



Full wwPDB EM Validation Report ⓘ

Mar 21, 2026 – 03:28 PM UTC

PDB ID : 9FGJ / pdb_00009fgj
EMDB ID : EMD-50408
Title : Cryo-EM structure of Legionella effector SdeC (PDE-mART domain)
Authors : Weng, T.-H.; Misra, M.; Chen, W.; Safarian, S.; Kudryashev, M.; Dikic, I.
Deposited on : 2024-05-24
Resolution : 3.80 Å(reported)
Based on initial model : .

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

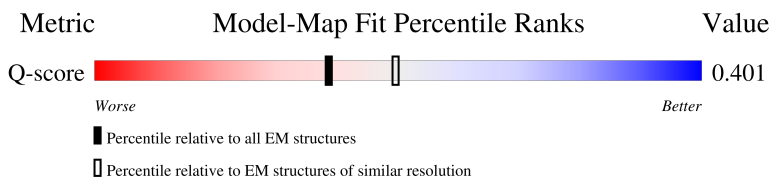
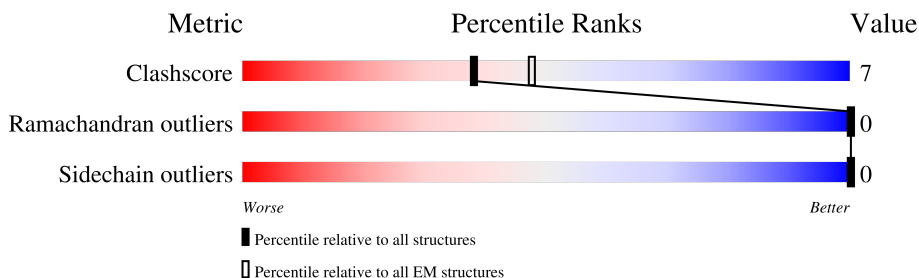
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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	10198 (3.30 - 4.30)

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	1764	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7021 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 SdeC.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	885	7021	4431	1210	1354	26	0	0

