



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 09:24 AM UTC

PDB ID : 8XMK / pdb_00008xmk
EMDB ID : EMD-38480
Title : Local refinement of SRCR5-9 domains
Authors : Xu, H.; Su, X.D.
Deposited on : 2023-12-27
Resolution : 3.03 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
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

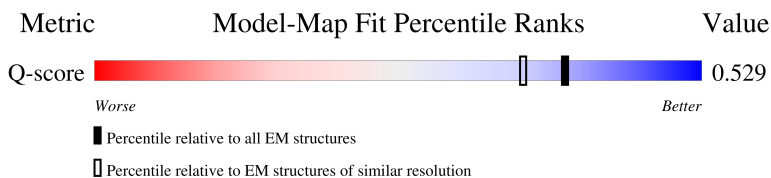
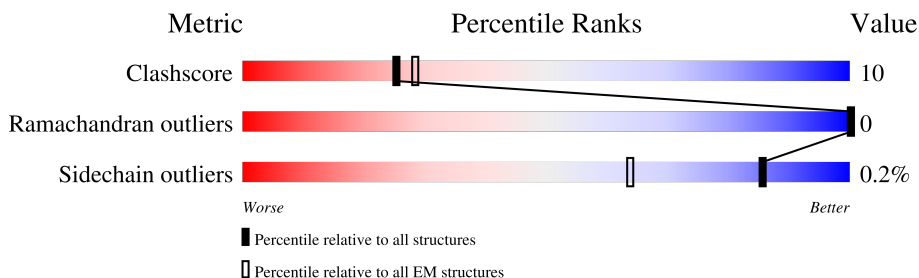
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.03 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	13929 (2.53 - 3.53)

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	D	1009	
1	E	1009	
1	F	1009	

2 Entry composition [i](#)

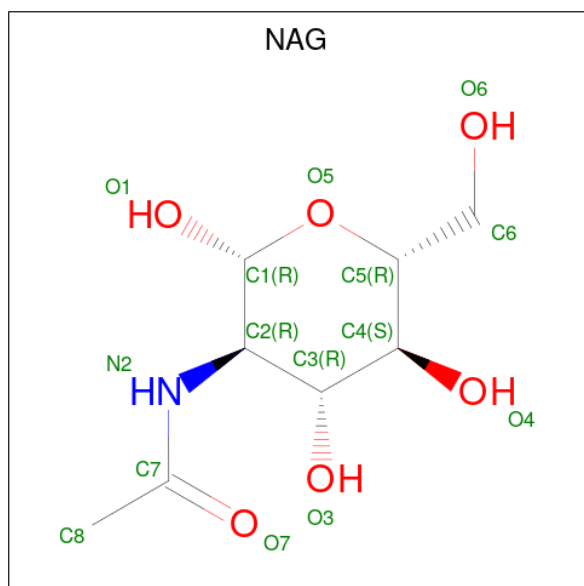
There are 3 unique types of molecules in this entry. The entry contains 11815 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Scavenger receptor cysteine-rich type 1 protein M130.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	522	Total	C	N	O	S	0	0
			3933	2412	716	761	44		
1	E	509	Total	C	N	O	S	0	0
			3847	2360	698	745	44		
1	F	522	Total	C	N	O	S	0	0
			3934	2412	716	762	44		

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
2	D	1	Total	C	N	O	0
			14	8	1	5	
2	D	1	Total	C	N	O	0
			14	8	1	5	
2	E	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
2	E	1	Total	C	N	O	0
			14	8	1	5	
2	F	1	Total	C	N	O	0
			14	8	1	5	
2	F	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
3	D	6	Total	Ca	0
			6	6	
3	E	5	Total	Ca	0
			5	5	
3	F	6	Total	Ca	0
			6	6	

N994	C835	GLU	V576	CYS	TRP	ILE	ARG	TRP	THR	GLY
E995	L839	SER	C577	ASP	GLY	TRP	PHE	PHE	ARG	TRP
V996		GLU	S578	HIS	GLY	GLN	GLN	GLN	GLY	GLY
	F842	VAL	R579	TYR	GLY	CYS	GLY	ASP	ASN	SER
E1002		ALA		GLU	GLU	LYS	TRP	LEU	MET	SER
W1006	W847	CYS	I583	GLU	ALA	HIS	TRP	ILE	ALA	ALA
A1010		ILE	G588	ALA	ASP	HIS	GLY	CYS	CYS	SER
R1011	D871	GLU	K589	ILE	VAL	TRP	THR	GLY	GLY	SER
R1012		SER	T590	THR	VAL	GLY	ILE	GLY	ARG	ARG
	S879	GLY		CYS	ARG	LYS	ASP	GLU	ILE	ARG
E1017		Q718	E593	S473	LEU	HIS	ASP	SER	GLU	ILE
	ASP	L719			GLN	TYR	GLY	ALA	ALA	TRP
	LYS		V596		GLY	CYS	TRP	TRP	LYS	TRP
H1020	ALA	G724		P478	CYS	ASN	ASP	TRP	PHE	ASP
K1021	MET		K599	R479	GLY	HIS	SER	TRP	GLN	VAL
E1022	S385	C728	T600	L480	SER	ASN	ASN	CYS	GLY	HIS
D1023		A729	L601	V481	ALA	GLU	ASP	LYS	ARG	SER
A1024	P896			C487	LEU	ASP	ALA	LYS	TRP	CYS
A1025		V732	W604	R490	LYS	ALA	ALA	GLN	HIS	ARG
N1027	P906	W740	S606	V491	SER	VAL	VAL	ARG	GLY	THR
N1028	S907				THR	THR	ALA	TRP	VAL	ASN
C1028					TYR	CYS	CYS	GLY	CYS	GLU
T1029	T921	V756	H618	D804	GLN	CYS	LYS	LYS	ASP	SER
D1030		C757	V619	S505	VAL	SER	GLN	HIS	ASP	ALA
ILE		R758		D506	TYR	ASP	LEU	ASP	ASN	ALA
SER	R930		V628		SER	GLY	GLY	CYS	PHE	TRP
VAL		A765		L515	LYS	SER	CYS	ASP	ASN	CYS
GLN	T936		M642	C516	ILE	ASP	PRO	HIS	ILE	CYS
LYS	S937	S771		R517	GLN	LEU	THR	ALA	ASP	LYS
THR			W646		ALA	GLU	GLU	GLU	HIS	ASP
PRO		G779	R647	V525	THR	LEU	VAL	ALA	ALA	HIS
GLN	E943			S526	ASN	ARG	THR	ALA	GLY	SER
LYS	I944	G790	C652	I527	THR	LEU	ILE	VAL	VAL	TRP
ALA	A945				TRP	ARG	ILE	VAL	ILE	GLY
THR		S800	H658	G830	LEU	GLY	GLY	ILE	CYS	LYS
THR	S949	H801	M659		PHE	GLY	ARG	ILE	ARG	HIS
GLY	W950			E535	LEU	GLY	CYS	CYS	ARG	GLN
ARG	G951	C808	V677	A542	SER	SER	VAL	SER	GLN	ASP
SER	T952	R809	A678	F543	SER	ARG	ALA	GLY	LEU	ASN
SER	W963	H810		F643	CYS	CYS	SER	ALA	CYS	THR
ARG	C954	K811	I681	E544	ASN	ALA	LYS	ASP	GLY	HIS
GLN	D955	E812			GLY	GLY	GLY	LEU	SER	GLN
SER	P956		L690	G549	ASN	THR	PHE	LEU	ALA	ASP
	S957	W816	S691	S552	THR	GLU	GLY	ARG	VAL	GLY
	W958	C818	S692	H553	GLU	VAL	ILE	LEU	SER	GLY
			CYS	L554	SER	GLU	TRP	VAL	PHE	GLY
			ASN		LEU	GLU	ASP	VAL	SER	VAL
			SER	R562	TRP	ILE	LEU	GLY	GLY	THR
	Q968	M822	SER		ASP	GLN	ASP	GLY	SER	SER
	Q969	S823	SER		CYS	ARG	SER	VAL	ASN	GLY
	L970		SER		LYS	LEU	THR	GLY	PHE	GLY
	F979	L826	LEU	T566	ASN	GLY	GLY	CYS	SER	SER
	K980	T897	GLY	C567	THR	LEU	LEU	VAL	GLY	ASN
		S828	PRO	S568	TRP	GLY	CYS	CYS	GLY	GLY
	G987	GLU	THR	H569	TRP	LYS	GLN	GLY	GLU	ASN
	T988	ALA	ARG	S570	TRP	CYS	GLY	GLY	SER	GLY
	G989	SER	PRO	R571	TRP	CYS	HIS	HIS	GLY	GLY
		ARG	THR	D572	GLY	ASP	GLU	LEU	GLY	MET
	Y992	GLU	ILE	V573	LEU	ASP	PRO	GLU	PRO	ARG
	I993	ALA			THR	CYS	ALA	VAL	ILE	THR

