



Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 04:18 AM UTC

PDB ID : 8Y6N / pdb_00008y6n
EMDB ID : EMD-38992
Title : The structure of Oryza sativa HKT1;5 salt tolerant variant
Authors : Yang, G.H.; Gao, R.
Deposited on : 2024-02-02
Resolution : 3.40 Å(reported)

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

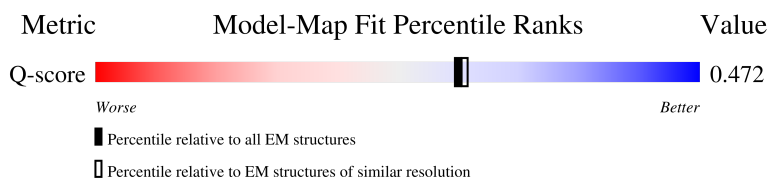
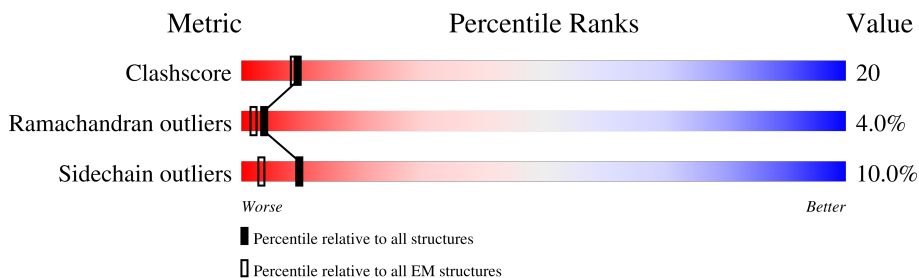
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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	640	
1	B	640	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5858 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 Sodium transporter HKT1.5, Soluble cytochrome b562.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	384	Total	C	N	O	S	0	0
			2929	1930	469	505	25		
1	B	384	Total	C	N	O	S	0	0
			2929	1930	469	505	25		

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	initiating methionine	UNP M1G2X2
A	-9	ASP	-	expression tag	UNP M1G2X2
A	-8	TYR	-	expression tag	UNP M1G2X2
A	-7	LYS	-	expression tag	UNP M1G2X2
A	-6	ASP	-	expression tag	UNP M1G2X2
A	-5	ASP	-	expression tag	UNP M1G2X2
A	-4	ASP	-	expression tag	UNP M1G2X2
A	-3	ASP	-	expression tag	UNP M1G2X2
A	-2	LYS	-	expression tag	UNP M1G2X2
A	-1	GLY	-	expression tag	UNP M1G2X2
A	0	SER	-	expression tag	UNP M1G2X2
A	116H	ARG	-	linker	UNP M1G2X2
A	116I	ARG	-	linker	UNP M1G2X2
A	116J	GLN	-	linker	UNP M1G2X2
A	116K	LEU	-	linker	UNP M1G2X2
A	116R	TRP	MET	conflict	UNP P0ABE7
A	120I	ILE	HIS	conflict	UNP P0ABE7
A	120M	LEU	-	linker	UNP P0ABE7
A	120N	GLU	-	linker	UNP P0ABE7
A	120O	ARG	-	linker	UNP P0ABE7
A	120P	ALA	-	linker	UNP P0ABE7
A	120Q	ARG	-	linker	UNP P0ABE7
A	120R	SER	-	linker	UNP P0ABE7
A	120S	THR	-	linker	UNP P0ABE7
A	120T	LEU	-	linker	UNP P0ABE7
A	555	GLY	-	expression tag	UNP M1G2X2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	556	SER	-	expression tag	UNP M1G2X2
A	557	ALA	-	expression tag	UNP M1G2X2
A	558	TRP	-	expression tag	UNP M1G2X2
A	559	SER	-	expression tag	UNP M1G2X2
A	560	HIS	-	expression tag	UNP M1G2X2
A	561	PRO	-	expression tag	UNP M1G2X2
A	562	GLN	-	expression tag	UNP M1G2X2
A	563	PHE	-	expression tag	UNP M1G2X2
A	564	GLU	-	expression tag	UNP M1G2X2
A	565	LYS	-	expression tag	UNP M1G2X2
A	566	GLY	-	expression tag	UNP M1G2X2
A	567	GLY	-	expression tag	UNP M1G2X2
A	568	GLY	-	expression tag	UNP M1G2X2
A	569	SER	-	expression tag	UNP M1G2X2
A	570	GLY	-	expression tag	UNP M1G2X2
A	571	GLY	-	expression tag	UNP M1G2X2
A	572	GLY	-	expression tag	UNP M1G2X2
A	573	SER	-	expression tag	UNP M1G2X2
A	574	GLY	-	expression tag	UNP M1G2X2
A	575	GLY	-	expression tag	UNP M1G2X2
A	576	SER	-	expression tag	UNP M1G2X2
A	577	ALA	-	expression tag	UNP M1G2X2
A	578	TRP	-	expression tag	UNP M1G2X2
A	579	SER	-	expression tag	UNP M1G2X2
A	580	HIS	-	expression tag	UNP M1G2X2
A	581	PRO	-	expression tag	UNP M1G2X2
A	582	GLN	-	expression tag	UNP M1G2X2
A	583	PHE	-	expression tag	UNP M1G2X2
A	584	GLU	-	expression tag	UNP M1G2X2
A	585	LYS	-	expression tag	UNP M1G2X2
B	-10	MET	-	initiating methionine	UNP M1G2X2
B	-9	ASP	-	expression tag	UNP M1G2X2
B	-8	TYR	-	expression tag	UNP M1G2X2
B	-7	LYS	-	expression tag	UNP M1G2X2
B	-6	ASP	-	expression tag	UNP M1G2X2
B	-5	ASP	-	expression tag	UNP M1G2X2
B	-4	ASP	-	expression tag	UNP M1G2X2
B	-3	ASP	-	expression tag	UNP M1G2X2
B	-2	LYS	-	expression tag	UNP M1G2X2
B	-1	GLY	-	expression tag	UNP M1G2X2
B	0	SER	-	expression tag	UNP M1G2X2
B	116H	ARG	-	linker	UNP M1G2X2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	116I	ARG	-	linker	UNP M1G2X2
B	116J	GLN	-	linker	UNP M1G2X2
B	116K	LEU	-	linker	UNP M1G2X2
B	116R	TRP	MET	conflict	UNP P0ABE7
B	120I	ILE	HIS	conflict	UNP P0ABE7
B	120M	LEU	-	linker	UNP P0ABE7
B	120N	GLU	-	linker	UNP P0ABE7
B	120O	ARG	-	linker	UNP P0ABE7
B	120P	ALA	-	linker	UNP P0ABE7
B	120Q	ARG	-	linker	UNP P0ABE7
B	120R	SER	-	linker	UNP P0ABE7
B	120S	THR	-	linker	UNP P0ABE7
B	120T	LEU	-	linker	UNP P0ABE7
B	555	GLY	-	expression tag	UNP M1G2X2
B	556	SER	-	expression tag	UNP M1G2X2
B	557	ALA	-	expression tag	UNP M1G2X2
B	558	TRP	-	expression tag	UNP M1G2X2
B	559	SER	-	expression tag	UNP M1G2X2
B	560	HIS	-	expression tag	UNP M1G2X2
B	561	PRO	-	expression tag	UNP M1G2X2
B	562	GLN	-	expression tag	UNP M1G2X2
B	563	PHE	-	expression tag	UNP M1G2X2
B	564	GLU	-	expression tag	UNP M1G2X2
B	565	LYS	-	expression tag	UNP M1G2X2
B	566	GLY	-	expression tag	UNP M1G2X2
B	567	GLY	-	expression tag	UNP M1G2X2
B	568	GLY	-	expression tag	UNP M1G2X2
B	569	SER	-	expression tag	UNP M1G2X2
B	570	GLY	-	expression tag	UNP M1G2X2
B	571	GLY	-	expression tag	UNP M1G2X2
B	572	GLY	-	expression tag	UNP M1G2X2
B	573	SER	-	expression tag	UNP M1G2X2
B	574	GLY	-	expression tag	UNP M1G2X2
B	575	GLY	-	expression tag	UNP M1G2X2
B	576	SER	-	expression tag	UNP M1G2X2
B	577	ALA	-	expression tag	UNP M1G2X2
B	578	TRP	-	expression tag	UNP M1G2X2
B	579	SER	-	expression tag	UNP M1G2X2
B	580	HIS	-	expression tag	UNP M1G2X2
B	581	PRO	-	expression tag	UNP M1G2X2
B	582	GLN	-	expression tag	UNP M1G2X2
B	583	PHE	-	expression tag	UNP M1G2X2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	584	GLU	-	expression tag	UNP M1G2X2
B	585	LYS	-	expression tag	UNP M1G2X2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	118956	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.962	Depositor
Minimum map value	-2.076	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.063	Depositor
Recommended contour level	0.5	Depositor
Map size ($\text{\AA}$)	277.12, 277.12, 277.12	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0825, 1.0825, 1.0825	Depositor

5 Model quality

5.1 Standard geometry

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	0.66	4/2993 (0.1%)	1.02	29/4066 (0.7%)
1	B	0.66	4/2993 (0.1%)	1.00	26/4066 (0.6%)
All	All	0.66	8/5986 (0.1%)	1.01	55/8132 (0.7%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	387	SER	CA-CB	-6.93	1.44	1.54
1	B	387	SER	CA-CB	-6.88	1.44	1.54
1	B	402	SER	CA-CB	-5.87	1.43	1.53
1	A	402	SER	CA-CB	-5.84	1.43	1.53
1	A	415	PRO	C-O	-5.80	1.18	1.24
1	B	415	PRO	C-O	-5.78	1.18	1.24
1	B	73	THR	C-O	-5.17	1.17	1.23
1	A	73	THR	C-O	-5.15	1.17	1.23