There are 231 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-230	MET	-	initiating methionine	UNP Q6RCQ8
A	-229	SER	-	expression tag	UNP Q6RCQ8
A	-228	PRO	-	expression tag	UNP Q6RCQ8
A	-227	ILE	-	expression tag	UNP Q6RCQ8
A	-226	LEU	-	expression tag	UNP Q6RCQ8
A	-225	GLY	-	expression tag	UNP Q6RCQ8
A	-224	TYR	-	expression tag	UNP Q6RCQ8
A	-223	TRP	-	expression tag	UNP Q6RCQ8
A	-222	LYS	-	expression tag	UNP Q6RCQ8
A	-221	ILE	-	expression tag	UNP Q6RCQ8
A	-220	LYS	-	expression tag	UNP Q6RCQ8
A	-219	GLY	-	expression tag	UNP Q6RCQ8
A	-218	LEU	-	expression tag	UNP Q6RCQ8
A	-217	VAL	-	expression tag	UNP Q6RCQ8
A	-216	GLN	-	expression tag	UNP Q6RCQ8
A	-215	PRO	-	expression tag	UNP Q6RCQ8
A	-214	THR	-	expression tag	UNP Q6RCQ8
A	-213	ARG	-	expression tag	UNP Q6RCQ8
A	-212	LEU	-	expression tag	UNP Q6RCQ8
A	-211	LEU	-	expression tag	UNP Q6RCQ8
A	-210	LEU	-	expression tag	UNP Q6RCQ8
A	-209	GLU	-	expression tag	UNP Q6RCQ8
A	-208	TYR	-	expression tag	UNP Q6RCQ8
A	-207	LEU	-	expression tag	UNP Q6RCQ8
A	-206	GLU	-	expression tag	UNP Q6RCQ8
A	-205	GLU	-	expression tag	UNP Q6RCQ8
A	-204	LYS	-	expression tag	UNP Q6RCQ8
A	-203	TYR	-	expression tag	UNP Q6RCQ8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-202	GLU	-	expression tag	UNP Q6RCQ8
A	-201	GLU	-	expression tag	UNP Q6RCQ8
A	-200	HIS	-	expression tag	UNP Q6RCQ8
A	-199	LEU	-	expression tag	UNP Q6RCQ8
A	-198	TYR	-	expression tag	UNP Q6RCQ8
A	-197	GLU	-	expression tag	UNP Q6RCQ8
A	-196	ARG	-	expression tag	UNP Q6RCQ8
A	-195	ASP	-	expression tag	UNP Q6RCQ8
A	-194	GLU	-	expression tag	UNP Q6RCQ8
A	-193	GLY	-	expression tag	UNP Q6RCQ8
A	-192	ASP	-	expression tag	UNP Q6RCQ8
A	-191	LYS	-	expression tag	UNP Q6RCQ8
A	-190	TRP	-	expression tag	UNP Q6RCQ8
A	-189	ARG	-	expression tag	UNP Q6RCQ8
A	-188	ASN	-	expression tag	UNP Q6RCQ8
A	-187	LYS	-	expression tag	UNP Q6RCQ8
A	-186	LYS	-	expression tag	UNP Q6RCQ8
A	-185	PHE	-	expression tag	UNP Q6RCQ8
A	-184	GLU	-	expression tag	UNP Q6RCQ8
A	-183	LEU	-	expression tag	UNP Q6RCQ8
A	-182	GLY	-	expression tag	UNP Q6RCQ8
A	-181	LEU	-	expression tag	UNP Q6RCQ8
A	-180	GLU	-	expression tag	UNP Q6RCQ8
A	-179	PHE	-	expression tag	UNP Q6RCQ8
A	-178	PRO	-	expression tag	UNP Q6RCQ8
A	-177	ASN	-	expression tag	UNP Q6RCQ8
A	-176	LEU	-	expression tag	UNP Q6RCQ8
A	-175	PRO	-	expression tag	UNP Q6RCQ8
A	-174	TYR	-	expression tag	UNP Q6RCQ8
A	-173	TYR	-	expression tag	UNP Q6RCQ8
A	-172	ILE	-	expression tag	UNP Q6RCQ8
A	-171	ASP	-	expression tag	UNP Q6RCQ8
A	-170	GLY	-	expression tag	UNP Q6RCQ8
A	-169	ASP	-	expression tag	UNP Q6RCQ8
A	-168	VAL	-	expression tag	UNP Q6RCQ8
A	-167	LYS	-	expression tag	UNP Q6RCQ8
A	-166	LEU	-	expression tag	UNP Q6RCQ8
A	-165	THR	-	expression tag	UNP Q6RCQ8
A	-164	GLN	-	expression tag	UNP Q6RCQ8
A	-163	SER	-	expression tag	UNP Q6RCQ8
A	-162	MET	-	expression tag	UNP Q6RCQ8
A	-161	ALA	-	expression tag	UNP Q6RCQ8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-160	ILE	-	expression tag	UNP Q6RCQ8
A	-159	ILE	-	expression tag	UNP Q6RCQ8
A	-158	ARG	-	expression tag	UNP Q6RCQ8
A	-157	TYR	-	expression tag	UNP Q6RCQ8
A	-156	ILE	-	expression tag	UNP Q6RCQ8
A	-155	ALA	-	expression tag	UNP Q6RCQ8
A	-154	ASP	-	expression tag	UNP Q6RCQ8
A	-153	LYS	-	expression tag	UNP Q6RCQ8
A	-152	HIS	-	expression tag	UNP Q6RCQ8
A	-151	ASN	-	expression tag	UNP Q6RCQ8
A	-150	MET	-	expression tag	UNP Q6RCQ8
A	-149	LEU	-	expression tag	UNP Q6RCQ8
A	-148	GLY	-	expression tag	UNP Q6RCQ8
A	-147	GLY	-	expression tag	UNP Q6RCQ8
A	-146	CYS	-	expression tag	UNP Q6RCQ8
A	-145	PRO	-	expression tag	UNP Q6RCQ8
A	-144	LYS	-	expression tag	UNP Q6RCQ8
A	-143	GLU	-	expression tag	UNP Q6RCQ8
A	-142	ARG	-	expression tag	UNP Q6RCQ8
A	-141	ALA	-	expression tag	UNP Q6RCQ8
A	-140	GLU	-	expression tag	UNP Q6RCQ8
A	-139	ILE	-	expression tag	UNP Q6RCQ8
A	-138	SER	-	expression tag	UNP Q6RCQ8
A	-137	MET	-	expression tag	UNP Q6RCQ8
A	-136	LEU	-	expression tag	UNP Q6RCQ8
A	-135	GLU	-	expression tag	UNP Q6RCQ8
A	-134	GLY	-	expression tag	UNP Q6RCQ8
A	-133	ALA	-	expression tag	UNP Q6RCQ8
A	-132	VAL	-	expression tag	UNP Q6RCQ8
A	-131	LEU	-	expression tag	UNP Q6RCQ8
A	-130	ASP	-	expression tag	UNP Q6RCQ8
A	-129	ILE	-	expression tag	UNP Q6RCQ8
A	-128	ARG	-	expression tag	UNP Q6RCQ8
A	-127	TYR	-	expression tag	UNP Q6RCQ8
A	-126	GLY	-	expression tag	UNP Q6RCQ8
A	-125	VAL	-	expression tag	UNP Q6RCQ8
A	-124	SER	-	expression tag	UNP Q6RCQ8
A	-123	ARG	-	expression tag	UNP Q6RCQ8
A	-122	ILE	-	expression tag	UNP Q6RCQ8
A	-121	ALA	-	expression tag	UNP Q6RCQ8
A	-120	TYR	-	expression tag	UNP Q6RCQ8
A	-119	SER	-	expression tag	UNP Q6RCQ8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-118	LYS	-	expression tag	UNP Q6RCQ8
A	-117	ASP	-	expression tag	UNP Q6RCQ8
A	-116	PHE	-	expression tag	UNP Q6RCQ8
A	-115	GLU	-	expression tag	UNP Q6RCQ8
A	-114	THR	-	expression tag	UNP Q6RCQ8
A	-113	LEU	-	expression tag	UNP Q6RCQ8
A	-112	LYS	-	expression tag	UNP Q6RCQ8
A	-111	VAL	-	expression tag	UNP Q6RCQ8
A	-110	ASP	-	expression tag	UNP Q6RCQ8
A	-109	PHE	-	expression tag	UNP Q6RCQ8
A	-108	LEU	-	expression tag	UNP Q6RCQ8
A	-107	SER	-	expression tag	UNP Q6RCQ8
A	-106	LYS	-	expression tag	UNP Q6RCQ8
A	-105	LEU	-	expression tag	UNP Q6RCQ8
A	-104	PRO	-	expression tag	UNP Q6RCQ8
A	-103	GLU	-	expression tag	UNP Q6RCQ8
A	-102	MET	-	expression tag	UNP Q6RCQ8
A	-101	LEU	-	expression tag	UNP Q6RCQ8
A	-100	LYS	-	expression tag	UNP Q6RCQ8
A	-99	MET	-	expression tag	UNP Q6RCQ8
A	-98	PHE	-	expression tag	UNP Q6RCQ8
A	-97	GLU	-	expression tag	UNP Q6RCQ8
A	-96	ASP	-	expression tag	UNP Q6RCQ8
A	-95	ARG	-	expression tag	UNP Q6RCQ8
A	-94	LEU	-	expression tag	UNP Q6RCQ8
A	-93	CYS	-	expression tag	UNP Q6RCQ8
A	-92	HIS	-	expression tag	UNP Q6RCQ8
A	-91	LYS	-	expression tag	UNP Q6RCQ8
A	-90	THR	-	expression tag	UNP Q6RCQ8
A	-89	TYR	-	expression tag	UNP Q6RCQ8
A	-88	LEU	-	expression tag	UNP Q6RCQ8
A	-87	ASN	-	expression tag	UNP Q6RCQ8
A	-86	GLY	-	expression tag	UNP Q6RCQ8
A	-85	ASP	-	expression tag	UNP Q6RCQ8
A	-84	HIS	-	expression tag	UNP Q6RCQ8
A	-83	VAL	-	expression tag	UNP Q6RCQ8
A	-82	THR	-	expression tag	UNP Q6RCQ8
A	-81	HIS	-	expression tag	UNP Q6RCQ8
A	-80	PRO	-	expression tag	UNP Q6RCQ8
A	-79	ASP	-	expression tag	UNP Q6RCQ8
A	-78	PHE	-	expression tag	UNP Q6RCQ8
A	-77	MET	-	expression tag	UNP Q6RCQ8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-76	LEU	-	expression tag	UNP Q6RCQ8
A	-75	TYR	-	expression tag	UNP Q6RCQ8
A	-74	ASP	-	expression tag	UNP Q6RCQ8
A	-73	ALA	-	expression tag	UNP Q6RCQ8
A	-72	LEU	-	expression tag	UNP Q6RCQ8
A	-71	ASP	-	expression tag	UNP Q6RCQ8
A	-70	VAL	-	expression tag	UNP Q6RCQ8
A	-69	VAL	-	expression tag	UNP Q6RCQ8
A	-68	LEU	-	expression tag	UNP Q6RCQ8
A	-67	TYR	-	expression tag	UNP Q6RCQ8
A	-66	MET	-	expression tag	UNP Q6RCQ8
A	-65	ASP	-	expression tag	UNP Q6RCQ8
A	-64	PRO	-	expression tag	UNP Q6RCQ8
A	-63	MET	-	expression tag	UNP Q6RCQ8
A	-62	CYS	-	expression tag	UNP Q6RCQ8
A	-61	LEU	-	expression tag	UNP Q6RCQ8
A	-60	ASP	-	expression tag	UNP Q6RCQ8
A	-59	ALA	-	expression tag	UNP Q6RCQ8
A	-58	PHE	-	expression tag	UNP Q6RCQ8
A	-57	PRO	-	expression tag	UNP Q6RCQ8
A	-56	LYS	-	expression tag	UNP Q6RCQ8
A	-55	LEU	-	expression tag	UNP Q6RCQ8
A	-54	VAL	-	expression tag	UNP Q6RCQ8
A	-53	CYS	-	expression tag	UNP Q6RCQ8
A	-52	PHE	-	expression tag	UNP Q6RCQ8
A	-51	LYS	-	expression tag	UNP Q6RCQ8
A	-50	LYS	-	expression tag	UNP Q6RCQ8
A	-49	ARG	-	expression tag	UNP Q6RCQ8
A	-48	ILE	-	expression tag	UNP Q6RCQ8
A	-47	GLU	-	expression tag	UNP Q6RCQ8
A	-46	ALA	-	expression tag	UNP Q6RCQ8
A	-45	ILE	-	expression tag	UNP Q6RCQ8
A	-44	PRO	-	expression tag	UNP Q6RCQ8
A	-43	GLN	-	expression tag	UNP Q6RCQ8
A	-42	ILE	-	expression tag	UNP Q6RCQ8
A	-41	ASP	-	expression tag	UNP Q6RCQ8
A	-40	LYS	-	expression tag	UNP Q6RCQ8
A	-39	TYR	-	expression tag	UNP Q6RCQ8
A	-38	LEU	-	expression tag	UNP Q6RCQ8
A	-37	LYS	-	expression tag	UNP Q6RCQ8
A	-36	SER	-	expression tag	UNP Q6RCQ8
A	-35	SER	-	expression tag	UNP Q6RCQ8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-34	LYS	-	expression tag	UNP Q6RCQ8
A	-33	TYR	-	expression tag	UNP Q6RCQ8
A	-32	ILE	-	expression tag	UNP Q6RCQ8
A	-31	ALA	-	expression tag	UNP Q6RCQ8
A	-30	TRP	-	expression tag	UNP Q6RCQ8
A	-29	PRO	-	expression tag	UNP Q6RCQ8
A	-28	LEU	-	expression tag	UNP Q6RCQ8
A	-27	GLN	-	expression tag	UNP Q6RCQ8
A	-26	GLY	-	expression tag	UNP Q6RCQ8
A	-25	TRP	-	expression tag	UNP Q6RCQ8
A	-24	GLN	-	expression tag	UNP Q6RCQ8
A	-23	ALA	-	expression tag	UNP Q6RCQ8
A	-22	THR	-	expression tag	UNP Q6RCQ8
A	-21	PHE	-	expression tag	UNP Q6RCQ8
A	-20	GLY	-	expression tag	UNP Q6RCQ8
A	-19	GLY	-	expression tag	UNP Q6RCQ8
A	-18	GLY	-	expression tag	UNP Q6RCQ8
A	-17	ASP	-	expression tag	UNP Q6RCQ8
A	-16	HIS	-	expression tag	UNP Q6RCQ8
A	-15	PRO	-	expression tag	UNP Q6RCQ8
A	-14	PRO	-	expression tag	UNP Q6RCQ8
A	-13	LYS	-	expression tag	UNP Q6RCQ8
A	-12	SER	-	expression tag	UNP Q6RCQ8
A	-11	ASP	-	expression tag	UNP Q6RCQ8
A	-10	LEU	-	expression tag	UNP Q6RCQ8
A	-9	GLU	-	expression tag	UNP Q6RCQ8
A	-8	VAL	-	expression tag	UNP Q6RCQ8
A	-7	LEU	-	expression tag	UNP Q6RCQ8
A	-6	PHE	-	expression tag	UNP Q6RCQ8
A	-5	GLN	-	expression tag	UNP Q6RCQ8
A	-4	GLY	-	expression tag	UNP Q6RCQ8
A	-3	PRO	-	expression tag	UNP Q6RCQ8
A	-2	LEU	-	expression tag	UNP Q6RCQ8
A	-1	GLY	-	expression tag	UNP Q6RCQ8
A	0	SER	-	expression tag	UNP Q6RCQ8



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	149762	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	33	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.837	Depositor
Minimum map value	-1.263	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	301.56, 301.56, 301.56	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.077, 1.077, 1.077	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	0.16	0/7151	0.38	0/9662

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	7021	0	7048	104	0
All	All	7021	0	7048	104	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 7.

