VAL	VAL	GLU	LEU	HIS	THR	ALA	ALA	ASP	GLY	THR	LEU	ILE	GLU	ALA	GLU	CYS	ASP	V330	R366	L341	L342	H360
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G364	D368	E369	G370	T371	M372	L378	N382	H391	H395	P396	L397	D403	V410	A413	T417	H418	G419	M420	M423	M424	R425	L426	T427	R431	M432	L433	P434	A443	V444	V440	M443	H450	P451	L455	M456	S457	L458	S462	D469	A470
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Y472	R473	W474	I475	K476	S477	V478		R482	P483	V484	K485	V486	GLU	GLY	GLY	GLY	ALA	ASP	THR	THR	ALA	ALA	THR	D497	C500	P501	A504	K505	VAL	ASP	GLU	ASP	GLN	PRO	PHE	PRO	PRO	ALA	ALA	VAL	PRO	PRO	LYS	TRP	S519	I520	K521	K522	K523	L524	S525	L526	PRO	GLY	GLU	THR	ARG	P532	A539	
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#541	MET	GLY	ASN	SER	L546	F549	K550	K551	Y552	W553	R561	L562	Q563	W568	D569	S574	LEU	ILE	LYS	TYP	ASP	GLU	ASN	ASN	ASN	ASP	ALA	SER	THR	TRP	PRO	PRO	ASP	PHE	PHE	GLY	GLY	ASP	THR	ASN	ASN	GLN	ARG	ARG	ARG	CYS	PHE	VAL	LEU	ALA	ALA	ASP	ARG	THR	PRO
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HIS	PRO	L617	A620	Q624	GLN	PHE	PHE	GLN	PHE	ARG	LEU	SER	GLY	GLN	THR	ILE	GLU	VAL	THR	SER	GLU	TYR	LEU	PHE	ARG	HIS	ASP	ASN	ASP	GLU	LEU	LEU	HIS	TRP	MET	VAL	ALA	ALA	LEU	ASP	GLY	LYS	PRO	PRO	VAL	VAL	LEU	ALA	SER	GLY	GLU	VAL	PRO	LEU	ASP	VAL	ALA	PRO	ALA	GLN
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LYS GLN LEU LEU ILE GLU LEU LEU PRO PRO LEU LEU PRO PRO GLN GLN PRO PRO GLU GLU SER SER ALA ALA GLY GLN LEU LEU TRP TRP LEU LEU THR THR VAL VAL ARG ARG VAL VAL VAL PRO GLN PRO ASN ASN ALA ALA THR THR ALA ALA TRP TRP SER SER GLU GLU ALA ALA GLY GLY HIS HIS ILE ILE SER SER LEU LEU ALA ALA TRP TRP GLN GLN GLN GLN TRP TRP ARG ARG LEU LEU ALA ALA GLU GLU ASN ASN LEU LEU SER SER VAL VAL THR THR LEU LEU PRO PRO ALA ALA ALA ALA HIS HIS

TLE	PRO	HIS	THR	THR	SER	GUR	MET	PHE	CYS	ILE	GLU	LEU	GLY	ASN	LVS	ARG	TRP	PHE	ASN	ARG	GLN	SER	GLY	PHE	LEU	SER	GLN	MET	TRP	ILE	GLY	ASP	LVS	LYS	GLN	GLN	ASP	LEU	LEU	THR	PRO	LEU	ARG	ALA	PRO	ILE	VAL	FED
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GLU	ALA	THR	ARG	ILE	ASP	PRO	ASN	ALA	ALA	ALA	ALA	GLY	HIS	TYR	GLN	GLU	ALA	ALA	LEU	LEU	GLN	CYS	THR	ALA	ASP	ASP	ALA	VAL	VAL	LEU	LEU	ILE	THR	THR	ALA	HIS	TRP	ALA	ALA	GLN	HIS	GLY	LYS	LEU	PHE	ILE	SER	ARG	LYS	THR	THR
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ARG	ASP	ILE	GLY	SER	GLY	GLN	MET	ALA	ALA	THR	VAL	ASP	VAL	GLU	VAL	VAL	ALA	ALA	SER	SER	ASP	THR	HIS	PRO	PRO	ALA	ALA	ARG	ILE	GLY	LEU	LEU	ASN	CYS	GLN	LEU	ALA	ALA	GLN	VAL	ALA	ALA	GLU	VAL	ARG	VAL	ASN	ASN	TRP	TRP	LEU	GLY	LEU	LEU	GLY	PRO	PRO	ASP	ASP	ARG	ARG	LEU	THR	ALA	ALA	CYS	PHE	ASP
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LEU	HIS	ALA	GLU	GLY	THR	TRP	LEU	ASN	ILE	ASP	GLY	PHE	HIS	MET	GLY	ILE	GLY	GLY	ASP	ASP	SER	SER	TRP	SER	PRO	SER	SER	VAL	SER	ALA	GLU	PHE	GLN	LEU	SER	ALA	GLY	ARG	TYR	HIS	TYR	GLN	LEU	VAL	TRP	CYS	GLN	LYS
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D2	Depositor
Number of particles used	463000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; As implemented in cryoSPARC	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	34	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.642	Depositor
Minimum map value	-2.596	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.158	Depositor
Map size (Å)	345.28, 345.28, 345.28	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.13	0/2579	0.39	0/3490
1	B	0.13	0/2579	0.39	0/3490
1	C	0.13	0/2579	0.39	0/3490
1	D	0.13	0/2579	0.39	0/3490
All	All	0.13	0/10316	0.39	0/13960

