



Full wwPDB EM Validation Report ⓘ

Aug 23, 2026 – 04:36 PM JST

PDB ID : 22EB / pdb_000022eb
EMDB ID : EMD-68192
Title : MERS-CoV RBD in complex with receptor DPP4
Authors : Wang, Y.J.; Sun, L.
Deposited on : 2026-01-07
Resolution : 2.88 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.dev133
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) : 2.50

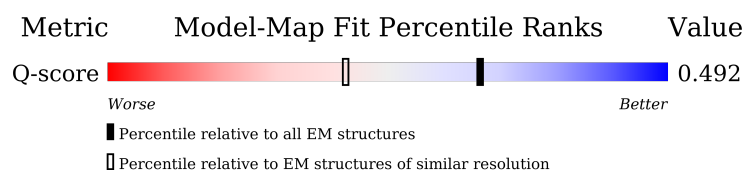
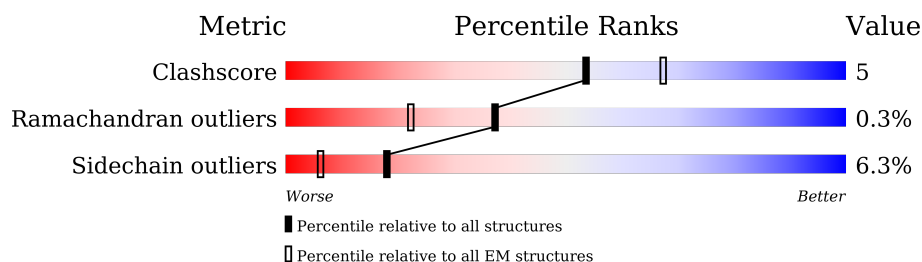
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.88 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	12111 (2.38 - 3.38)

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	C	1340	
1	L	1340	
2	A	791	
2	B	791	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15158 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L	209	Total	C	N	O	S	0	0
			1616	1030	257	318	11		
1	C	209	Total	C	N	O	S	0	0
			1616	1030	257	318	11		

There are 98 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	1292	GLY	-	expression tag	UNP K9N5Q8
L	1293	SER	-	expression tag	UNP K9N5Q8
L	1294	GLY	-	expression tag	UNP K9N5Q8
L	1295	TYR	-	expression tag	UNP K9N5Q8
L	1296	ILE	-	expression tag	UNP K9N5Q8
L	1297	PRO	-	expression tag	UNP K9N5Q8
L	1298	GLU	-	expression tag	UNP K9N5Q8
L	1299	ALA	-	expression tag	UNP K9N5Q8
L	1300	PRO	-	expression tag	UNP K9N5Q8
L	1301	ARG	-	expression tag	UNP K9N5Q8
L	1302	ASP	-	expression tag	UNP K9N5Q8
L	1303	GLY	-	expression tag	UNP K9N5Q8
L	1304	GLN	-	expression tag	UNP K9N5Q8
L	1305	ALA	-	expression tag	UNP K9N5Q8
L	1306	TYR	-	expression tag	UNP K9N5Q8
L	1307	VAL	-	expression tag	UNP K9N5Q8
L	1308	ARG	-	expression tag	UNP K9N5Q8
L	1309	LYS	-	expression tag	UNP K9N5Q8
L	1310	ASP	-	expression tag	UNP K9N5Q8
L	1311	GLY	-	expression tag	UNP K9N5Q8
L	1312	GLU	-	expression tag	UNP K9N5Q8
L	1313	TRP	-	expression tag	UNP K9N5Q8
L	1314	VAL	-	expression tag	UNP K9N5Q8
L	1315	LEU	-	expression tag	UNP K9N5Q8
L	1316	LEU	-	expression tag	UNP K9N5Q8
L	1317	SER	-	expression tag	UNP K9N5Q8

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Chain	Residue	Modelled	Actual	Comment	Reference
L	1318	THR	-	expression tag	UNP K9N5Q8
L	1319	PHE	-	expression tag	UNP K9N5Q8
L	1320	LEU	-	expression tag	UNP K9N5Q8
L	1321	GLY	-	expression tag	UNP K9N5Q8
L	1322	ARG	-	expression tag	UNP K9N5Q8
L	1323	SER	-	expression tag	UNP K9N5Q8
L	1324	LEU	-	expression tag	UNP K9N5Q8
L	1325	GLU	-	expression tag	UNP K9N5Q8
L	1326	VAL	-	expression tag	UNP K9N5Q8
L	1327	LEU	-	expression tag	UNP K9N5Q8
L	1328	PHE	-	expression tag	UNP K9N5Q8
L	1329	GLN	-	expression tag	UNP K9N5Q8
L	1330	GLY	-	expression tag	UNP K9N5Q8
L	1331	PRO	-	expression tag	UNP K9N5Q8
L	1332	GLY	-	expression tag	UNP K9N5Q8
L	1333	HIS	-	expression tag	UNP K9N5Q8
L	1334	HIS	-	expression tag	UNP K9N5Q8
L	1335	HIS	-	expression tag	UNP K9N5Q8
L	1336	HIS	-	expression tag	UNP K9N5Q8
L	1337	HIS	-	expression tag	UNP K9N5Q8
L	1338	HIS	-	expression tag	UNP K9N5Q8
L	1339	HIS	-	expression tag	UNP K9N5Q8
L	1340	HIS	-	expression tag	UNP K9N5Q8
C	1292	GLY	-	expression tag	UNP K9N5Q8
C	1293	SER	-	expression tag	UNP K9N5Q8
C	1294	GLY	-	expression tag	UNP K9N5Q8
C	1295	TYR	-	expression tag	UNP K9N5Q8
C	1296	ILE	-	expression tag	UNP K9N5Q8
C	1297	PRO	-	expression tag	UNP K9N5Q8
C	1298	GLU	-	expression tag	UNP K9N5Q8
C	1299	ALA	-	expression tag	UNP K9N5Q8
C	1300	PRO	-	expression tag	UNP K9N5Q8
C	1301	ARG	-	expression tag	UNP K9N5Q8
C	1302	ASP	-	expression tag	UNP K9N5Q8
C	1303	GLY	-	expression tag	UNP K9N5Q8
C	1304	GLN	-	expression tag	UNP K9N5Q8
C	1305	ALA	-	expression tag	UNP K9N5Q8
C	1306	TYR	-	expression tag	UNP K9N5Q8
C	1307	VAL	-	expression tag	UNP K9N5Q8
C	1308	ARG	-	expression tag	UNP K9N5Q8
C	1309	LYS	-	expression tag	UNP K9N5Q8
C	1310	ASP	-	expression tag	UNP K9N5Q8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1311	GLY	-	expression tag	UNP K9N5Q8
C	1312	GLU	-	expression tag	UNP K9N5Q8
C	1313	TRP	-	expression tag	UNP K9N5Q8
C	1314	VAL	-	expression tag	UNP K9N5Q8
C	1315	LEU	-	expression tag	UNP K9N5Q8
C	1316	LEU	-	expression tag	UNP K9N5Q8
C	1317	SER	-	expression tag	UNP K9N5Q8
C	1318	THR	-	expression tag	UNP K9N5Q8
C	1319	PHE	-	expression tag	UNP K9N5Q8
C	1320	LEU	-	expression tag	UNP K9N5Q8
C	1321	GLY	-	expression tag	UNP K9N5Q8
C	1322	ARG	-	expression tag	UNP K9N5Q8
C	1323	SER	-	expression tag	UNP K9N5Q8
C	1324	LEU	-	expression tag	UNP K9N5Q8
C	1325	GLU	-	expression tag	UNP K9N5Q8
C	1326	VAL	-	expression tag	UNP K9N5Q8
C	1327	LEU	-	expression tag	UNP K9N5Q8
C	1328	PHE	-	expression tag	UNP K9N5Q8
C	1329	GLN	-	expression tag	UNP K9N5Q8
C	1330	GLY	-	expression tag	UNP K9N5Q8
C	1331	PRO	-	expression tag	UNP K9N5Q8
C	1332	GLY	-	expression tag	UNP K9N5Q8
C	1333	HIS	-	expression tag	UNP K9N5Q8
C	1334	HIS	-	expression tag	UNP K9N5Q8
C	1335	HIS	-	expression tag	UNP K9N5Q8
C	1336	HIS	-	expression tag	UNP K9N5Q8
C	1337	HIS	-	expression tag	UNP K9N5Q8
C	1338	HIS	-	expression tag	UNP K9N5Q8
C	1339	HIS	-	expression tag	UNP K9N5Q8
C	1340	HIS	-	expression tag	UNP K9N5Q8

- Molecule 2 is a protein called Dipeptidyl peptidase 4 membrane form.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	728	Total	C	N	O	S	0	0
			5963	3827	982	1128	26		
2	B	728	Total	C	N	O	S	0	0
			5963	3827	982	1128	26		