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	105	THR	N-CA-C	-10.58	101.12	114.56
1	A	105	THR	N-CA-C	-10.54	101.17	114.56
1	A	528	LYS	N-CA-C	-9.73	101.91	113.88
1	B	549	GLN	N-CA-C	-8.73	101.61	113.30
1	A	549	GLN	N-CA-C	-8.71	101.62	113.30
1	B	528	LYS	N-CA-C	-8.70	102.79	113.41
1	A	387	SER	N-CA-C	-8.32	102.56	114.12
1	B	387	SER	N-CA-C	-8.31	102.57	114.12
1	A	403	ALA	N-CA-C	-7.93	103.74	113.41
1	B	403	ALA	N-CA-C	-7.91	103.76	113.41
1	B	362	GLU	CB-CA-C	-7.66	95.17	110.42
1	A	362	GLU	CB-CA-C	-7.65	95.19	110.42
1	A	384	ALA	N-CA-C	-7.62	105.94	114.62
1	B	384	ALA	N-CA-C	-7.61	105.95	114.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	411	MET	N-CA-C	-7.60	101.17	113.19
1	B	411	MET	N-CA-C	-7.59	101.19	113.19
1	B	340	THR	N-CA-C	-7.33	102.58	112.26
1	A	340	THR	N-CA-C	-7.32	102.60	112.26
1	B	397	LEU	N-CA-C	-7.26	104.45	112.72
1	A	397	LEU	N-CA-C	-7.23	104.48	112.72
1	B	336	PRO	CB-CA-C	-7.00	101.78	110.95
1	A	336	PRO	CB-CA-C	-6.99	101.79	110.95
1	B	353	ALA	N-CA-C	-6.93	104.44	113.17
1	A	353	ALA	N-CA-C	-6.91	104.46	113.17
1	B	105	THR	CB-CA-C	6.79	119.72	109.13
1	B	368	LEU	N-CA-C	-6.76	103.41	112.94
1	A	368	LEU	N-CA-C	-6.75	103.43	112.94
1	A	74	VAL	N-CA-C	6.71	123.29	109.34
1	B	74	VAL	N-CA-C	6.70	123.27	109.34
1	A	105	THR	CB-CA-C	6.67	119.53	109.13
1	A	522	LYS	N-CA-C	-6.66	101.56	111.81
1	A	340	THR	CB-CA-C	6.50	121.60	111.13
1	B	340	THR	CB-CA-C	6.50	121.60	111.13
1	B	394	VAL	N-CA-C	-6.25	106.23	112.17
1	B	389	HIS	CA-C-O	-6.22	115.42	121.02
1	A	394	VAL	N-CA-C	-6.22	106.26	112.17
1	A	389	HIS	CA-C-O	-6.13	115.50	121.02
1	A	408	TYR	CA-C-O	-6.10	114.37	120.90
1	B	408	TYR	CA-C-O	-6.10	114.38	120.90
1	B	105	THR	CA-CB-OG1	-6.00	100.60	109.60
1	B	412	MET	N-CA-C	-5.99	103.92	112.13
1	A	412	MET	N-CA-C	-5.96	103.96	112.13
1	A	105	THR	CA-CB-OG1	-5.91	100.73	109.60
1	A	343	LEU	N-CA-C	-5.76	108.06	114.62
1	B	343	LEU	N-CA-C	-5.76	108.06	114.62
1	B	396	ASP	N-CA-C	-5.48	101.19	109.85
1	A	396	ASP	N-CA-C	-5.48	101.19	109.85
1	A	355	LEU	N-CA-C	-5.44	105.43	111.36
1	B	355	LEU	N-CA-C	-5.41	105.46	111.36
1	A	354	GLN	N-CA-C	-5.24	107.02	113.41
1	A	522	LYS	CB-CA-C	5.22	120.11	111.23
1	B	354	GLN	N-CA-C	-5.22	107.04	113.41
1	A	343	LEU	CB-CA-C	5.14	116.12	109.28
1	B	343	LEU	CB-CA-C	5.14	116.11	109.28
1	A	526	GLN	N-CA-C	-5.02	107.43	113.21

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	2929	0	3034	123	0
1	B	2929	0	3034	126	0
All	All	5858	0	6068	242	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 20.