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	432933	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.904	Depositor
Minimum map value	-2.426	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.044	Depositor
Recommended contour level	0.2	Depositor
Map size ($\text{\AA}$)	385.2, 385.2, 385.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.07, 1.07, 1.07	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, NAG

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	D	0.17	0/4025	0.31	0/5453
1	E	0.15	0/3935	0.29	0/5330
1	F	0.17	0/4026	0.31	0/5454
All	All	0.16	0/11986	0.30	0/16237

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	D	3933	0	3661	85	0
1	E	3847	0	3578	81	0
1	F	3934	0	3661	78	0
2	D	28	0	26	0	0
2	E	28	0	26	0	0
2	F	28	0	26	0	0
3	D	6	0	0	0	0
3	E	5	0	0	0	0
3	F	6	0	0	0	0
All	All	11815	0	10978	238	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 10.

All (238) 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:E:808:CYS:SG	1:F:1021:LYS:NZ	2.62	0.72
1:D:781:ILE:HB	1:D:806:GLN:HG3	1.71	0.72
1:E:779:GLY:O	1:E:810:HIS:NE2	2.20	0.72
1:F:593:GLU:HB2	1:F:681:ILE:HA	1.73	0.70
1:F:779:GLY:O	1:F:810:HIS:NE2	2.21	0.70
1:D:968:GLN:NE2	1:D:1002:GLU:O	2.26	0.68
1:D:590:THR:HG22	1:D:592:CYS:H	1.59	0.67
1:F:517:ARG:NH2	1:F:549:GLY:O	2.26	0.67
1:D:517:ARG:NH2	1:D:549:GLY:O	2.28	0.66
1:F:527:ILE:H	1:F:949:SER:HB3	1.61	0.65
1:D:487:CYS:HB3	1:D:577:CYS:HB2	1.78	0.65
1:D:938:CYS:HB3	1:D:1028:CYS:HB2	1.77	0.65
1:E:901:THR:OG1	1:E:904:GLN:NE2	2.30	0.65
1:E:955:ASP:HB2	1:E:980:LYS:HG2	1.80	0.64
1:E:583:ILE:HG21	1:E:659:MET:HG3	1.80	0.63
1:E:670:SER:HA	1:E:909:PRO:HB3	1.81	0.63
1:D:954:CYS:HB3	1:D:994:ASN:HB3	1.82	0.62
1:D:601:LEU:HD21	1:D:894:GLN:HB3	1.81	0.62
1:F:979:PHE:HE2	1:F:1027:ASN:HB2	1.65	0.62
1:D:953:VAL:HG13	1:D:993:LEU:HB2	1.82	0.62
1:E:720:ARG:HG2	1:E:733:GLU:HB2	1.83	0.61
1:D:846:ALA:HB3	1:D:889:TRP:HZ2	1.66	0.61
1:F:952:THR:HG21	1:F:987:GLY:HA3	1.82	0.61
1:E:958:TRP:O	1:E:980:LYS:NZ	2.30	0.61
1:E:517:ARG:NH2	1:E:549:GLY:O	2.34	0.60
1:E:996:VAL:HA	1:E:1010:ALA:HB2	1.82	0.60
1:F:758:ARG:NH2	1:F:790:GLY:O	2.35	0.60
1:D:720:ARG:HG2	1:D:733:GLU:HB2	1.83	0.60
1:D:744:CYS:O	1:D:745:ASP:HB3	2.02	0.59
1:F:968:GLN:NE2	1:F:1002:GLU:O	2.35	0.59
1:D:979:PHE:HB2	1:D:1025:ALA:HB3	1.83	0.59
1:E:938:CYS:HB3	1:E:1028:CYS:HB2	1.84	0.59
1:F:987:GLY:N	1:F:1023:ASP:OD2	2.36	0.58
1:E:478:PRO:HB2	1:E:515:LEU:HD13	1.85	0.58
1:E:864:CYS:HB3	1:E:870:ALA:HB3	1.86	0.58
1:E:509:LEU:HA	1:E:527:ILE:HD11	1.84	0.58
1:D:592:CYS:HB3	1:D:682:CYS:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:875:ILE:HD13	1:D:923:ILE:HG22	1.87	0.57
1:E:571:ARG:HH12	1:E:988:THR:HA	1.69	0.57
1:F:989:GLY:O	1:F:1020:HIS:NE2	2.28	0.56
1:D:587:ASN:ND2	1:D:638:PHE:O	2.38	0.56
1:F:618:HIS:HB3	1:F:690:LEU:HD11	1.86	0.56
1:D:506:ASP:HB2	1:D:544:GLU:HA	1.87	0.56
1:D:1011:ARG:NH2	1:D:1015:HIS:O	2.37	0.56
1:D:647:ARG:NH1	1:D:907:SER:O	2.38	0.56
1:E:728:CYS:HB3	1:E:818:CYS:HB2	1.88	0.55
1:E:889:TRP:HB3	1:E:910:TRP:CE3	2.42	0.55
1:D:1021:LYS:NZ	1:F:808:CYS:SG	2.80	0.55
1:F:1006:TRP:O	1:F:1012:ARG:NH1	2.39	0.55
1:D:823:SER:HB3	1:D:842:PHE:HB3	1.89	0.55
1:F:480:LEU:HD21	1:F:515:LEU:HD21	1.89	0.55
1:E:896:PRO:HD3	1:E:906:PRO:HD2	1.89	0.54
1:E:944:ILE:HD11	1:E:992:TRP:HB2	1.90	0.54
1:D:629:ALA:HA	1:D:682:CYS:HA	1.89	0.54
1:E:526:SER:HB3	1:E:865:ARG:HH12	1.72	0.54
1:F:929:ILE:HG12	1:F:970:LEU:HD11	1.89	0.54
1:F:957:SER:HB3	1:F:995:GLU:HA	1.90	0.54
1:F:800:SER:OG	1:F:801:HIS:N	2.40	0.54
1:D:746:ASP:OD2	1:E:977:LYS:NZ	2.29	0.53
1:D:952:THR:HG21	1:D:987:GLY:HA3	1.90	0.53
1:E:889:TRP:HB3	1:E:910:TRP:HE3	1.73	0.53
1:F:647:ARG:NH2	1:F:907:SER:O	2.41	0.53
1:F:590:THR:HB	1:F:593:GLU:OE1	2.08	0.53
1:F:955:ASP:HB2	1:F:980:LYS:HG2	1.90	0.53
1:F:938:CYS:HB3	1:F:1028:CYS:HB2	1.88	0.53
1:E:477:GLU:HB3	1:E:494:LYS:HE2	1.91	0.53
1:E:822:MET:HA	1:E:842:PHE:O	2.09	0.53
1:F:601:LEU:HD22	1:F:896:PRO:HB3	1.91	0.53
1:F:826:LEU:HD12	1:F:835:CYS:HB3	1.90	0.53
1:D:744:CYS:O	1:D:744:CYS:SG	2.67	0.52
1:F:506:ASP:HB3	1:F:544:GLU:HA	1.92	0.52
1:F:628:VAL:HG12	1:F:690:LEU:HG	1.91	0.52
1:D:871:ASP:HB3	1:D:945:TRP:NE1	2.25	0.52
1:F:954:CYS:SG	1:F:955:ASP:N	2.83	0.52
1:D:743:ILE:HB	1:D:814:ALA:HB3	1.92	0.52
1:D:548:GLU:OE1	1:D:550:HIS:ND1	2.37	0.51
1:D:955:ASP:O	1:D:980:LYS:HE3	2.11	0.51
1:D:589:LYS:N	1:D:593:GLU:OE2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:668:GLY:H	1:D:907:SER:HG	1.57	0.51
1:E:595:ARG:NH2	1:E:597:GLU:OE2	2.28	0.51
1:E:941:ARG:NH1	1:E:986:GLN:O	2.43	0.51
1:F:823:SER:HB3	1:F:842:PHE:HB3	1.92	0.51
1:E:966:VAL:HG11	1:E:1026:VAL:HG21	1.93	0.51
1:F:728:CYS:HB3	1:F:818:CYS:HB2	1.93	0.51
1:D:733:GLU:OE2	1:D:742:THR:OG1	2.29	0.51
1:D:891:ASP:OD1	1:D:892:ASN:N	2.41	0.51
1:D:536:GLY:O	1:D:569:HIS:ND1	2.43	0.50
1:D:889:TRP:HB3	1:D:910:TRP:HE3	1.76	0.50
1:D:986:GLN:HB3	1:D:1020:HIS:HB3	1.93	0.50
1:D:767:ASN:HB2	1:D:817:ILE:HB	1.92	0.50
1:E:853:SER:OG	1:E:892:ASN:OD1	2.28	0.50
1:E:836:ALA:HB1	1:E:924:THR:HG22	1.93	0.50
1:D:728:CYS:HB3	1:D:818:CYS:HB2	1.94	0.49
1:E:794:ARG:HB2	1:E:797:GLN:HG3	1.94	0.49
1:F:955:ASP:O	1:F:980:LYS:NZ	2.37	0.49
1:F:491:VAL:HB	1:F:573:VAL:HG13	1.94	0.49
1:D:1006:TRP:O	1:D:1012:ARG:NH2	2.41	0.49
1:F:839:LEU:HB3	1:F:921:THR:HG23	1.93	0.49
1:D:989:GLY:O	1:D:1020:HIS:NE2	2.37	0.49
1:E:951:GLY:HA3	1:E:992:TRP:CD1	2.48	0.49
1:D:954:CYS:SG	1:D:955:ASP:N	2.85	0.49
1:F:606:SER:HB3	1:F:677:VAL:HG13	1.95	0.49
1:F:771:SER:HA	1:F:812:GLU:HA	1.94	0.49
1:D:509:LEU:HA	1:D:527:ILE:HD11	1.95	0.48
1:F:542:ALA:HB2	1:F:566:THR:HB	1.95	0.48
1:F:930:ARG:HG3	1:F:943:GLU:HB2	1.95	0.48
1:F:478:PRO:HB3	1:F:554:LEU:HD12	1.95	0.48
1:F:958:TRP:CE2	1:F:1024:ALA:HB1	2.48	0.48
1:D:889:TRP:HB3	1:D:910:TRP:CE3	2.49	0.48
1:E:941:ARG:HH11	1:E:987:GLY:HA2	1.78	0.48
1:F:481:VAL:O	1:F:490:ARG:N	2.42	0.48
1:E:848:GLY:HA3	1:E:889:TRP:CD1	2.48	0.48
1:E:583:ILE:HD12	1:E:598:LEU:HD12	1.94	0.48
1:F:599:LYS:HD2	1:F:604:TRP:CE2	2.48	0.48
