



wwPDB EM Validation Summary Report ⓘ

Mar 10, 2026 – 12:07 AM UTC

PDB ID : 9JWG / pdb_00009jwg
EMDB ID : EMD-61852
Title : Cryo-EM Focused Refined Map of Human RNF213 E3 module and IpaH1.4 LRR domain
Authors : Zhang, H.
Deposited on : 2024-10-10
Resolution : 3.47 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
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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

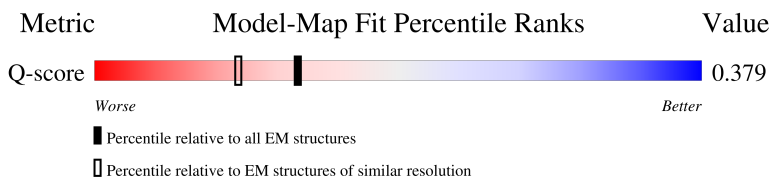
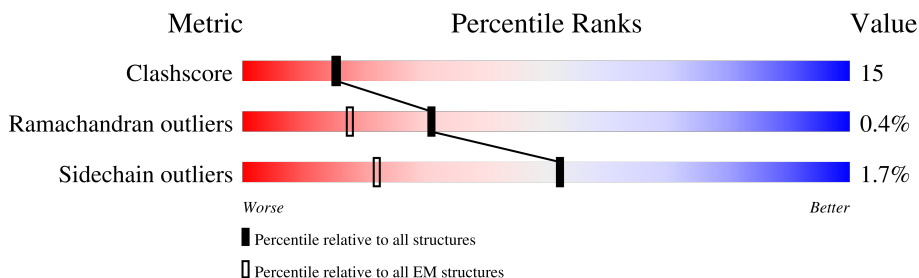
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.47 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	13733 (2.97 - 3.97)

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	B	579	
2	A	4841	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11647 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 E3 ubiquitin-protein ligase IpaH1.4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	235	Total	C	N	O	S	0	0
			1872	1199	322	346	5		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP A0A0H2USG1
B	-2	PRO	-	expression tag	UNP A0A0H2USG1
B	-1	GLY	-	expression tag	UNP A0A0H2USG1
B	0	SER	-	expression tag	UNP A0A0H2USG1
B	37	MET	CYS	conflict	UNP A0A0H2USG1
B	267	ARG	GLN	conflict	UNP A0A0H2USG1

- Molecule 2 is a protein called Ring finger protein 213.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	1221	Total	C	N	O	S	0	0
			9775	6222	1702	1792	59		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	367	GLY	-	expression tag	UNP A0A0A0MTR7
A	368	PRO	-	expression tag	UNP A0A0A0MTR7
A	369	GLY	-	expression tag	UNP A0A0A0MTR7
A	370	THR	-	expression tag	UNP A0A0A0MTR7





V3952	F3953	Q3880	H3756	PHE	ILE	GLU	LEU	ARG	ALA	GLU	THR	THR	ALA	THR	ALA	HIS	ILE	LYS	GLU	LYS	ASP	ASP	LYS	ASP	TRP	ALA	ARG	LEU
F3953	F3954	Q3884	G3757	ILE	GLN	GLU	ARG	ASP	ASP	MET	THR	THR	LEU	THR	GLY	GLN	VAL	TYR	ILE	GLY	GLY	GLY	GLY	MET	ALA	PHE	ARG	VAL
L3955	L3955	L3885	P3759	SER	ASN	GLN	ASN	GLN	ASN	GLU	VAL	VAL	GLU	GLU	GLY	VAL	GLU	ASP	PHE	GLY	GLY	GLY	GLY	LYS	PRO	GLN	GLY	GLY
D3956	D3956	Q3760	Q3760	ASP	GLN	THR	GLU	THR	THR	GLU	PHE	PHE	GLY	GLY	GLY	GLU	GLU	GLY	LEU	LEU	LEU	LEU	LEU	LEU	ALA	ASP	GLY	GLY
K3957	K3957	L3889	Q3761	THR	MET	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
C3958	C3958	S3890	E3762	MET	GLU	SER	ALA	CYS	ALA	SER	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
L3959	L3959	M3891	C3766	LEU	LEU	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
R3960	R3960	P3892	C3766	LEU	GLN	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU
		L3893	K3769	ASN	ALA	GLY	ASN	ASN	GLY	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
S3963	S3963	E3894	K3795	ILE	ILE	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
D3964	D3964	L3895	K3795	PRO	GLY	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU
T3967	T3967	L3896	K3795	LEU	LEU	THR	ARG	ARG	VAL	VAL	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
		C3897	M3789	VAL	MET	PHE	ARG	ARG	VAL	VAL	PHE	PHE	ASP	ASP	ASP	ASN	ASN	CYS	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
P3970	P3970	M3902	M3789	MET	ASN	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
F3971	F3971	L3902	C3794	ASN	ASN	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
E3972	E3972	M3902	T3795	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU
A3973	A3973	S3905	R3796	ARG	ARG	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
V3974	V3974	L3908	K3797	HIS	HIS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS
M3975	M3975	A3909	L3798	LYS	GLY	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU
		L3978	H3815	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
C3979	C3979	V3912	L3816	MET	ALA	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
E3980	E3980	I3913	L3816	ALA	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
C3981	C3981	R3914	Q3819	TYR	TYR	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
K3982	K3982	E3915	R3820	ILE	ILE	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
E3983	E3983	V3916	F3821	VAL	VAL	PRO	CYS	CYS	ALA	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU
T3984	T3984	S3925	N3827	VAL	VAL	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU
A3985	A3985	Q3919	S3823	GLN	GLN	LEU	ALA	ALA	ALA	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
S3986	S3986	L3922	R3824	ASN	ASN	ALA	ALA	ALA	ALA	LYS	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
K3987	K3987	I3923	L3825	HIS	HIS	SER	PHE	PHE	THR	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU
T3988	T3988	F3924	Q3826	MET	MET	LEU	LEU	LEU	LEU	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
L3989	L3989	S3924	N3827	ILE	ILE	ARG	ARG	ARG	ARG	SER	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
S3990	S3990	F3925	F3828	SER	SER	VAL	VAL	VAL	VAL	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU
R3991	R3991	T3926	S3829	PHE	PHE	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU
F3992	F3992	A3927	R3830	ILE	ILE	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
		L3928	T3833	ASP	ASP	MET	MET	MET	MET	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
S3998	S3998	F3929	T3833	ARG	ARG	ARG	ARG	ARG	ARG	SER	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN
T3999	T3999	V3930	L3842	ASP	ASP	GLY	GLY	GLY	GLY	VAL	PHE	PHE	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU
C4000	C4000	L4001	L3842	ASN	ASN	ASN	ASN	ASN	ASN	SER	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
G4002	G4002	V3933	A3845	LEU	LEU	LEU	PHE	PHE	LEU	ILE	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO
D4003	D4003	L3934	A3845	GLU	GLU	GLU	LEU	LEU	LEU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
A4004	A4004	G3956	N3848	LEU	LEU	LEU	LEU	LEU	LEU	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
K4005	K4005	T3937	G3853	LEU	LEU	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
D4006	D4006	E3938	T3729	THR	THR	GLN	GLN	GLN	GLN	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE
P4007	P4007	S3939	T3730	ARG	ARG	GLU	GLU	GLU	GLU	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
		R3940	T3730	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU
		V3941	M3856	GLY	GLY	SER	SER	SER	SER	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
C4012	C4012	P3942	P3736	ASP	ASP	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
D4013	D4013	F3942	K3737	GLN	GLN	ARG	ARG	ARG	ARG	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE
H4014	H4014	E3943	K3738	PHE	PHE	SER	SER	SER	SER	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
V4015	V4015	L3944	M3864	HIS	HIS	CYS	CYS	CYS	CYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS
H4016	H4016	Q3945	Q3745	PRO	PRO	VAL	VAL	VAL	VAL	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG
C4017	C4017	G3946	T3746	LEU	LEU	GLN	GLN	GLN	GLN	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
L4018	L4018	L3947	T3867	ALA	ALA	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
R4019	R4019	T3948	K3876	ASP	ASP	GLY	GLY	GLY	GLY	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
C4020	C4020	T3949	P3877	LEU	LEU	LEU	LEU	LEU	LEU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
L4021	L4021	E3960	R3750	THR	THR	ALA	ALA	ALA	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
R4022	R4022	H3951	L3755	ARG	ARG	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	137886	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 ($e^-/\text{\AA}^2$)	49.41	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.542	Depositor
Minimum map value	-1.493	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.048	Depositor
Recommended contour level	0.18	Depositor
Map size (Å)	527.5, 527.5, 527.5	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.055, 1.055, 1.055	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	B	0.12	0/1916	0.33	0/2615
2	A	0.54	22/9978 (0.2%)	0.67	27/13512 (0.2%)
All	All	0.50	22/11894 (0.2%)	0.62	27/16127 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	0	3