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2508	0	2394	76	0
1	B	2508	0	2394	75	0
1	C	2508	0	2394	81	0
1	D	2508	0	2394	83	0
All	All	10032	0	9576	265	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (265) 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:C:473:ARG:NH2	1:D:469:ASP:O	2.08	0.87
1:C:469:ASP:O	1:D:473:ARG:NH2	2.08	0.86
1:A:473:ARG:NH2	1:B:469:ASP:O	2.10	0.84
1:A:469:ASP:O	1:B:473:ARG:NH2	2.10	0.84
1:B:444:VAL:HG21	1:B:475:ILE:HG12	1.67	0.75
1:A:444:VAL:HG21	1:A:475:ILE:HG12	1.67	0.74
1:C:444:VAL:HG21	1:C:475:ILE:HG12	1.67	0.74
1:D:444:VAL:HG21	1:D:475:ILE:HG12	1.67	0.74
1:A:476:LYS:NZ	1:A:482:ARG:O	2.22	0.72
1:B:476:LYS:NZ	1:B:482:ARG:O	2.22	0.72
1:D:476:LYS:NZ	1:D:482:ARG:O	2.22	0.69
1:C:476:LYS:NZ	1:C:482:ARG:O	2.22	0.69
1:A:200:GLN:O	1:A:204:ARG:NH2	2.27	0.68
1:A:440:VAL:HG11	1:A:471:LEU:HB3	1.75	0.68
1:B:200:GLN:O	1:B:204:ARG:NH2	2.27	0.68
1:B:440:VAL:HG11	1:B:471:LEU:HB3	1.75	0.67
1:C:200:GLN:O	1:C:204:ARG:NH2	2.27	0.67
1:D:200:GLN:O	1:D:204:ARG:NH2	2.27	0.67
1:A:147:ASN:ND2	1:A:205:MET:O	2.27	0.67
1:B:147:ASN:ND2	1:B:205:MET:O	2.27	0.67
1:C:147:ASN:ND2	1:C:205:MET:O	2.27	0.66
1:D:147:ASN:ND2	1:D:205:MET:O	2.27	0.66
1:D:440:VAL:HG11	1:D:471:LEU:HB3	1.75	0.66
1:C:440:VAL:HG11	1:C:471:LEU:HB3	1.76	0.66
1:A:199:ASP:O	1:A:418:HIS:ND1	2.30	0.65
1:B:199:ASP:O	1:B:418:HIS:ND1	2.30	0.65
1:C:199:ASP:O	1:C:418:HIS:ND1	2.30	0.65
1:D:199:ASP:O	1:D:418:HIS:ND1	2.30	0.65
1:A:368:ASP:OD2	1:A:371:THR:OG1	2.14	0.64
1:B:368:ASP:OD2	1:B:371:THR:OG1	2.14	0.64
1:A:473:ARG:NH2	1:B:473:ARG:HG2	2.13	0.64
1:A:473:ARG:HG2	1:B:473:ARG:NH2	2.13	0.64
1:A:561:ARG:HB2	1:D:525:SER:HB2	1.81	0.62
1:B:561:ARG:HB2	1:C:525:SER:HB2	1.81	0.62
1:A:525:SER:HB2	1:D:561:ARG:HB2	1.82	0.61
1:B:525:SER:HB2	1:C:561:ARG:HB2	1.82	0.61
1:C:473:ARG:HG2	1:D:473:ARG:NH2	2.15	0.61
1:A:410:VAL:HG22	1:A:455:ILE:HB	1.83	0.61
1:B:410:VAL:HG22	1:B:455:ILE:HB	1.83	0.61
1:C:473:ARG:NH2	1:D:473:ARG:HG2	2.15	0.61
1:D:410:VAL:HG22	1:D:455:ILE:HB	1.83	0.61
1:C:410:VAL:HG22	1:C:455:ILE:HB	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:ARG:HH21	1:B:473:ARG:HG2	1.66	0.61
1:A:473:ARG:HG2	1:B:473:ARG:HH21	1.66	0.60
1:A:473:ARG:HA	1:A:476:LYS:HB2	1.83	0.60
1:B:473:ARG:HA	1:B:476:LYS:HB2	1.84	0.60
1:A:458:LEU:HD12	1:A:486:TYR:HB2	1.84	0.60
1:B:458:LEU:HD12	1:B:486:TYR:HB2	1.84	0.60
1:C:368:ASP:OD2	1:C:371:THR:OG1	2.14	0.60
1:D:368:ASP:OD2	1:D:371:THR:OG1	2.14	0.60
1:C:473:ARG:HA	1:C:476:LYS:HB2	1.84	0.59
1:D:473:ARG:HA	1:D:476:LYS:HB2	1.84	0.59
1:D:458:LEU:HD12	1:D:486:TYR:HB2	1.84	0.59
1:C:458:LEU:HD12	1:C:486:TYR:HB2	1.84	0.59
1:B:469:ASP:HA	1:B:472:TYR:HB3	1.85	0.58
1:A:469:ASP:HA	1:A:472:TYR:HB3	1.85	0.58
1:C:472:TYR:HD1	1:C:484:VAL:HB	1.68	0.58
1:C:434:PRO:HB3	1:D:434:PRO:HB3	1.84	0.58
1:D:472:TYR:HD1	1:D:484:VAL:HB	1.68	0.58
1:A:472:TYR:HD1	1:A:484:VAL:HB	1.68	0.57
1:B:472:TYR:HD1	1:B:484:VAL:HB	1.68	0.57
1:C:473:ARG:HG2	1:D:473:ARG:HH21	1.69	0.57
1:C:473:ARG:HH21	1:D:473:ARG:HG2	1.69	0.57
1:D:469:ASP:HA	1:D:472:TYR:HB3	1.85	0.57
1:A:458:LEU:HD11	1:A:472:TYR:HB2	1.87	0.56
1:C:450:HIS:O	1:C:482:ARG:NH2	2.38	0.56
1:C:469:ASP:HA	1:C:472:TYR:HB3	1.85	0.56
1:D:450:HIS:O	1:D:482:ARG:NH2	2.38	0.56
1:B:458:LEU:HD11	1:B:472:TYR:HB2	1.87	0.56
1:D:504:ALA:O	1:D:552:TYR:OH	2.23	0.56
1:A:474:TRP:O	1:A:478:VAL:HB	2.06	0.56
1:B:474:TRP:O	1:B:478:VAL:HB	2.06	0.56
1:C:458:LEU:HD11	1:C:472:TYR:HB2	1.87	0.56
1:D:458:LEU:HD11	1:D:472:TYR:HB2	1.87	0.55
1:A:434:PRO:HB3	1:B:434:PRO:HB3	1.86	0.55
1:C:437:SER:HA	1:C:471:LEU:HD11	1.88	0.55
1:D:437:SER:HA	1:D:471:LEU:HD11	1.88	0.55
1:D:474:TRP:O	1:D:478:VAL:HB	2.06	0.55
1:C:474:TRP:O	1:C:478:VAL:HB	2.06	0.55
1:B:521:LYS:HD3	1:C:521:LYS:NZ	2.21	0.55
1:A:521:LYS:NZ	1:D:521:LYS:HD3	2.22	0.55
1:B:521:LYS:NZ	1:C:521:LYS:HD3	2.22	0.55
1:A:450:HIS:O	1:A:482:ARG:NH2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:LYS:HD3	1:D:521:LYS:NZ	2.21	0.54
1:B:450:HIS:O	1:B:482:ARG:NH2	2.38	0.54
1:A:437:SER:HA	1:A:471:LEU:HD11	1.88	0.54
1:B:437:SER:HA	1:B:471:LEU:HD11	1.88	0.54
1:C:372:MET:HE1	1:C:395:HIS:HB3	1.88	0.54
1:D:372:MET:HE1	1:D:395:HIS:HB3	1.88	0.54
1:B:372:MET:HE1	1:B:395:HIS:HB3	1.88	0.54
1:A:425:ARG:O	1:A:425:ARG:NH1	2.41	0.54
1:B:425:ARG:NH1	1:B:425:ARG:O	2.41	0.54
1:A:372:MET:HE1	1:A:395:HIS:HB3	1.88	0.53
1:C:425:ARG:O	1:C:425:ARG:NH1	2.41	0.53
1:D:425:ARG:O	1:D:425:ARG:NH1	2.41	0.53
1:C:425:ARG:C	1:C:425:ARG:HH11	2.16	0.53
1:D:425:ARG:C	1:D:425:ARG:HH11	2.16	0.53
1:B:425:ARG:C	1:B:425:ARG:HH11	2.16	0.53
1:A:425:ARG:C	1:A:425:ARG:HH11	2.16	0.53
1:C:336:ARG:HA	1:C:336:ARG:NE	2.24	0.53
1:A:336:ARG:HA	1:A:336:ARG:NE	2.24	0.53
1:B:336:ARG:HA	1:B:336:ARG:NE	2.24	0.53
1:D:336:ARG:HA	1:D:336:ARG:NE	2.24	0.52
1:C:473:ARG:HH22	1:D:469:ASP:C	2.15	0.52
1:C:469:ASP:HB3	1:D:473:ARG:HH12	1.74	0.52
1:C:473:ARG:HH12	1:D:469:ASP:HB3	1.74	0.52
1:C:469:ASP:C	1:D:473:ARG:HH22	2.15	0.52
1:A:472:TYR:CD1	1:A:484:VAL:HB	2.46	0.51
1:B:167:LEU:HD11	1:B:443:MET:HB2	1.92	0.51
1:A:167:LEU:HD11	1:A:443:MET:HB2	1.92	0.51
1:B:472:TYR:CD1	1:B:484:VAL:HB	2.46	0.51
1:C:472:TYR:HD2	1:D:473:ARG:NH2	2.08	0.51
1:C:473:ARG:NH2	1:D:472:TYR:HD2	2.08	0.51
1:C:167:LEU:HD11	1:C:443:MET:HB2	1.92	0.50
1:A:473:ARG:HH22	1:B:469:ASP:C	2.16	0.50
1:A:574:SER:O	1:A:574:SER:OG	2.29	0.50
1:C:342:LEU:H	1:C:563:GLN:NE2	2.09	0.50
1:D:167:LEU:HD11	1:D:443:MET:HB2	1.92	0.50
1:A:89:ASN:ND2	1:A:205:MET:SD	2.84	0.50
1:B:574:SER:O	1:B:574:SER:OG	2.29	0.50
1:D:342:LEU:H	1:D:563:GLN:NE2	2.09	0.50
1:D:472:TYR:HA	1:D:484:VAL:HG11	1.94	0.50
1:C:472:TYR:CD1	1:C:484:VAL:HB	2.46	0.50
1:C:472:TYR:HA	1:C:484:VAL:HG11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:ASN:ND2	1:B:205:MET:SD	2.84	0.50
1:D:472:TYR:CD1	1:D:484:VAL:HB	2.46	0.50
1:A:504:ALA:O	1:A:552:TYR:OH	2.23	0.50
1:A:469:ASP:C	1:B:473:ARG:HH22	2.16	0.50
1:A:472:TYR:HA	1:A:484:VAL:HG11	1.94	0.50