1:F:951:GLY:HA3	1:F:992:TRP:CD1	2.48	0.48
1:F:504:ASP:N	1:F:504:ASP:OD1	2.44	0.48
1:E:618:HIS:HB3	1:E:690:LEU:HD11	1.95	0.48
1:E:504:ASP:HA	1:E:573:VAL:HB	1.96	0.48
1:F:579:ARG:HD3	1:F:658:HIS:CG	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:736:HIS:HE2	1:D:782:TRP:CD1	2.32	0.47
1:D:805:GLN:O	1:D:807:ASN:ND2	2.47	0.47
1:F:871:ASP:HB3	1:F:945:TRP:NE1	2.29	0.47
1:E:855:MET:HE3	1:E:921:THR:HG21	1.97	0.47
1:D:869:CYS:O	1:D:928:LYS:HG2	2.14	0.47
1:D:976:LEU:N	1:D:1027:ASN:O	2.47	0.47
1:F:936:THR:HG23	1:F:938:CYS:H	1.79	0.47
1:E:855:MET:HG2	1:E:875:ILE:HD11	1.96	0.47
1:E:954:CYS:HB3	1:E:994:ASN:HB3	1.96	0.47
1:F:542:ALA:HB1	1:F:562:ARG:HG2	1.97	0.47
1:D:951:GLY:HA3	1:D:992:TRP:CD1	2.50	0.47
1:F:530:GLY:HA2	1:F:571:ARG:HA	1.97	0.47
1:E:835:CYS:SG	1:E:925:CYS:HB2	2.54	0.46
1:F:566:THR:HG23	1:F:567:CYS:N	2.29	0.46
1:F:822:MET:HA	1:F:842:PHE:O	2.14	0.46
1:D:595:ARG:HD2	1:D:677:VAL:HG21	1.97	0.46
1:F:506:ASP:OD1	1:F:562:ARG:NH2	2.46	0.46
1:F:606:SER:O	1:F:646:TRP:N	2.42	0.46
1:E:608:CYS:HA	1:E:678:ALA:H	1.79	0.46
1:D:721:LEU:HD13	1:D:760:LEU:HD11	1.97	0.46
1:D:994:ASN:HD21	1:D:1011:ARG:NH1	2.14	0.46
1:E:934:GLY:HA3	1:E:939:SER:O	2.15	0.46
1:E:598:LEU:HD21	1:E:600:THR:HG23	1.97	0.46
1:E:893:VAL:HG11	1:E:902:LEU:HD11	1.97	0.46
1:F:588:GLY:HA3	1:F:593:GLU:O	2.16	0.46
1:D:1018:CYS:HA	1:F:811:LYS:NZ	2.31	0.46
1:E:871:ASP:HB2	1:E:945:TRP:NE1	2.31	0.46
1:E:599:LYS:HB2	1:E:604:TRP:CD2	2.50	0.45
1:E:732:VAL:HG23	1:E:815:GLY:HA2	1.97	0.45
1:F:979:PHE:HB2	1:F:1025:ALA:HB3	1.99	0.45
1:D:476:ARG:NH2	1:D:543:GLU:OE2	2.49	0.45
1:D:848:GLY:HA3	1:D:889:TRP:CD1	2.51	0.45
1:F:954:CYS:HB3	1:F:994:ASN:HB3	1.98	0.45
1:E:579:ARG:HD3	1:E:658:HIS:CG	2.51	0.45
1:E:668:GLY:HA2	1:E:908:SER:O	2.17	0.45
1:E:766:ILE:HG12	1:E:845:GLY:HA3	1.98	0.45
1:E:926:ASP:OD1	1:E:926:ASP:N	2.45	0.44
1:F:842:PHE:HB2	1:F:847:TRP:CD2	2.52	0.44
1:D:668:GLY:HA2	1:D:908:SER:O	2.17	0.44
1:D:994:ASN:HD21	1:D:1011:ARG:HH11	1.64	0.44
1:E:599:LYS:HB2	1:E:604:TRP:CE3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:859:THR:HA	1:E:895:CYS:HB2	2.00	0.44
1:D:583:ILE:HG21	1:D:659:MET:HG3	1.99	0.44
1:D:958:TRP:CD1	1:D:978:ALA:HB1	2.51	0.44
1:E:995:GLU:HG2	1:E:997:LYS:HE2	1.99	0.44
1:E:871:ASP:HB2	1:E:945:TRP:CE2	2.51	0.44
1:F:535:GLU:HB3	1:F:569:HIS:HB3	1.99	0.44
1:D:598:LEU:HD21	1:D:600:THR:HG23	1.99	0.44
1:F:504:ASP:HA	1:F:573:VAL:HB	1.98	0.44
1:F:618:HIS:CG	1:F:690:LEU:HD21	2.53	0.44
1:F:993:LEU:HD23	1:F:1012:ARG:HA	2.00	0.44
1:F:619:VAL:HG21	1:F:652:CYS:HB3	1.99	0.44
1:E:809:ARG:HG2	1:F:1017:GLU:HG3	1.99	0.43
1:E:842:PHE:HB2	1:E:847:TRP:CD2	2.53	0.43
1:D:612:TRP:HD1	1:D:632:THR:HG21	1.83	0.43
1:D:783:LEU:HD12	1:D:783:LEU:HA	1.89	0.43
1:E:494:LYS:HD3	1:E:499:TRP:CZ2	2.53	0.43
1:E:756:VAL:HG12	1:E:795:ILE:HB	2.01	0.43
1:D:855:MET:HE3	1:D:921:THR:HG21	2.01	0.43
1:D:992:TRP:HE3	1:D:1013:TRP:HA	1.83	0.43
1:E:475:HIS:O	1:E:476:ARG:NH1	2.51	0.43
1:F:718:GLN:HG3	1:F:740:TRP:CH2	2.53	0.43
1:E:823:SER:HB3	1:E:842:PHE:HB3	2.00	0.43
1:F:896:PRO:HD3	1:F:906:PRO:HD2	2.00	0.43
1:F:954:CYS:HB3	1:F:994:ASN:CB	2.49	0.43
1:E:979:PHE:HB2	1:E:1025:ALA:HB3	2.01	0.43
1:F:596:VAL:HG22	1:F:678:ALA:O	2.19	0.43
1:F:724:GLY:HA3	1:F:729:ALA:O	2.19	0.43
1:D:956:ASP:OD2	1:F:811:LYS:HE3	2.18	0.43
1:F:525:VAL:HB	1:F:576:VAL:HG12	2.01	0.43
1:D:735:TYR:HB2	1:D:740:TRP:CD2	2.54	0.42
1:E:649:MET:HE2	1:E:669:ALA:HB2	2.00	0.42
1:D:752:ASP:OD1	1:D:788:CYS:N	2.51	0.42
1:E:608:CYS:HA	1:E:678:ALA:N	2.34	0.42
1:E:842:PHE:HB2	1:E:847:TRP:CE3	2.54	0.42
1:F:765:ALA:HA	1:F:818:CYS:HA	2.01	0.42
1:D:871:ASP:CG	1:D:950:TRP:HE1	2.28	0.42
1:E:734:ILE:HD11	1:E:796:TRP:HE3	1.83	0.42
1:D:481:VAL:O	1:D:490:ARG:N	2.48	0.42
1:D:504:ASP:HA	1:D:573:VAL:HB	2.01	0.42
1:D:943:GLU:HG2	1:D:952:THR:HG22	2.02	0.42
1:E:756:VAL:HG21	1:E:816:VAL:HG11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:850:VAL:HG13	1:E:890:VAL:HG13	2.00	0.42
1:D:504:ASP:OD1	1:D:504:ASP:N	2.49	0.42
1:D:595:ARG:NH2	1:D:597:GLU:OE2	2.46	0.42
1:D:619:VAL:HG21	1:D:652:CYS:HB3	2.02	0.42
1:D:742:THR:HG22	1:D:743:ILE:N	2.34	0.42
1:D:756:VAL:HG11	1:D:816:VAL:HG11	2.02	0.42
1:D:478:PRO:HB3	1:D:554:LEU:HD12	2.01	0.41
1:E:588:GLY:HA3	1:E:593:GLU:O	2.20	0.41
1:E:785:GLU:HG3	1:E:801:HIS:CE1	2.55	0.41
1:E:960:LEU:O	1:E:964:GLN:HG2	2.20	0.41
1:F:552:SER:OG	1:F:553:HIS:ND1	2.41	0.41
1:D:996:VAL:HG12	1:D:1010:ALA:HB2	2.02	0.41
1:D:579:ARG:NH2	1:D:661:ASP:OD2	2.52	0.41
1:F:955:ASP:OD1	1:F:1022:GLU:HB3	2.21	0.41
1:F:996:VAL:HG12	1:F:1010:ALA:HB2	2.02	0.41
1:D:893:VAL:HG11	1:D:902:LEU:HD11	2.01	0.41
1:E:741:GLY:HA3	1:E:782:TRP:CD1	2.56	0.41
1:E:848:GLY:HA2	1:E:886:ILE:HG22	2.02	0.41
1:E:1011:ARG:NH1	1:E:1015:HIS:O	2.53	0.41
1:F:938:CYS:O	1:F:1028:CYS:HB2	2.21	0.41
1:E:567:CYS:SG	1:E:568:SER:N	2.78	0.41
1:E:601:LEU:HD22	1:E:896:PRO:HB3	2.03	0.41
1:E:993:LEU:HD23	1:E:996:VAL:HG11	2.03	0.41
1:D:736:HIS:HE2	1:D:782:TRP:CG	2.38	0.41
1:D:960:LEU:HD12	1:D:963:ALA:HB3	2.02	0.41
1:E:607:LEU:HD12	1:E:646:TRP:O	2.21	0.41
1:E:959:ASP:OD1	1:E:959:ASP:N	2.53	0.41
1:F:719:LEU:HD11	1:F:732:VAL:HG13	2.03	0.41
1:F:756:VAL:HG21	1:F:816:VAL:HG11	2.03	0.41
1:F:583:ILE:HG21	1:F:659:MET:HG3	2.03	0.41
1:D:488:SER:HB2	1:D:576:VAL:HG22	2.03	0.40
1:E:753:ALA:HA	1:E:756:VAL:HG22	2.03	0.40
1:D:608:CYS:HA	1:D:678:ALA:H	1.86	0.40
1:F:487:CYS:HB3	1:F:577:CYS:HB2	2.02	0.40
1:D:504:ASP:OD1	1:D:571:ARG:HB3	2.21	0.40
1:D:592:CYS:SG	1:D:684:GLY:HA2	2.61	0.40
1:E:504:ASP:OD1	1:E:504:ASP:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	514/1009 (51%)	492 (96%)	22 (4%)	0	100	100
1	E	497/1009 (49%)	480 (97%)	17 (3%)	0	100	100
1	F	514/1009 (51%)	496 (96%)	18 (4%)	0	100	100
All	All	1525/3027 (50%)	1468 (96%)	57 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	425/823 (52%)	424 (100%)	1 (0%)	87	90
1	E	419/823 (51%)	419 (100%)	0	100	100
1	F	426/823 (52%)	425 (100%)	1 (0%)	87	90
All	All	1270/2469 (51%)	1268 (100%)	2 (0%)	85	90