All (104) 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:297:MET:SD	1:A:414:GLN:NE2	2.58	0.72
1:A:644:MET:HE3	1:A:644:MET:HA	1.72	0.71
1:A:867:ASP:OD2	1:A:896:LYS:NZ	2.24	0.69
1:A:244:ILE:HD11	1:A:291:MET:HE1	1.75	0.67
1:A:685:ASP:OD1	1:A:689:ASN:ND2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1142:ARG:NH1	1:A:1170:GLU:OE2	2.30	0.65
1:A:747:LYS:NZ	1:A:751:ASP:OD1	2.27	0.64
1:A:632:GLU:HG3	1:A:735:VAL:HG11	1.80	0.64
1:A:835:PHE:HD2	1:A:892:LEU:HD11	1.62	0.64
1:A:259:PRO:HD3	1:A:344:ASP:HB3	1.82	0.61
1:A:719:VAL:HG22	1:A:738:THR:HG22	1.82	0.61
1:A:800:LYS:HB2	1:A:1135:LEU:HD21	1.84	0.60
1:A:912:PRO:O	1:A:916:MET:HG3	2.02	0.60
1:A:690:ARG:HG2	1:A:691:ILE:HD13	1.82	0.60
1:A:821:ASN:HB3	1:A:824:LEU:HD12	1.85	0.59
1:A:701:MET:SD	1:A:701:MET:N	2.76	0.59
1:A:664:ARG:O	1:A:664:ARG:NE	2.37	0.58
1:A:746:ASN:O	1:A:750:ILE:HG12	2.03	0.58
1:A:612:MET:HE3	1:A:612:MET:HA	1.87	0.57
1:A:1135:LEU:O	1:A:1139:VAL:HG22	2.03	0.57
1:A:599:MET:HE3	1:A:910:VAL:HG21	1.86	0.57
1:A:698:VAL:HA	1:A:701:MET:HG2	1.87	0.57
1:A:472:ALA:HB1	1:A:476:PRO:HD2	1.86	0.56
1:A:307:ARG:NH1	1:A:787:GLU:OE2	2.38	0.56
1:A:595:ARG:NH2	1:A:866:GLU:OE2	2.39	0.55
1:A:1052:GLN:HB3	1:A:1080:PRO:HD3	1.88	0.55
1:A:256:TYR:CD1	1:A:344:ASP:HA	2.42	0.55
1:A:468:VAL:HB	1:A:544:LEU:HB2	1.88	0.55
1:A:298:ILE:HD12	1:A:328:LEU:HD13	1.89	0.55
1:A:924:ALA:HB2	1:A:1102:VAL:HG21	1.89	0.55
1:A:808:SER:OG	1:A:870:LEU:O	2.25	0.55
1:A:1163:ASP:HA	1:A:1166:ASN:ND2	2.23	0.54
1:A:256:TYR:CE2	1:A:279:ARG:HG2	2.43	0.54
1:A:452:LYS:HB2	1:A:790:LEU:HB2	1.90	0.53
1:A:532:ASP:N	1:A:532:ASP:OD1	2.42	0.53
1:A:598:ASN:HB2	1:A:601:GLU:HG3	1.91	0.53
1:A:502:LYS:HA	1:A:505:LEU:HD13	1.91	0.52
1:A:467:LEU:HD13	1:A:546:ALA:HB2	1.91	0.51
1:A:230:ASP:HA	1:A:299:GLU:OE1	2.11	0.50
1:A:256:TYR:CD2	1:A:279:ARG:HG2	2.46	0.50
1:A:921:VAL:HG13	1:A:1057:LEU:HD22	1.93	0.50
1:A:712:ASP:HA	1:A:716:PHE:HB3	1.93	0.50
1:A:617:CYS:HB3	1:A:624:LEU:O	2.13	0.49
1:A:804:LEU:HD11	1:A:1169:GLN:HB3	1.93	0.49
1:A:667:LYS:HA	1:A:684:GLY:HA3	1.95	0.49
1:A:841:ASP:HB2	1:A:843:LEU:HG	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:905:GLU:OE1	1:A:905:GLU:N	2.45	0.49
1:A:663:MET:HE2	1:A:741:MET:HE1	1.94	0.48
1:A:1063:ALA:O	1:A:1067:GLN:N	2.46	0.48
1:A:657:LYS:HE2	1:A:657:LYS:HB3	1.70	0.48
1:A:1182:HIS:CG	1:A:1189:VAL:HG12	2.50	0.47
1:A:612:MET:SD	1:A:740:LEU:HD11	2.55	0.47
1:A:1048:MET:SD	1:A:1049:LEU:N	2.87	0.47
1:A:913:PHE:O	1:A:917:GLN:HG2	2.14	0.46
1:A:1175:ARG:NH2	1:A:1195:GLU:OE2	2.44	0.46
1:A:1052:GLN:HA	1:A:1078:LYS:HZ2	1.80	0.46
1:A:395:ILE:HG12	1:A:409:HIS:CE1	2.50	0.46
1:A:735:VAL:O	1:A:739:THR:HG22	2.15	0.46
1:A:865:PRO:HG2	1:A:868:VAL:HB	1.97	0.46
1:A:899:ASP:OD2	1:A:1131:ARG:NH2	2.34	0.46
1:A:917:GLN:HB3	1:A:1106:LEU:HD11	1.97	0.46
1:A:899:ASP:OD1	1:A:1180:ARG:NH1	2.48	0.46
1:A:656:ILE:HA	1:A:659:ILE:HD12	1.98	0.46
1:A:655:ASP:O	1:A:659:ILE:HG13	2.15	0.46
1:A:758:PRO:HG3	1:A:860:PHE:HE2	1.80	0.46
1:A:326:GLU:HG3	1:A:330:LYS:HE3	1.97	0.45
1:A:1053:ILE:HD13	1:A:1099:ILE:HD13	1.98	0.45
1:A:385:ASP:OD1	1:A:387:LYS:N	2.50	0.45
1:A:428:GLU:OE2	1:A:428:GLU:N	2.40	0.44
1:A:1204:VAL:O	1:A:1208:LEU:HG	2.18	0.44
1:A:899:ASP:O	1:A:1180:ARG:NH1	2.51	0.44
1:A:385:ASP:OD1	1:A:385:ASP:C	2.61	0.44
1:A:1132:TYR:HB2	1:A:1177:GLU:OE2	2.18	0.44
1:A:431:LEU:HD11	1:A:451:LEU:HD13	1.99	0.44
1:A:673:SER:O	1:A:718:ARG:NH2	2.51	0.44
1:A:839:ASP:OD1	1:A:839:ASP:N	2.50	0.44
1:A:1163:ASP:HA	1:A:1166:ASN:HD21	1.83	0.44
1:A:344:ASP:OD1	1:A:344:ASP:C	2.61	0.43
1:A:475:ASP:N	1:A:476:PRO:HD3	2.33	0.43
1:A:1106:LEU:HD13	1:A:1106:LEU:HA	1.84	0.43
1:A:1058:THR:O	1:A:1062:GLU:HG3	2.19	0.43
1:A:1057:LEU:HA	1:A:1060:CYS:SG	2.59	0.43
1:A:612:MET:SD	1:A:740:LEU:HD21	2.59	0.43
1:A:823:LYS:HA	1:A:826:THR:HG22	2.00	0.43
1:A:782:ILE:HG21	1:A:872:PRO:HD2	2.01	0.43
1:A:925:LEU:O	1:A:929:GLU:HG3	2.18	0.42
1:A:261:LYS:HB3	1:A:261:LYS:HE2	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:597:PRO:HB3	1:A:646:VAL:HG11	2.02	0.42
1:A:718:ARG:NH1	1:A:730:SER:OG	2.51	0.42
1:A:331:ILE:HG21	1:A:411:LEU:HD23	2.02	0.42
1:A:585:GLY:HA2	1:A:795:SER:HB2	2.00	0.42
1:A:256:TYR:CE1	1:A:344:ASP:HA	2.55	0.42
1:A:285:ALA:HB1	1:A:461:THR:HG21	2.01	0.42
1:A:1048:MET:HE1	1:A:1053:ILE:CD1	2.50	0.42
1:A:491:PHE:CG	1:A:505:LEU:HD23	2.54	0.41
1:A:228:SER:OG	1:A:230:ASP:OD1	2.25	0.41
1:A:320:LEU:O	1:A:323:VAL:HG22	2.21	0.41
1:A:807:PHE:HE1	1:A:835:PHE:HE2	1.69	0.41
1:A:1080:PRO:O	1:A:1103:LYS:NZ	2.47	0.41
1:A:659:ILE:HD11	1:A:744:LEU:HD22	2.02	0.41
1:A:468:VAL:HG21	1:A:544:LEU:HD12	2.03	0.40
1:A:644:MET:HB2	1:A:863:TYR:OH	2.22	0.40
1:A:261:LYS:NZ	1:A:268:GLU:O	2.36	0.40
1:A:663:MET:CE	1:A:741:MET:HE1	2.52	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	A	881/1764 (50%)	860 (98%)	21 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	770/1539 (50%)	770 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	A	409	HIS
1	A	754	HIS
1	A	773	ASN
1	A	777	ASN
1	A	1052	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.