All (242) 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:343:LEU:HB2	1:A:419:THR:CG2	1.37	1.53
1:B:343:LEU:CG	1:B:419:THR:HG22	1.41	1.51
1:A:343:LEU:CG	1:A:419:THR:HG22	1.41	1.50
1:B:343:LEU:HB2	1:B:419:THR:CG2	1.37	1.48
1:B:343:LEU:CB	1:B:419:THR:HG22	1.49	1.43
1:A:343:LEU:CB	1:A:419:THR:HG22	1.49	1.42
1:B:343:LEU:CB	1:B:419:THR:CG2	2.03	1.34
1:A:343:LEU:CB	1:A:419:THR:CG2	2.03	1.30
1:A:343:LEU:CG	1:A:419:THR:CG2	2.16	1.22
1:B:343:LEU:CG	1:B:419:THR:CG2	2.16	1.19
1:A:343:LEU:HG	1:A:419:THR:CG2	1.73	1.17
1:B:343:LEU:HG	1:B:419:THR:CG2	1.73	1.14
1:A:286:MET:HG3	1:A:385:VAL:HG21	1.28	1.14
1:B:286:MET:HG3	1:B:385:VAL:HG21	1.28	1.09
1:B:343:LEU:HB2	1:B:419:THR:CB	1.83	1.08
1:A:343:LEU:CD2	1:A:419:THR:HG22	1.85	1.06
1:A:343:LEU:HB2	1:A:419:THR:CB	1.83	1.05
1:B:343:LEU:CD2	1:B:419:THR:HG22	1.85	1.05
1:B:69:VAL:HG11	1:B:532:MET:HE1	1.46	0.96
1:A:69:VAL:HG11	1:A:532:MET:HE1	1.46	0.94
1:A:343:LEU:CB	1:A:419:THR:HG21	1.96	0.94
1:B:343:LEU:HB2	1:B:419:THR:HG21	1.49	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:LEU:CB	1:B:419:THR:HG21	1.96	0.93
1:A:343:LEU:HB2	1:A:419:THR:HG21	1.49	0.90
1:B:77:MET:HE1	1:B:490:ALA:HB2	1.54	0.89
1:A:77:MET:HE1	1:A:490:ALA:HB2	1.54	0.89
1:B:294:THR:HG21	1:B:388:ARG:HG3	1.61	0.83
1:B:77:MET:HE2	1:B:531:LEU:HD21	1.62	0.81
1:B:263:CYS:SG	1:B:264:GLY:N	2.53	0.81
1:B:343:LEU:HB2	1:B:419:THR:HG22	1.17	0.81
1:B:371:LEU:HB3	1:B:375:GLN:HB2	1.63	0.81
1:A:263:CYS:SG	1:A:264:GLY:N	2.53	0.81
1:A:77:MET:HE2	1:A:531:LEU:HD21	1.62	0.81
1:A:294:THR:HG21	1:A:388:ARG:HG3	1.61	0.80
1:A:371:LEU:HB3	1:A:375:GLN:HB2	1.63	0.80
1:A:343:LEU:HB2	1:A:419:THR:HG22	1.17	0.79
1:A:343:LEU:HD23	1:A:419:THR:HG22	1.63	0.76
1:B:343:LEU:HD23	1:B:419:THR:HG22	1.64	0.76
1:A:264:GLY:HA2	1:A:392:GLU:HG2	1.68	0.75
1:B:94:THR:HG23	1:B:257:VAL:HG11	1.69	0.75
1:A:343:LEU:HB2	1:A:419:THR:HB	1.70	0.74
1:B:343:LEU:HB2	1:B:419:THR:HB	1.69	0.74
1:A:94:THR:HG23	1:A:257:VAL:HG11	1.69	0.74
1:B:264:GLY:HA2	1:B:392:GLU:HG2	1.68	0.73
1:A:298:VAL:HA	1:A:340:THR:HG23	1.71	0.73
1:B:298:VAL:HA	1:B:340:THR:HG23	1.71	0.72
1:A:520:SER:HG	1:A:523:TRP:CG	2.08	0.72
1:B:520:SER:HG	1:B:523:TRP:CG	2.08	0.71
1:B:398:SER:HB3	1:B:504:ARG:NH1	2.07	0.70
1:A:398:SER:HB3	1:A:504:ARG:NH1	2.07	0.69
1:A:209:MET:HE2	1:A:209:MET:N	2.08	0.68
1:B:209:MET:N	1:B:209:MET:HE2	2.08	0.68
1:A:66:PHE:CZ	1:A:528:LYS:HB3	2.30	0.67
1:A:69:VAL:HG11	1:A:532:MET:CE	2.24	0.66
1:B:66:PHE:CZ	1:B:528:LYS:HB3	2.31	0.65
1:B:405:VAL:CG2	1:B:481:LEU:HD21	2.27	0.65
1:A:405:VAL:CG2	1:A:481:LEU:HD21	2.27	0.65
1:A:107:ILE:HD13	1:A:213:MET:HG2	1.80	0.64
1:B:107:ILE:HD13	1:B:213:MET:HG2	1.80	0.64
1:A:383:MET:HG3	1:A:394:VAL:HG12	1.81	0.63
1:A:405:VAL:HG21	1:A:481:LEU:HD21	1.81	0.63
1:A:391:GLY:HA2	1:A:494:VAL:HG12	1.81	0.63
1:A:253:ILE:O	1:A:257:VAL:HG12	1.99	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:MET:HG3	1:B:394:VAL:HG12	1.81	0.63
1:B:253:ILE:O	1:B:257:VAL:HG12	1.99	0.63
1:B:69:VAL:HG11	1:B:532:MET:CE	2.24	0.63
1:B:405:VAL:HG21	1:B:481:LEU:HD21	1.81	0.62
1:B:391:GLY:HA2	1:B:494:VAL:HG12	1.81	0.62
1:B:393:MET:HE2	1:B:397:LEU:HG	1.81	0.62
1:B:107:ILE:HD11	1:B:212:VAL:HG12	1.82	0.62
1:A:393:MET:HE2	1:A:397:LEU:HG	1.81	0.61
1:A:75:SER:CB	1:A:535:MET:HG2	2.30	0.61
1:B:75:SER:CB	1:B:535:MET:HG2	2.30	0.61
1:A:107:ILE:HD11	1:A:212:VAL:HG12	1.82	0.60
1:A:45:MET:CE	1:A:92:LEU:HD13	2.33	0.59
1:B:547:GLY:O	1:B:548:GLY:C	2.46	0.58
1:A:547:GLY:O	1:A:548:GLY:C	2.46	0.58
1:B:45:MET:CE	1:B:92:LEU:HD13	2.33	0.57
1:A:480:VAL:HG21	1:B:402:SER:HB3	1.87	0.57
1:B:341:ARG:C	1:B:343:LEU:H	2.12	0.57
1:A:343:LEU:CD2	1:A:419:THR:CG2	2.72	0.57
1:B:343:LEU:HG	1:B:419:THR:HG21	1.80	0.57
1:B:358:PHE:HD1	1:B:404:VAL:HG11	1.69	0.57
1:B:36:LEU:O	1:B:36:LEU:HD23	2.05	0.57
1:A:341:ARG:C	1:A:343:LEU:H	2.12	0.56
1:A:358:PHE:HD1	1:A:404:VAL:HG11	1.69	0.56
1:B:343:LEU:HD23	1:B:419:THR:CG2	2.34	0.56
1:A:36:LEU:HD23	1:A:36:LEU:O	2.05	0.56
1:A:391:GLY:HA3	1:A:494:VAL:O	2.06	0.56
1:A:479:SER:O	1:A:482:ASN:N	2.40	0.55
1:A:402:SER:HB3	1:B:480:VAL:HG21	1.88	0.55
1:A:343:LEU:HG	1:A:419:THR:HG21	1.80	0.54
1:A:413:TYR:CE1	1:A:453:LEU:HG	2.42	0.54
1:B:479:SER:O	1:B:482:ASN:N	2.40	0.54
1:A:465:ILE:HA	1:B:361:MET:SD	2.47	0.54
1:B:413:TYR:CE1	1:B:453:LEU:HG	2.42	0.54
1:A:388:ARG:O	1:A:389:HIS:CG	2.61	0.54
1:B:391:GLY:HA3	1:B:494:VAL:O	2.06	0.54
1:A:343:LEU:HD23	1:A:419:THR:CG2	2.34	0.54
1:B:388:ARG:O	1:B:389:HIS:CG	2.61	0.53
1:A:93:ILE:O	1:A:97:MET:N	2.42	0.53
1:B:93:ILE:O	1:B:97:MET:N	2.42	0.52
1:A:293:ASN:O	1:A:417:TYR:HE2	1.93	0.52
1:A:532:MET:HE3	1:A:532:MET:HA	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:532:MET:HE3	1:B:532:MET:HA	1.91	0.52
1:A:104:PHE:HB2	1:A:216:HIS:NE2	2.26	0.51
1:B:402:SER:HA	1:B:405:VAL:HG22	1.93	0.51
1:A:519:PHE:O	1:A:520:SER:OG	2.29	0.51
1:B:391:GLY:CA	1:B:494:VAL:HG12	2.41	0.50
1:A:268:THR:HG22	1:A:270:GLU:H	1.77	0.50
1:B:75:SER:HB2	1:B:535:MET:HG2	1.93	0.50
1:B:293:ASN:O	1:B:417:TYR:HE2	1.93	0.50
1:A:361:MET:SD	1:B:465:ILE:HA	2.51	0.50
1:B:268:THR:HG22	1:B:270:GLU:H	1.77	0.50
1:A:391:GLY:CA	1:A:494:VAL:HG12	2.41	0.50
1:A:402:SER:HA	1:A:405:VAL:HG22	1.93	0.49
1:A:350:LEU:HG	1:A:411:MET:HE1	1.95	0.49
1:A:75:SER:HB2	1:A:535:MET:HG2	1.93	0.49
1:B:519:PHE:O	1:B:520:SER:OG	2.29	0.49
1:B:348:ALA:O	1:B:349:VAL:C	2.55	0.49
1:B:520:SER:O	1:B:523:TRP:N	2.37	0.49
1:B:350:LEU:HG	1:B:411:MET:HE1	1.95	0.49
1:A:358:PHE:CD1	1:A:404:VAL:HG11	2.48	0.48
1:A:348:ALA:O	1:A:349:VAL:C	2.55	0.48
1:B:104:PHE:HB2	1:B:216:HIS:NE2	2.27	0.48
1:A:208:LEU:HA	1:A:211:VAL:HG12	1.95	0.48
1:A:520:SER:O	1:A:523:TRP:N	2.42	0.48
1:B:358:PHE:CD1	1:B:404:VAL:HG11	2.48	0.48
1:A:262:ASN:HB3	1:A:389:HIS:O	2.14	0.48
1:B:286:MET:SD	1:B:382:PHE:HD1	2.37	0.48
1:B:383:MET:HE3	1:B:383:MET:HB3	1.73	0.48
1:B:208:LEU:HA	1:B:211:VAL:HG12	1.95	0.47
1:A:286:MET:SD	1:A:382:PHE:HD1	2.37	0.47
1:A:522:LYS:HB3	1:A:522:LYS:HE3	1.39	0.47
1:B:262:ASN:HB3	1:B:389:HIS:O	2.14	0.47
1:A:78:VAL:HG12	1:A:80:VAL:O	2.15	0.47
1:A:527:GLY:HA2	1:A:530:THR:OG1	2.14	0.47
1:B:78:VAL:HG12	1:B:80:VAL:O	2.15	0.47
1:A:269:ASN:HB2	1:A:517:VAL:HG21	1.96	0.47
1:B:468:ARG:O	1:B:469:ARG:HG2	2.15	0.47
1:B:528:LYS:O	1:B:531:LEU:HB3	2.14	0.47
1:B:269:ASN:HB2	1:B:517:VAL:HG21	1.96	0.47
1:B:527:GLY:HA2	1:B:530:THR:OG1	2.15	0.46
1:B:413:TYR:O	1:B:414:LEU:C	2.58	0.46
1:A:413:TYR:O	1:A:414:LEU:C	2.58	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:VAL:HG12	1:A:244:LYS:NZ	2.31	0.46
1:A:528:LYS:O	1:A:531:LEU:HB3	2.16	0.46
1:A:541:LYS:O	1:A:545:LEU:N	2.49	0.46
1:A:388:ARG:NE	1:A:388:ARG:HA	2.26	0.46
1:A:468:ARG:O	1:A:469:ARG:HG2	2.15	0.46
1:B:343:LEU:HG	1:B:419:THR:HG23	1.85	0.46
1:B:231:LEU:HD13	1:B:281:LEU:HD11	1.96	0.46
1:B:541:LYS:O	1:B:545:LEU:N	2.49	0.46
1:A:39:SER:HB2	1:A:69:VAL:HG22	1.98	0.46
1:A:507:ARG:CG	1:A:507:ARG:O	2.64	0.46
1:A:231:LEU:HD13	1:A:281:LEU:HD11	1.97	0.45
1:B:390:SER:HB3	1:B:391:GLY:H	1.56	0.45
1:B:240:VAL:HG12	1:B:244:LYS:NZ	2.31	0.45
1:B:507:ARG:CG	1:B:507:ARG:O	2.64	0.45
1:B:39:SER:HB2	1:B:69:VAL:HG22	1.98	0.45
1:B:388:ARG:NE	1:B:388:ARG:HA	2.26	0.45
1:B:521:GLY:HA3	1:B:528:LYS:HG2	1.99	0.45
1:B:76:SER:O	1:B:77:MET:C	2.59	0.45
1:A:341:ARG:C	1:A:343:LEU:N	2.75	0.45
1:B:107:ILE:HD13	1:B:213:MET:CG	2.46	0.45
1:B:520:SER:OG	1:B:523:TRP:CG	2.70	0.45
1:A:107:ILE:HD13	1:A:213:MET:CG	2.46	0.44
1:A:293:ASN:OD1	1:A:294:THR:N	2.51	0.44
1:A:214:GLY:O	1:A:218:VAL:HG23	2.18	0.43
1:A:270:GLU:O	1:A:273:VAL:N	2.51	0.43
1:A:269:ASN:O	1:A:517:VAL:HG11	2.18	0.43
1:B:293:ASN:OD1	1:B:294:THR:N	2.51	0.43
1:A:529:LEU:O	1:A:532:MET:HB2	2.19	0.43
1:B:393:MET:H	1:B:393:MET:HG3	1.45	0.43
1:B:345:LEU:O	1:B:348:ALA:HB3	2.19	0.43
1:A:76:SER:O	1:A:77:MET:C	2.59	0.43
1:B:270:GLU:O	1:B:273:VAL:N	2.51	0.43
1:A:52:LYS:NZ	1:A:244:LYS:O	2.52	0.43
1:B:214:GLY:O	1:B:218:VAL:HG23	2.18	0.43
1:B:393:MET:HG2	1:B:496:PHE:CD1	2.54	0.43
1:B:529:LEU:O	1:B:532:MET:HB2	2.19	0.43
1:A:357:LEU:HD21	1:A:403:ALA:O	2.19	0.43
1:B:75:SER:O	1:B:76:SER:C	2.62	0.43
1:A:396:ASP:HB3	1:A:398:SER:H	1.84	0.42
1:A:520:SER:OG	1:A:523:TRP:CG	2.71	0.42
1:B:357:LEU:HD21	1:B:403:ALA:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:LEU:HD13	1:B:377:LEU:HA	1.80	0.42
1:A:286:MET:CG	1:A:385:VAL:HG21	2.21	0.42
1:B:355:LEU:HD12	1:B:355:LEU:HA	1.86	0.42
1:B:408:TYR:C	1:B:410:VAL:H	2.27	0.42
1:A:345:LEU:O	1:A:348:ALA:HB3	2.19	0.42
1:A:393:MET:HG2	1:A:496:PHE:CD1	2.54	0.42
1:B:269:ASN:O	1:B:517:VAL:HG11	2.18	0.42
1:B:520:SER:HG	1:B:523:TRP:CD1	2.38	0.42
1:A:75:SER:O	1:A:76:SER:C	2.62	0.42
1:B:38:ILE:HG21	1:B:99:LEU:HD22	2.01	0.42
1:B:358:PHE:O	1:B:359:CYS:C	2.63	0.42
1:A:361:MET:HE2	1:A:361:MET:HB3	1.60	0.42
1:A:408:TYR:C	1:A:410:VAL:H	2.28	0.42
1:A:486:GLU:HG2	1:A:522:LYS:NZ	2.35	0.42
1:A:551:TRP:HA	1:B:419:THR:O	2.20	0.42
1:A:102:GLU:OE1	1:A:539:ARG:NH1	2.51	0.42
1:A:532:MET:HE3	1:A:532:MET:CA	2.50	0.41
1:B:372:THR:H	1:B:375:GLN:HG3	1.85	0.41
1:B:525:LYS:C	1:B:527:GLY:H	2.28	0.41
1:A:404:VAL:O	1:A:406:VAL:N	2.53	0.41
1:A:516:TRP:CD1	1:A:516:TRP:C	2.98	0.41
1:A:519:PHE:CD2	1:A:521:GLY:O	2.73	0.41
1:B:102:GLU:OE1	1:B:539:ARG:NH1	2.51	0.41
1:B:396:ASP:HB3	1:B:398:SER:H	1.84	0.41
1:B:519:PHE:CD2	1:B:521:GLY:O	2.73	0.41
1:B:532:MET:HE3	1:B:532:MET:CA	2.50	0.41
1:A:38:ILE:HG21	1:A:99:LEU:HD22	2.01	0.41
1:A:377:LEU:C	1:A:379:GLY:H	2.29	0.41
1:A:45:MET:HE1	1:A:92:LEU:HD13	2.02	0.41
1:A:52:LYS:O	1:A:55:MET:HG2	2.20	0.41
1:A:407:LEU:O	1:A:410:VAL:HG12	2.20	0.41
1:A:525:LYS:C	1:A:527:GLY:H	2.28	0.41
1:B:52:LYS:NZ	1:B:244:LYS:O	2.52	0.41
1:B:77:MET:HE3	1:B:486:GLU:HG3	2.02	0.41
1:B:374:GLY:O	1:B:375:GLN:C	2.64	0.41
1:A:77:MET:HE3	1:A:486:GLU:HG3	2.02	0.41
1:A:358:PHE:O	1:A:359:CYS:C	2.63	0.41
1:A:419:THR:O	1:B:551:TRP:HA	2.21	0.41
1:B:377:LEU:C	1:B:379:GLY:H	2.29	0.41
1:B:522:LYS:C	1:B:524:SER:N	2.78	0.41
1:A:521:GLY:HA3	1:A:528:LYS:HG2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:LYS:O	1:B:55:MET:HG2	2.21	0.41
1:B:342:PHE:O	1:B:419:THR:HB	2.21	0.41
1:A:372:THR:H	1:A:375:GLN:HG3	1.85	0.41
1:A:412:MET:O	1:A:413:TYR:C	2.64	0.41
1:A:463:ILE:CD1	1:A:487:VAL:HG22	2.51	0.41
1:A:480:VAL:HG21	1:B:481:LEU:HD22	2.03	0.41
1:B:341:ARG:C	1:B:343:LEU:N	2.75	0.41
1:B:407:LEU:O	1:B:410:VAL:HG12	2.20	0.41
1:B:390:SER:O	1:B:494:VAL:HA	2.21	0.40
1:B:404:VAL:O	1:B:406:VAL:N	2.53	0.40
1:A:98:LEU:HD13	1:A:220:HIS:HE1	1.87	0.40
1:B:389:HIS:HE1	1:B:412:MET:O	2.05	0.40
1:B:368:LEU:O	1:B:369:ARG:C	2.64	0.40
1:A:374:GLY:O	1:A:375:GLN:C	2.64	0.40
1:B:348:ALA:O	1:B:352:VAL:HG23	2.22	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	376/640 (59%)	307 (82%)	54 (14%)	15 (4%)	2	15
1	B	376/640 (59%)	307 (82%)	54 (14%)	15 (4%)	2	15
All	All	752/1280 (59%)	614 (82%)	108 (14%)	30 (4%)	4	15