1:B:504:ALA:O	1:B:552:TYR:OH	2.23	0.50
1:B:342:LEU:H	1:B:563:GLN:NE2	2.09	0.49
1:B:472:TYR:HA	1:B:484:VAL:HG11	1.94	0.49
1:A:342:LEU:H	1:A:563:GLN:NE2	2.09	0.49
1:A:469:ASP:HB3	1:B:473:ARG:HH12	1.78	0.49
1:A:473:ARG:HH12	1:B:469:ASP:HB3	1.78	0.49
1:D:165:SER:OG	1:D:198:GLU:OE2	2.23	0.49
1:A:472:TYR:HD2	1:B:473:ARG:NH2	2.11	0.49
1:C:165:SER:OG	1:C:198:GLU:OE2	2.23	0.49
1:C:341:LEU:HG	1:C:563:GLN:HE22	1.78	0.49
1:C:504:ALA:O	1:C:552:TYR:OH	2.23	0.49
1:D:341:LEU:HG	1:D:563:GLN:HE22	1.78	0.49
1:C:469:ASP:HB3	1:D:473:ARG:NH1	2.27	0.49
1:A:473:ARG:NH2	1:B:472:TYR:HD2	2.11	0.49
1:C:89:ASN:ND2	1:C:205:MET:SD	2.84	0.49
1:C:473:ARG:NH1	1:D:469:ASP:HB3	2.27	0.49
1:D:89:ASN:ND2	1:D:205:MET:SD	2.84	0.49
1:D:403:ASP:HB2	1:D:451:PRO:HG2	1.95	0.48
1:C:403:ASP:HB2	1:C:451:PRO:HG2	1.95	0.48
1:A:341:LEU:HG	1:A:563:GLN:HE22	1.78	0.48
1:A:549:PHE:HE2	1:A:620:ALA:HA	1.79	0.48
1:B:341:LEU:HG	1:B:563:GLN:HE22	1.78	0.48
1:B:549:PHE:HE2	1:B:620:ALA:HA	1.79	0.48
1:A:403:ASP:HB2	1:A:451:PRO:HG2	1.95	0.48
1:B:403:ASP:HB2	1:B:451:PRO:HG2	1.95	0.48
1:C:369:GLU:HG3	1:C:397:LEU:HD21	1.97	0.47
1:C:549:PHE:HE2	1:C:620:ALA:HA	1.79	0.47
1:D:369:GLU:HG3	1:D:397:LEU:HD21	1.97	0.47
1:C:472:TYR:CD2	1:D:473:ARG:NH2	2.82	0.47
1:C:200:GLN:NE2	1:C:202:MET:SD	2.88	0.47
1:C:473:ARG:NH2	1:D:472:TYR:CD2	2.82	0.47
1:D:549:PHE:HE2	1:D:620:ALA:HA	1.79	0.47
1:D:200:GLN:NE2	1:D:202:MET:SD	2.88	0.47
1:B:199:ASP:HB3	1:B:418:HIS:HD1	1.80	0.47
1:D:501:PRO:HB3	1:D:523:TRP:CD2	2.50	0.47
1:A:199:ASP:HB3	1:A:418:HIS:HD1	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:501:PRO:HB3	1:C:523:TRP:CD2	2.50	0.47
1:A:200:GLN:NE2	1:A:202:MET:SD	2.88	0.47
1:B:200:GLN:NE2	1:B:202:MET:SD	2.88	0.47
1:B:501:PRO:HB3	1:B:523:TRP:CD2	2.50	0.47
1:A:501:PRO:HB3	1:A:523:TRP:CD2	2.50	0.46
1:A:521:LYS:HD3	1:D:521:LYS:HZ3	1.80	0.46
1:B:369:GLU:HG3	1:B:397:LEU:HD21	1.97	0.46
1:C:574:SER:O	1:C:574:SER:OG	2.29	0.46
1:D:360:HIS:N	1:D:364:GLY:O	2.44	0.46
1:A:369:GLU:HG3	1:A:397:LEU:HD21	1.97	0.46
1:A:469:ASP:HB3	1:B:473:ARG:NH1	2.30	0.46
1:D:199:ASP:HB3	1:D:418:HIS:HD1	1.80	0.46
1:D:574:SER:O	1:D:574:SER:OG	2.29	0.46
1:C:199:ASP:HB3	1:C:418:HIS:HD1	1.80	0.46
1:C:378:LEU:O	1:C:382:ASN:ND2	2.46	0.46
1:A:473:ARG:NH1	1:B:469:ASP:HB3	2.30	0.46
1:D:199:ASP:HB2	1:D:417:THR:HA	1.97	0.46
1:C:199:ASP:HB2	1:C:417:THR:HA	1.98	0.46
1:C:360:HIS:N	1:C:364:GLY:O	2.44	0.46
1:D:378:LEU:O	1:D:382:ASN:ND2	2.46	0.46
1:A:472:TYR:CD2	1:B:473:ARG:NH2	2.85	0.45
1:B:568:TRP:HA	1:B:569:ASP:HA	1.80	0.45
1:A:473:ARG:NH2	1:B:472:TYR:CD2	2.85	0.45
1:A:199:ASP:HB2	1:A:417:THR:HA	1.97	0.45
1:B:199:ASP:HB2	1:B:417:THR:HA	1.97	0.45
1:A:568:TRP:HA	1:A:569:ASP:HA	1.81	0.44
1:B:342:LEU:H	1:B:563:GLN:HE22	1.65	0.44
1:A:342:LEU:H	1:A:563:GLN:HE22	1.66	0.44
1:B:521:LYS:HD3	1:C:521:LYS:HZ3	1.82	0.44
1:B:360:HIS:N	1:B:364:GLY:O	2.44	0.44
1:A:360:HIS:N	1:A:364:GLY:O	2.44	0.43
1:A:378:LEU:O	1:A:382:ASN:ND2	2.46	0.43
1:B:378:LEU:O	1:B:382:ASN:ND2	2.46	0.43
1:A:521:LYS:HZ2	1:D:521:LYS:HD3	1.82	0.43
1:C:342:LEU:H	1:C:563:GLN:HE22	1.65	0.43
1:D:456:TRP:HB2	1:D:484:VAL:HG22	2.01	0.43
1:C:456:TRP:HB2	1:C:484:VAL:HG22	2.01	0.43
1:D:342:LEU:H	1:D:563:GLN:HE22	1.66	0.43
1:D:520:ILE:HD13	1:D:520:ILE:HA	1.95	0.42
1:A:21:VAL:O	1:A:163:GLN:NE2	2.52	0.42
1:C:469:ASP:CB	1:D:473:ARG:HH12	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:VAL:O	1:B:163:GLN:NE2	2.52	0.42
1:C:473:ARG:HH12	1:D:469:ASP:CB	2.32	0.42
1:C:568:TRP:HA	1:C:569:ASP:HA	1.80	0.42
1:A:456:TRP:HB2	1:A:484:VAL:HG22	2.01	0.42
1:B:456:TRP:HB2	1:B:484:VAL:HG22	2.00	0.42
1:C:21:VAL:O	1:C:163:GLN:NE2	2.52	0.42
1:C:427:THR:HG21	1:C:462:SER:HB2	2.02	0.42
1:C:520:ILE:HD13	1:C:520:ILE:HA	1.95	0.42
1:D:427:THR:HG21	1:D:462:SER:HB2	2.02	0.42
1:D:21:VAL:O	1:D:163:GLN:NE2	2.52	0.42
1:A:427:THR:HG21	1:A:462:SER:HB2	2.02	0.41
1:A:520:ILE:HD13	1:A:520:ILE:HA	1.95	0.41
1:B:427:THR:HG21	1:B:462:SER:HB2	2.02	0.41
1:B:521:LYS:HZ2	1:C:521:LYS:HD3	1.83	0.41
1:C:553:TRP:CZ2	1:C:624:GLN:HG2	2.55	0.41
1:D:553:TRP:CZ2	1:D:624:GLN:HG2	2.55	0.41
1:A:413:ALA:HB3	1:A:458:LEU:O	2.21	0.41
1:B:413:ALA:HB3	1:B:458:LEU:O	2.21	0.41
1:C:433:LEU:HD23	1:D:437:SER:HB2	2.01	0.41
1:D:413:ALA:HB3	1:D:458:LEU:O	2.21	0.41
1:B:520:ILE:HD13	1:B:520:ILE:HA	1.95	0.41
1:D:568:TRP:HA	1:D:569:ASP:HA	1.80	0.41
1:C:413:ALA:HB3	1:C:458:LEU:O	2.21	0.41
1:C:420:MET:H	1:C:420:MET:HG2	1.64	0.41
1:B:431:ARG:NH1	1:B:431:ARG:HG2	2.36	0.41
1:A:147:ASN:HB2	1:A:209:PHE:CZ	2.56	0.41
1:B:147:ASN:HB2	1:B:209:PHE:CZ	2.56	0.41
1:A:431:ARG:NH1	1:A:431:ARG:HG2	2.36	0.41
1:C:437:SER:HB2	1:D:433:LEU:HD23	2.02	0.41
1:A:370:GLN:O	1:A:374:GLN:HG2	2.21	0.41
1:B:200:GLN:OE1	1:B:391:HIS:HB3	2.21	0.41
1:B:204:ARG:HA	1:B:204:ARG:HD3	1.82	0.41
1:B:370:GLN:O	1:B:374:GLN:HG2	2.21	0.41
1:C:200:GLN:OE1	1:C:391:HIS:HB3	2.21	0.41
1:D:420:MET:H	1:D:420:MET:HG2	1.65	0.41
1:A:200:GLN:OE1	1:A:391:HIS:HB3	2.21	0.41
1:B:192:SER:OG	1:B:193:ASP:N	2.54	0.41
1:D:147:ASN:HB2	1:D:209:PHE:CZ	2.56	0.41
1:D:200:GLN:OE1	1:D:391:HIS:HB3	2.21	0.41
1:D:539:ALA:HB1	1:D:546:LEU:HD23	2.03	0.41
1:A:192:SER:OG	1:A:193:ASP:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:GLU:HG3	1:B:439:ARG:HH12	1.86	0.40
1:C:147:ASN:HB2	1:C:209:PHE:CZ	2.56	0.40
1:A:553:TRP:CZ2	1:A:624:GLN:HG2	2.55	0.40
1:C:473:ARG:CA	1:C:476:LYS:HB2	2.50	0.40
1:C:539:ALA:HB1	1:C:546:LEU:HD23	2.03	0.40
1:D:370:GLN:OE1	1:D:370:GLN:N	2.46	0.40
1:D:431:ARG:HG2	1:D:431:ARG:NH1	2.36	0.40
1:A:198:GLU:HG3	1:A:439:ARG:HH12	1.87	0.40
1:A:204:ARG:HA	1:A:204:ARG:HD3	1.82	0.40
1:B:553:TRP:CZ2	1:B:624:GLN:HG2	2.55	0.40
1:C:370:GLN:OE1	1:C:370:GLN:N	2.46	0.40
1:C:166:ARG:CZ	1:C:202:MET:HE1	2.52	0.40
1:C:431:ARG:HG2	1:C:431:ARG:NH1	2.36	0.40
1:D:473:ARG:CA	1:D:476:LYS:HB2	2.50	0.40
1:D:476:LYS:HZ3	1:D:484:VAL:HG23	1.86	0.40
1:D:503:TYR:HH	1:D:568:TRP:CD1	2.39	0.40
1:A:378:LEU:HD23	1:A:378:LEU:HA	1.91	0.40
1:D:166:ARG:CZ	1:D:202:MET:HE1	2.52	0.40