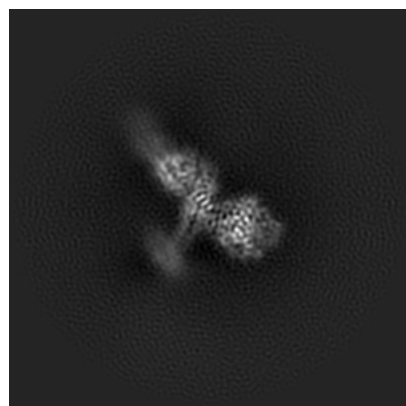
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50408. These allow visual inspection of the internal detail of the map and identification of artifacts.

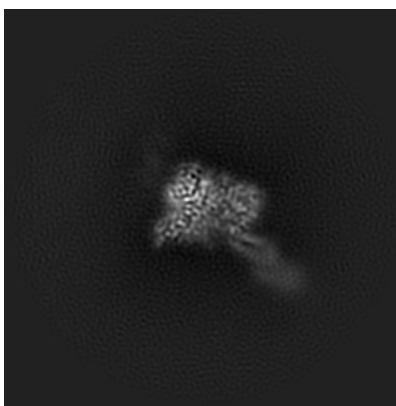
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

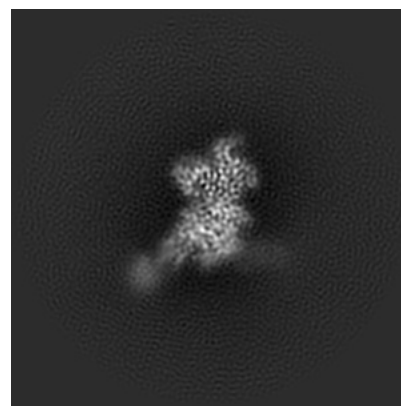
6.1.1 Primary map



X

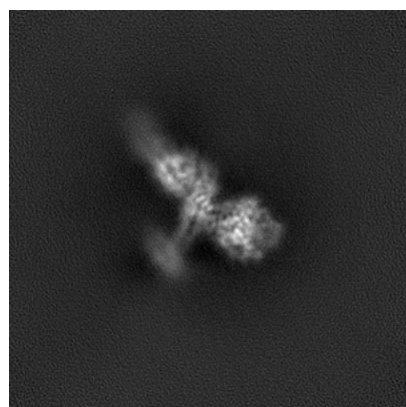


Y

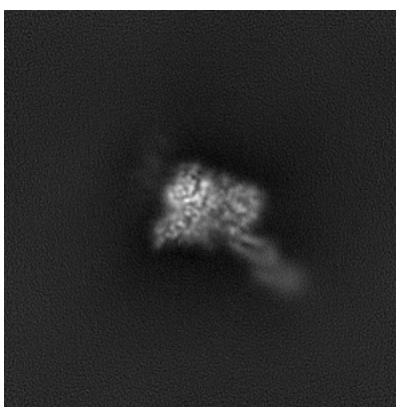


Z

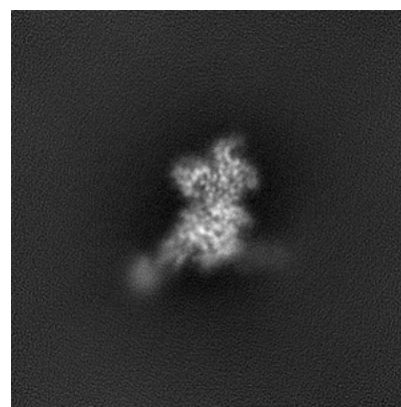
6.1.2 Raw map



X



Y

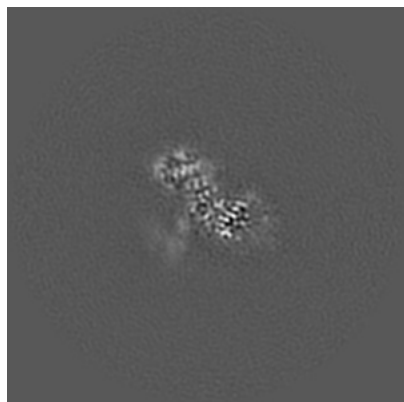


Z

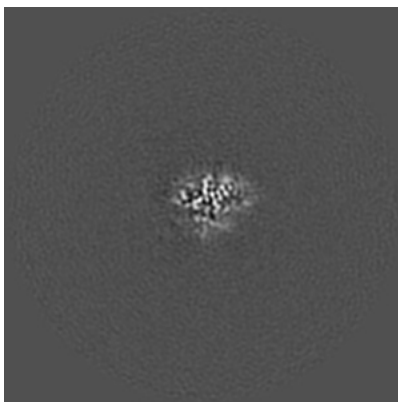
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

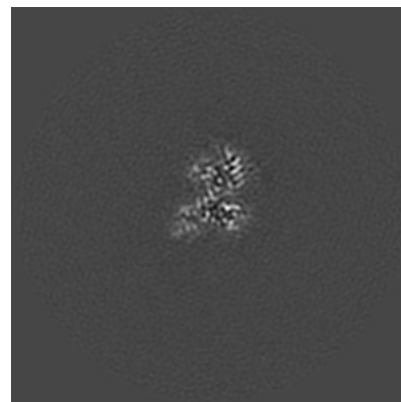
6.2.1 Primary map



X Index: 140

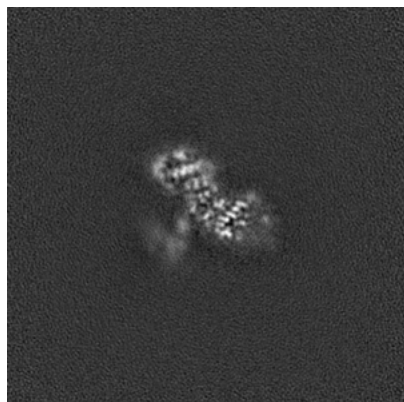


Y Index: 140

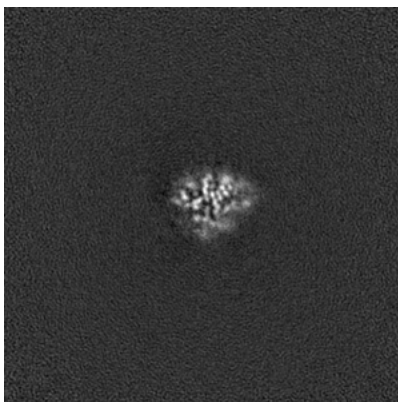


Z Index: 140

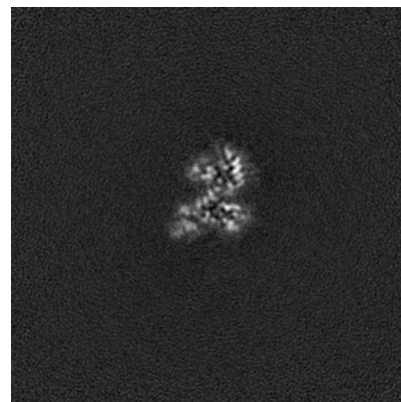
6.2.2 Raw map



X Index: 140



Y Index: 140

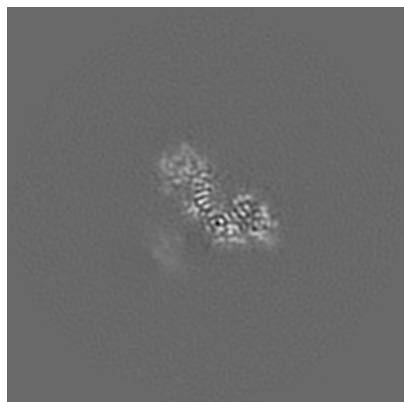


Z Index: 140

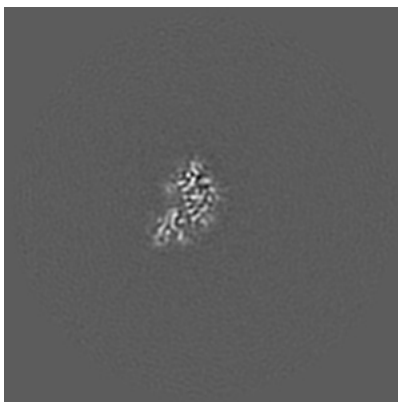
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