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3934	LEU	CA-C	-11.75	1.36	1.52
2	A	3929	PHE	CA-C	-11.07	1.37	1.52
2	A	3926	THR	CA-C	-9.73	1.39	1.52
2	A	4926	GLU	CA-C	-8.92	1.40	1.52
2	A	3935	LEU	CA-C	-7.79	1.41	1.52

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3939	SER	N-CA-C	-13.61	96.52	111.36
2	A	3929	PHE	N-CA-C	-9.38	99.42	112.45
2	A	3935	LEU	N-CA-C	-8.73	101.46	112.90
2	A	4925	VAL	N-CA-C	8.44	119.22	110.62
2	A	3938	GLU	N-CA-CB	-7.89	98.50	110.73

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	3972	GLU	Mainchain
2	A	4079	LYS	Peptide
2	A	4268	ILE	Peptide

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	B	1872	0	1900	33	0
2	A	9775	0	9858	313	0
All	All	11647	0	11758	343	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 15.

The worst 5 of 343 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)
2:A:3928:LEU:HD13	2:A:4072:LEU:HB3	1.61	0.82
2:A:4428:PRO:HB2	2:A:4595:SER:HB3	1.64	0.78
2:A:4908:TYR:HB3	2:A:4969:PRO:HD2	1.64	0.78
2:A:4308:LYS:HB3	2:A:4310:VAL:HG12	1.66	0.77
2:A:4976:ILE:HG13	2:A:4977:PRO:HD2	1.66	0.77

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	B	233/579 (40%)	228 (98%)	5 (2%)	0	100	100
2	A	1207/4841 (25%)	1077 (89%)	124 (10%)	6 (0%)	24	58
All	All	1440/5420 (27%)	1305 (91%)	129 (9%)	6 (0%)	31	62

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	4901	LEU
2	A	4003	ASP
2	A	4927	ARG
2	A	3989	LEU
2	A	4900	LYS

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	B	214/503 (42%)	213 (100%)	1 (0%)	81	80
2	A	1093/4330 (25%)	1072 (98%)	21 (2%)	50	67
All	All	1307/4833 (27%)	1285 (98%)	22 (2%)	52	69

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	4061	PHE
2	A	4800	ASN
2	A	4329	VAL
2	A	4924	GLU
2	A	3986	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	4587	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	4599	GLN
2	A	4936	ASN
2	A	4691	HIS
2	A	4728	HIS

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.

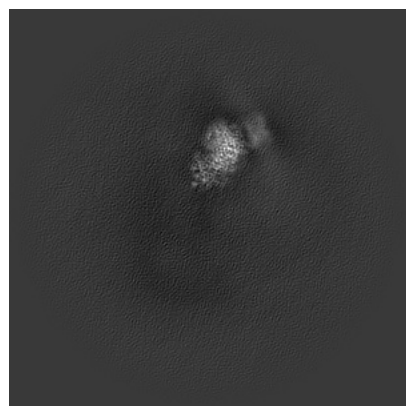
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61852. These allow visual inspection of the internal detail of the map and identification of artifacts.

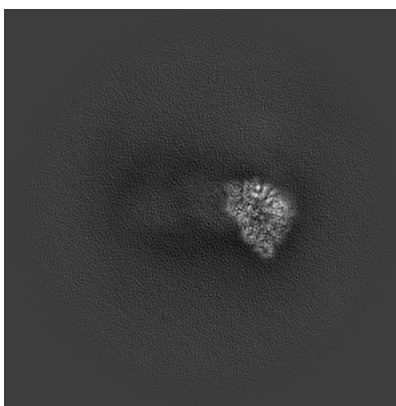
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