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	279/1024 (27%)	263 (94%)	16 (6%)	0	100	100
1	B	279/1024 (27%)	263 (94%)	16 (6%)	0	100	100
1	C	279/1024 (27%)	263 (94%)	16 (6%)	0	100	100
1	D	279/1024 (27%)	264 (95%)	15 (5%)	0	100	100
All	All	1116/4096 (27%)	1053 (94%)	63 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	265/876 (30%)	255 (96%)	10 (4%)	29	56
1	B	265/876 (30%)	255 (96%)	10 (4%)	29	56
1	C	265/876 (30%)	255 (96%)	10 (4%)	29	56
1	D	265/876 (30%)	254 (96%)	11 (4%)	26	52
All	All	1060/3504 (30%)	1019 (96%)	41 (4%)	30	55

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	165	SER
1	A	192	SER
1	A	368	ASP
1	A	423	MET
1	A	472	TYR
1	A	476	LYS
1	A	478	VAL
1	A	500	CYS
1	A	551	LYS
1	B	24	LEU
1	B	165	SER
1	B	192	SER
1	B	368	ASP
1	B	423	MET
1	B	472	TYR
1	B	476	LYS
1	B	478	VAL
1	B	500	CYS
1	B	551	LYS
1	C	24	LEU
1	C	165	SER
1	C	192	SER
1	C	368	ASP

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Mol	Chain	Res	Type
1	C	423	MET
1	C	472	TYR
1	C	476	LYS
1	C	478	VAL
1	C	500	CYS
1	C	551	LYS
1	D	24	LEU
1	D	165	SER
1	D	192	SER
1	D	200	GLN
1	D	368	ASP
1	D	423	MET
1	D	472	TYR
1	D	476	LYS
1	D	478	VAL
1	D	500	CYS
1	D	551	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	558	GLN
1	A	563	GLN
1	B	558	GLN
1	B	563	GLN
1	C	558	GLN
1	C	563	GLN
1	D	558	GLN
1	D	563	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

There are no ligands in this entry.

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.

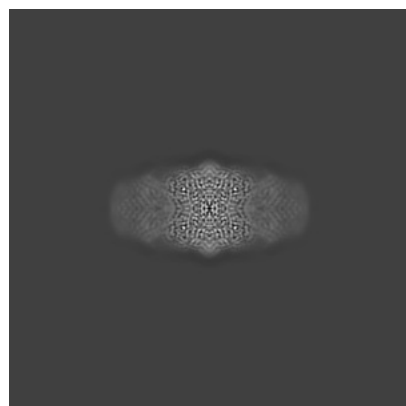
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18244. These allow visual inspection of the internal detail of the map and identification of artifacts.

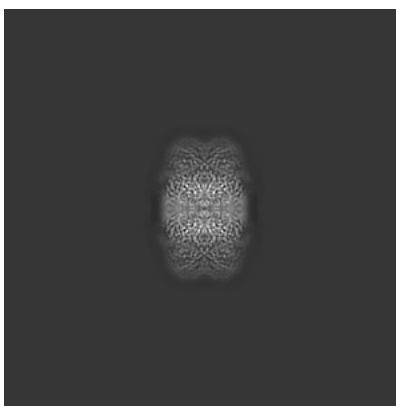
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

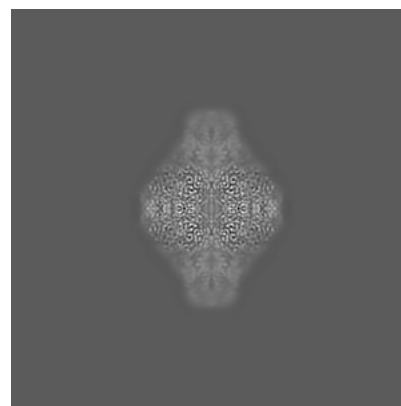
6.1.1 Primary map



X

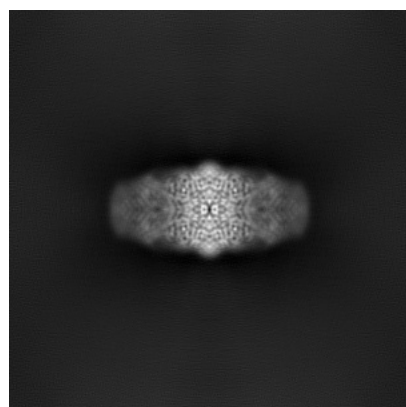


Y

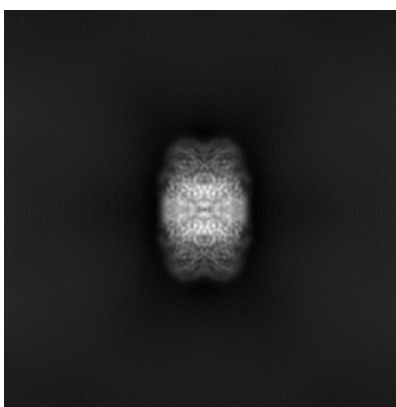


Z

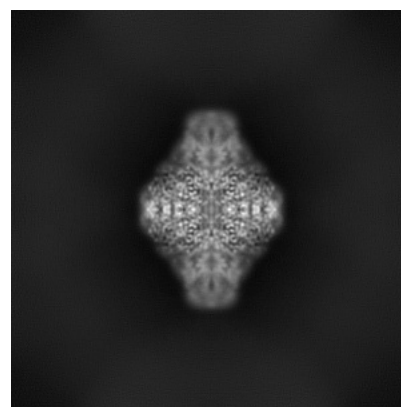
6.1.2 Raw map



X



Y

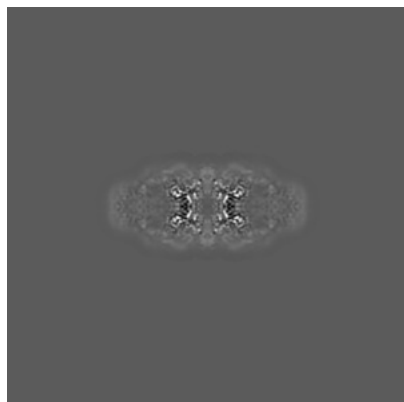


Z

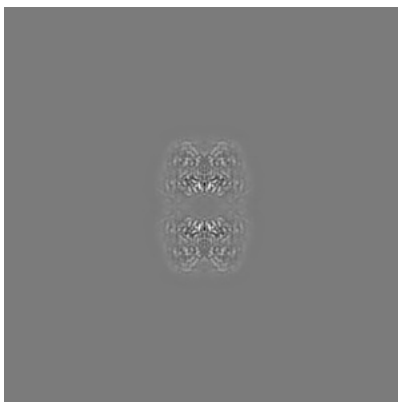
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