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	74	VAL
1	A	76	SER
1	A	372	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	74	VAL
1	B	76	SER
1	B	372	THR
1	A	77	MET
1	A	362	GLU
1	A	369	ARG
1	A	405	VAL
1	A	548	GLY
1	B	77	MET
1	B	362	GLU
1	B	369	ARG
1	B	548	GLY
1	A	388	ARG
1	B	388	ARG
1	B	405	VAL
1	A	356	ALA
1	B	356	ALA
1	A	357	LEU
1	A	409	VAL
1	B	357	LEU
1	B	409	VAL
1	A	395	VAL
1	B	395	VAL
1	A	347	VAL
1	B	347	VAL
1	A	414	LEU
1	B	414	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	321/530 (61%)	288 (90%)	33 (10%)	7	24
1	B	321/530 (61%)	290 (90%)	31 (10%)	8	28
All	All	642/1060 (61%)	578 (90%)	64 (10%)	9	26

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	THR
1	A	77	MET
1	A	103	VAL
1	A	105	THR
1	A	343	LEU
1	A	345	LEU
1	A	350	LEU
1	A	351	VAL
1	A	352	VAL
1	A	365	SER
1	A	366	ASP
1	A	375	GLN
1	A	376	LYS
1	A	377	LEU
1	A	378	VAL
1	A	383	MET
1	A	388	ARG
1	A	393	MET
1	A	395	VAL
1	A	396	ASP
1	A	397	LEU
1	A	398	SER
1	A	399	THR
1	A	402	SER
1	A	405	VAL
1	A	409	VAL
1	A	411	MET
1	A	414	LEU
1	A	418	THR
1	A	522	LYS
1	A	525	LYS
1	A	526	GLN
1	A	549	GLN
1	B	73	THR
1	B	77	MET
1	B	103	VAL
1	B	105	THR
1	B	343	LEU
1	B	345	LEU
1	B	350	LEU
1	B	351	VAL
1	B	352	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	365	SER
1	B	366	ASP
1	B	375	GLN
1	B	376	LYS
1	B	377	LEU
1	B	378	VAL
1	B	383	MET
1	B	388	ARG
1	B	393	MET
1	B	395	VAL
1	B	396	ASP
1	B	397	LEU
1	B	398	SER
1	B	399	THR
1	B	402	SER
1	B	405	VAL
1	B	409	VAL
1	B	411	MET
1	B	414	LEU
1	B	418	THR
1	B	526	GLN
1	B	549	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	262	ASN
1	A	549	GLN
1	B	262	ASN
1	B	549	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.

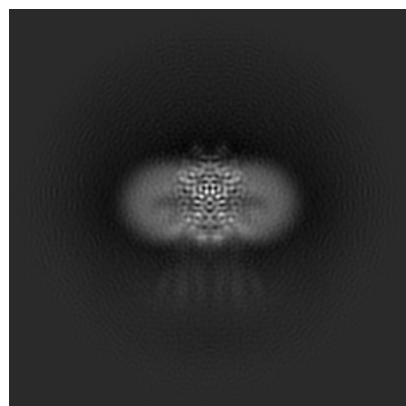
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38992. These allow visual inspection of the internal detail of the map and identification of artifacts.

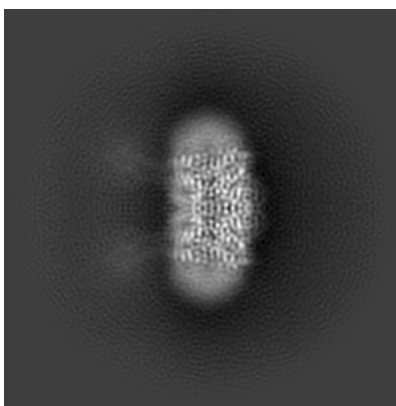
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