There are 106 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	MET	-	initiating methionine	UNP P27487
A	-13	LEU	-	expression tag	UNP P27487
A	-12	LEU	-	expression tag	UNP P27487
A	-11	VAL	-	expression tag	UNP P27487
A	-10	ASN	-	expression tag	UNP P27487
A	-9	GLN	-	expression tag	UNP P27487
A	-8	SER	-	expression tag	UNP P27487
A	-7	HIS	-	expression tag	UNP P27487
A	-6	GLN	-	expression tag	UNP P27487
A	-5	GLY	-	expression tag	UNP P27487
A	-4	PHE	-	expression tag	UNP P27487
A	-3	ASN	-	expression tag	UNP P27487
A	-2	LYS	-	expression tag	UNP P27487
A	-1	GLU	-	expression tag	UNP P27487
A	0	HIS	-	expression tag	UNP P27487
A	1	THR	-	expression tag	UNP P27487
A	2	SER	-	expression tag	UNP P27487
A	3	LYS	-	expression tag	UNP P27487
A	4	MET	-	expression tag	UNP P27487
A	5	VAL	-	expression tag	UNP P27487
A	6	SER	-	expression tag	UNP P27487
A	7	ALA	-	expression tag	UNP P27487
A	8	ILE	-	expression tag	UNP P27487
A	9	VAL	-	expression tag	UNP P27487
A	10	LEU	-	expression tag	UNP P27487
A	11	TYR	-	expression tag	UNP P27487
A	12	VAL	-	expression tag	UNP P27487
A	13	LEU	-	expression tag	UNP P27487
A	14	LEU	-	expression tag	UNP P27487
A	15	ALA	-	expression tag	UNP P27487
A	16	ALA	-	expression tag	UNP P27487
A	17	ALA	-	expression tag	UNP P27487
A	18	ALA	-	expression tag	UNP P27487
A	19	HIS	-	expression tag	UNP P27487
A	20	SER	-	expression tag	UNP P27487
A	21	ALA	-	expression tag	UNP P27487
A	22	PHE	-	expression tag	UNP P27487
A	23	ALA	-	expression tag	UNP P27487
A	24	ALA	-	expression tag	UNP P27487
A	25	ASP	-	expression tag	UNP P27487
A	26	MET	-	expression tag	UNP P27487
A	27	GLY	-	expression tag	UNP P27487
A	28	SER	-	expression tag	UNP P27487

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Chain	Residue	Modelled	Actual	Comment	Reference
A	767	GLY	-	expression tag	UNP P27487
A	768	SER	-	expression tag	UNP P27487
A	769	HIS	-	expression tag	UNP P27487
A	770	HIS	-	expression tag	UNP P27487
A	771	HIS	-	expression tag	UNP P27487
A	772	HIS	-	expression tag	UNP P27487
A	773	HIS	-	expression tag	UNP P27487
A	774	HIS	-	expression tag	UNP P27487
A	775	HIS	-	expression tag	UNP P27487
A	776	HIS	-	expression tag	UNP P27487
B	-14	MET	-	initiating methionine	UNP P27487
B	-13	LEU	-	expression tag	UNP P27487
B	-12	LEU	-	expression tag	UNP P27487
B	-11	VAL	-	expression tag	UNP P27487
B	-10	ASN	-	expression tag	UNP P27487
B	-9	GLN	-	expression tag	UNP P27487
B	-8	SER	-	expression tag	UNP P27487
B	-7	HIS	-	expression tag	UNP P27487
B	-6	GLN	-	expression tag	UNP P27487
B	-5	GLY	-	expression tag	UNP P27487
B	-4	PHE	-	expression tag	UNP P27487
B	-3	ASN	-	expression tag	UNP P27487
B	-2	LYS	-	expression tag	UNP P27487
B	-1	GLU	-	expression tag	UNP P27487
B	0	HIS	-	expression tag	UNP P27487
B	1	THR	-	expression tag	UNP P27487
B	2	SER	-	expression tag	UNP P27487
B	3	LYS	-	expression tag	UNP P27487
B	4	MET	-	expression tag	UNP P27487
B	5	VAL	-	expression tag	UNP P27487
B	6	SER	-	expression tag	UNP P27487
B	7	ALA	-	expression tag	UNP P27487
B	8	ILE	-	expression tag	UNP P27487
B	9	VAL	-	expression tag	UNP P27487
B	10	LEU	-	expression tag	UNP P27487
B	11	TYR	-	expression tag	UNP P27487
B	12	VAL	-	expression tag	UNP P27487
B	13	LEU	-	expression tag	UNP P27487
B	14	LEU	-	expression tag	UNP P27487
B	15	ALA	-	expression tag	UNP P27487
B	16	ALA	-	expression tag	UNP P27487
B	17	ALA	-	expression tag	UNP P27487

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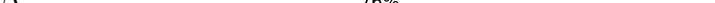
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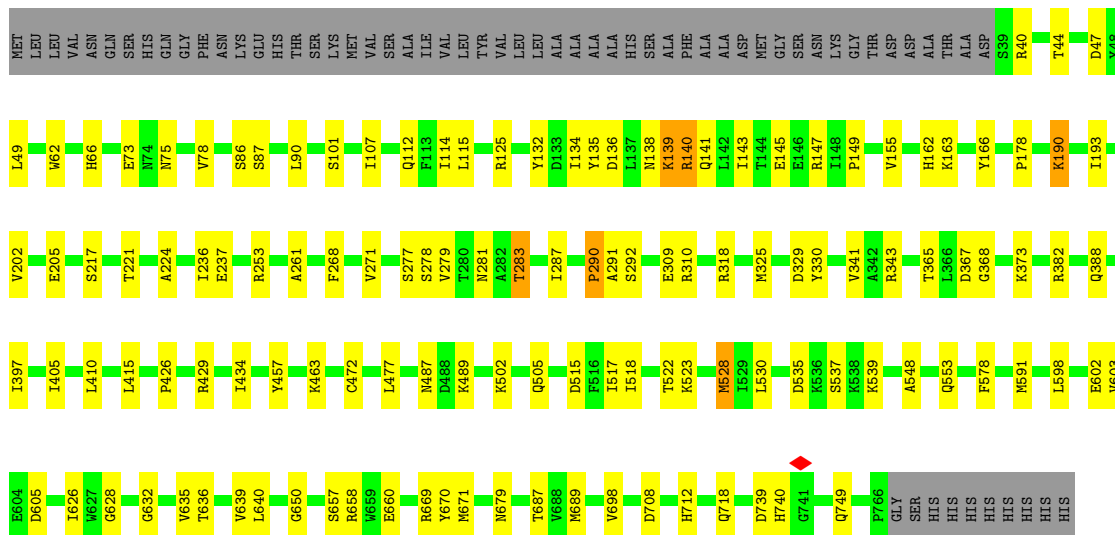
Chain	Residue	Modelled	Actual	Comment	Reference
B	18	ALA	-	expression tag	UNP P27487
B	19	HIS	-	expression tag	UNP P27487
B	20	SER	-	expression tag	UNP P27487
B	21	ALA	-	expression tag	UNP P27487
B	22	PHE	-	expression tag	UNP P27487
B	23	ALA	-	expression tag	UNP P27487
B	24	ALA	-	expression tag	UNP P27487
B	25	ASP	-	expression tag	UNP P27487
B	26	MET	-	expression tag	UNP P27487
B	27	GLY	-	expression tag	UNP P27487
B	28	SER	-	expression tag	UNP P27487
B	767	GLY	-	expression tag	UNP P27487
B	768	SER	-	expression tag	UNP P27487
B	769	HIS	-	expression tag	UNP P27487
B	770	HIS	-	expression tag	UNP P27487
B	771	HIS	-	expression tag	UNP P27487
B	772	HIS	-	expression tag	UNP P27487
B	773	HIS	-	expression tag	UNP P27487
B	774	HIS	-	expression tag	UNP P27487
B	775	HIS	-	expression tag	UNP P27487
B	776	HIS	-	expression tag	UNP P27487



[illegible]

- Molecule 2: Dipeptidyl peptidase 4 membrane form

Chain A:  76% 15% 8%



- Molecule 2: Dipeptidyl peptidase 4 membrane form



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	133001	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.241	Depositor
Minimum map value	-0.510	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.044	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	279.6, 279.6, 279.6	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93200004, 0.93200004, 0.93200004	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	C	0.52	0/1656	0.80	0/2260
1	L	0.49	0/1656	0.81	0/2260
2	A	0.30	0/6135	0.44	0/8344
2	B	0.09	0/6135	0.28	0/8344
All	All	0.31	0/15582	0.49	0/21208

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	C	1616	0	1570	19	0
1	L	1616	0	1570	32	0
2	A	5963	0	5685	68	0
2	B	5963	0	5685	54	0
All	All	15158	0	14510	155	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 5.