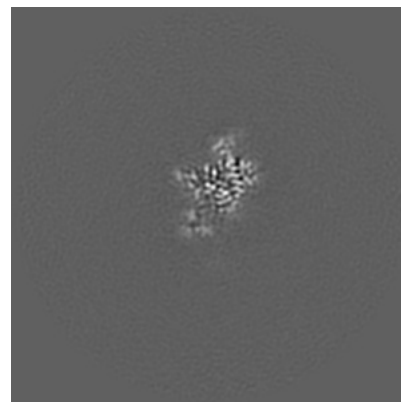
6.3.1 Primary map



X Index: 150

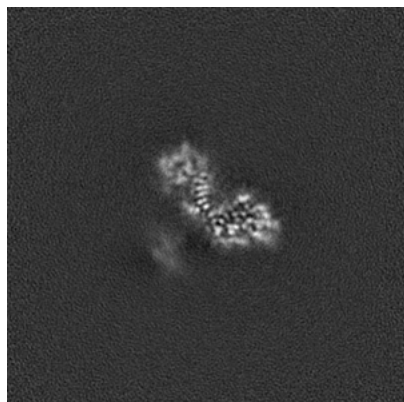


Y Index: 166

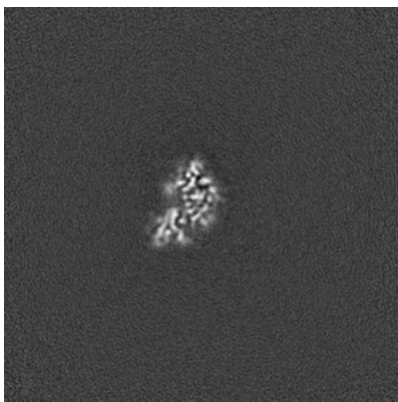


Z Index: 130

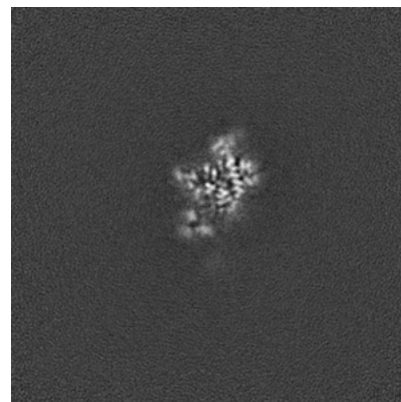
6.3.2 Raw map



X Index: 151



Y Index: 166

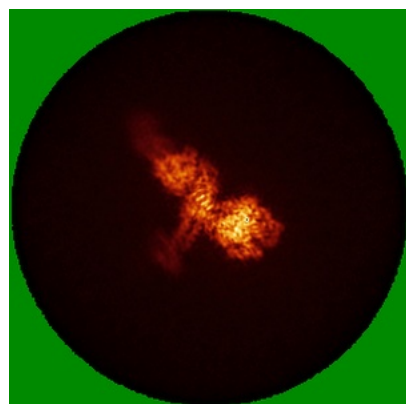


Z Index: 130

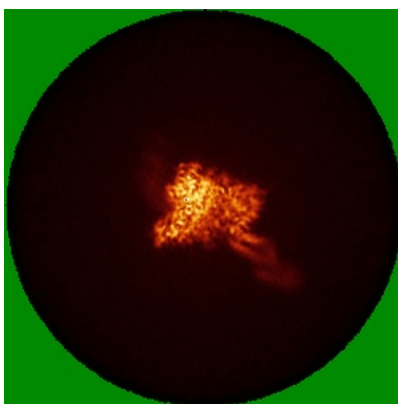
The images above show the largest variance slices of the map in three orthogonal directions.

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

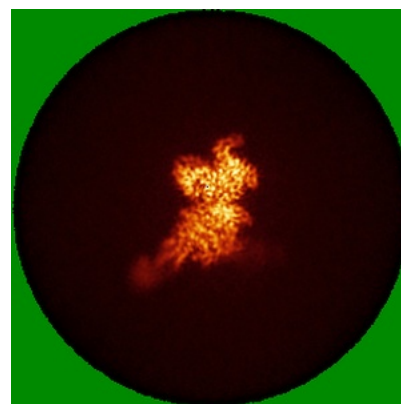
6.4.1 Primary map



X

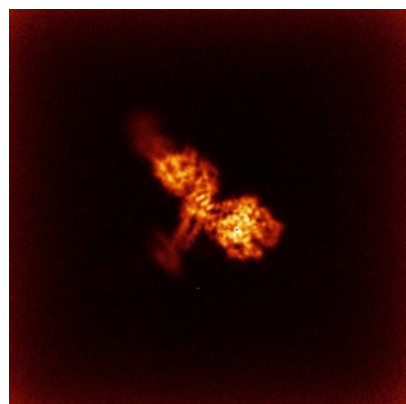


Y



Z

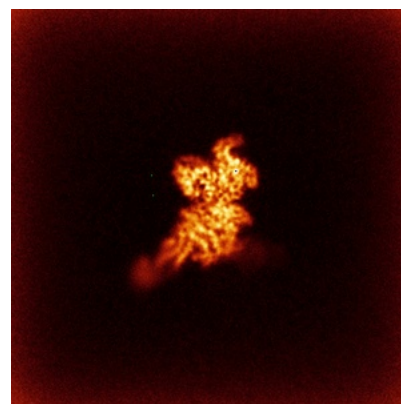
6.4.2 Raw map



X



Y

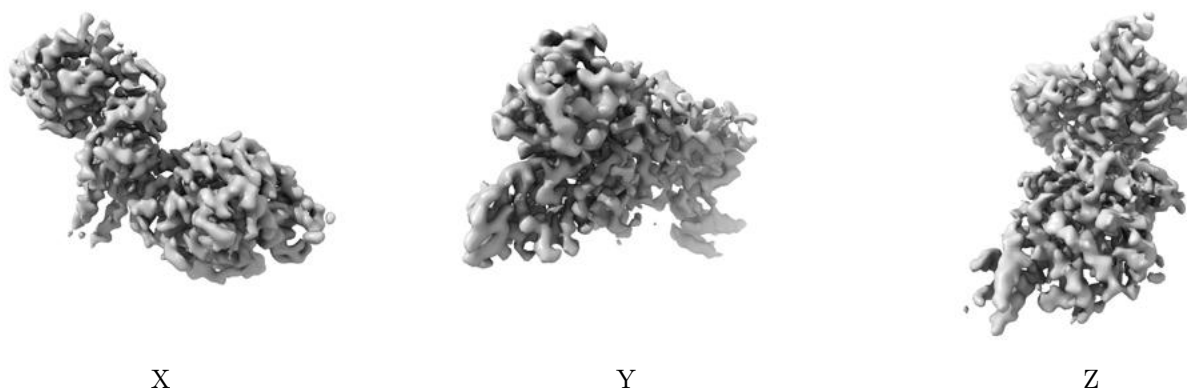


Z

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.