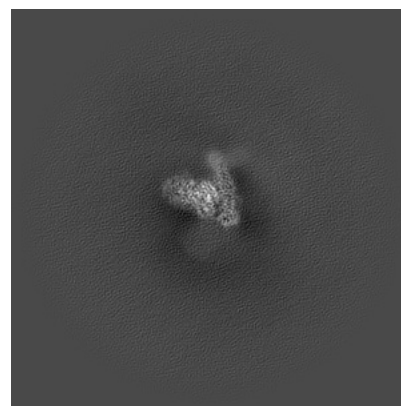
6.1.1 Primary map



X

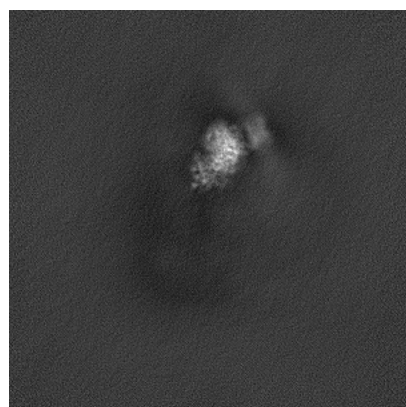


Y

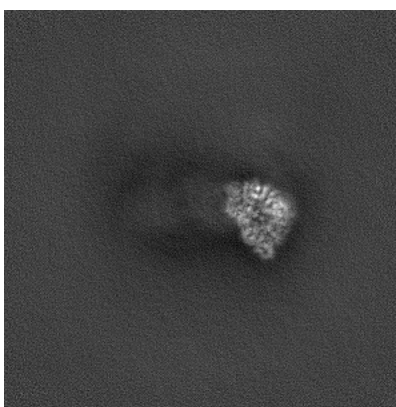


Z

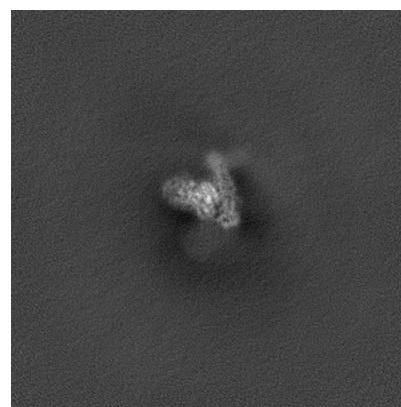
6.1.2 Raw map



X



Y



Z

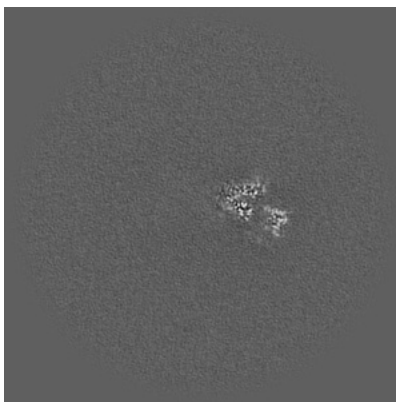
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

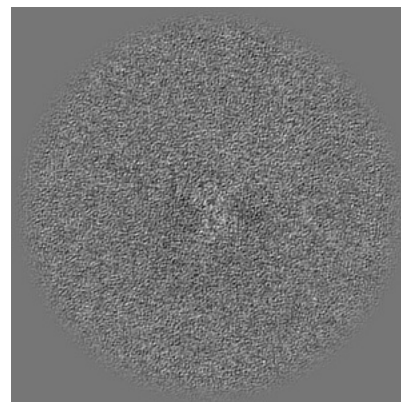
6.2.1 Primary map



X Index: 250



Y Index: 250

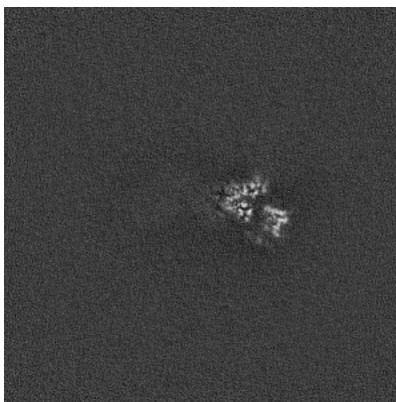


Z Index: 250

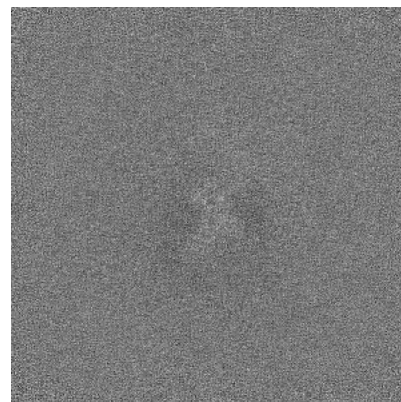
6.2.2 Raw map



X Index: 250



Y Index: 250



Z Index: 250

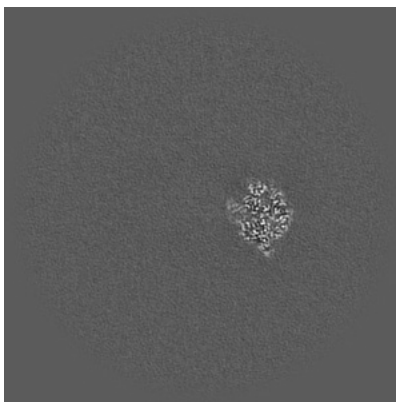
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