All (155) 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:L:513:GLU:HB3	2:A:341:VAL:HG21	1.57	0.86
1:L:502:LYS:HE2	2:A:290:PRO:HA	1.60	0.84
1:L:513:GLU:HB3	2:A:341:VAL:CG2	2.07	0.83
1:L:513:GLU:OE2	2:A:341:VAL:HB	1.88	0.74
2:A:253:ARG:HH21	2:B:253:ARG:HH22	1.41	0.69
1:L:513:GLU:CB	2:A:341:VAL:HG21	2.23	0.68
1:L:513:GLU:CD	2:A:341:VAL:CG2	2.68	0.66
2:A:640:LEU:HB3	2:A:698:VAL:HG21	1.78	0.66
1:L:513:GLU:CD	2:A:341:VAL:HG23	2.22	0.64
1:L:513:GLU:CG	2:A:341:VAL:HG21	2.28	0.64
2:B:548:ALA:HB3	2:B:635:VAL:HG21	1.79	0.63
2:A:548:ALA:HB3	2:A:635:VAL:HG21	1.79	0.63
2:B:263:ASN:ND2	2:B:299:TYR:OH	2.32	0.62
1:L:422:ASP:HB3	1:L:481:LEU:HB2	1.80	0.62
2:A:325:MET:SD	2:A:373:LYS:NZ	2.68	0.62
2:A:271:VAL:HG23	2:A:283:THR:H	1.67	0.59
1:L:513:GLU:CB	2:A:341:VAL:CG2	2.80	0.59
2:A:62:TRP:O	2:A:463:LYS:NZ	2.36	0.59
2:B:640:LEU:HB3	2:B:698:VAL:HG21	1.84	0.58
2:A:329:ASP:OD2	2:A:343:ARG:NH1	2.36	0.58
1:L:388:LEU:HD21	1:L:443:LEU:HD22	1.86	0.57
2:B:301:CYS:O	2:B:358:ARG:NH2	2.37	0.57
2:A:410:LEU:HD13	2:A:415:LEU:HD12	1.86	0.57
2:A:535:ASP:OD2	2:A:537:SER:OG	2.20	0.57
2:B:329:ASP:OD2	2:B:343:ARG:NH1	2.37	0.57
2:B:193:ILE:HG22	2:B:194:ILE:HG12	1.87	0.56
1:C:388:LEU:HD21	1:C:443:LEU:HD22	1.86	0.56
2:A:626:ILE:HG23	2:A:636:THR:HG23	1.86	0.56
2:A:136:ASP:HB3	2:A:139:LYS:HG2	1.88	0.56
1:L:513:GLU:CG	2:A:341:VAL:CG2	2.83	0.56
2:B:640:LEU:HD11	2:B:650:GLY:HA3	1.87	0.56
2:B:535:ASP:OD2	2:B:537:SER:OG	2.21	0.55
2:A:49:LEU:HB3	2:A:749:GLN:HG2	1.88	0.55
2:B:658:ARG:HD3	2:B:660:GLU:HB2	1.89	0.55
1:C:433:ILE:HG13	1:C:478:CYS:SG	2.48	0.54
1:L:513:GLU:CD	2:A:341:VAL:HB	2.32	0.54
2:A:310:ARG:NH1	2:A:368:GLY:O	2.39	0.54
2:B:626:ILE:HG23	2:B:636:THR:HG23	1.89	0.54
2:B:429:ARG:NH2	2:B:553:GLN:OE1	2.41	0.54
2:B:671:MET:O	2:B:679:ASN:ND2	2.37	0.54
1:C:543:LYS:HB3	1:C:554:LEU:HB3	1.90	0.54
2:A:237:GLU:HG2	2:A:253:ARG:HG2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:543:LYS:HB3	1:L:554:LEU:HB3	1.90	0.53
2:B:44:THR:OG1	2:B:47:ASP:OD1	2.25	0.53
2:B:258:LYS:NZ	2:B:661:TYR:O	2.41	0.53
2:A:190:LYS:HB3	2:A:193:ILE:HB	1.89	0.53
2:B:184:ARG:NH1	2:B:186:THR:O	2.38	0.53
2:A:261:ALA:O	2:A:318:ARG:NH2	2.41	0.53
1:L:468:ASN:ND2	1:L:500:ILE:O	2.34	0.53
2:B:382:ARG:HH21	2:B:591:MET:HE1	1.74	0.52
1:C:468:ASN:ND2	1:C:500:ILE:O	2.34	0.52
2:B:478:PRO:O	2:B:497:ASN:ND2	2.43	0.52
1:L:433:ILE:HG13	1:L:478:CYS:SG	2.50	0.52
2:B:237:GLU:OE2	2:B:253:ARG:NH1	2.43	0.52
2:A:689:MET:N	2:A:689:MET:SD	2.83	0.52
2:B:90:LEU:HD21	2:B:95:PHE:HE2	1.74	0.51
2:B:261:ALA:O	2:B:318:ARG:NH2	2.42	0.51
2:A:44:THR:OG1	2:A:47:ASP:OD1	2.28	0.51
2:A:640:LEU:HD11	2:A:650:GLY:HA3	1.93	0.51
2:B:175:LYS:NZ	2:B:180:LEU:O	2.44	0.50
1:L:497:TYR:HB2	1:L:561:VAL:HB	1.94	0.50
2:B:49:LEU:HB3	2:B:749:GLN:HG2	1.94	0.50
1:L:513:GLU:OE1	2:A:341:VAL:HG23	2.12	0.50
2:A:134:ILE:HG21	2:A:178:PRO:HB3	1.93	0.50
2:A:658:ARG:HD3	2:A:660:GLU:HB2	1.93	0.50
2:B:149:PRO:O	2:B:152:THR:OG1	2.29	0.50
2:A:114:ILE:HG23	2:A:135:TYR:HB3	1.94	0.49
2:B:310:ARG:NH1	2:B:368:GLY:O	2.46	0.49
2:B:689:MET:SD	2:B:689:MET:N	2.85	0.49
2:B:726:VAL:HG23	2:B:728:VAL:HG23	1.93	0.49
2:B:628:GLY:HA3	2:B:632:GLY:HA3	1.93	0.49
1:C:497:TYR:HB2	1:C:561:VAL:HB	1.94	0.48
2:A:365:THR:OG1	2:A:367:ASP:OD1	2.31	0.48
2:A:628:GLY:HA3	2:A:632:GLY:HA3	1.94	0.48
2:B:426:PRO:O	2:B:553:GLN:NE2	2.46	0.48
2:A:382:ARG:HH21	2:A:591:MET:HE1	1.77	0.48
2:A:236:ILE:HG12	2:A:712:HIS:CE1	2.49	0.48
2:A:73:GLU:O	2:A:75:ASN:ND2	2.47	0.48
2:A:708:ASP:HA	2:A:739:ASP:HA	1.96	0.48
2:B:708:ASP:HA	2:B:739:ASP:HA	1.96	0.47
2:A:598:LEU:HD11	2:A:670:TYR:HB2	1.94	0.47
2:B:376:SER:HA	2:B:382:ARG:HA	1.96	0.47
2:B:236:ILE:HG12	2:B:712:HIS:CE1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:485:PRO:HD2	1:C:488:LEU:HD13	1.95	0.47
2:A:487:ASN:HB2	2:A:489:LYS:HE3	1.97	0.47
2:B:594:ILE:HG22	2:B:601:PHE:HB2	1.97	0.47
1:L:494:PRO:HD2	1:L:567:LEU:HD13	1.97	0.46
2:A:217:SER:OG	2:A:221:THR:N	2.47	0.46
2:A:429:ARG:HB2	2:A:457:TYR:H	1.80	0.46
2:B:297:ASP:HB2	2:B:318:ARG:HB2	1.97	0.46
1:C:494:PRO:HD2	1:C:567:LEU:HD13	1.97	0.46
2:A:429:ARG:NH2	2:A:553:GLN:OE1	2.47	0.46
2:A:669:ARG:HD2	2:A:670:TYR:CZ	2.50	0.46
2:B:289:ALA:HB3	2:B:294:LEU:HD21	1.96	0.46
2:A:40:ARG:NH1	2:A:505:GLN:O	2.49	0.46
2:A:718:GLN:NE2	2:B:242:SER:O	2.36	0.46
2:B:114:ILE:HG23	2:B:135:TYR:HB3	1.97	0.46
2:B:115:LEU:HD11	2:B:132:TYR:HB3	1.97	0.46
2:A:155:VAL:HG23	2:A:166:TYR:HB3	1.98	0.46
2:A:149:PRO:HD2	2:A:166:TYR:CE2	2.52	0.45
2:A:224:ALA:HB1	2:A:268:PHE:CZ	2.52	0.45
2:B:388:GLN:HB3	2:B:391:LYS:HB2	1.99	0.45
2:A:115:LEU:HD11	2:A:132:TYR:HB3	1.97	0.44
2:B:267:LYS:HD3	1:C:538:GLY:HA3	1.98	0.44
1:C:529:ILE:HD12	1:C:529:ILE:HA	1.86	0.44
1:C:387:PRO:HB2	1:C:402:LEU:HD11	1.99	0.44
1:L:506:PHE:HB2	2:A:291:ALA:HB1	2.00	0.44
1:C:427:GLN:HB2	1:C:476:PRO:HA	2.00	0.44
1:C:531:PRO:HB3	1:C:535:TRP:CZ3	2.52	0.44
1:L:485:PRO:HD2	1:L:488:LEU:HD13	1.99	0.44
1:L:531:PRO:HB3	1:L:535:TRP:CZ3	2.52	0.44
2:A:125:ARG:NH2	2:A:205:GLU:OE2	2.52	0.43
2:B:154:TRP:CE2	2:B:212:SER:HB3	2.53	0.43
1:L:582:ASN:OD1	1:L:582:ASN:N	2.50	0.43
2:A:112:GLN:HB3	2:A:138:ASN:HD21	1.83	0.43
2:A:140:ARG:HA	2:A:140:ARG:HD2	1.59	0.43
2:A:603:VAL:HG13	2:A:639:VAL:HG22	2.00	0.43
2:A:578:PHE:HE2	2:A:605:ASP:HB3	1.84	0.43
2:A:657:SER:HB2	2:A:689:MET:SD	2.59	0.43
1:C:404:PHE:HB2	1:C:441:LEU:HB3	2.01	0.43
2:A:397:ILE:HD12	2:A:434:ILE:HD13	2.01	0.43
1:L:404:PHE:HB2	1:L:441:LEU:HB3	2.01	0.43
2:B:134:ILE:HG21	2:B:178:PRO:HB3	1.99	0.43
1:C:470:LYS:HB3	1:C:470:LYS:HE2	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:428:ILE:HB	1:L:476:PRO:HB3	2.01	0.43
2:A:671:MET:O	2:A:679:ASN:ND2	2.42	0.42
2:B:410:LEU:HD13	2:B:415:LEU:HD12	2.00	0.42
1:C:394:PRO:HG3	1:C:400:LYS:HG3	2.00	0.42
1:C:476:PRO:HD2	1:C:575:VAL:O	2.19	0.42
2:A:687:THR:HB	2:A:689:MET:HE2	2.01	0.42
2:B:269:PHE:HB3	2:B:284:SER:HB3	2.01	0.42
2:B:91:GLU:HG3	2:B:93:SER:H	1.85	0.42
1:L:529:ILE:HD12	1:L:529:ILE:HA	1.86	0.42
1:C:402:LEU:HB3	1:C:404:PHE:CZ	2.54	0.42
2:B:687:THR:HB	2:B:689:MET:HE2	2.01	0.42
1:L:394:PRO:HG3	1:L:400:LYS:HG3	2.01	0.42
2:A:309:GLU:HB3	2:A:330:TYR:HB3	2.02	0.42
2:A:426:PRO:O	2:A:553:GLN:NE2	2.50	0.42
1:C:385:PHE:HB3	1:C:414:LEU:HD13	2.01	0.42
2:B:704:HIS:NE2	2:B:711:VAL:O	2.50	0.41
2:B:761:GLN:HE21	2:B:761:GLN:HB3	1.64	0.41
1:L:470:LYS:HB3	1:L:470:LYS:HE2	1.79	0.41
1:L:483:THR:HG23	1:L:568:GLN:HG2	2.02	0.41
2:A:405:ILE:HG13	2:A:429:ARG:HD2	2.01	0.41
2:B:297:ASP:HB2	2:B:318:ARG:HD2	2.03	0.41
2:B:531:PRO:HD3	2:B:574:ILE:HG12	2.02	0.41
1:L:513:GLU:CD	2:A:341:VAL:CB	2.92	0.41
2:A:528:MET:HE3	2:A:530:LEU:HD21	2.03	0.41
2:B:49:LEU:HD22	2:B:749:GLN:HA	2.02	0.41
1:L:406:ASN:N	1:L:584:VAL:HG22	2.36	0.41
1:L:513:GLU:HG2	2:A:341:VAL:HG21	1.99	0.41
1:C:406:ASN:N	1:C:584:VAL:HG22	2.36	0.41
2:B:657:SER:HB2	2:B:689:MET:SD	2.61	0.41
2:B:397:ILE:HD12	2:B:434:ILE:HD13	2.02	0.40
2:B:297:ASP:OD2	2:B:318:ARG:NH1	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	207/1340 (15%)	197 (95%)	7 (3%)	3 (1%)	9	28
1	L	207/1340 (15%)	194 (94%)	11 (5%)	2 (1%)	12	35
2	A	726/791 (92%)	699 (96%)	26 (4%)	1 (0%)	48	74
2	B	726/791 (92%)	711 (98%)	15 (2%)	0	100	100
All	All	1866/4262 (44%)	1801 (96%)	59 (3%)	6 (0%)	37	62