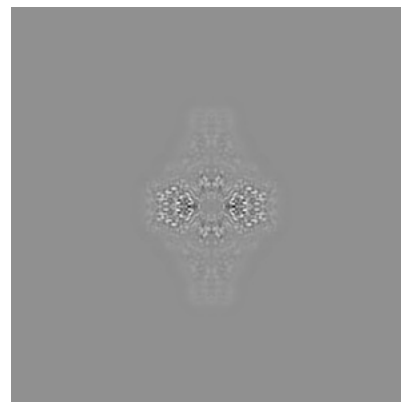
6.2.1 Primary map



X Index: 208

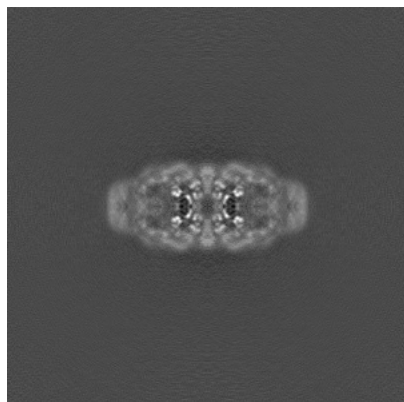


Y Index: 208

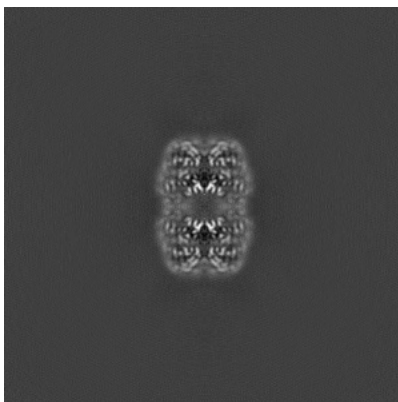


Z Index: 208

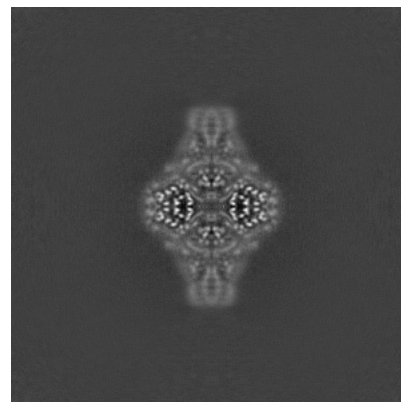
6.2.2 Raw map



X Index: 208



Y Index: 208

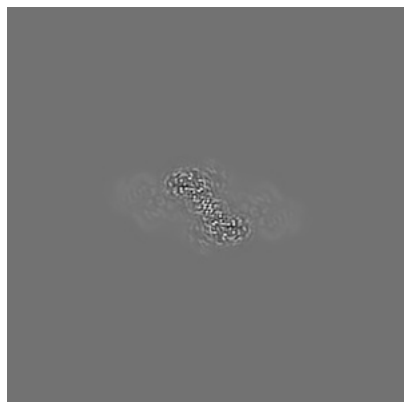


Z Index: 208

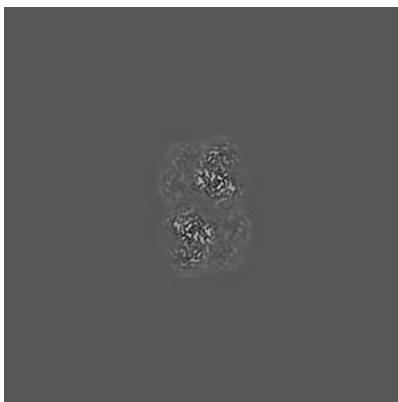
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

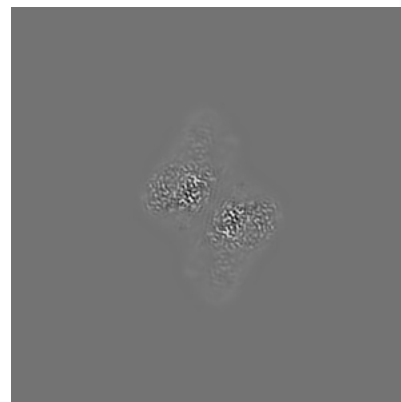
6.3.1 Primary map



X Index: 185

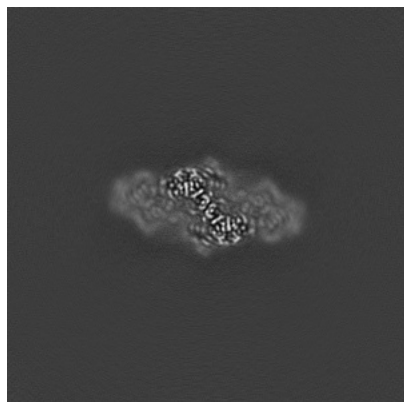


Y Index: 215

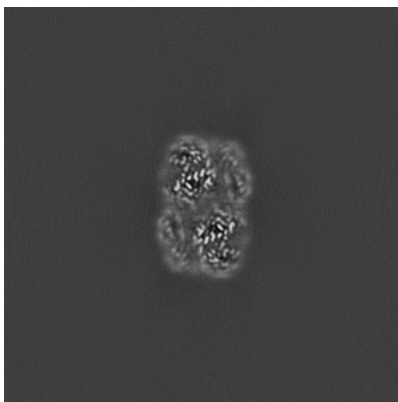


Z Index: 192

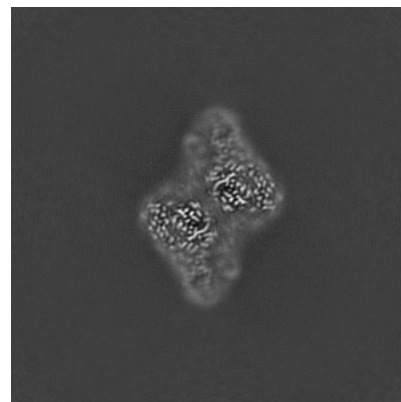
6.3.2 Raw map



X Index: 187



Y Index: 201

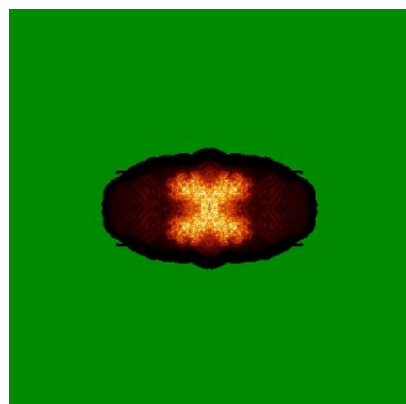


Z Index: 223

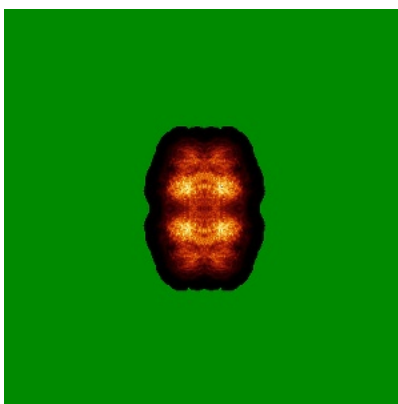
The images above show the largest variance slices of the map in three orthogonal directions.

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

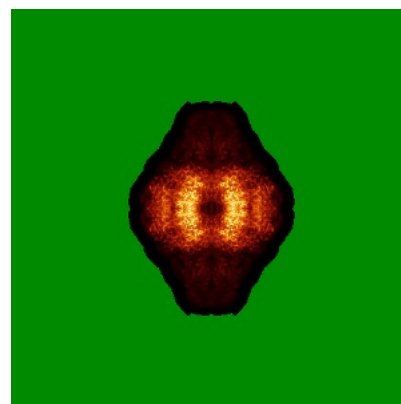
6.4.1 Primary map



X

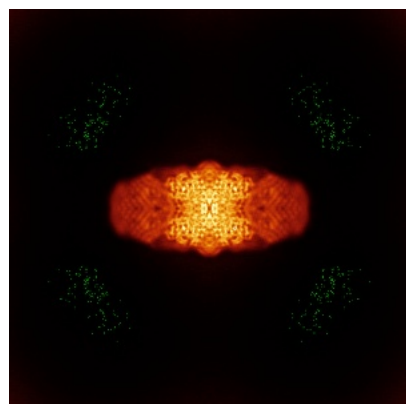


Y

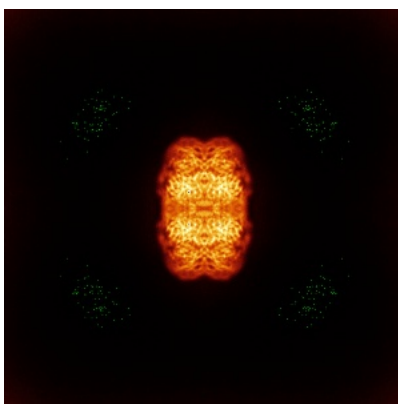


Z

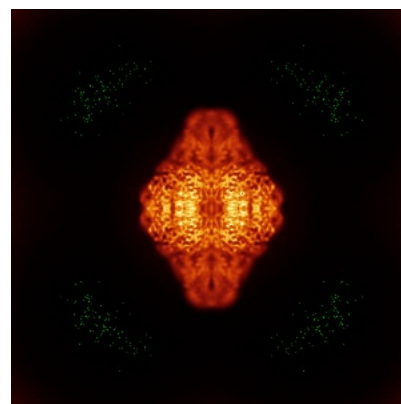
6.4.2 Raw map



X



Y

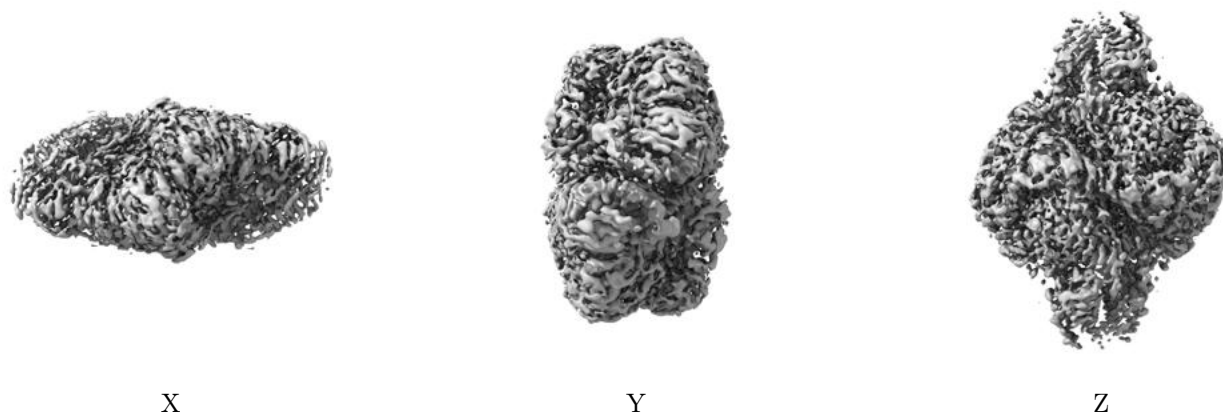


Z

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.