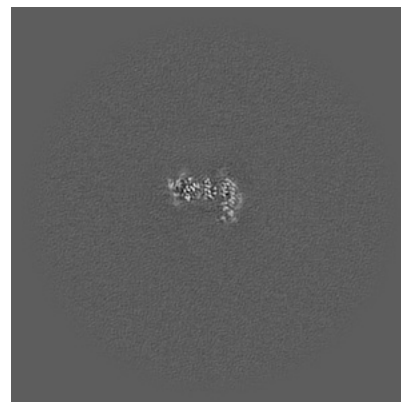
6.3.1 Primary map



X Index: 247

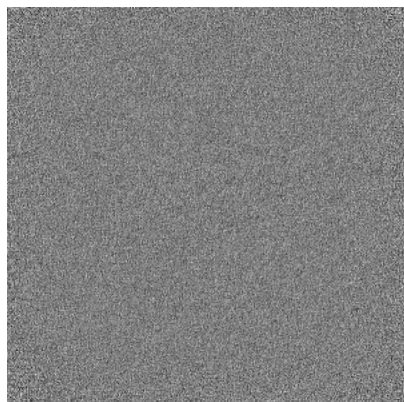


Y Index: 269

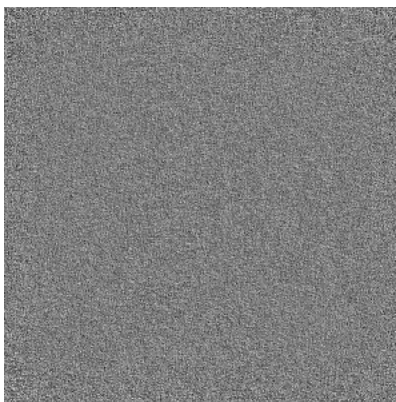


Z Index: 316

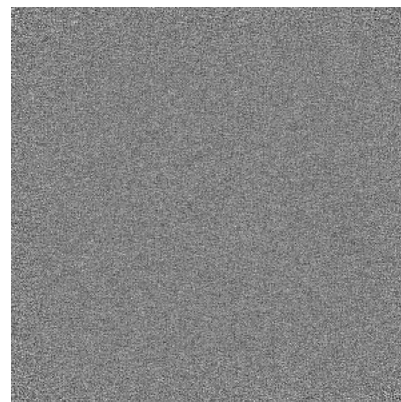
6.3.2 Raw map



X Index: 0



Y Index: 0

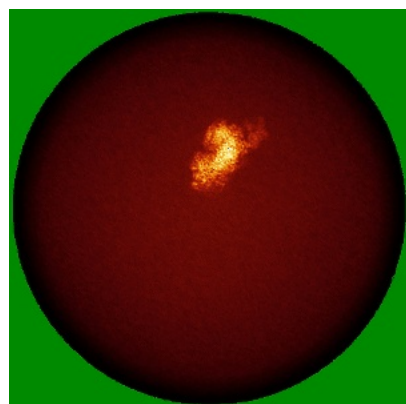


Z Index: 0

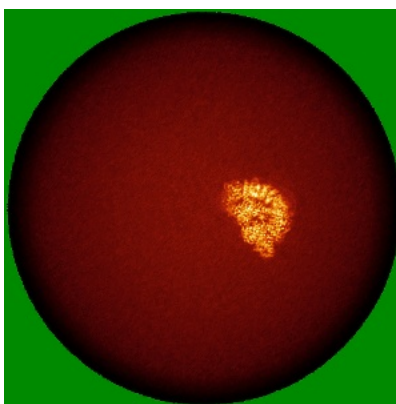
The images above show the largest variance slices of the map in three orthogonal directions.

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

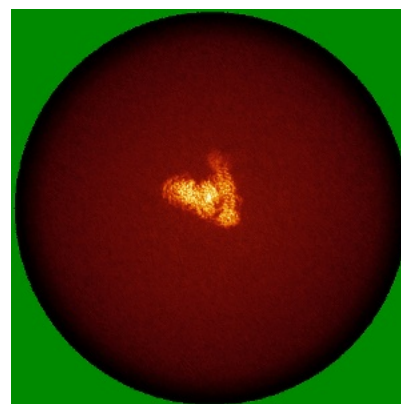
6.4.1 Primary map



X

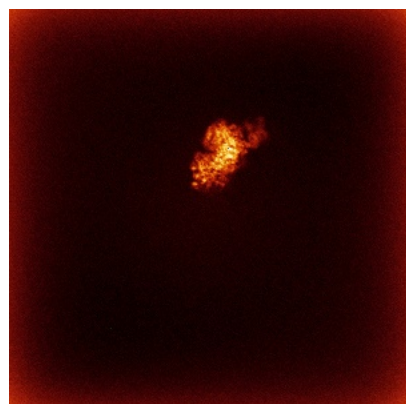


Y

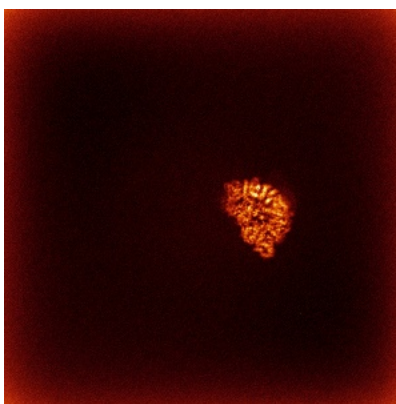


Z

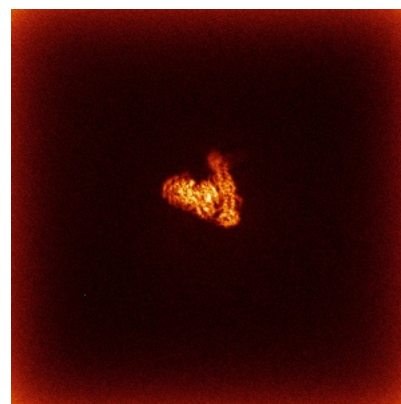
6.4.2 Raw map



X



Y

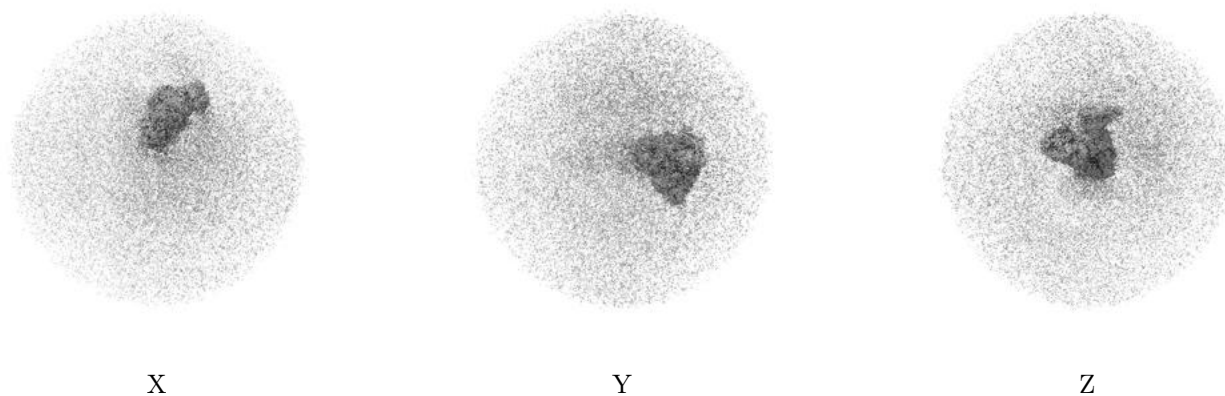


Z

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.