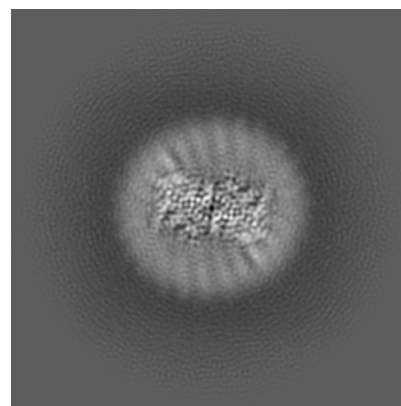
6.1.1 Primary map



X

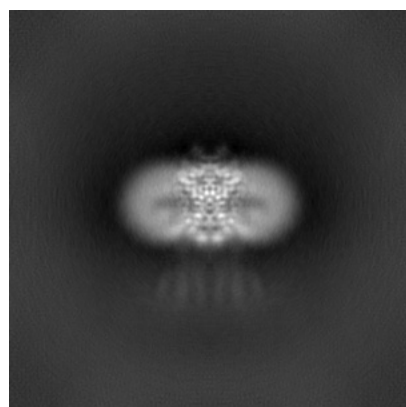


Y

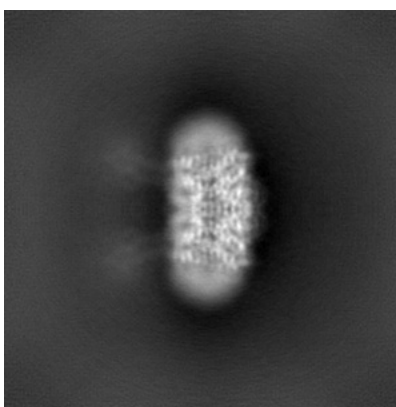


Z

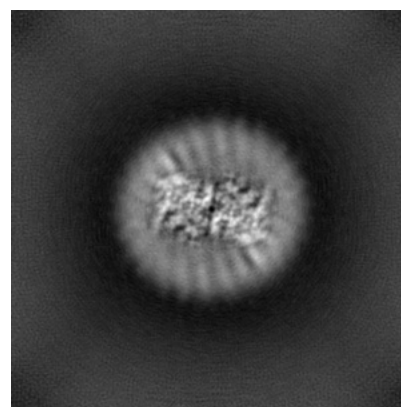
6.1.2 Raw map



X



Y

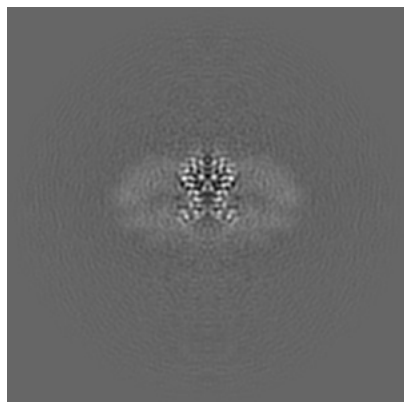


Z

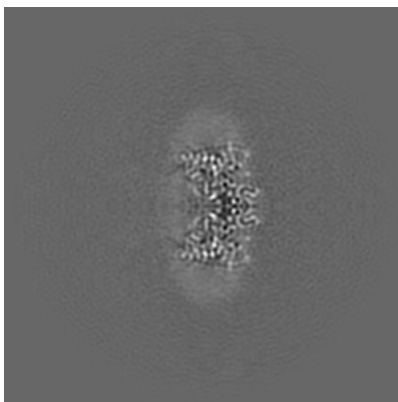
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

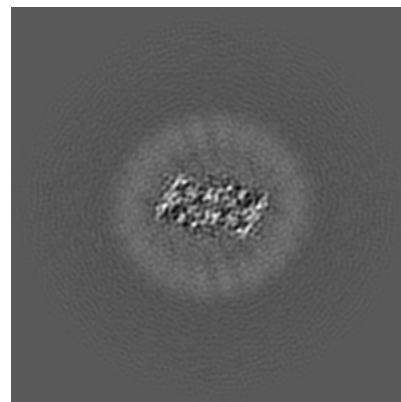
6.2.1 Primary map



X Index: 128

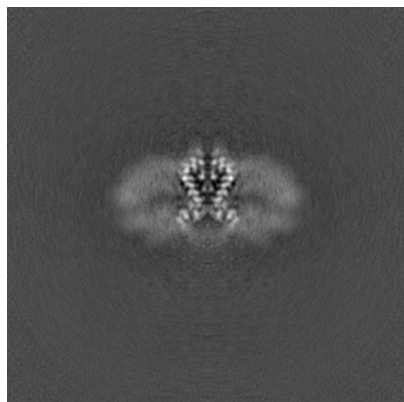


Y Index: 128

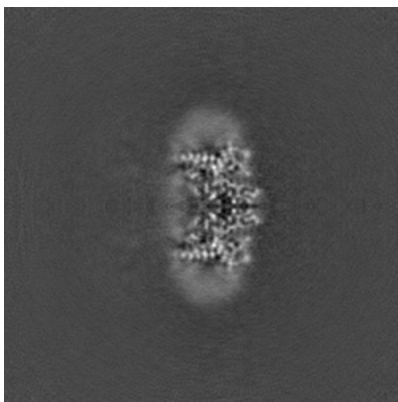


Z Index: 128

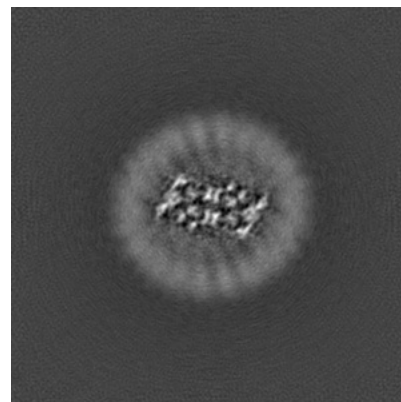
6.2.2 Raw map



X Index: 128



Y Index: 128

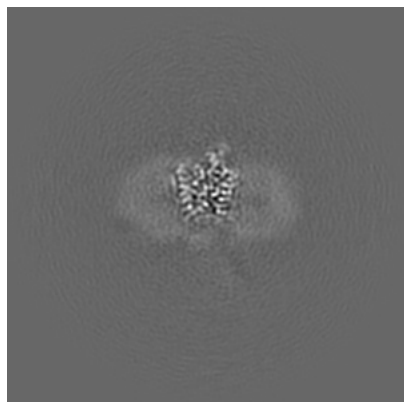


Z Index: 128

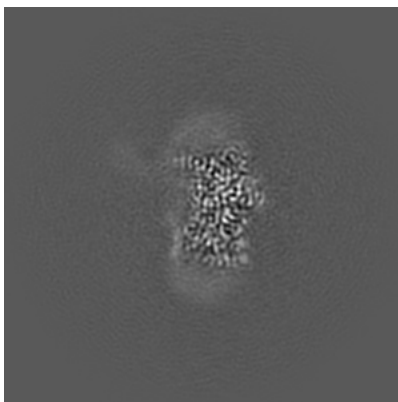
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

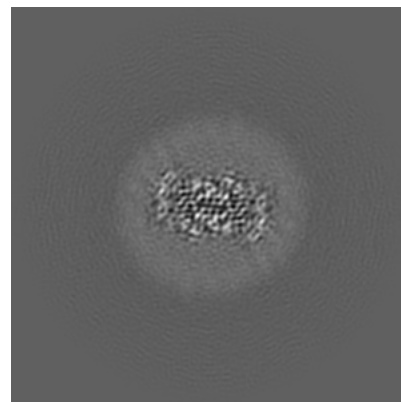
6.3.1 Primary map



X Index: 117

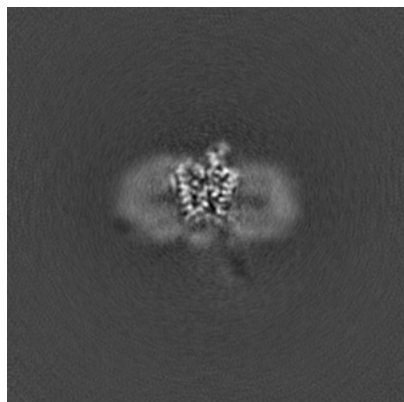


Y Index: 122

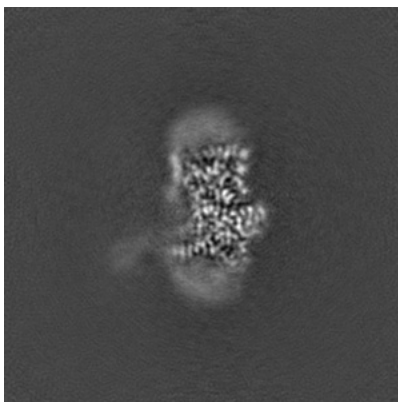


Z Index: 141

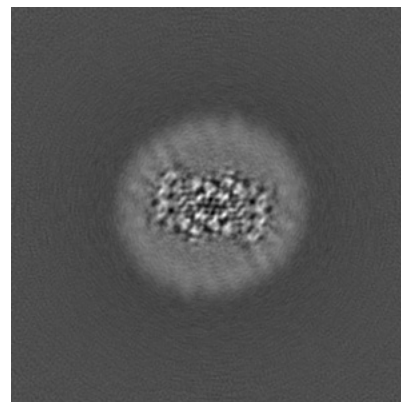
6.3.2 Raw map



X Index: 117



Y Index: 134

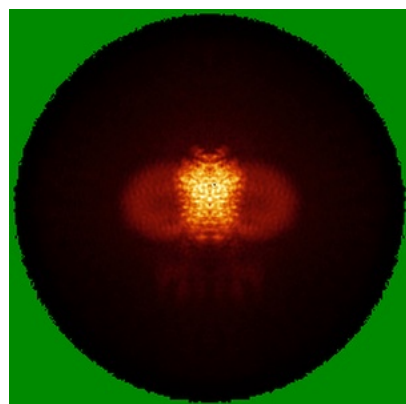


Z Index: 141

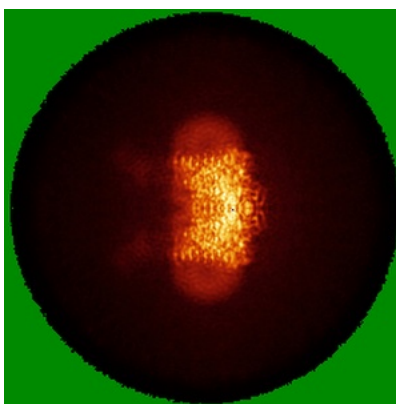
The images above show the largest variance slices of the map in three orthogonal directions.