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	290	PRO
1	L	382	GLU
1	C	382	GLU
1	L	511	ARG
1	C	511	ARG
1	C	428	ILE

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	C	190/1159 (16%)	161 (85%)	29 (15%)	3	8
1	L	190/1159 (16%)	160 (84%)	30 (16%)	2	7
2	A	653/702 (93%)	616 (94%)	37 (6%)	18	47
2	B	653/702 (93%)	643 (98%)	10 (2%)	57	82
All	All	1686/3722 (45%)	1580 (94%)	106 (6%)	18	42

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	379	GLU
1	L	381	VAL

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Mol	Chain	Res	Type
1	L	389	LEU
1	L	392	THR
1	L	400	LYS
1	L	402	LEU
1	L	405	THR
1	L	411	LEU
1	L	412	THR
1	L	417	LEU
1	L	424	THR
1	L	428	ILE
1	L	429	SER
1	L	433	ILE
1	L	441	LEU
1	L	470	LYS
1	L	472	SER
1	L	480	ILE
1	L	483	THR
1	L	491	ILE
1	L	492	THR
1	L	493	LYS
1	L	495	LEU
1	L	507	LEU
1	L	508	SER
1	L	511	ARG
1	L	532	SER
1	L	533	THR
1	L	536	GLU
1	L	573	ILE
2	A	66	HIS
2	A	78	VAL
2	A	86	SER
2	A	87	SER
2	A	90	LEU
2	A	101	SER
2	A	107	ILE
2	A	139	LYS
2	A	140	ARG
2	A	141	GLN
2	A	143	ILE
2	A	145	GLU
2	A	147	ARG
2	A	162	HIS

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Mol	Chain	Res	Type
2	A	163	LYS
2	A	190	LYS
2	A	202	VAL
2	A	277	SER
2	A	278	SER
2	A	279	VAL
2	A	281	ASN
2	A	283	THR
2	A	287	ILE
2	A	292	SER
2	A	388	GLN
2	A	472	CYS
2	A	477	LEU
2	A	502	LYS
2	A	515	ASP
2	A	517	ILE
2	A	518	ILE
2	A	522	THR
2	A	523	LYS
2	A	528	MET
2	A	539	LYS
2	A	602	GLU
2	A	740	HIS
2	B	57	LEU
2	B	78	VAL
2	B	214	LEU
2	B	287	ILE
2	B	341	VAL
2	B	487	ASN
2	B	502	LYS
2	B	602	GLU
2	B	740	HIS
2	B	742	ILE
1	C	379	GLU
1	C	381	VAL
1	C	389	LEU
1	C	392	THR
1	C	400	LYS
1	C	402	LEU
1	C	405	THR
1	C	411	LEU
1	C	412	THR

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Mol	Chain	Res	Type
1	C	424	THR
1	C	428	ILE
1	C	429	SER
1	C	433	ILE
1	C	441	LEU
1	C	470	LYS
1	C	472	SER
1	C	480	ILE
1	C	483	THR
1	C	491	ILE
1	C	492	THR
1	C	493	LYS
1	C	495	LEU
1	C	507	LEU
1	C	508	SER
1	C	511	ARG
1	C	532	SER
1	C	533	THR
1	C	536	GLU
1	C	573	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	408	ASN
1	L	410	ASN
1	L	466	GLN
2	A	123	GLN
2	A	138	ASN
2	A	169	ASN
2	A	179	ASN
2	A	281	ASN
2	A	314	GLN
2	A	344	GLN
2	A	505	GLN
2	A	586	GLN
2	A	621	ASN
2	A	731	GLN
2	A	748	HIS
2	B	66	HIS
2	B	123	GLN
2	B	263	ASN

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Mol	Chain	Res	Type
2	B	272	ASN
2	B	314	GLN
2	B	344	GLN
2	B	497	ASN
2	B	505	GLN
2	B	586	GLN
2	B	748	HIS
2	B	761	GLN
1	C	427	GLN
1	C	466	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](#)

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.

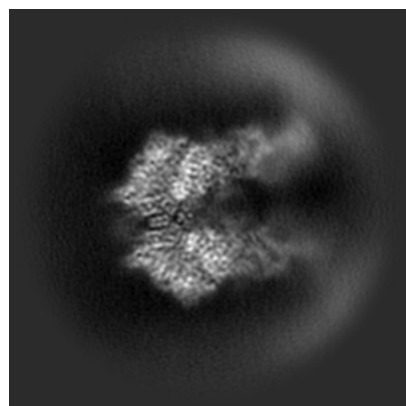
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-68192. These allow visual inspection of the internal detail of the map and identification of artifacts.

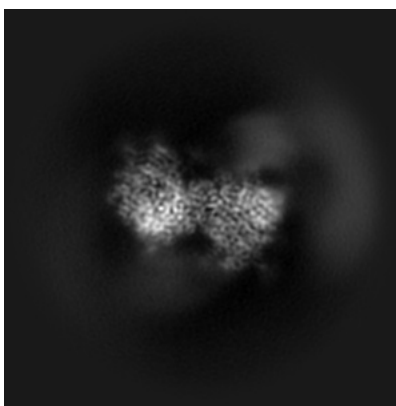
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

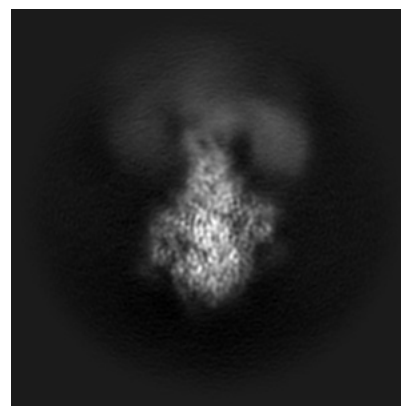
6.1.1 Primary map



X

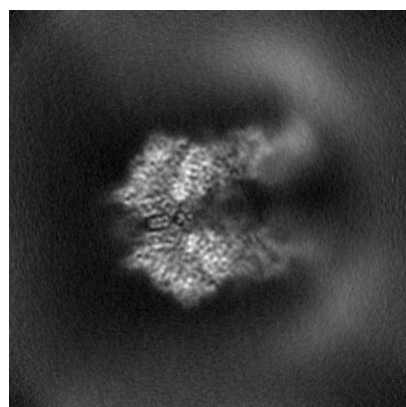


Y

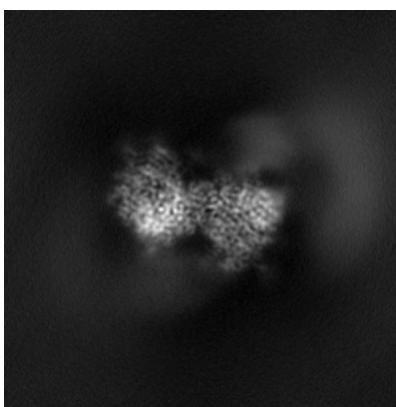


Z

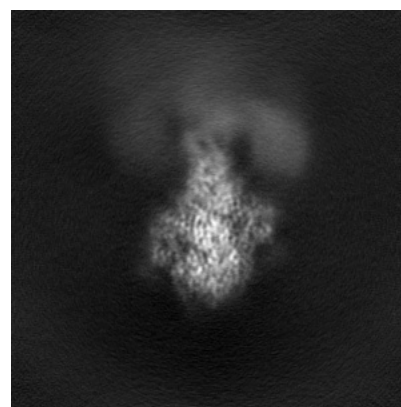
6.1.2 Raw map



X



Y

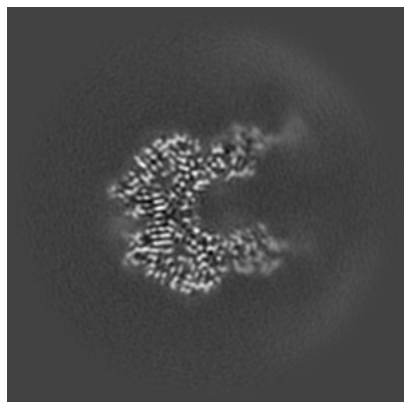


Z

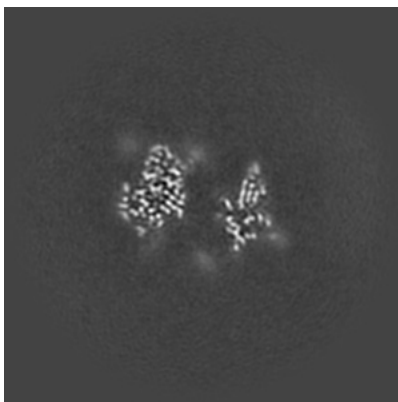
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