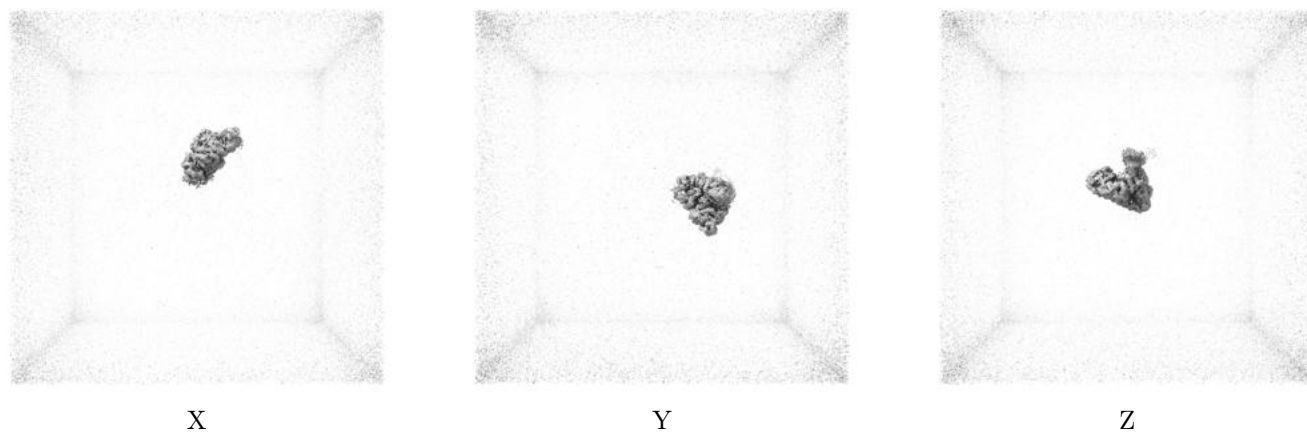
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.18. 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.

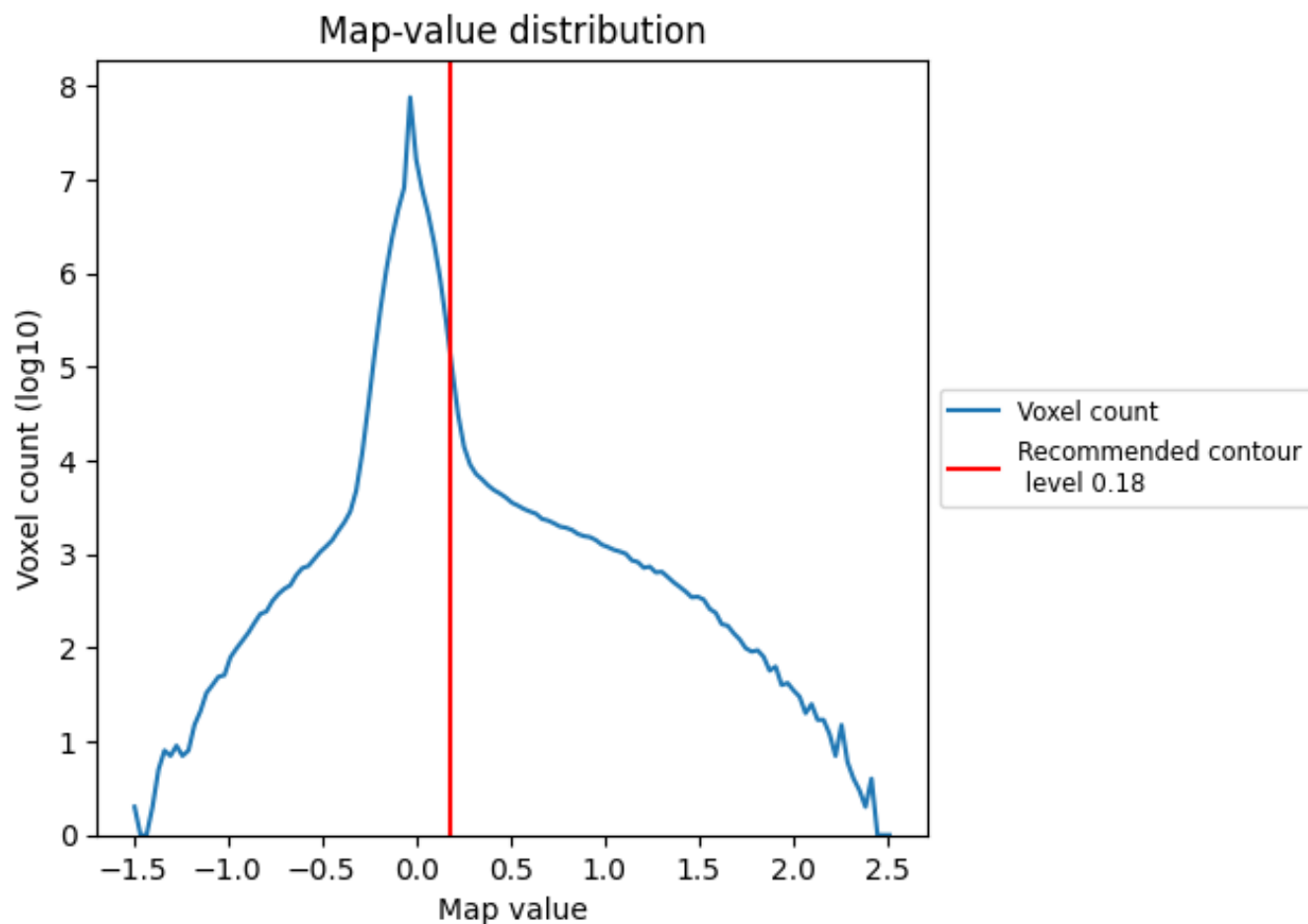
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