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

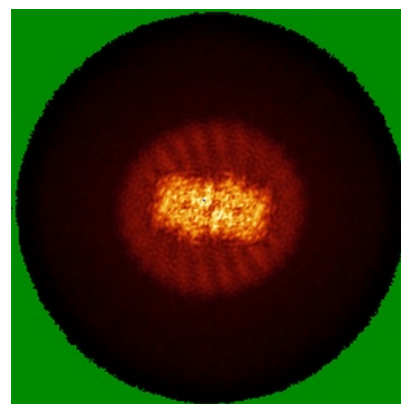
6.4.1 Primary map



X

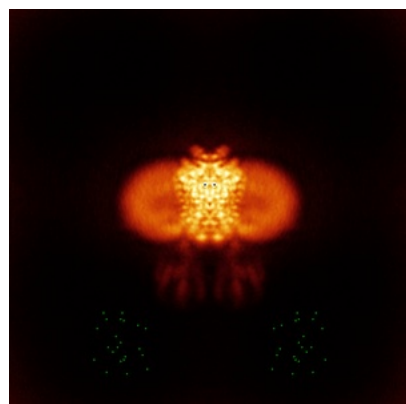


Y

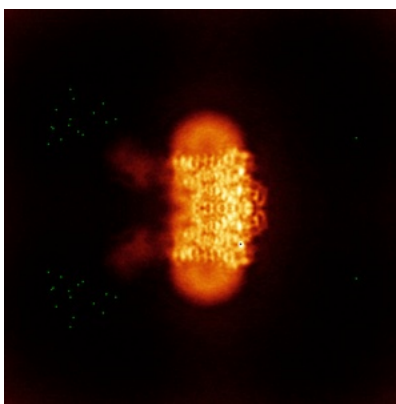


Z

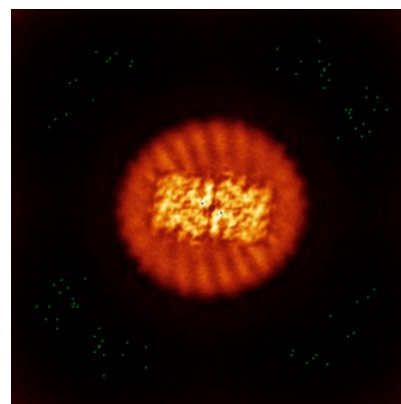
6.4.2 Raw map



X



Y

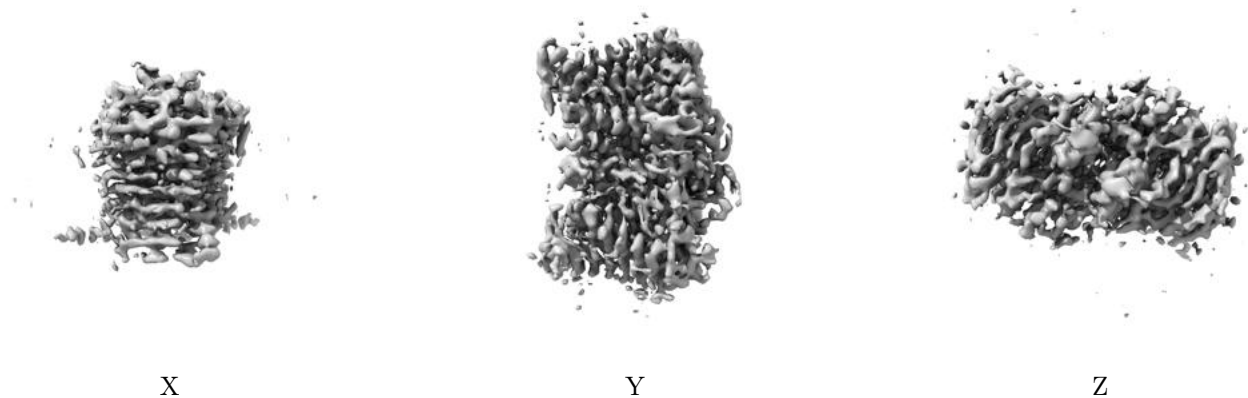


Z

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.

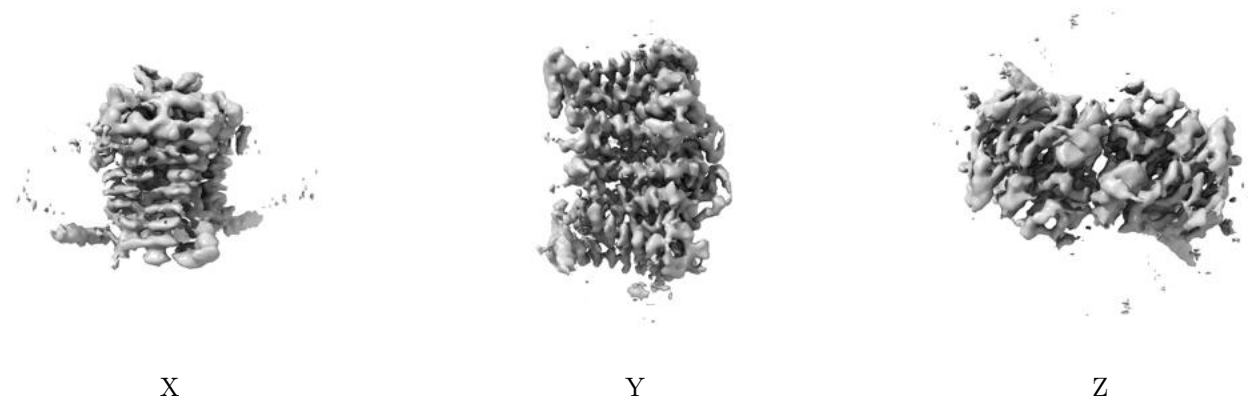
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. 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.

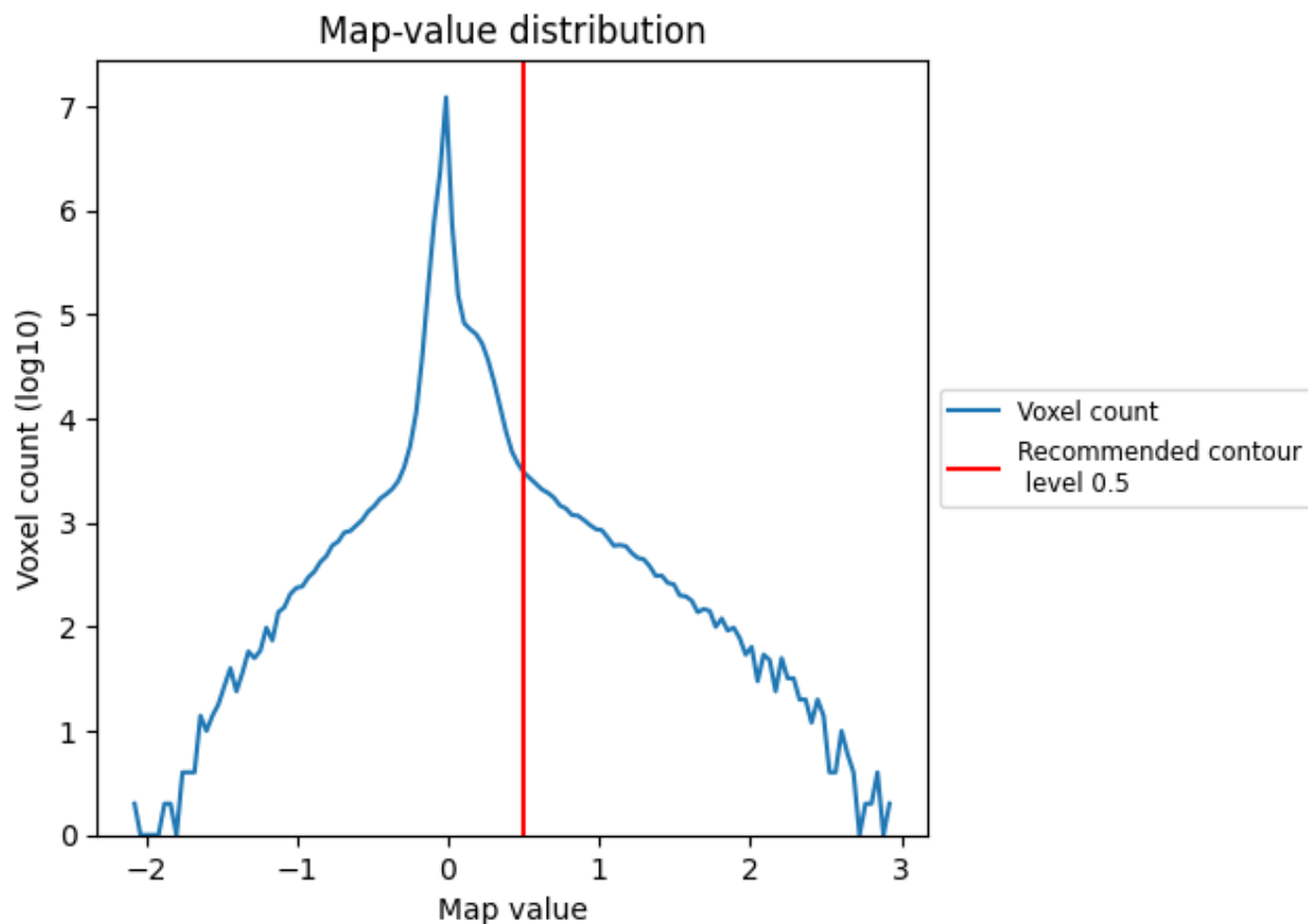
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