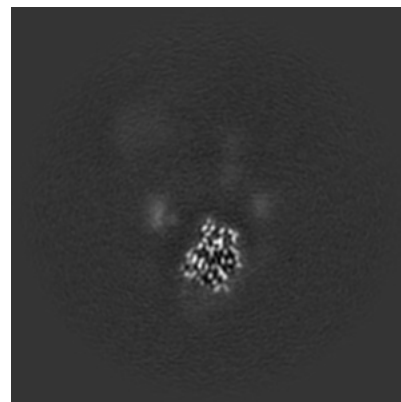
6.2.1 Primary map



X Index: 150

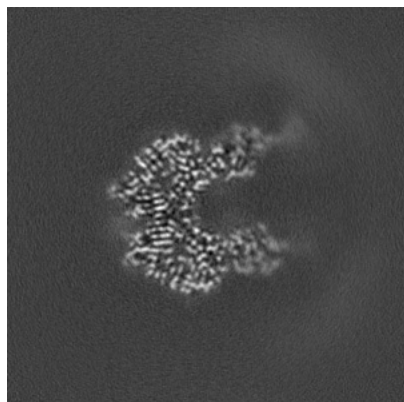


Y Index: 150

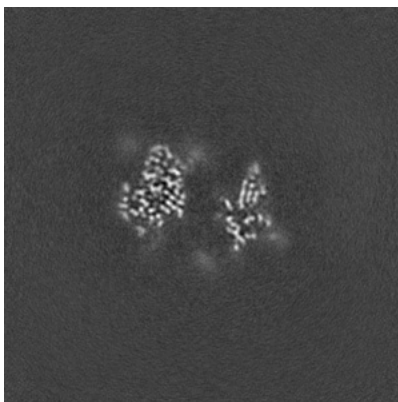


Z Index: 150

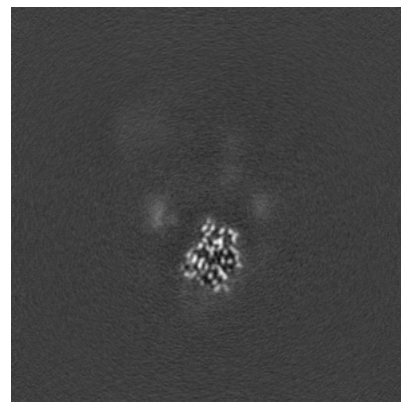
6.2.2 Raw map



X Index: 150



Y Index: 150

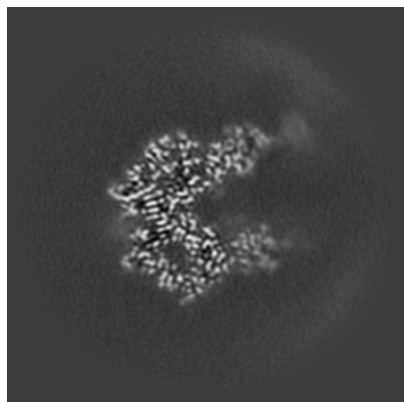


Z Index: 150

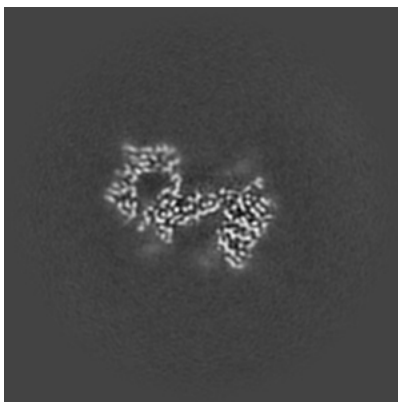
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

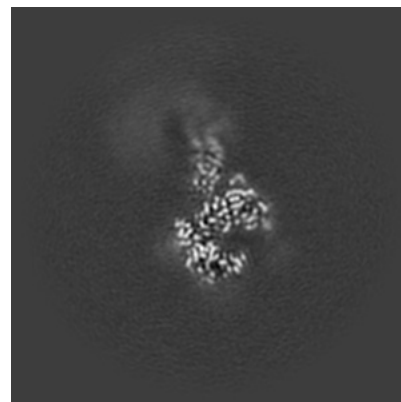
6.3.1 Primary map



X Index: 153

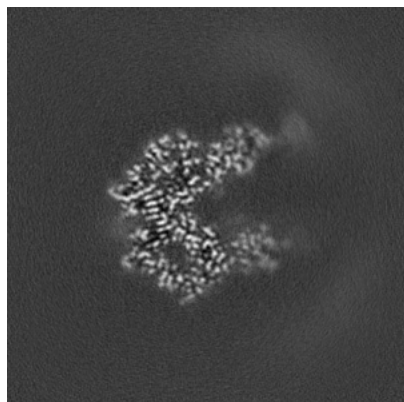


Y Index: 135

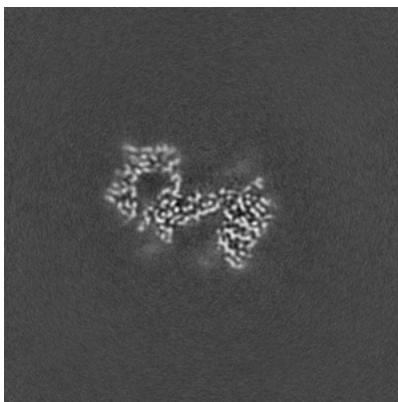


Z Index: 123

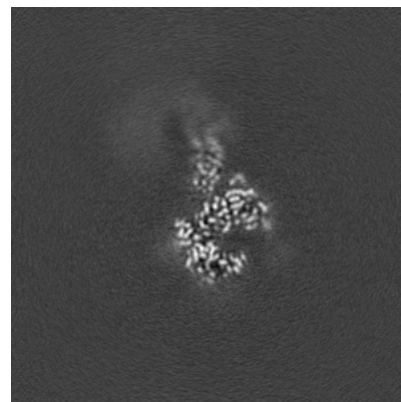
6.3.2 Raw map



X Index: 153



Y Index: 135

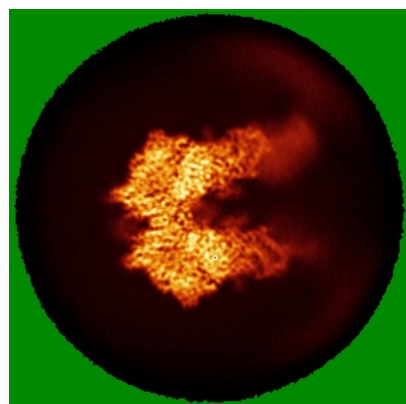


Z Index: 123

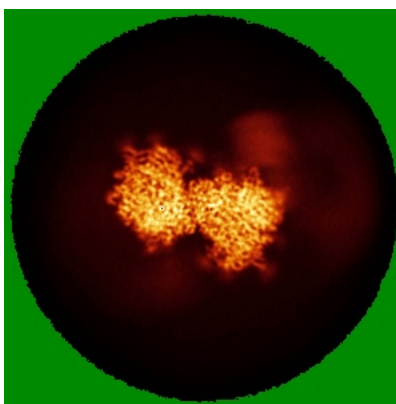
The images above show the largest variance slices of the map in three orthogonal directions.