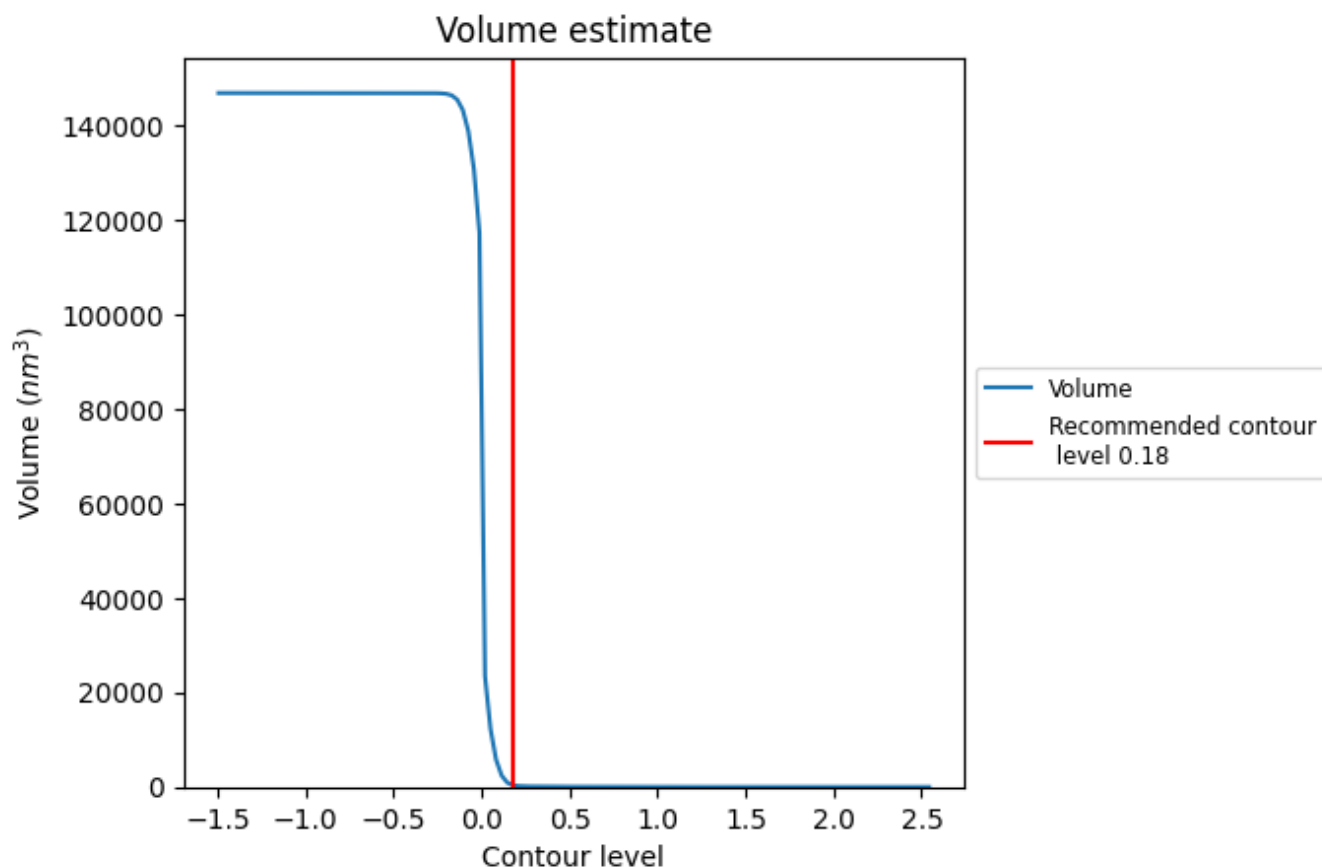
This section contains the results of statistical analysis of the map.

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.

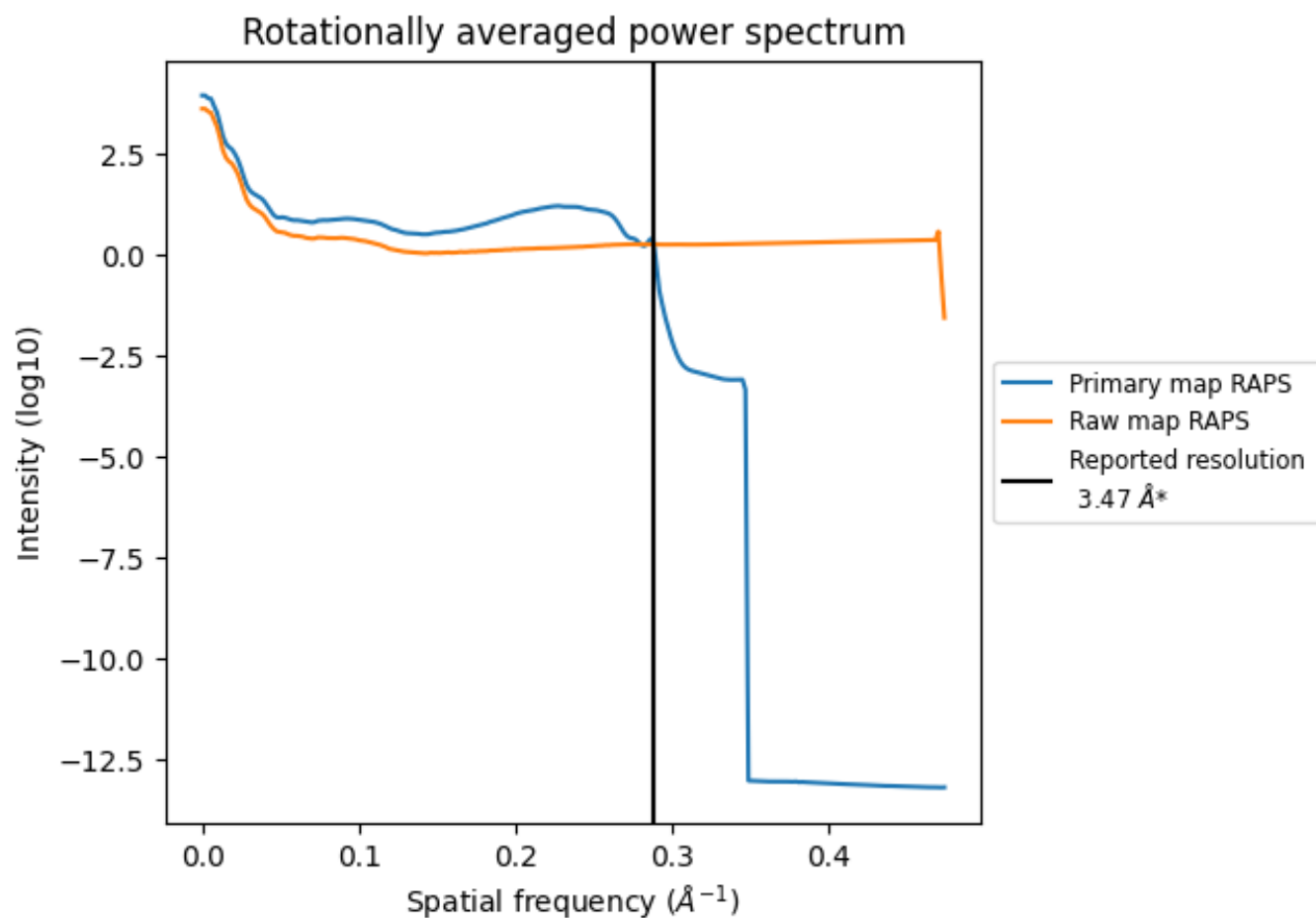
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 362 nm^3 ; this corresponds to an approximate mass of 327 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 ⓘ