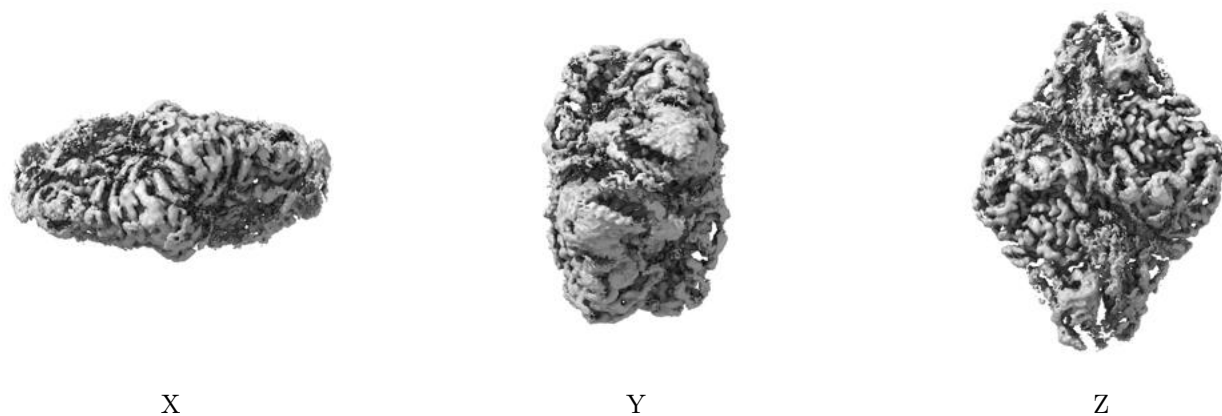
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.158. 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.

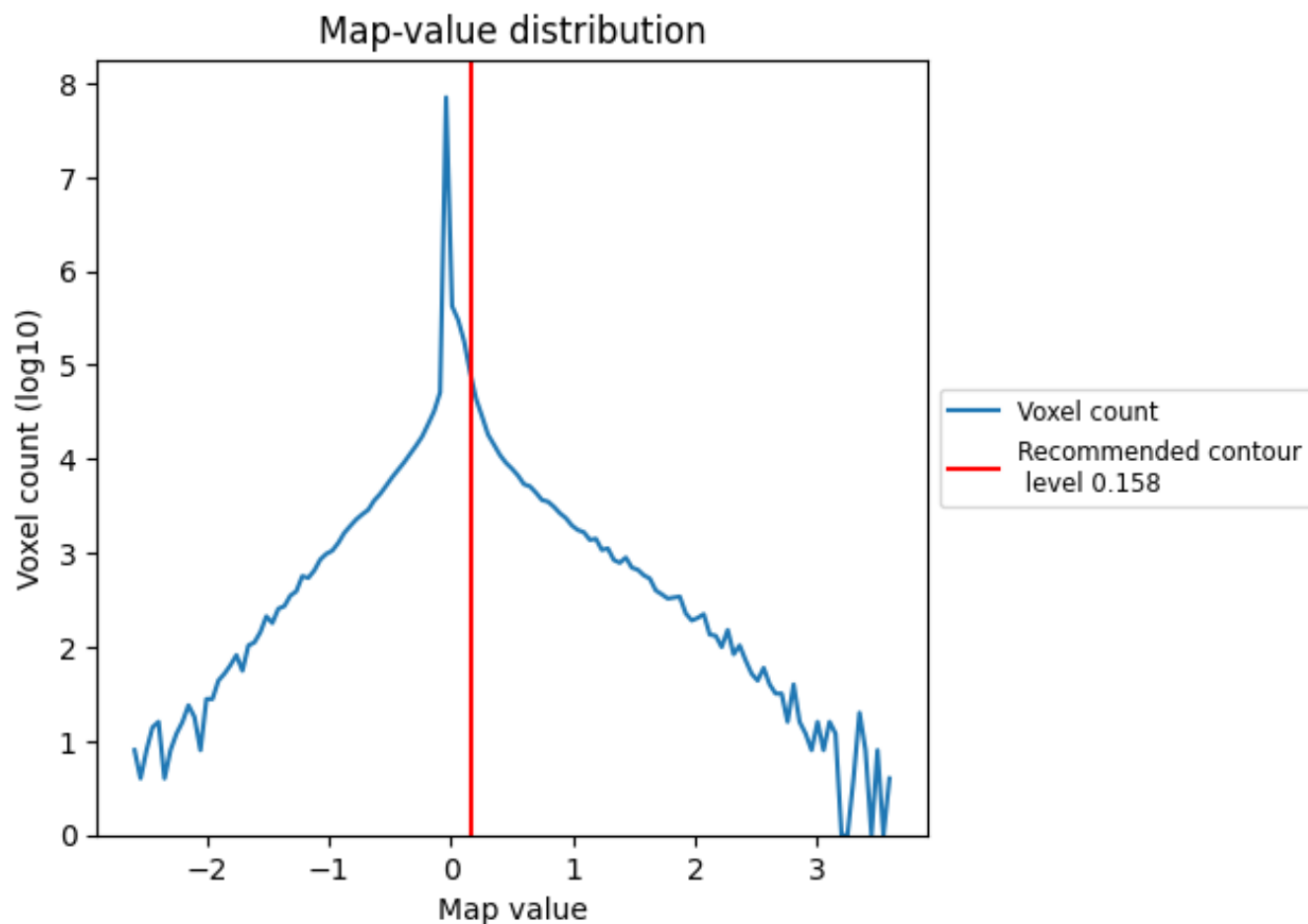
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

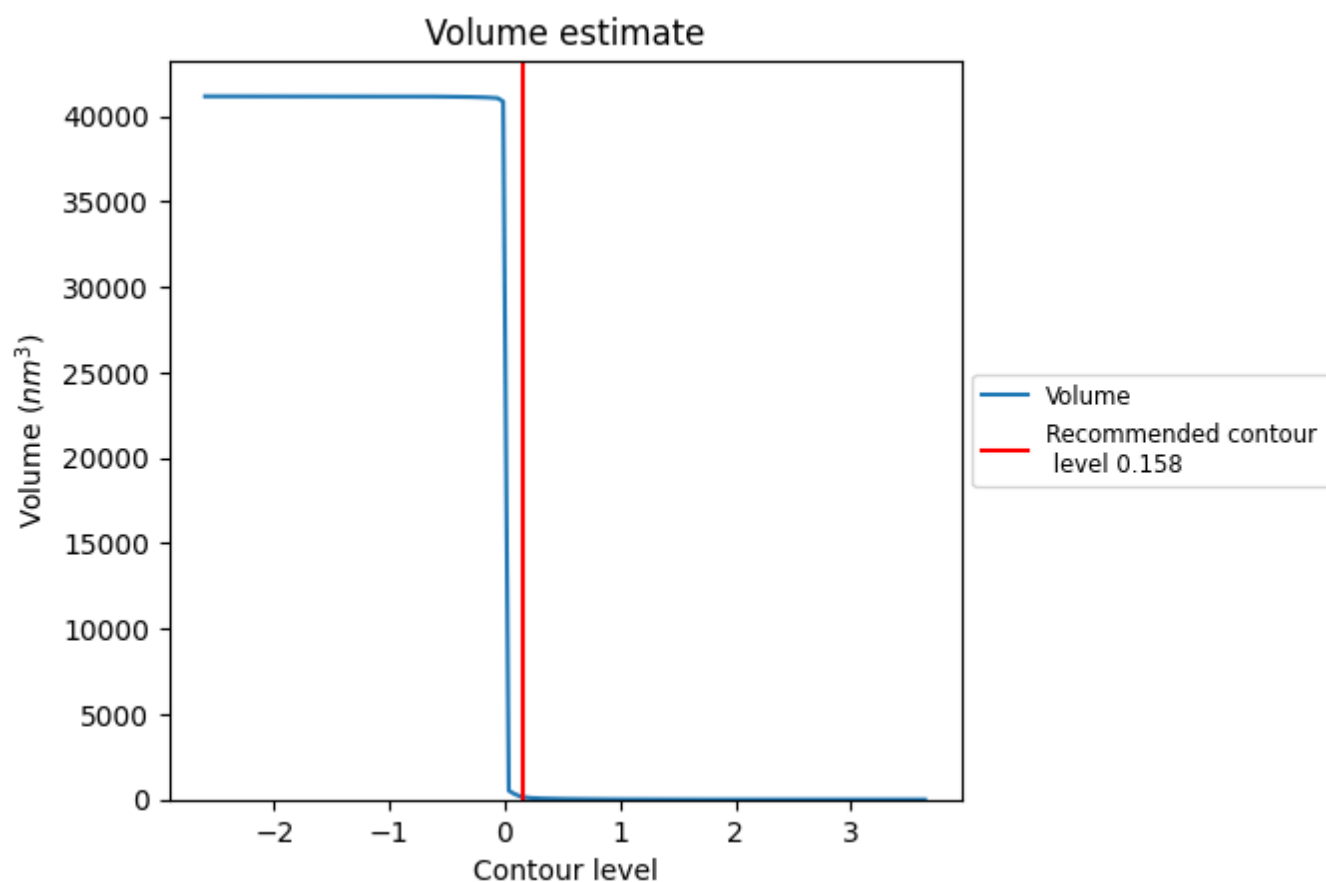
This section contains the results of statistical analysis of the map.