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

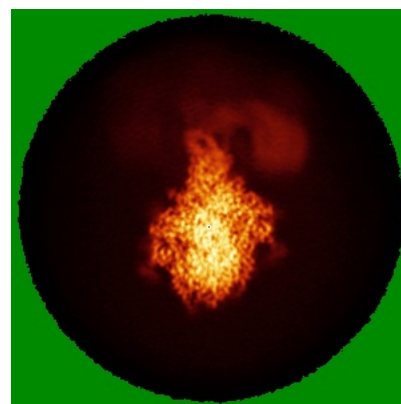
6.4.1 Primary map



X

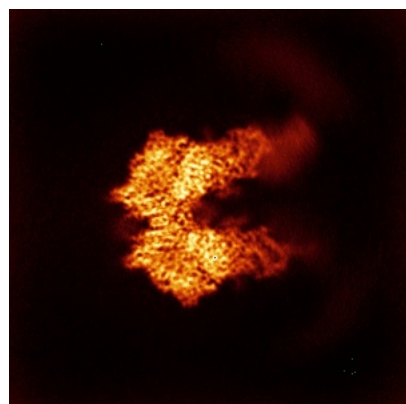


Y

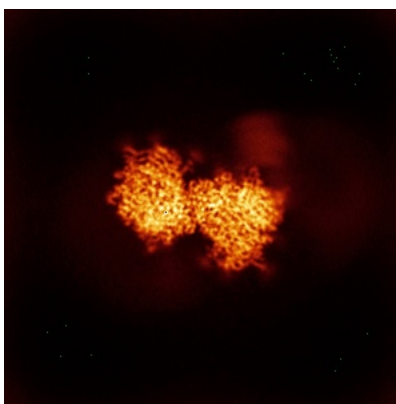


Z

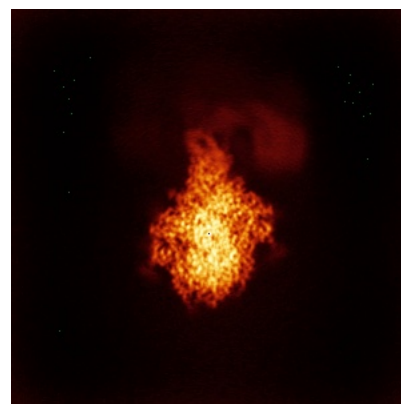
6.4.2 Raw map



X



Y

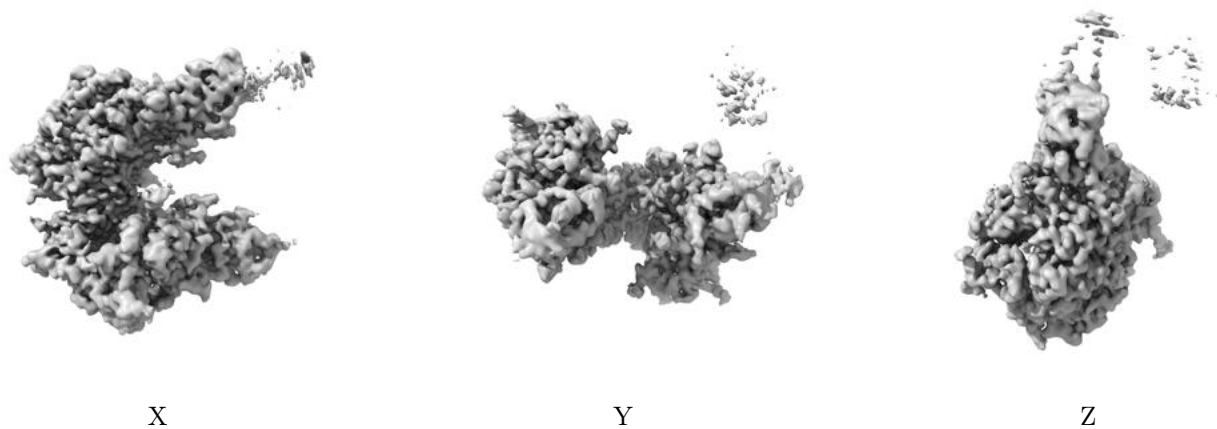


Z

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.

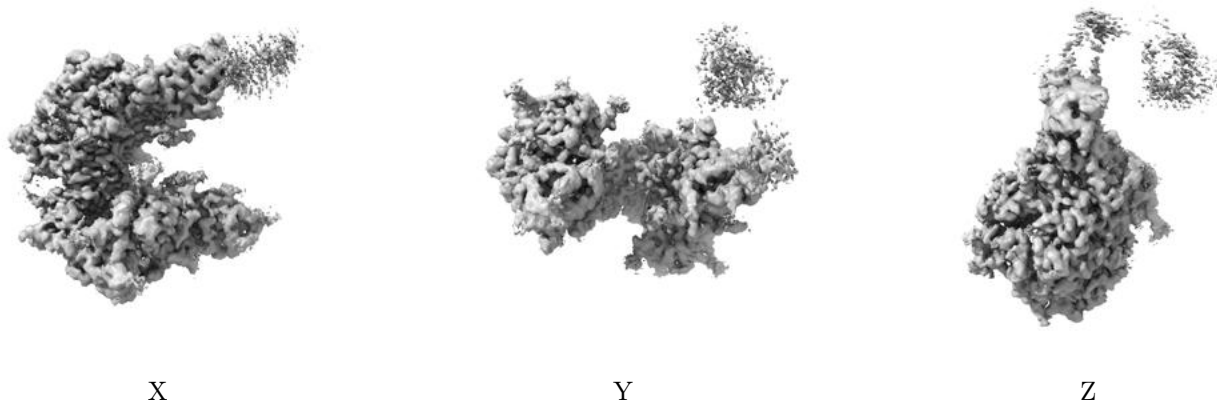
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

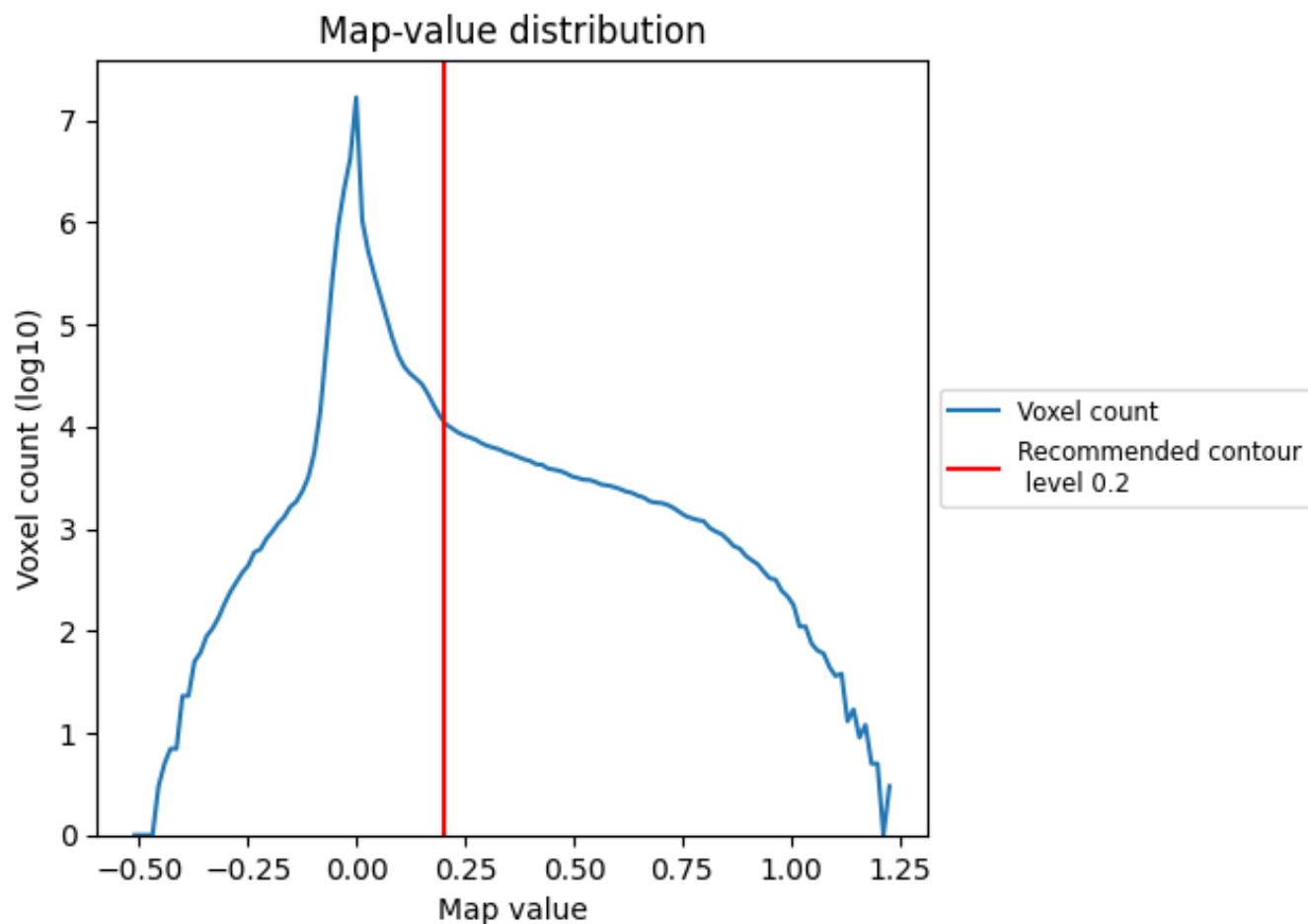
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