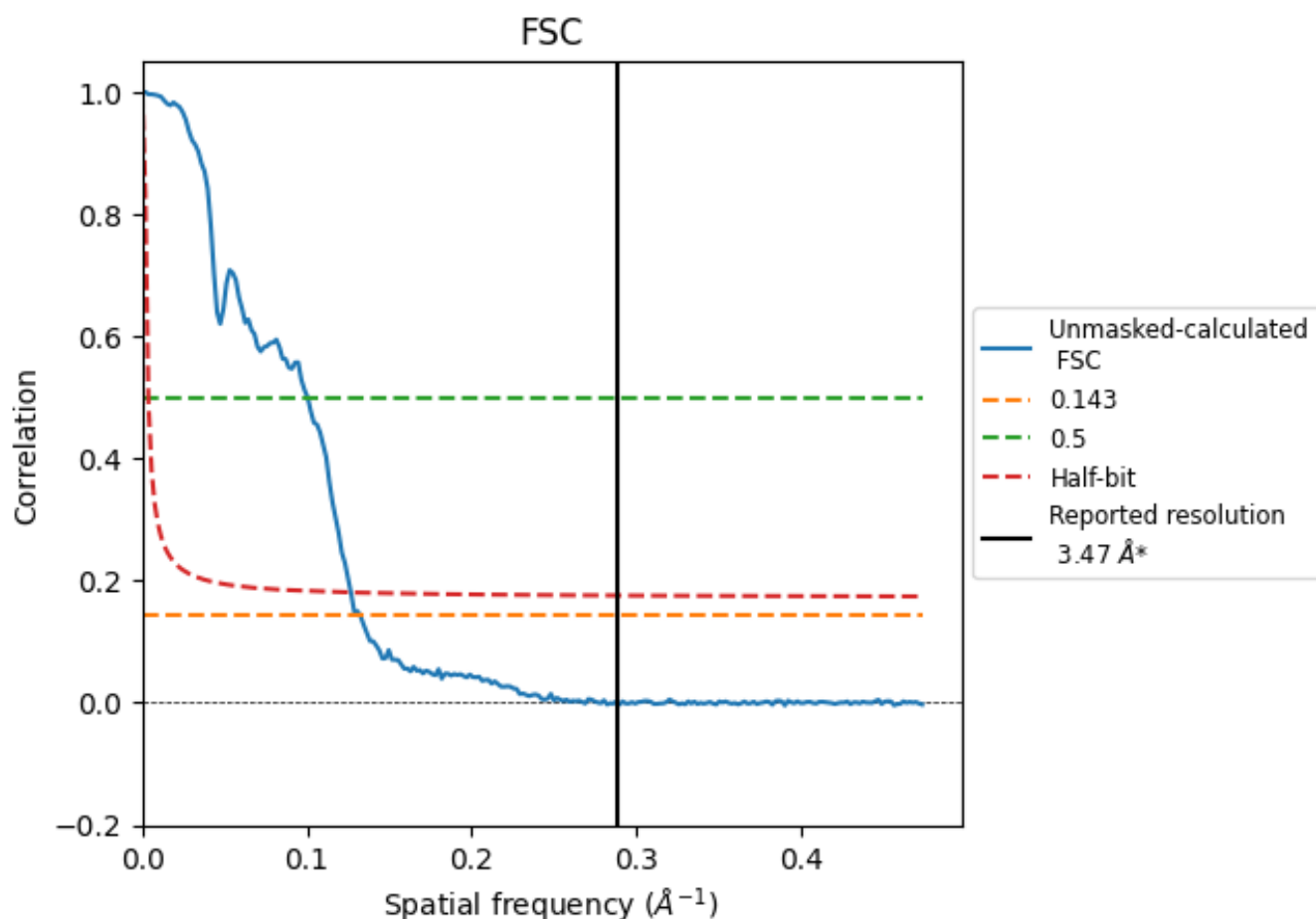


*Reported resolution corresponds to spatial frequency of 0.288 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.288 Å⁻¹

8.2 Resolution estimates [i](#)

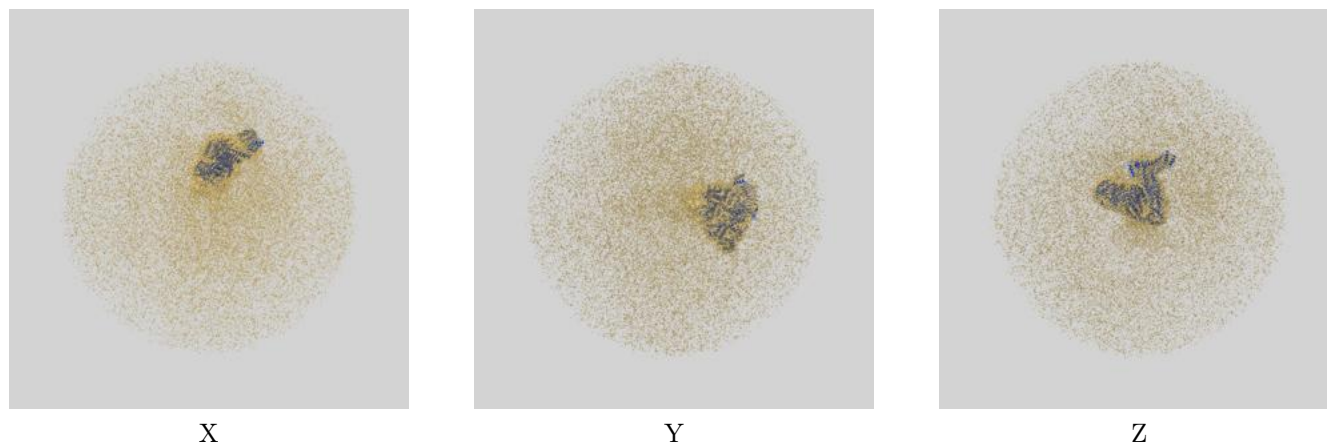
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.47	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.56	9.95	7.89

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

9 Map-model fit [i](#)

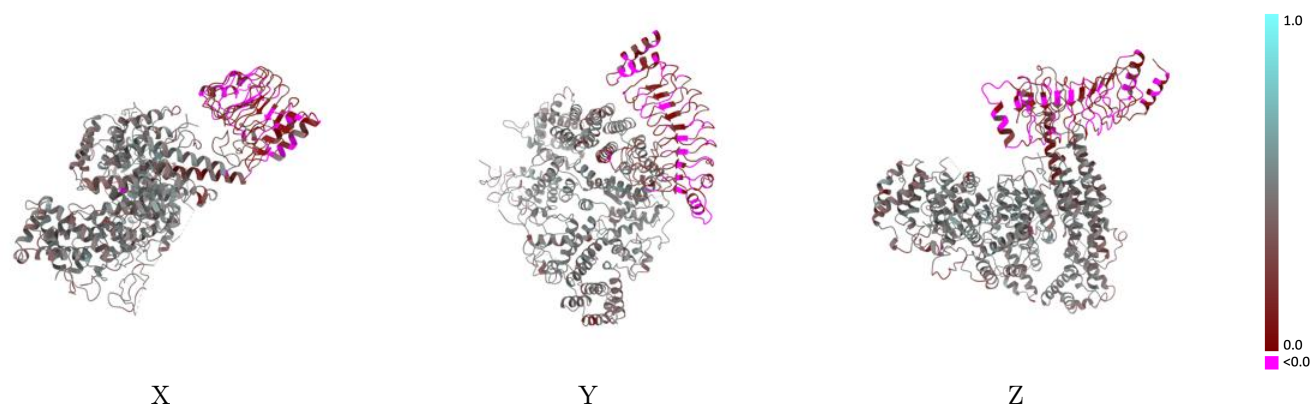
This section contains information regarding the fit between EMDB map EMD-61852 and PDB model 9JWG. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