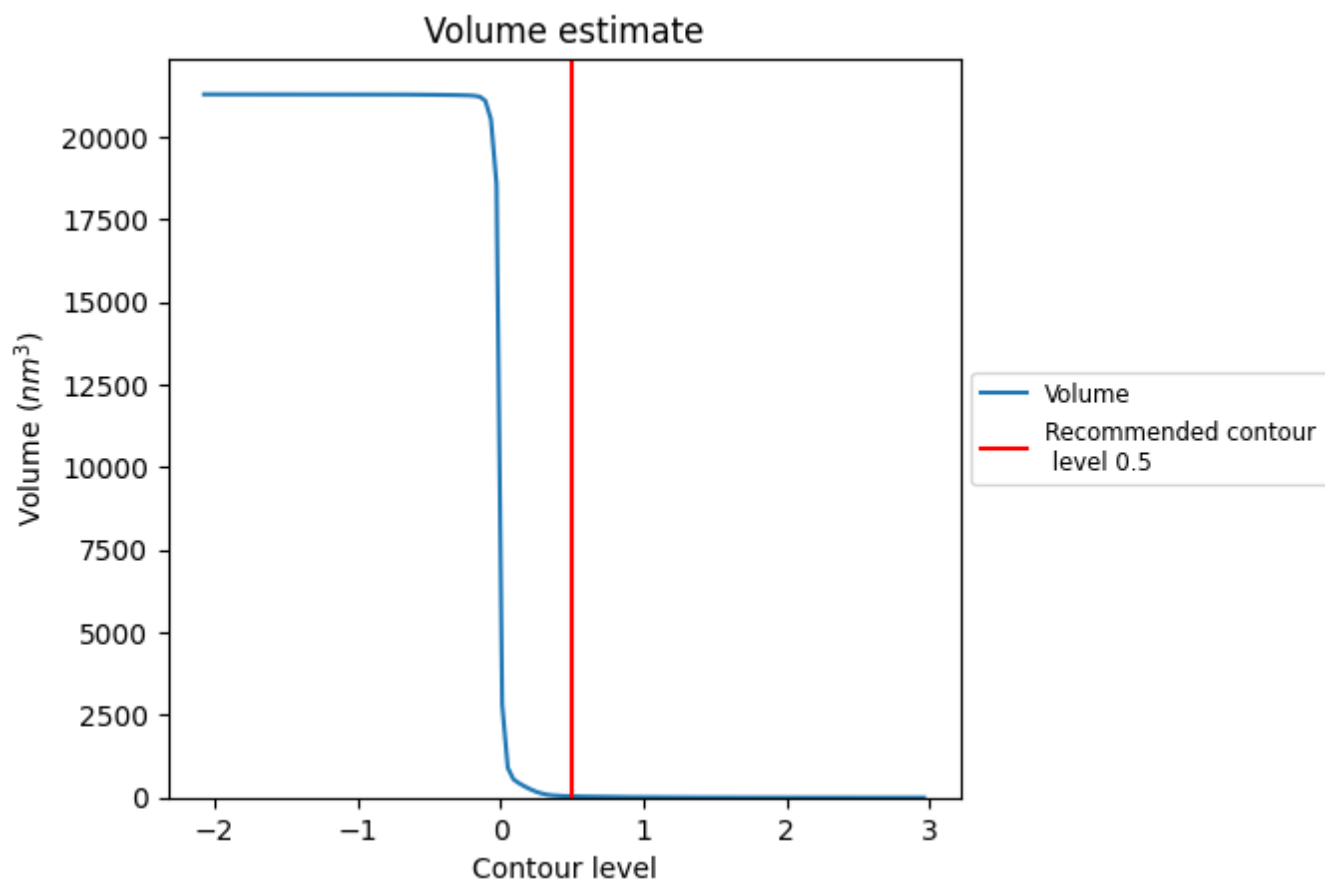
This section contains the results of statistical analysis of the map.

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.

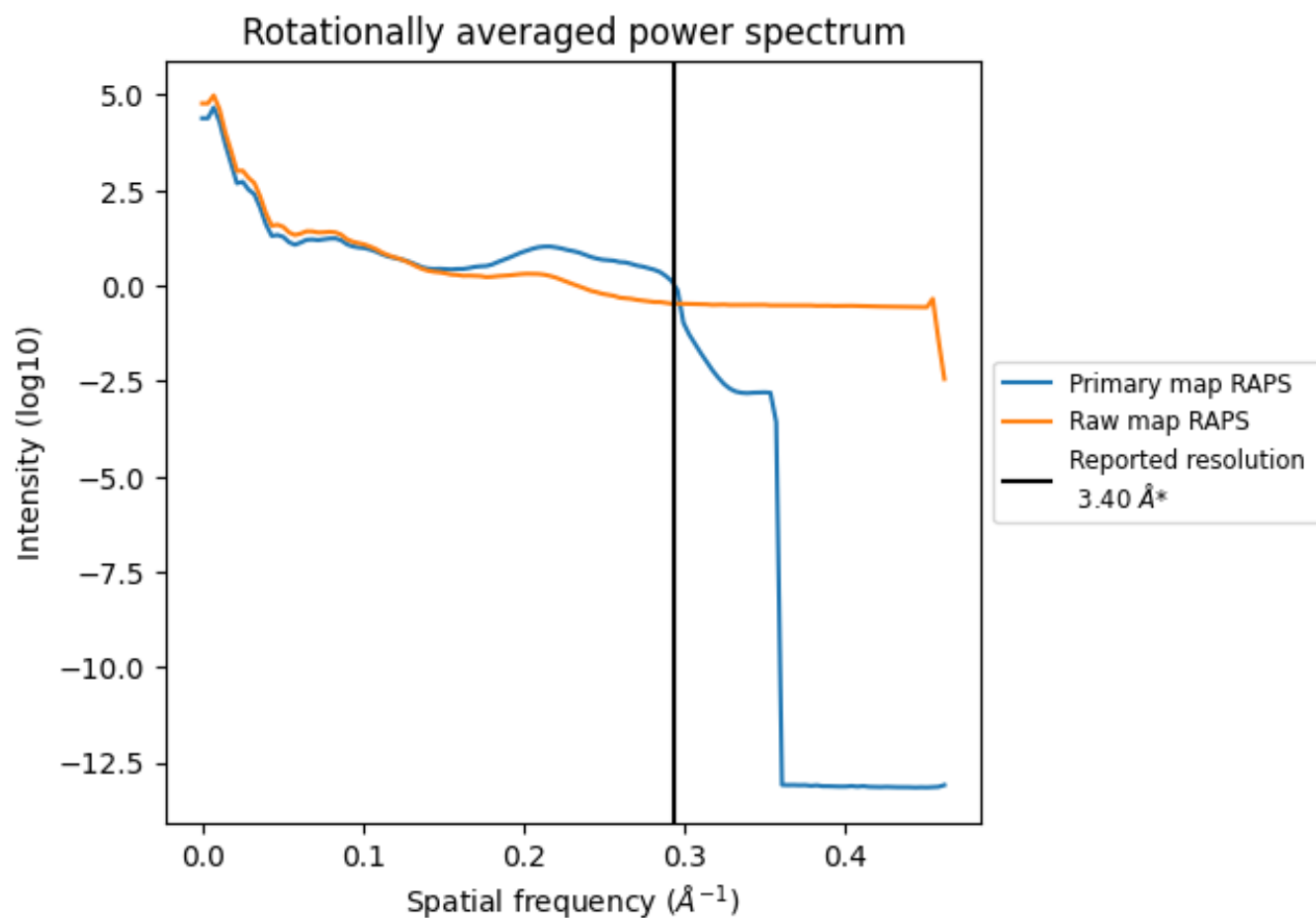
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 39 nm³; this corresponds to an approximate mass of 35 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 ⓘ

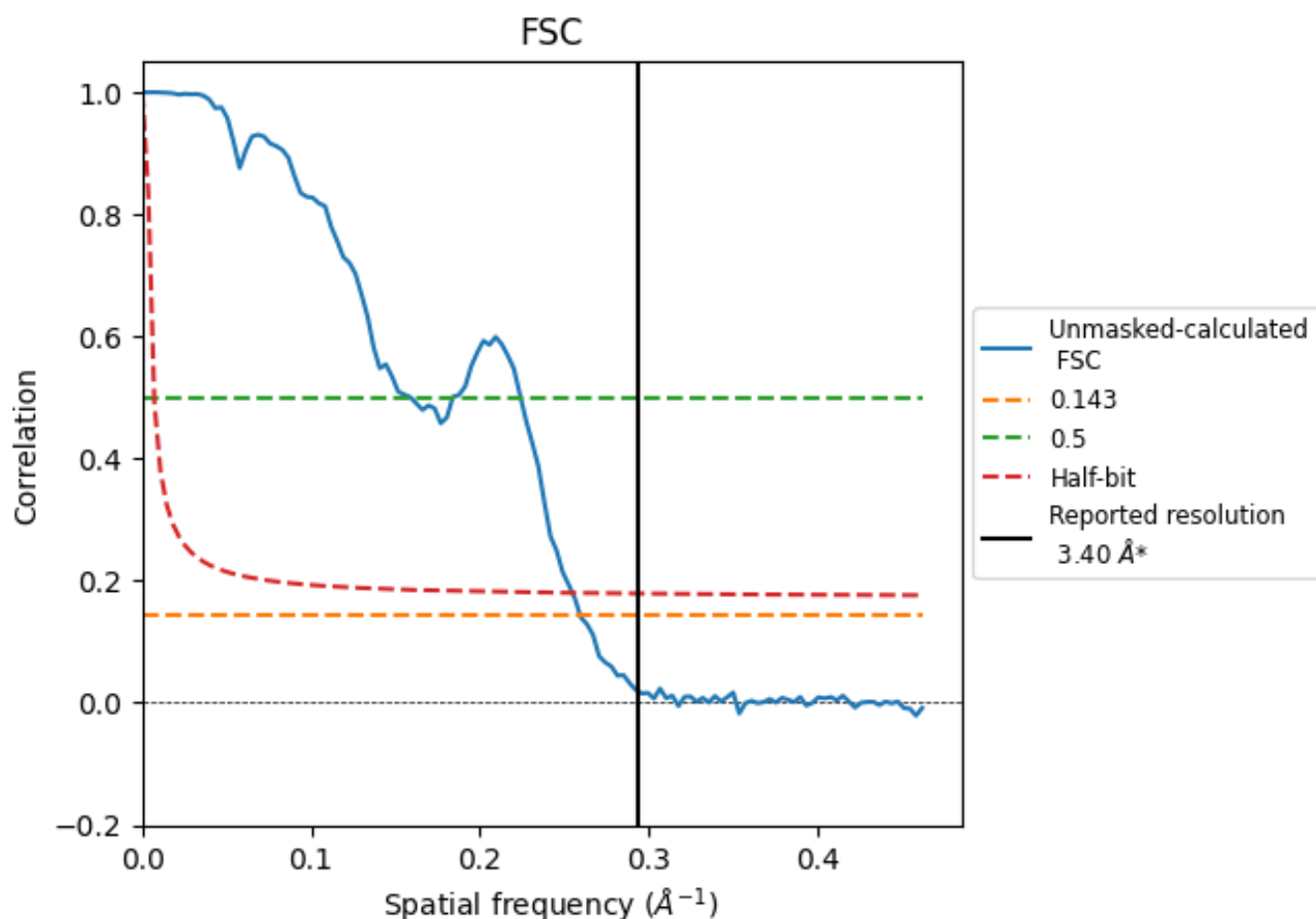


*Reported resolution corresponds to spatial frequency of 0.294 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