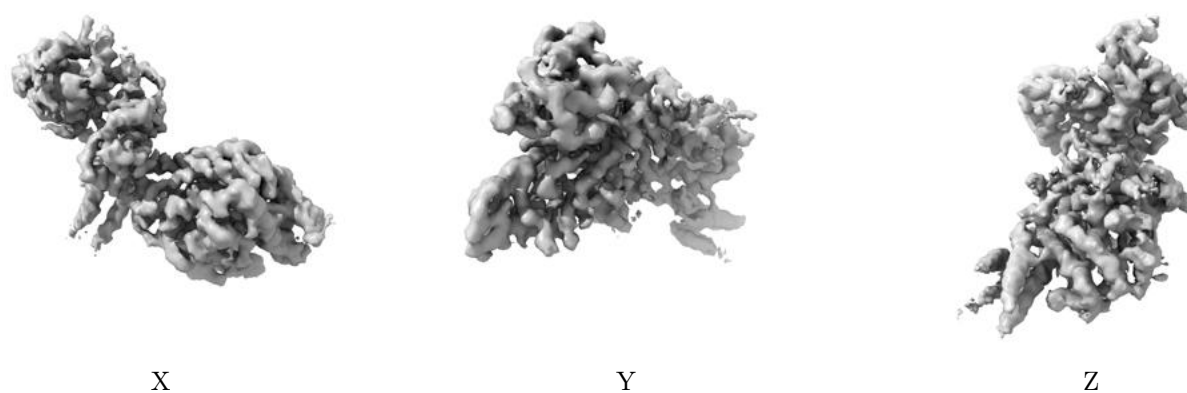
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.35. 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.

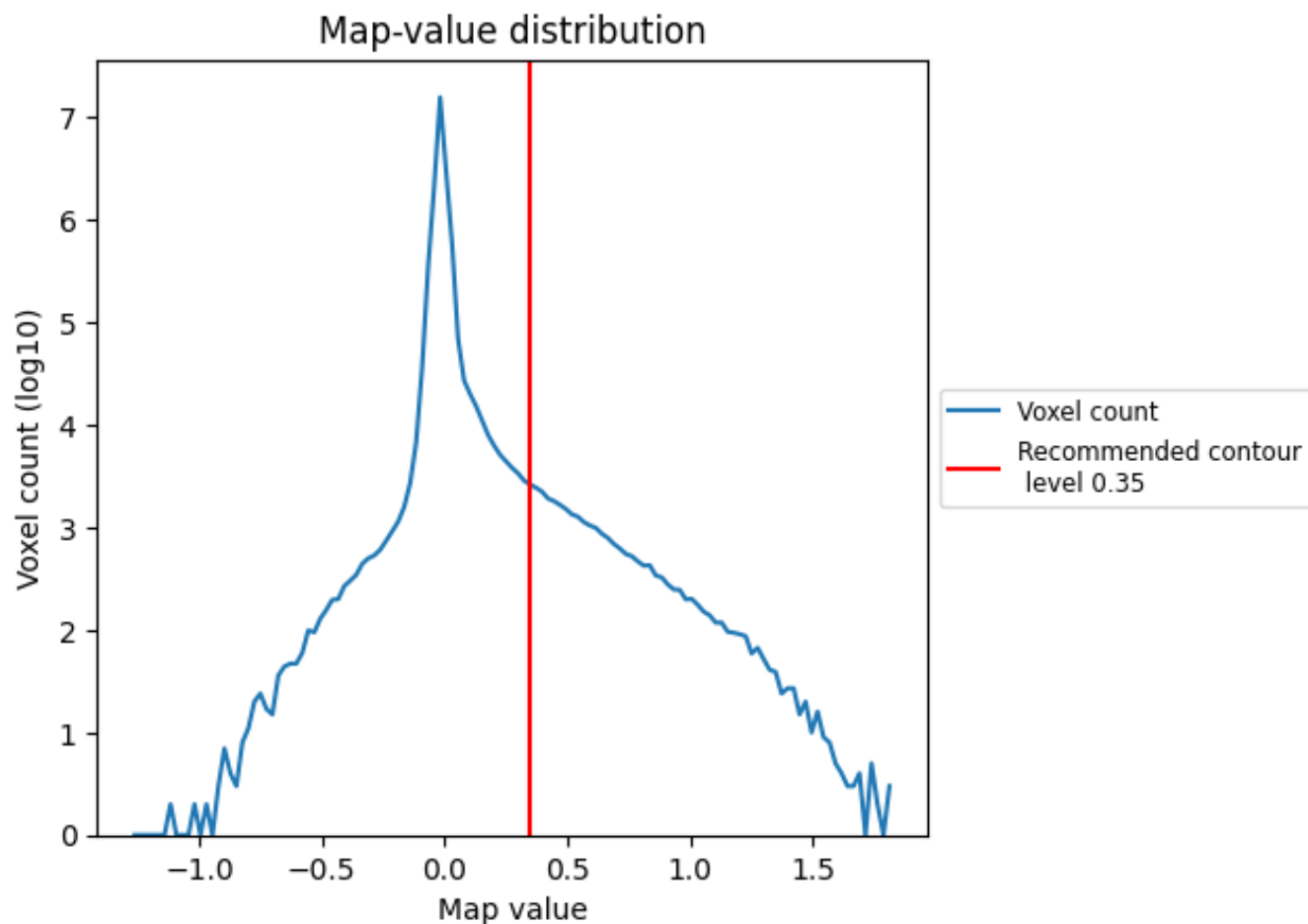
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

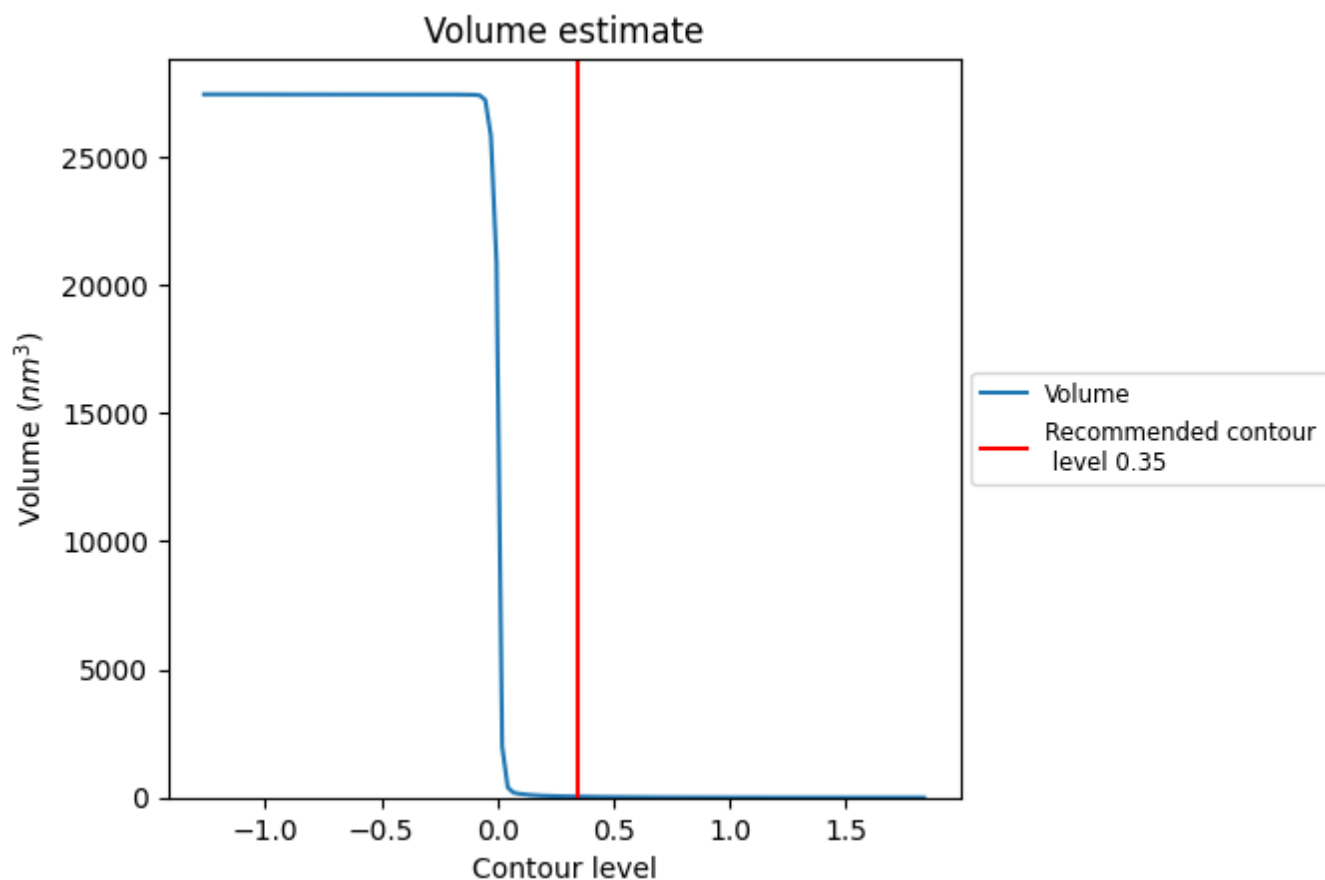
This section contains the results of statistical analysis of the map.

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.