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	745	ASP
1	F	811	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	648	HIS
1	D	688	GLN
1	D	773	HIS
1	D	892	ASN
1	D	986	GLN
1	E	475	HIS
1	E	805	GLN
1	E	946	HIS
1	F	611	HIS
1	F	773	HIS
1	F	932	GLN
1	F	968	GLN
1	F	986	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](#)

Of 23 ligands modelled in this entry, 17 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	F	1102	1	14,14,15	0.21	0	17,19,21	0.41	0
2	NAG	D	1102	1	14,14,15	0.24	0	17,19,21	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	D	1101	1	14,14,15	0.21	0	17,19,21	0.44	0
2	NAG	F	1101	1	14,14,15	0.21	0	17,19,21	0.43	0
2	NAG	E	1102	1	14,14,15	0.25	0	17,19,21	0.47	0
2	NAG	E	1101	1	14,14,15	0.21	0	17,19,21	0.48	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	F	1102	1	-	0/6/23/26	0/1/1/1
2	NAG	D	1102	1	-	2/6/23/26	0/1/1/1
2	NAG	D	1101	1	-	0/6/23/26	0/1/1/1
2	NAG	F	1101	1	-	0/6/23/26	0/1/1/1
2	NAG	E	1102	1	-	4/6/23/26	0/1/1/1
2	NAG	E	1101	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1101	NAG	C4-C5-C6-O6
2	E	1102	NAG	O5-C5-C6-O6
2	E	1101	NAG	O5-C5-C6-O6
2	E	1102	NAG	C4-C5-C6-O6
2	E	1102	NAG	C8-C7-N2-C2
2	E	1102	NAG	O7-C7-N2-C2
2	D	1102	NAG	C4-C5-C6-O6
2	D	1102	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

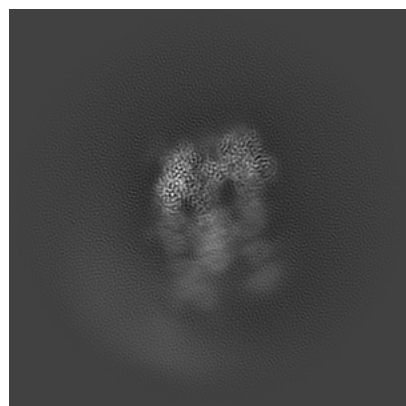
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38480. These allow visual inspection of the internal detail of the map and identification of artifacts.