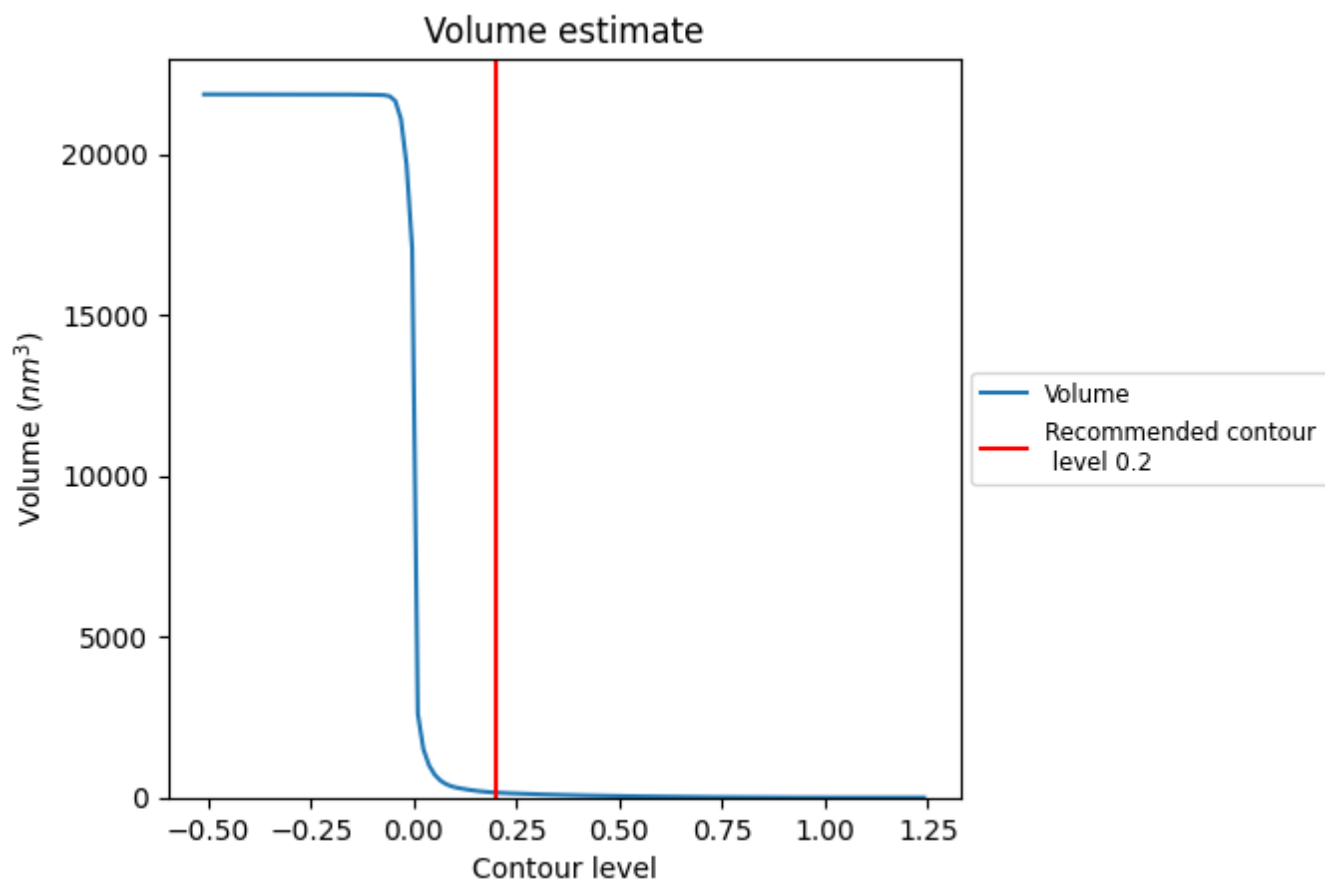
This section contains the results of statistical analysis of the map.

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.

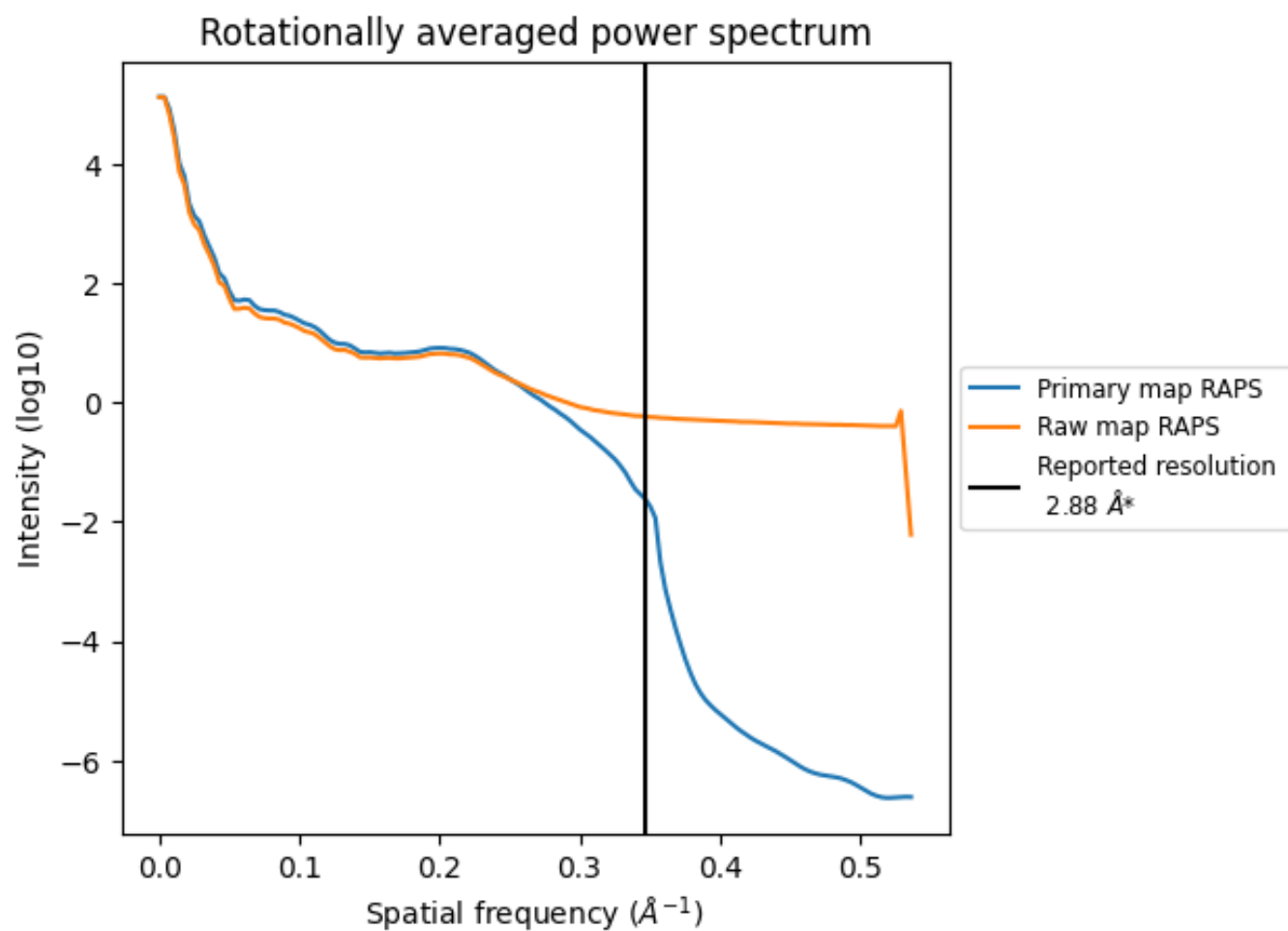
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 154 nm³; this corresponds to an approximate mass of 139 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 ⓘ

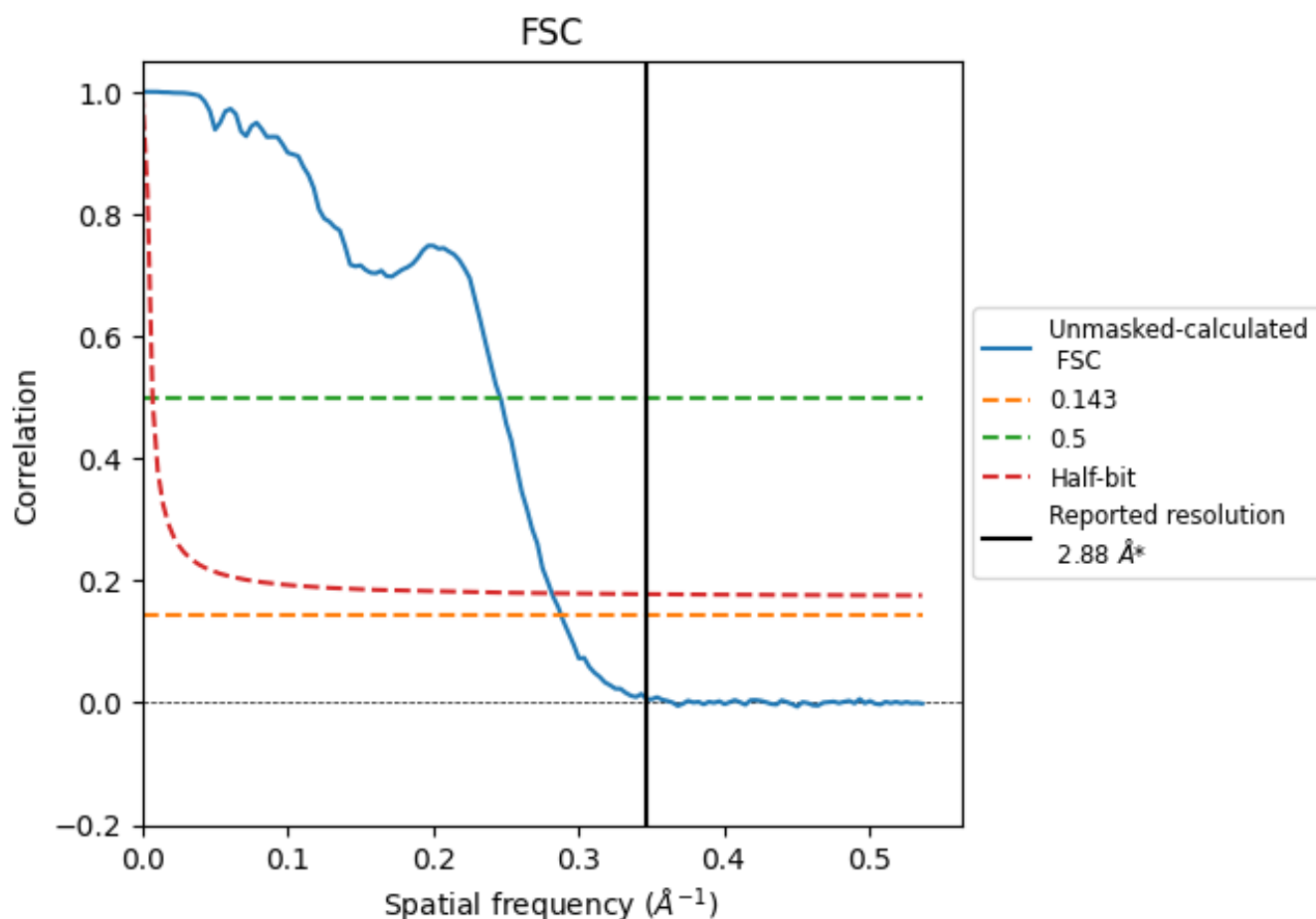


*Reported resolution corresponds to spatial frequency of $0.347 \text{ \AA}^{-1}$