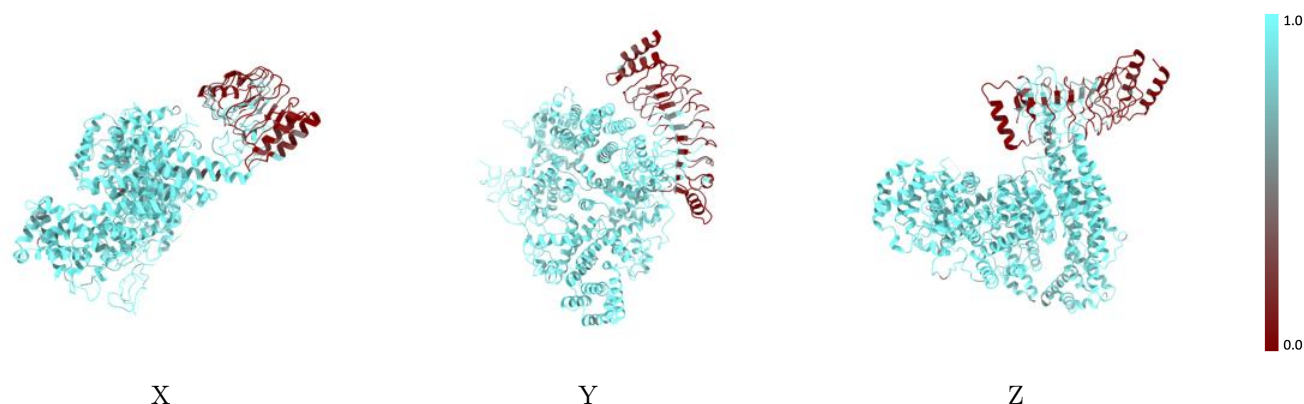
The images above show the 3D surface view of the map at the recommended contour level 0.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



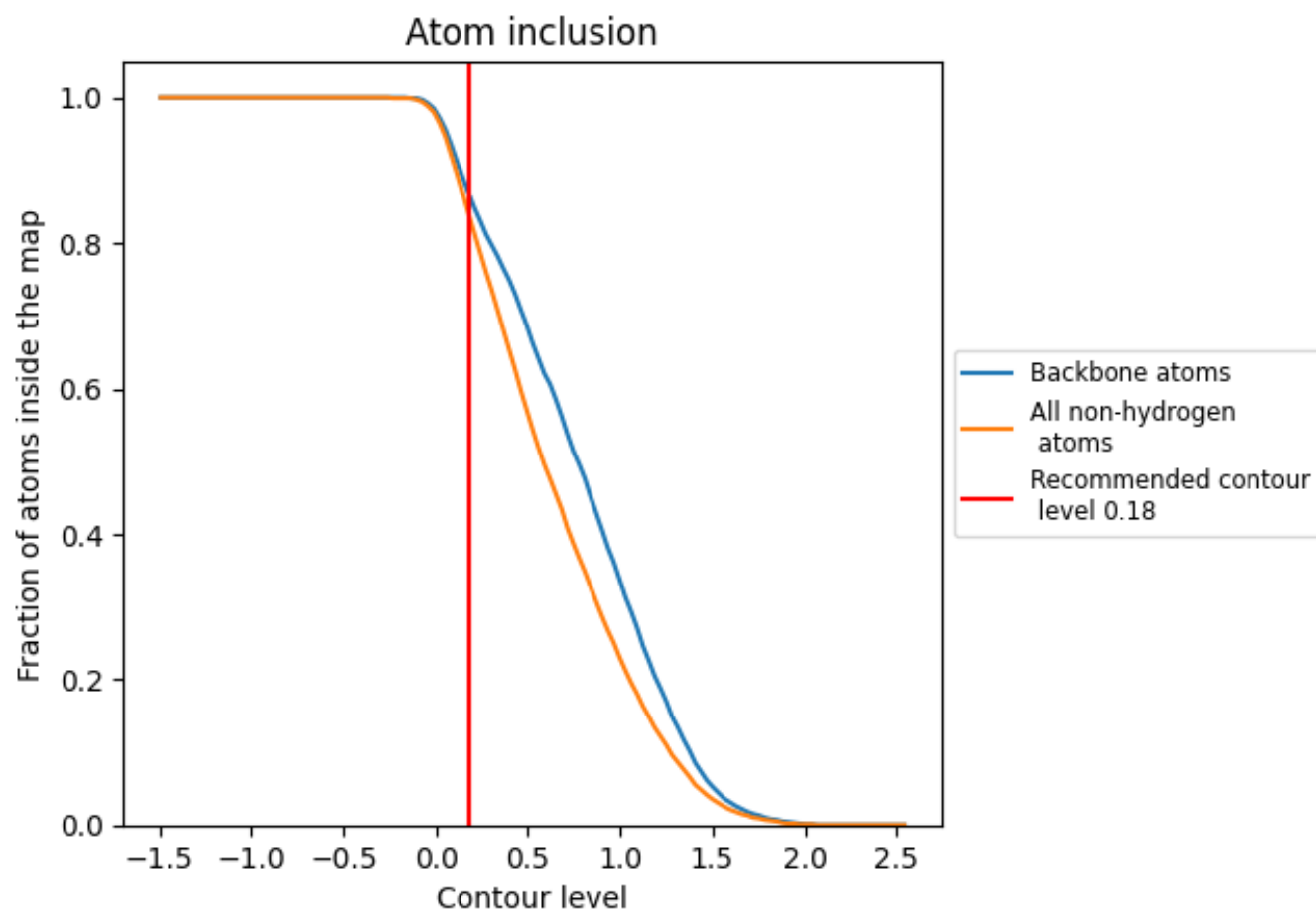
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.18).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 84% 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 (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8400	0.3790
A	0.9500	0.4410
B	0.2740	0.0530