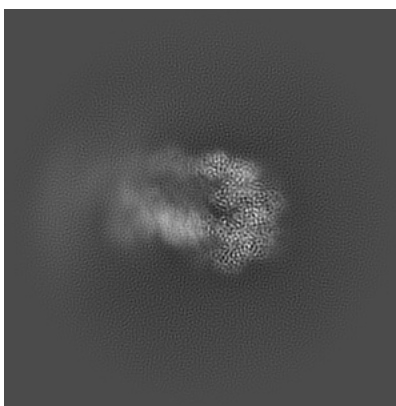
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

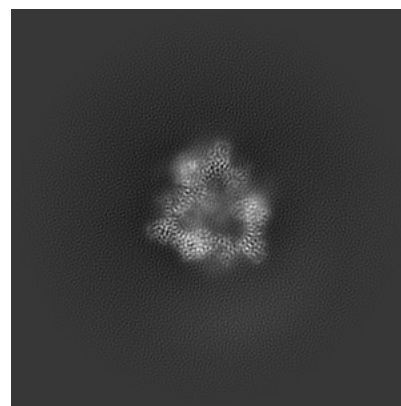
6.1.1 Primary map



X

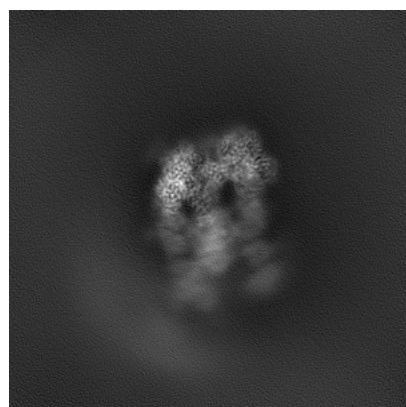


Y

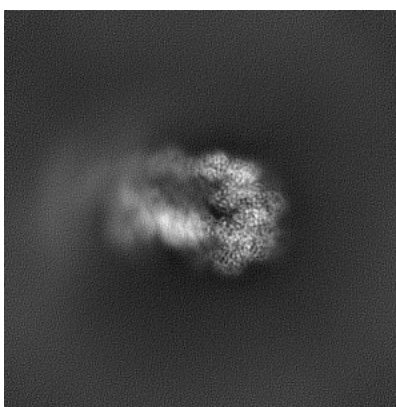


Z

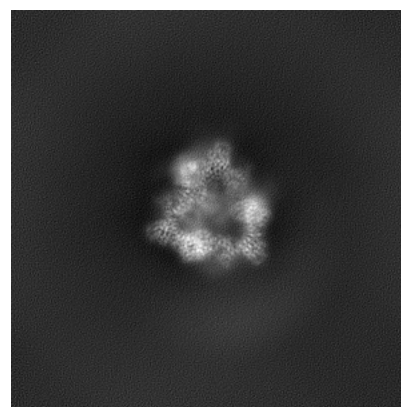
6.1.2 Raw map



X



Y



Z

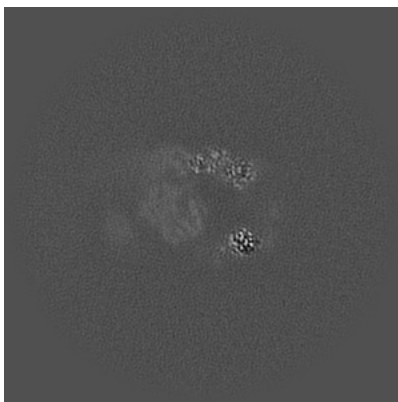
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

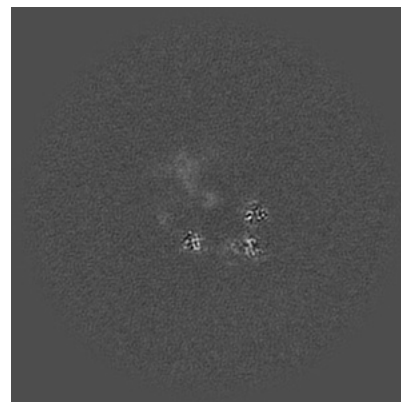
6.2.1 Primary map



X Index: 180



Y Index: 180

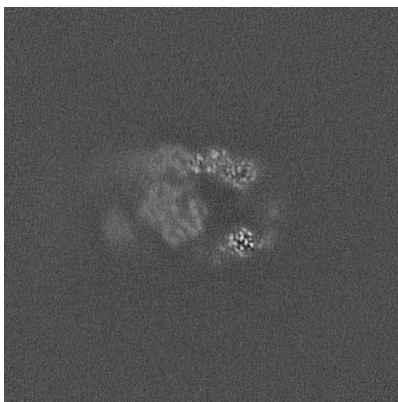


Z Index: 180

6.2.2 Raw map



X Index: 180



Y Index: 180



Z Index: 180

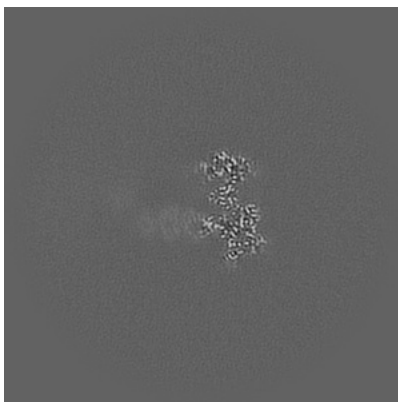
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

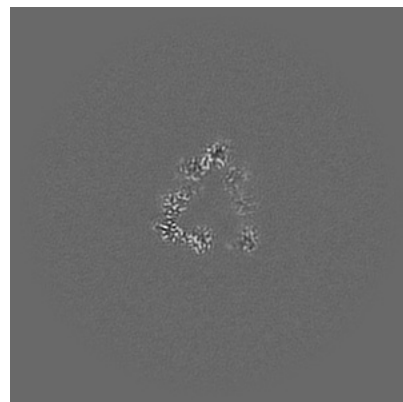
6.3.1 Primary map



X Index: 159



Y Index: 150

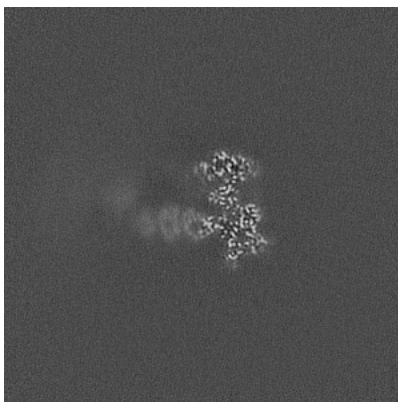


Z Index: 218

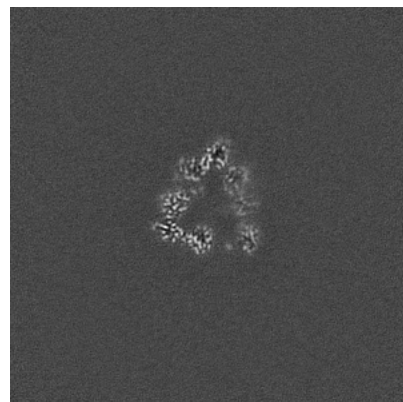
6.3.2 Raw map



X Index: 159



Y Index: 150

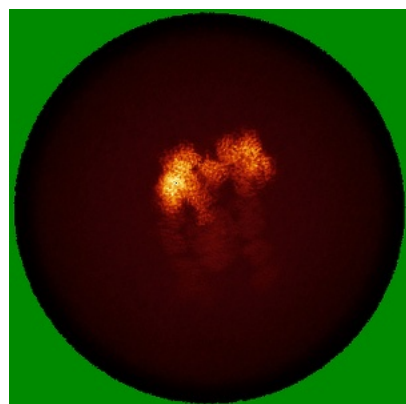


Z Index: 218

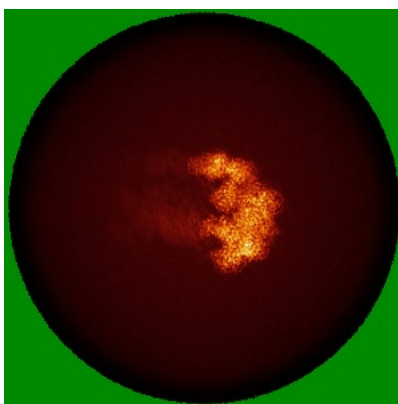
The images above show the largest variance slices of the map in three orthogonal directions.