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.

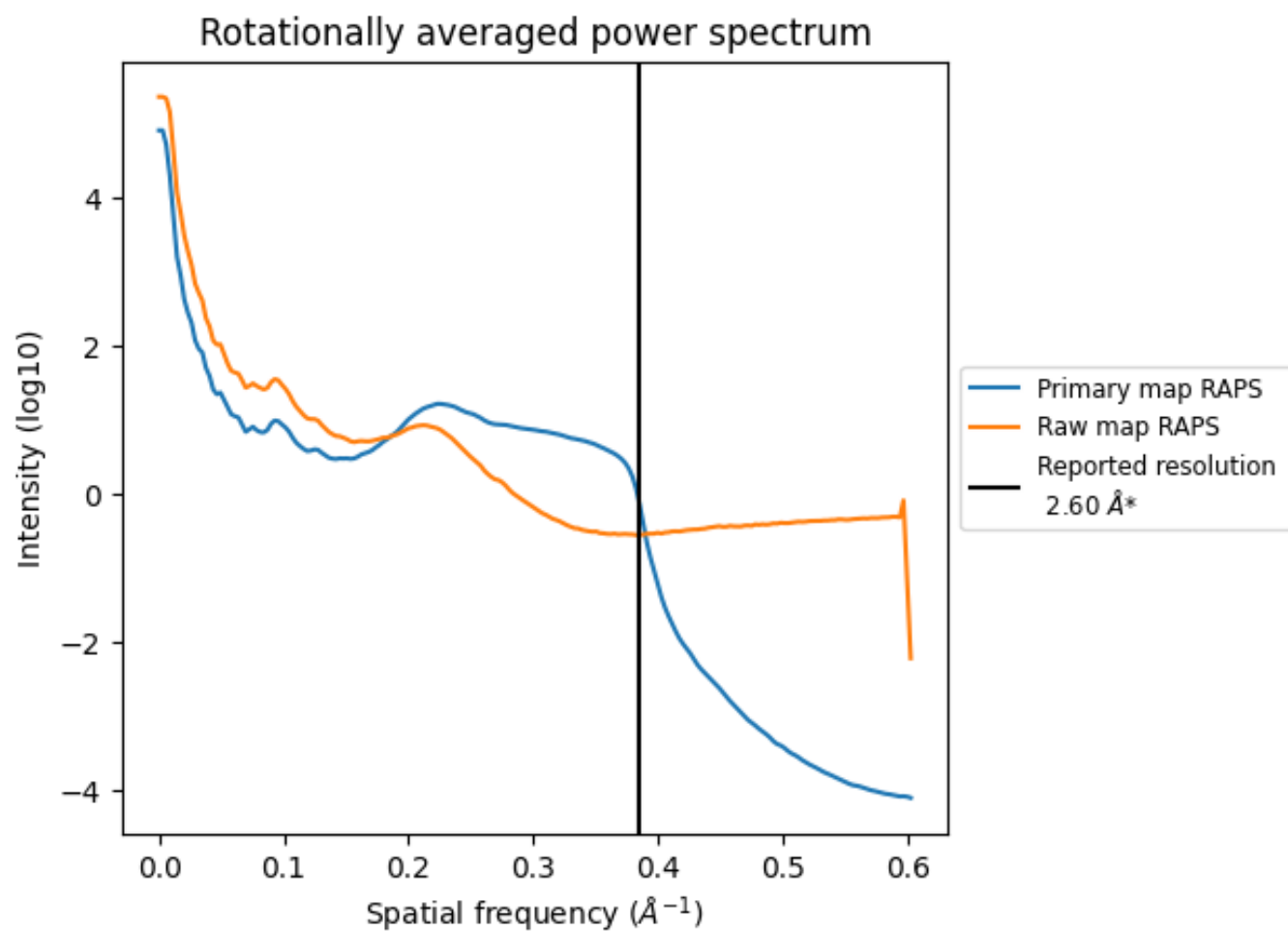
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 158 nm³; this corresponds to an approximate mass of 143 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 ⓘ

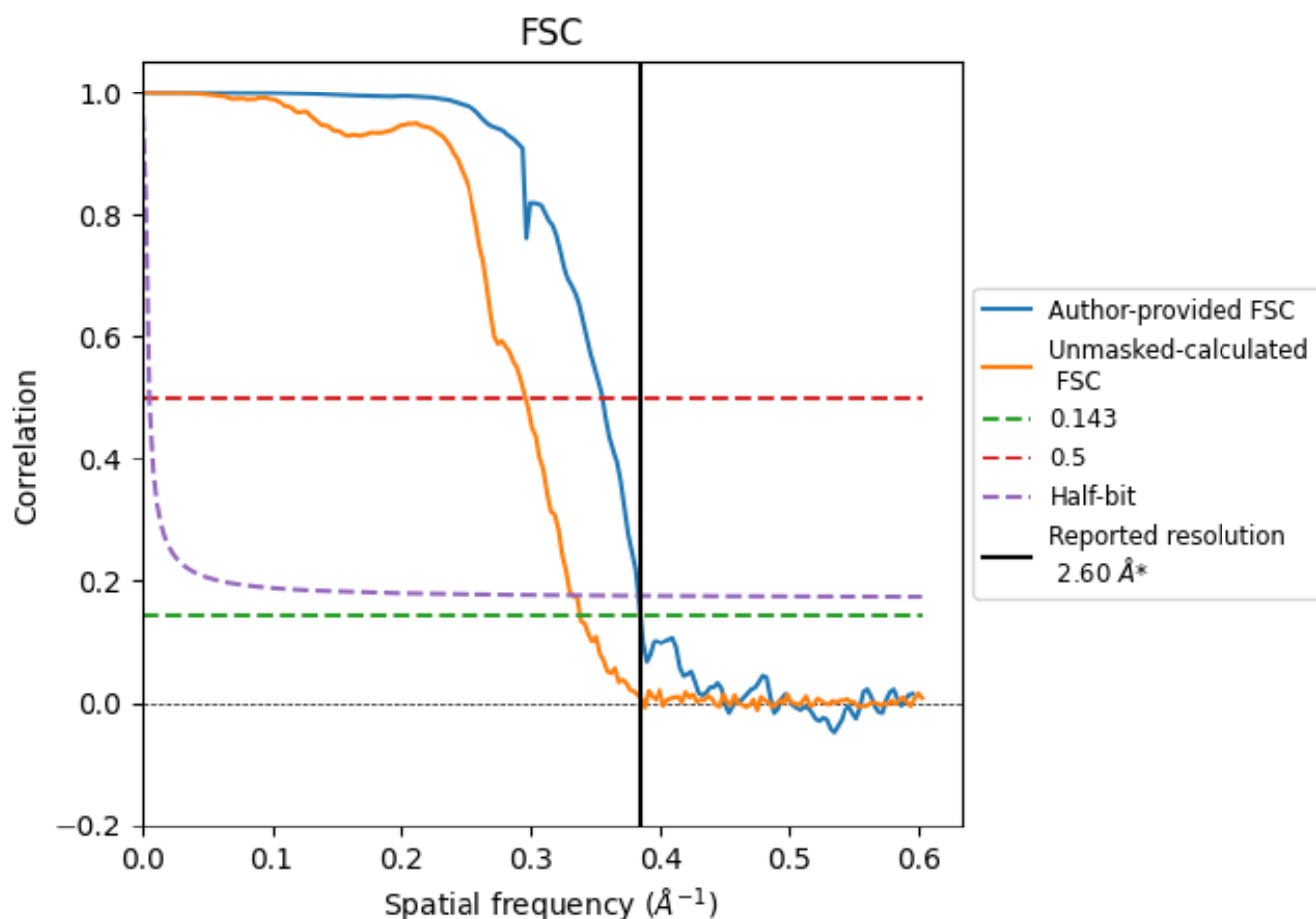


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

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 0.385 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

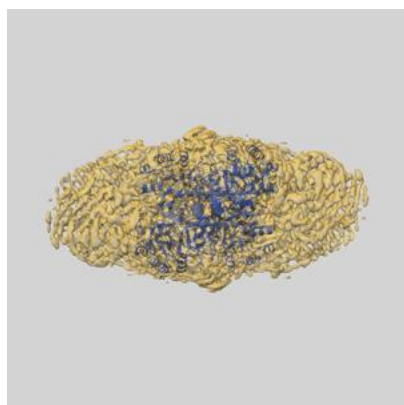
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.60	2.81	2.61
Unmasked-calculated*	2.96	3.38	3.01