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 $0.347 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

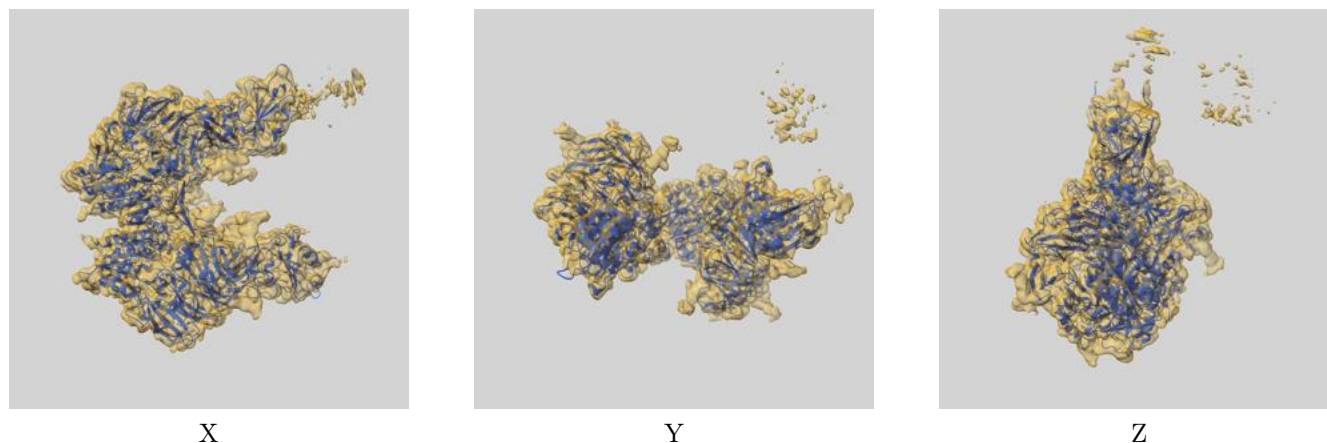
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.88	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.47	4.06	3.55

*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 3.47 differs from the reported value 2.88 by more than 10 %

9 Map-model fit [i](#)

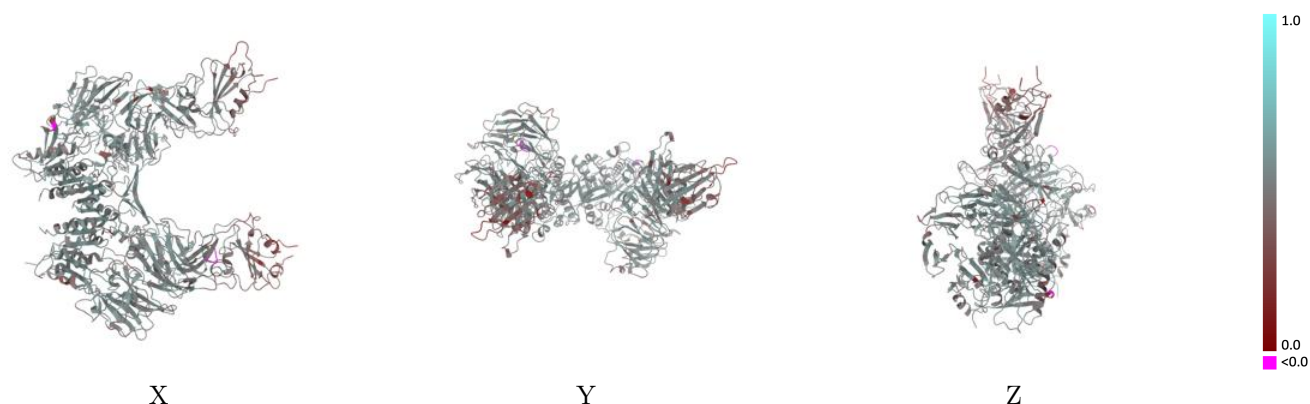
This section contains information regarding the fit between EMDB map EMD-68192 and PDB model 22EB. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

9.1 Map-model overlay [i](#)



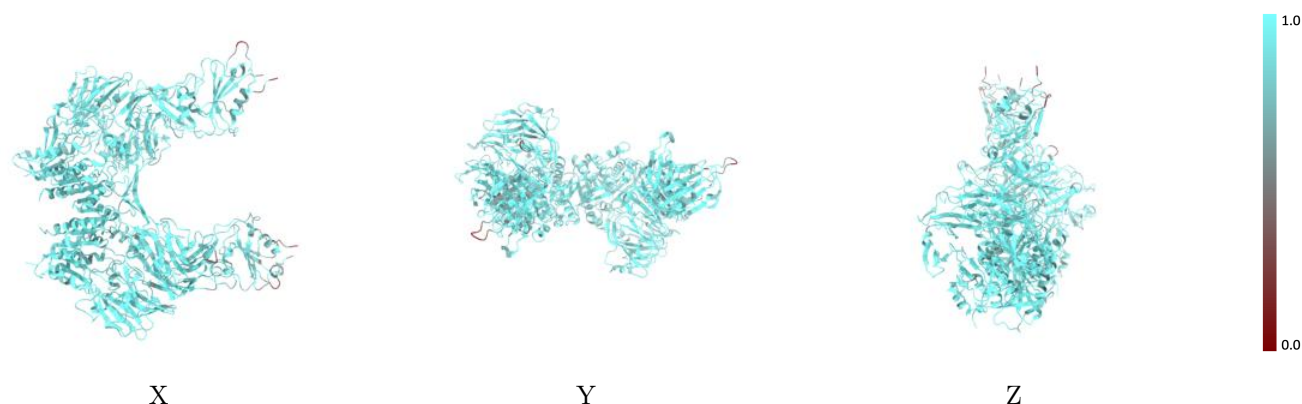
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



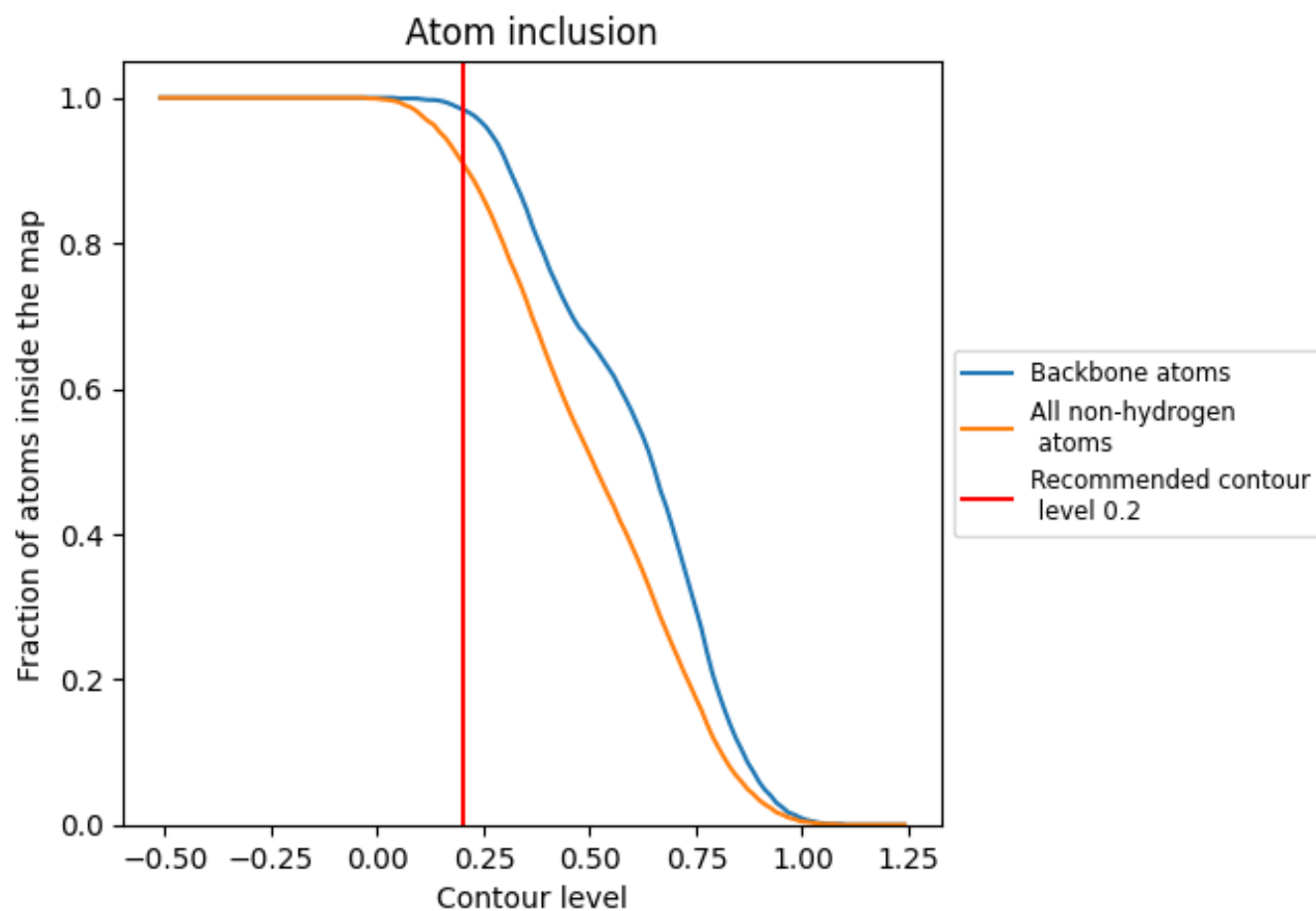
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 91% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9110	0.4920
A	0.9310	0.5110
B	0.9320	0.5120
C	0.8020	0.4010
L	0.8700	0.4410