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

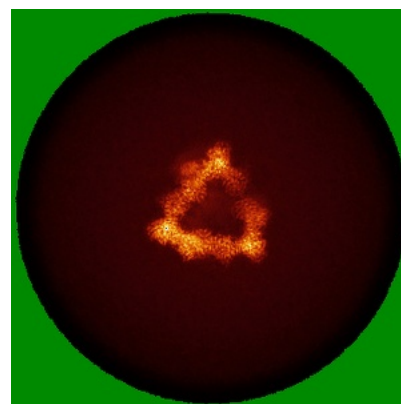
6.4.1 Primary map



X

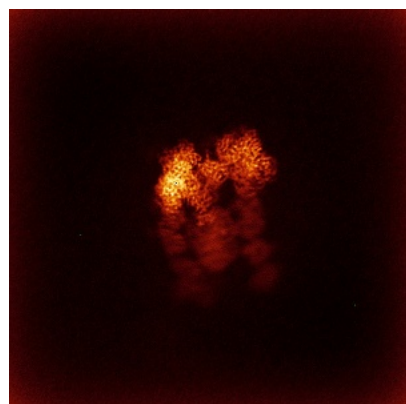


Y

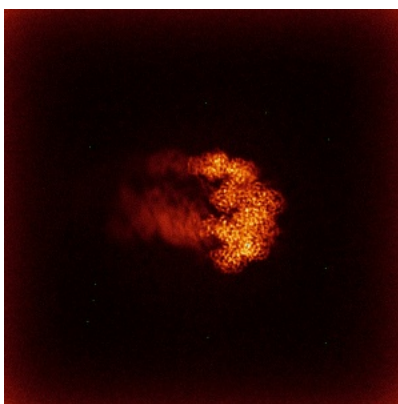


Z

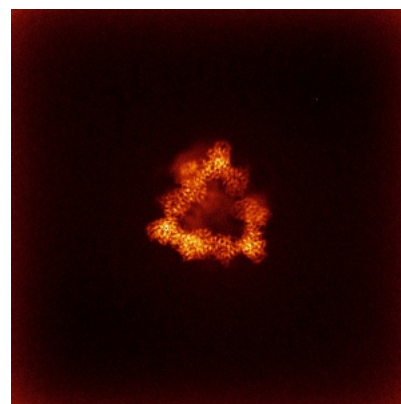
6.4.2 Raw map



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.

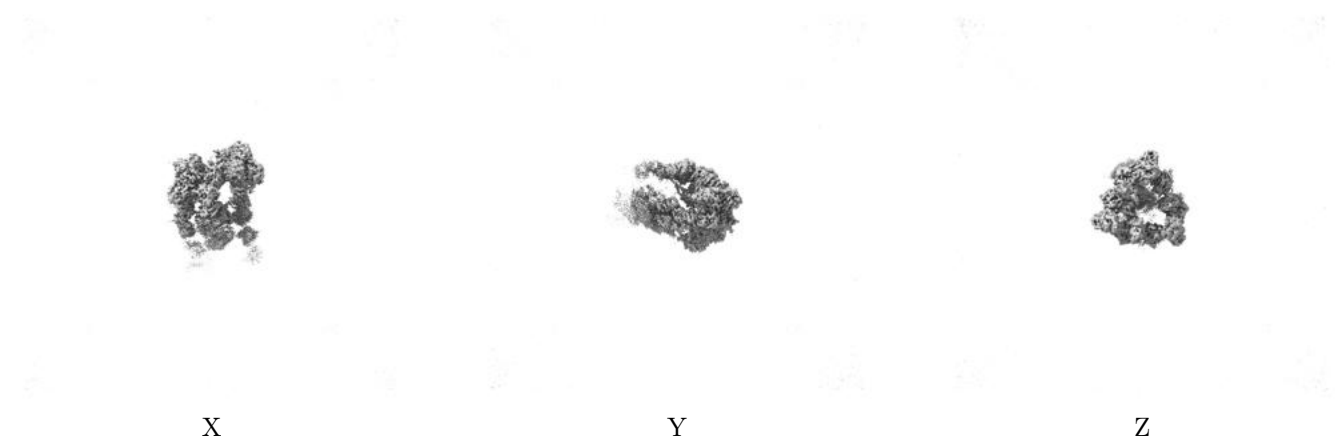
6.5 Orthogonal surface views [i](#)

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.

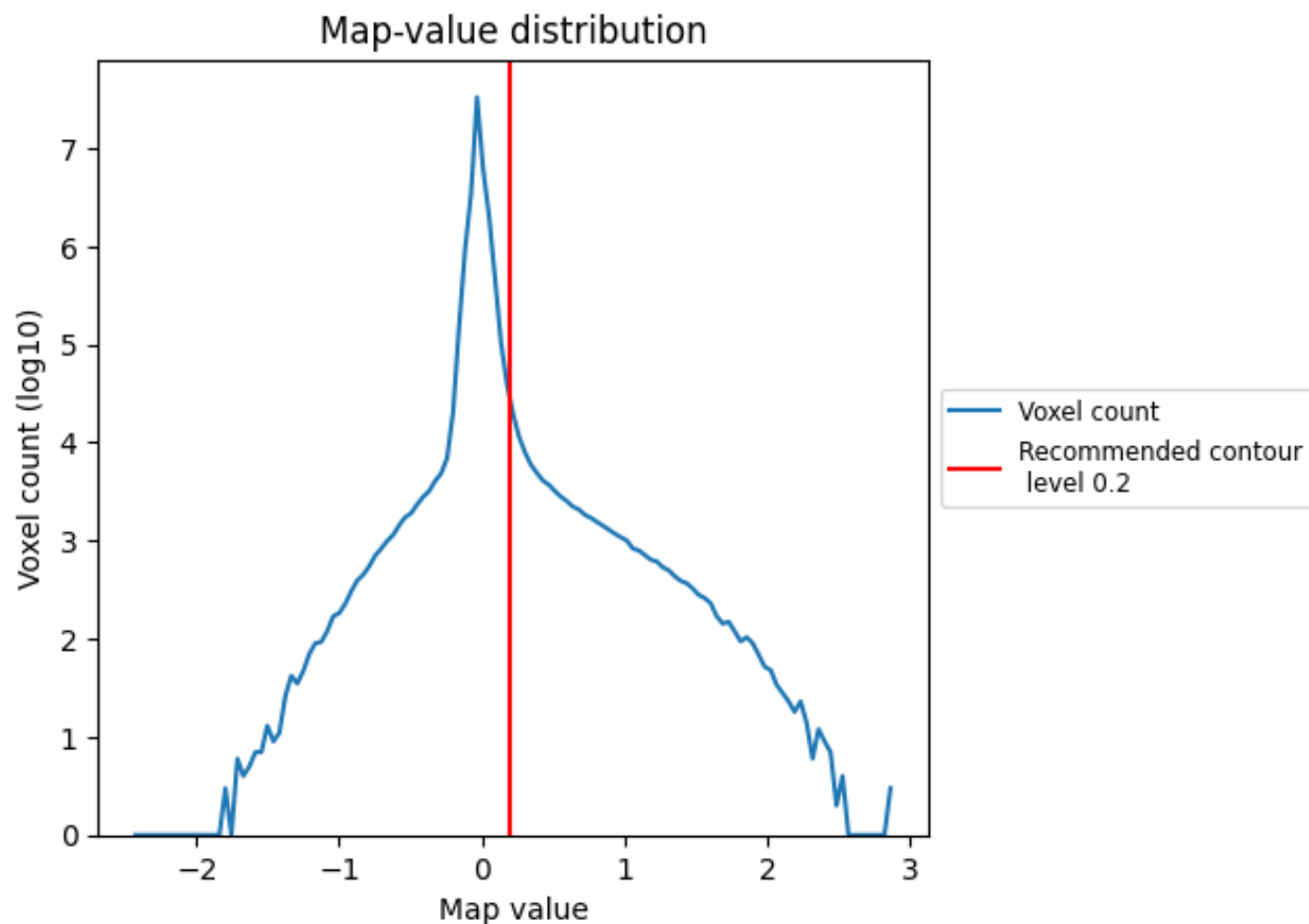
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