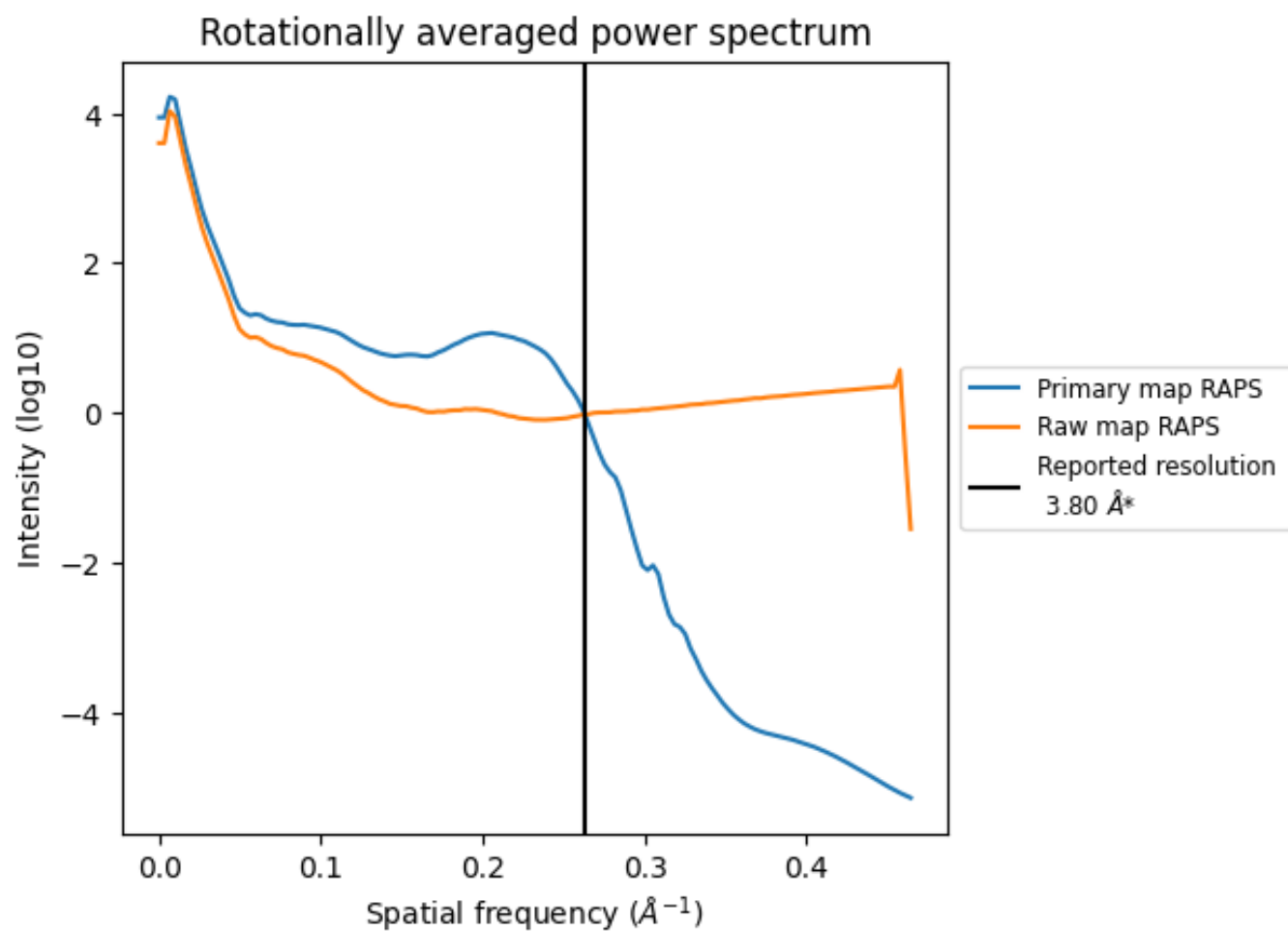
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 36 nm³; this corresponds to an approximate mass of 32 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 ⓘ

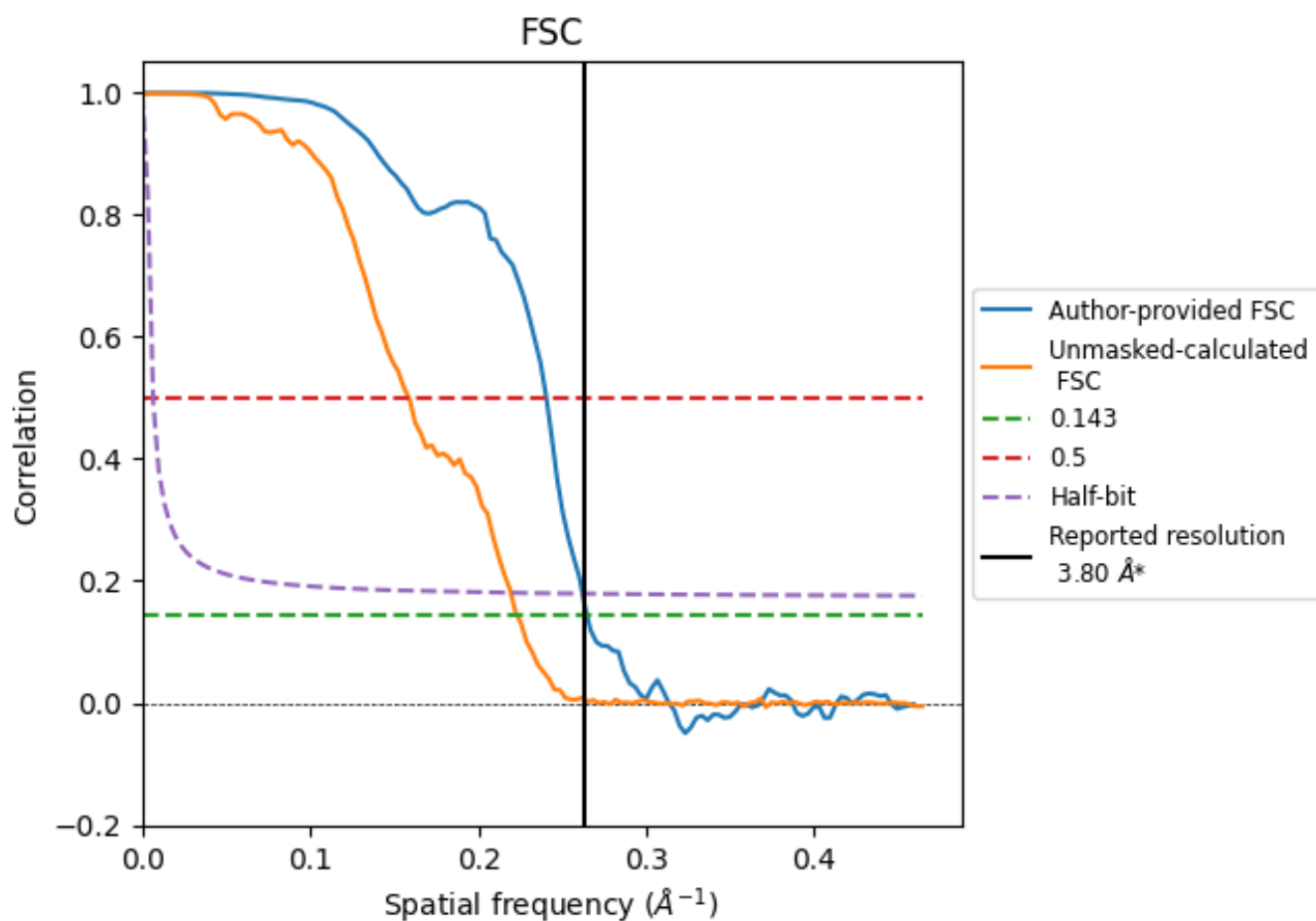


*Reported resolution corresponds to spatial frequency of $0.263 \text{ \AA}^{-1}$

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 0.263 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

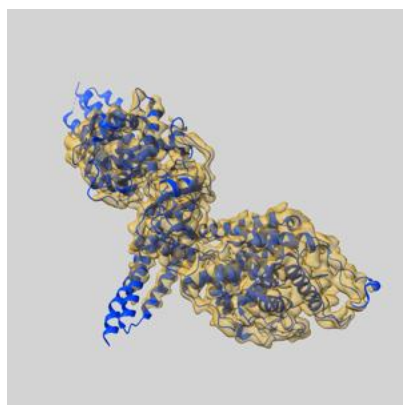
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.78	4.16	3.82
Unmasked-calculated*	4.48	6.30	4.56

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.48 differs from the reported value 3.8 by more than 10 %

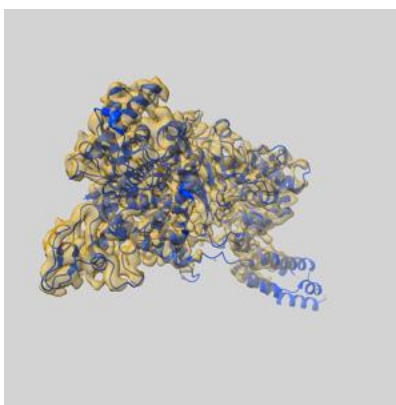
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-50408 and PDB model 9FGJ. Per-residue inclusion information can be found in section 3 on page 9.