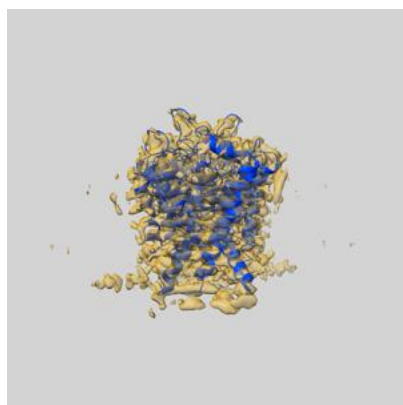
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.86	6.29	3.92

*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 3.86 differs from the reported value 3.4 by more than 10 %

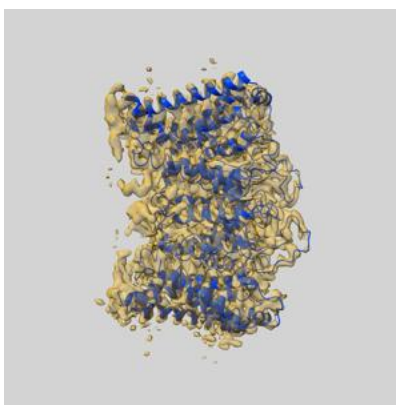
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38992 and PDB model 8Y6N. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

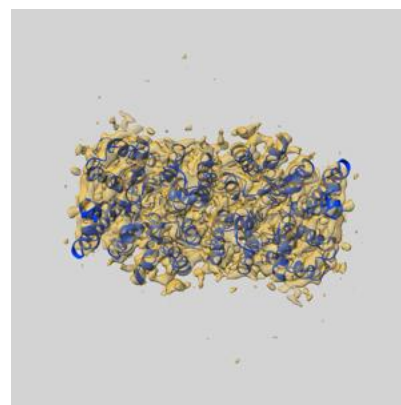
9.1 Map-model overlay [i](#)



X



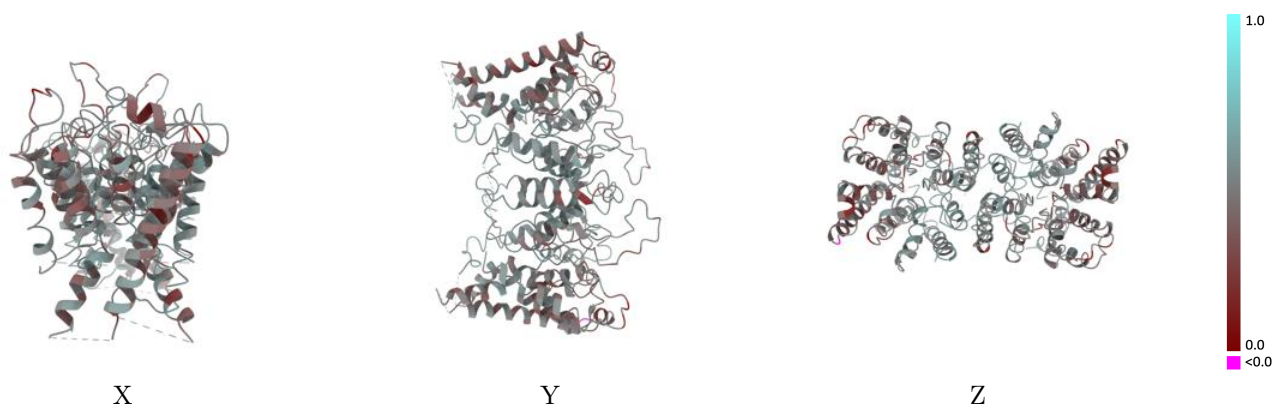
Y



Z

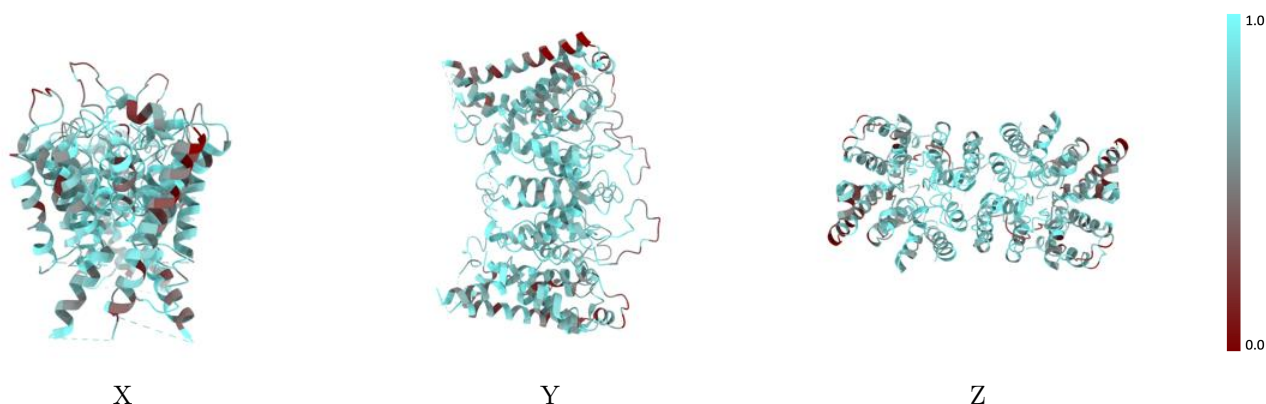
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



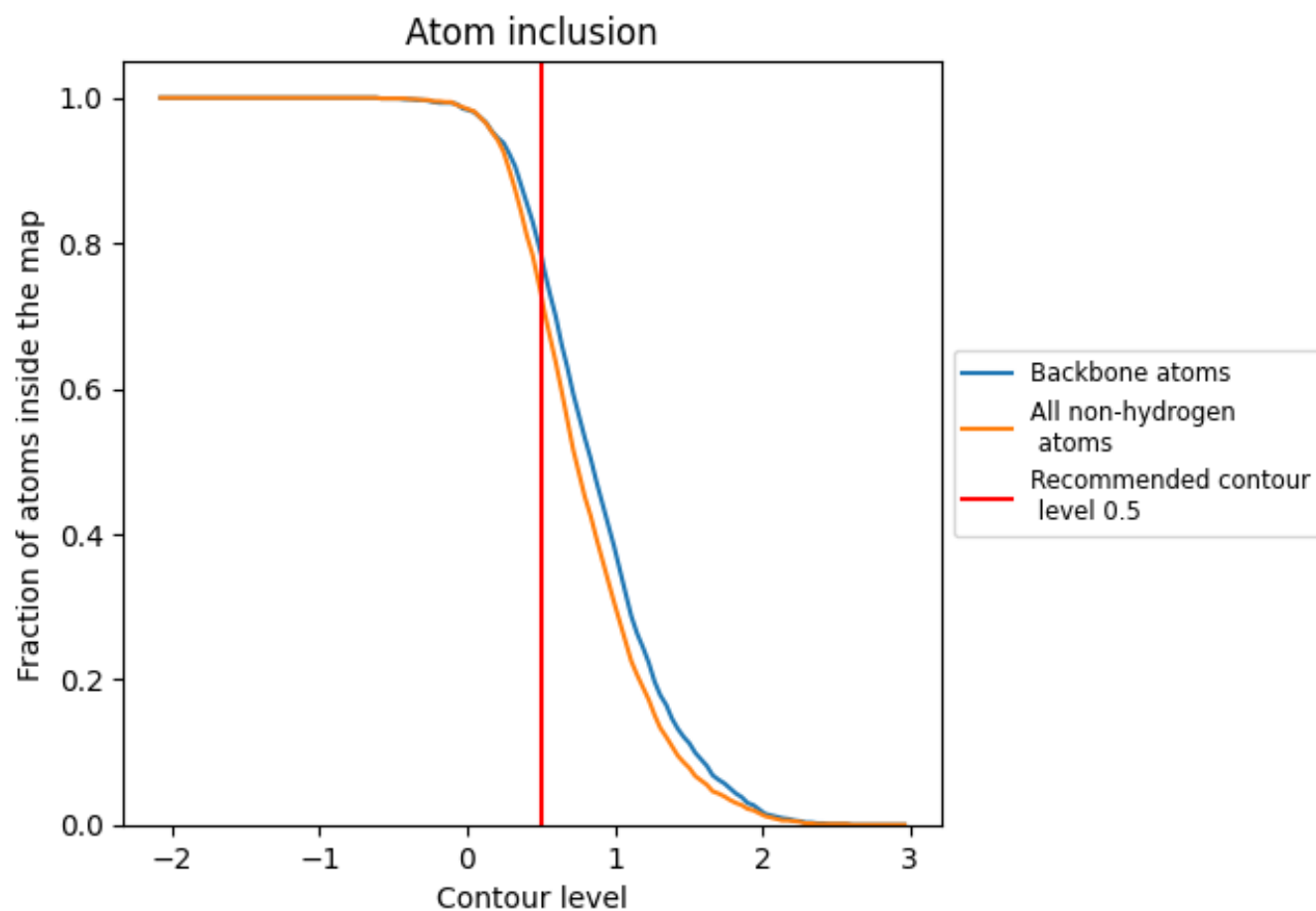
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7310	0.4720
A	0.7310	0.4720
B	0.7310	0.4720