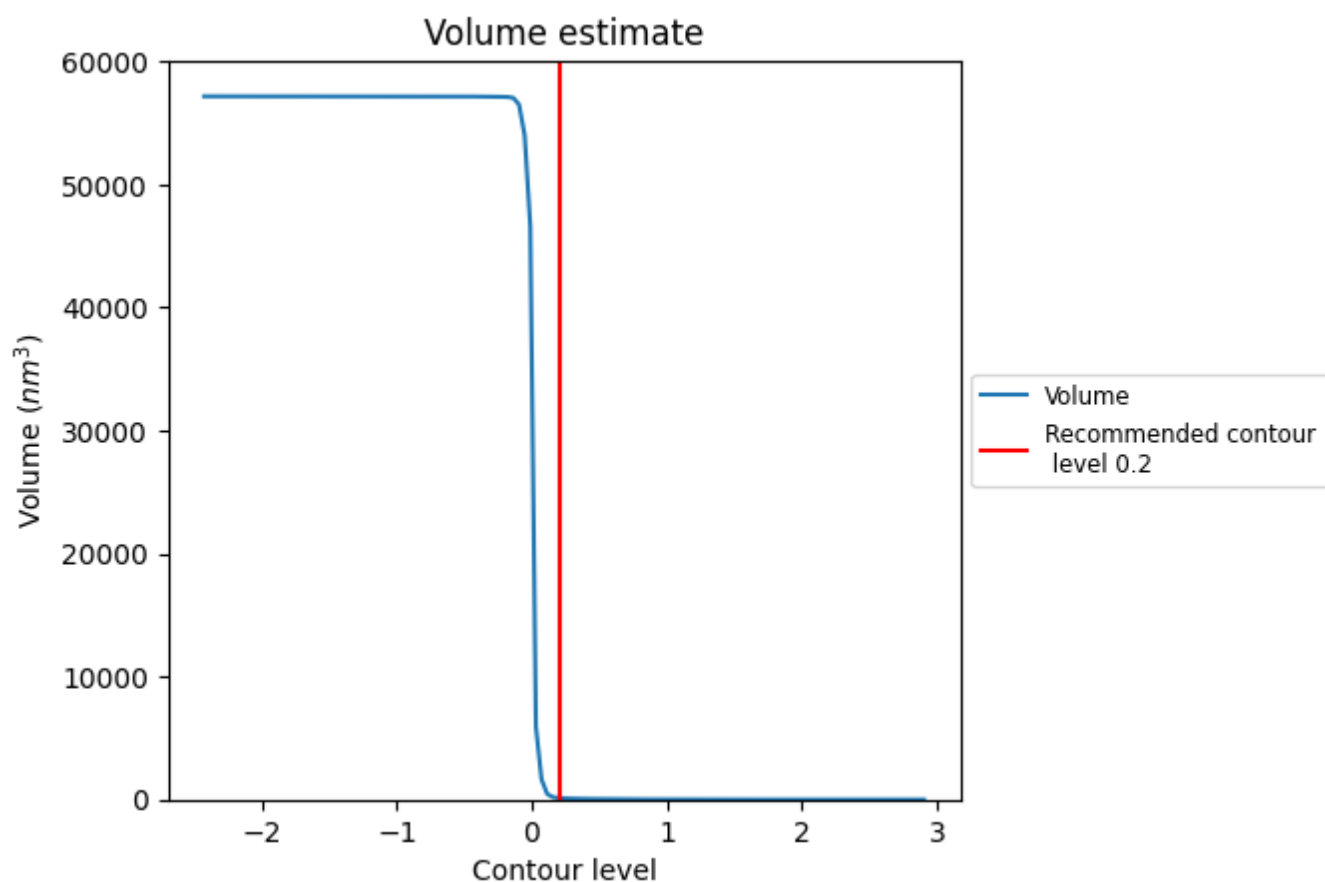
This section contains the results of statistical analysis of the map.

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.

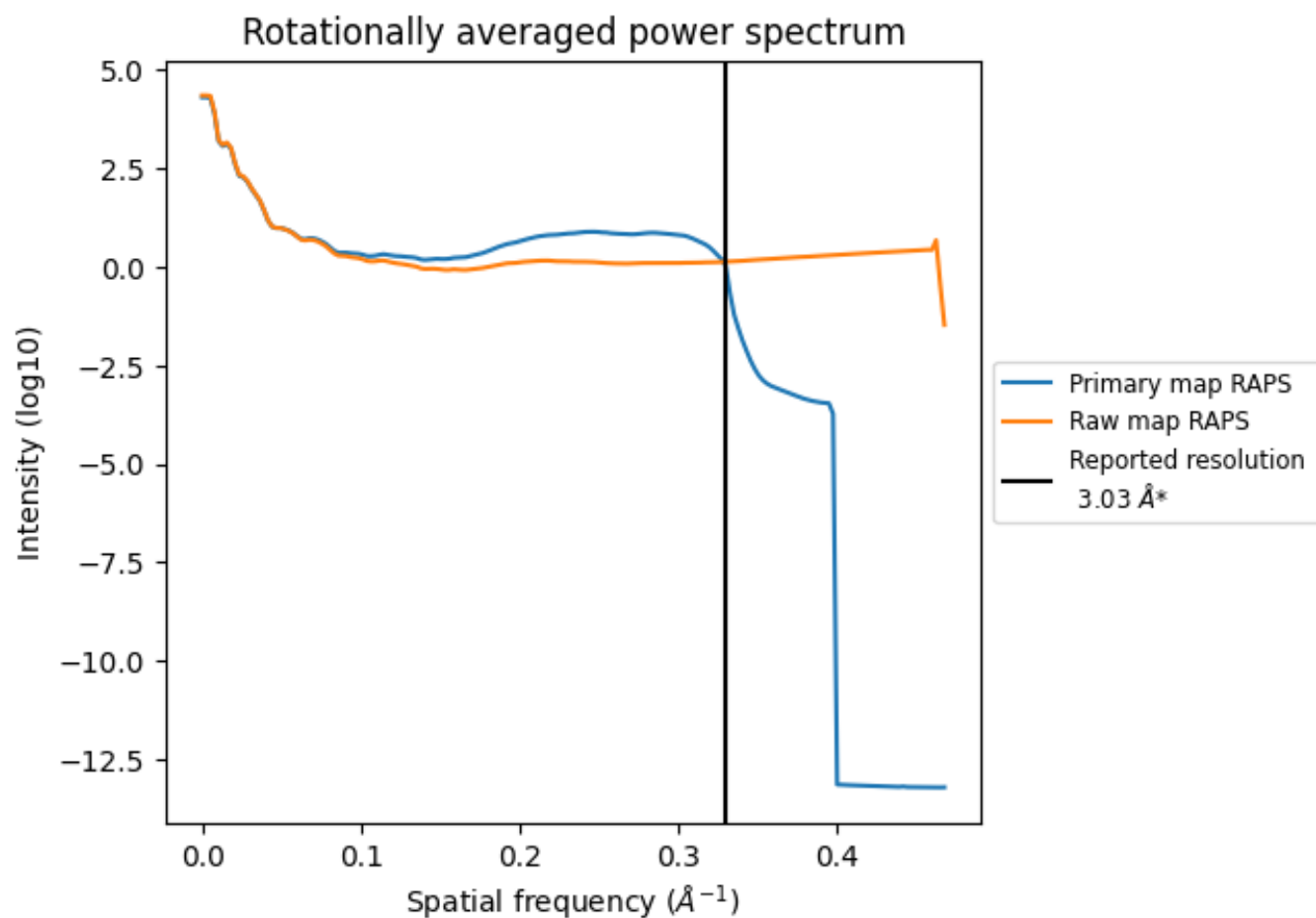
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 127 nm³; this corresponds to an approximate mass of 115 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 ⓘ