*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 2.96 differs from the reported value 2.6 by more than 10 %

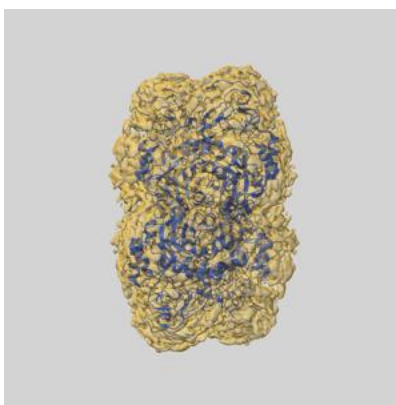
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-18244 and PDB model 8Q7Y. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

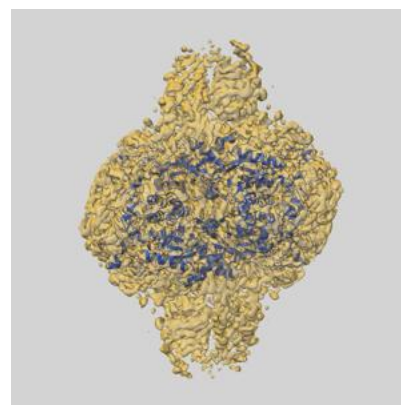
9.1 Map-model overlay [i](#)



X



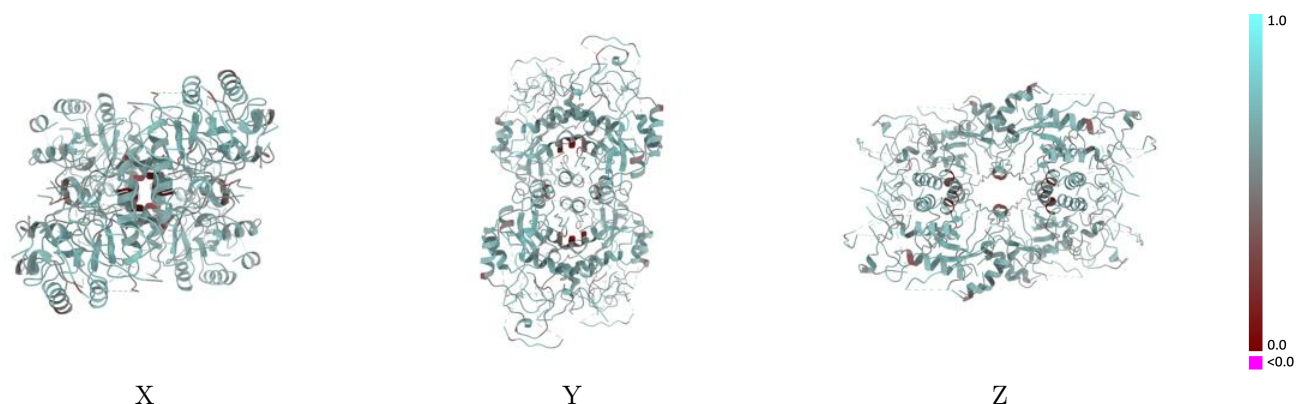
Y



Z

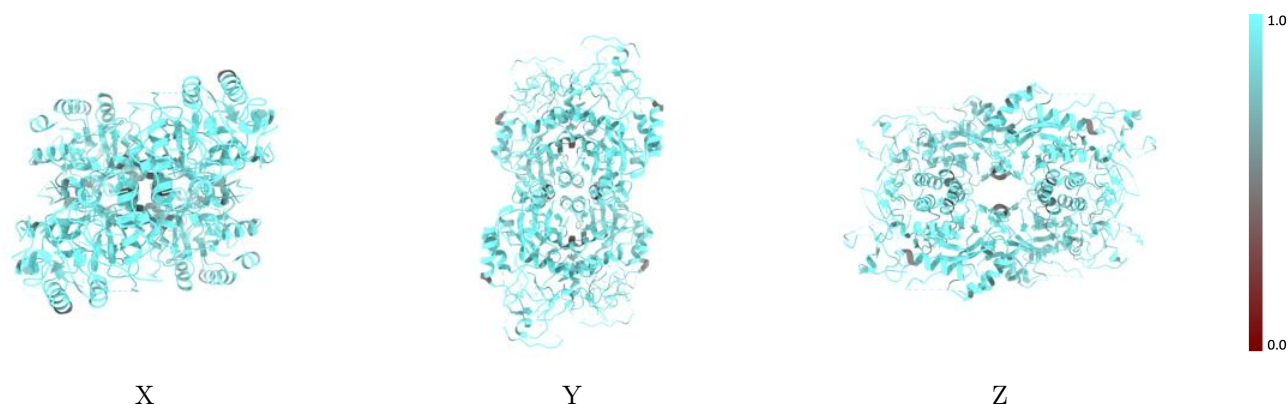
The images above show the 3D surface view of the map at the recommended contour level 0.158 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



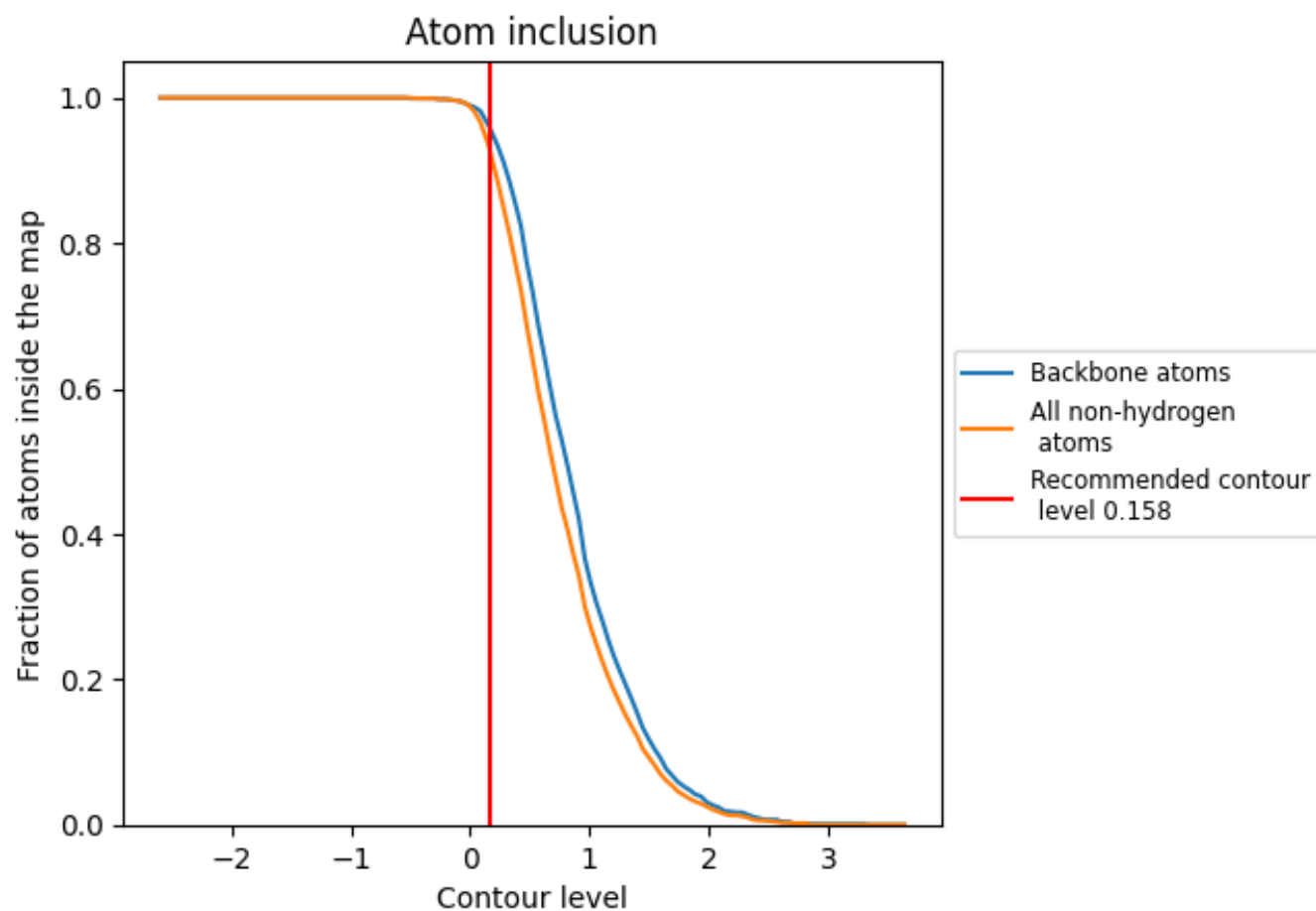
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.158).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 93% 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 (0.158) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9330	0.5900
A	0.9330	0.5910
B	0.9320	0.5890
C	0.9340	0.5900
D	0.9330	0.5910