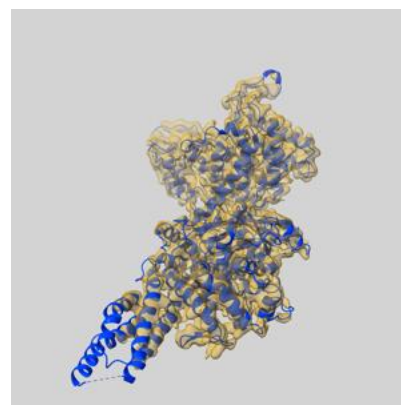
9.1 Map-model overlay [i](#)



X



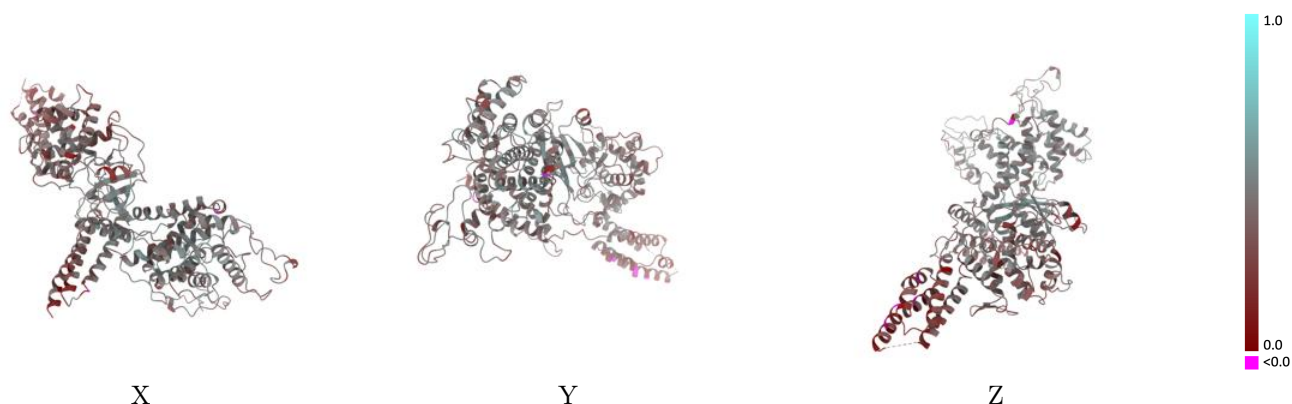
Y



Z

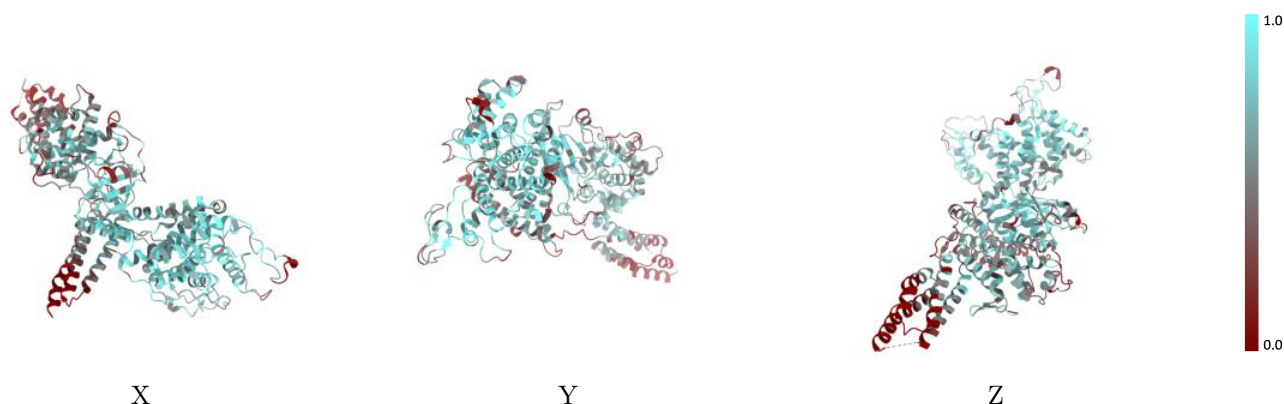
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



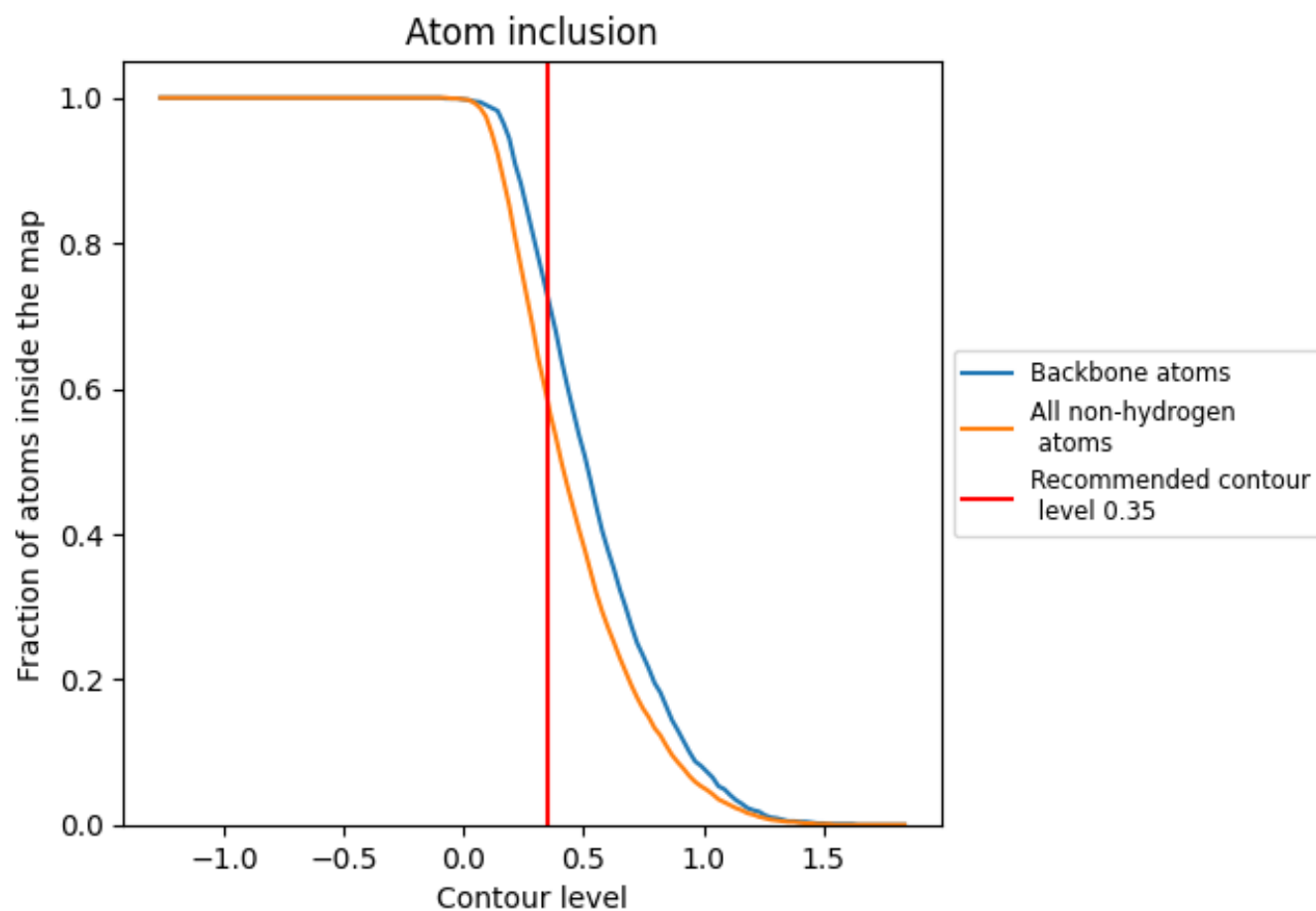
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.35).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 58% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5840	0.4010
A	0.5840	0.4010