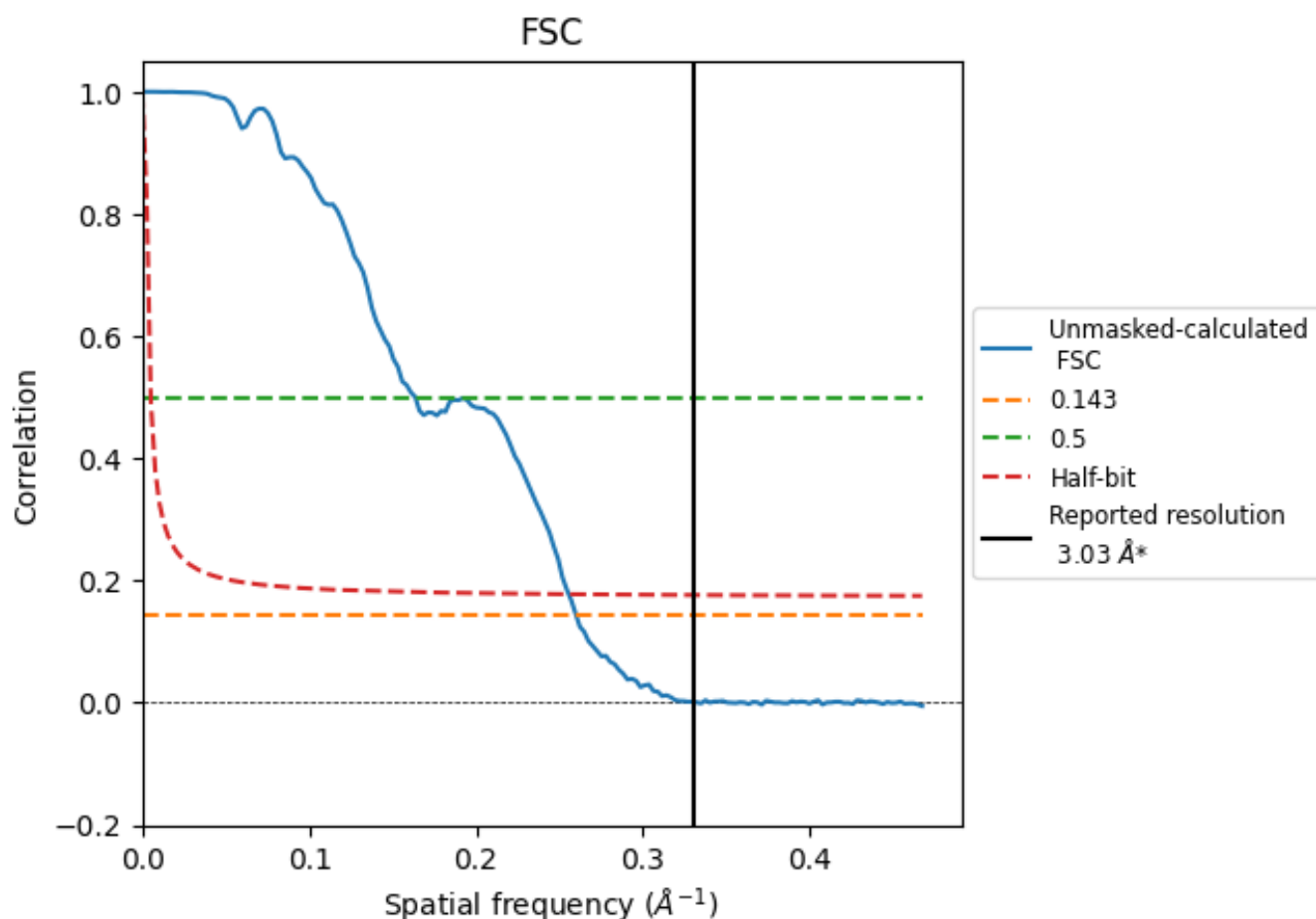


*Reported resolution corresponds to spatial frequency of 0.330 $\text{\AA}^{-1}$

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 $0.330 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

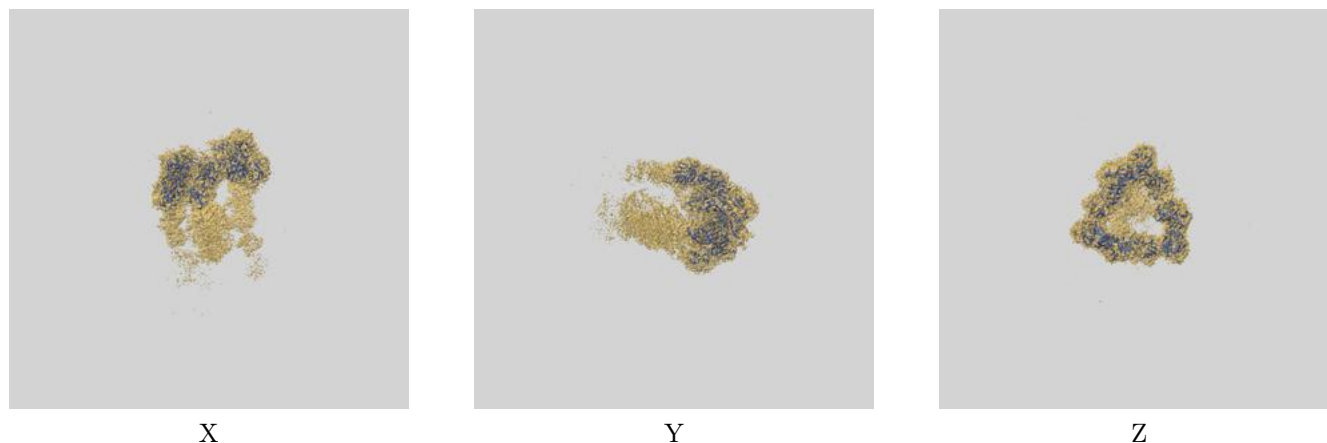
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.03	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.85	6.11	3.91

*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 3.85 differs from the reported value 3.03 by more than 10 %

9 Map-model fit [i](#)

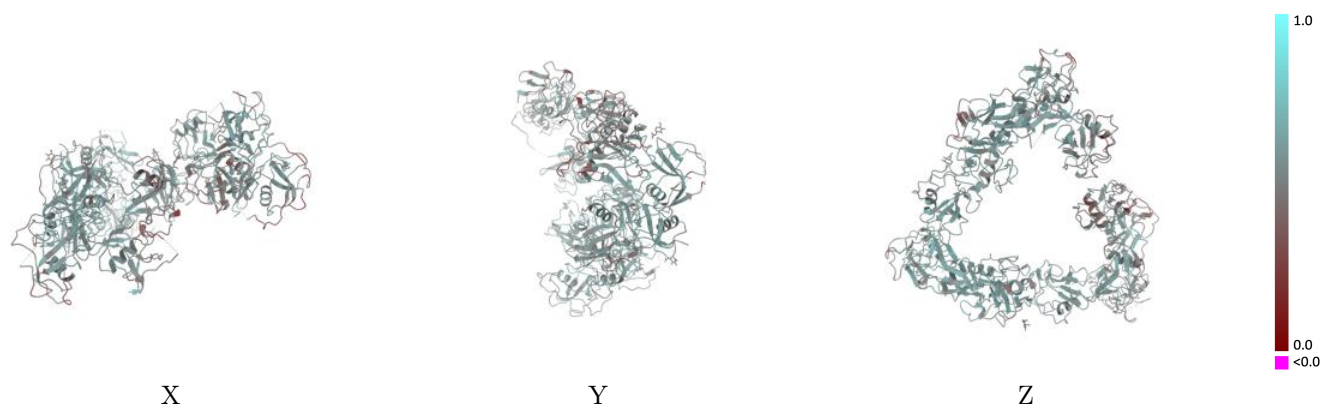
This section contains information regarding the fit between EMDB map EMD-38480 and PDB model 8XMK. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



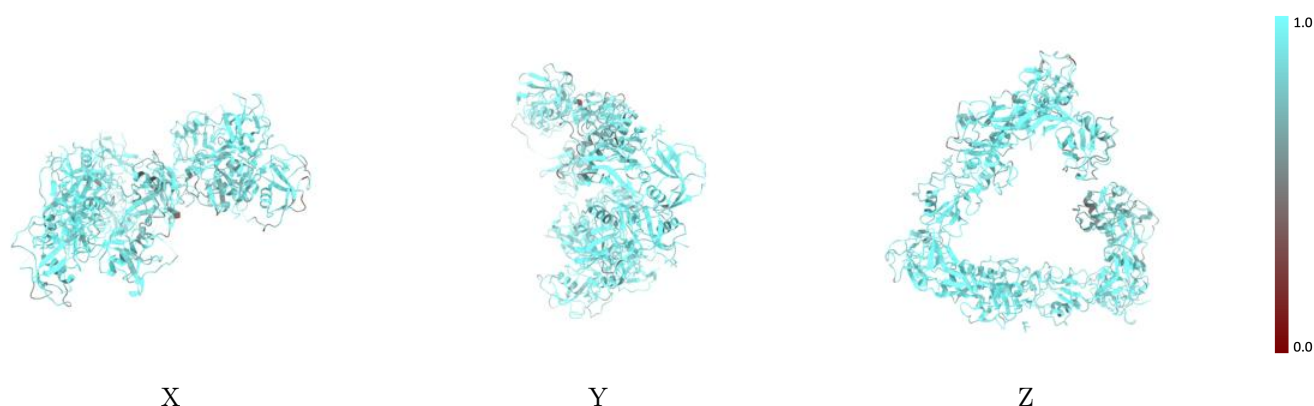
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



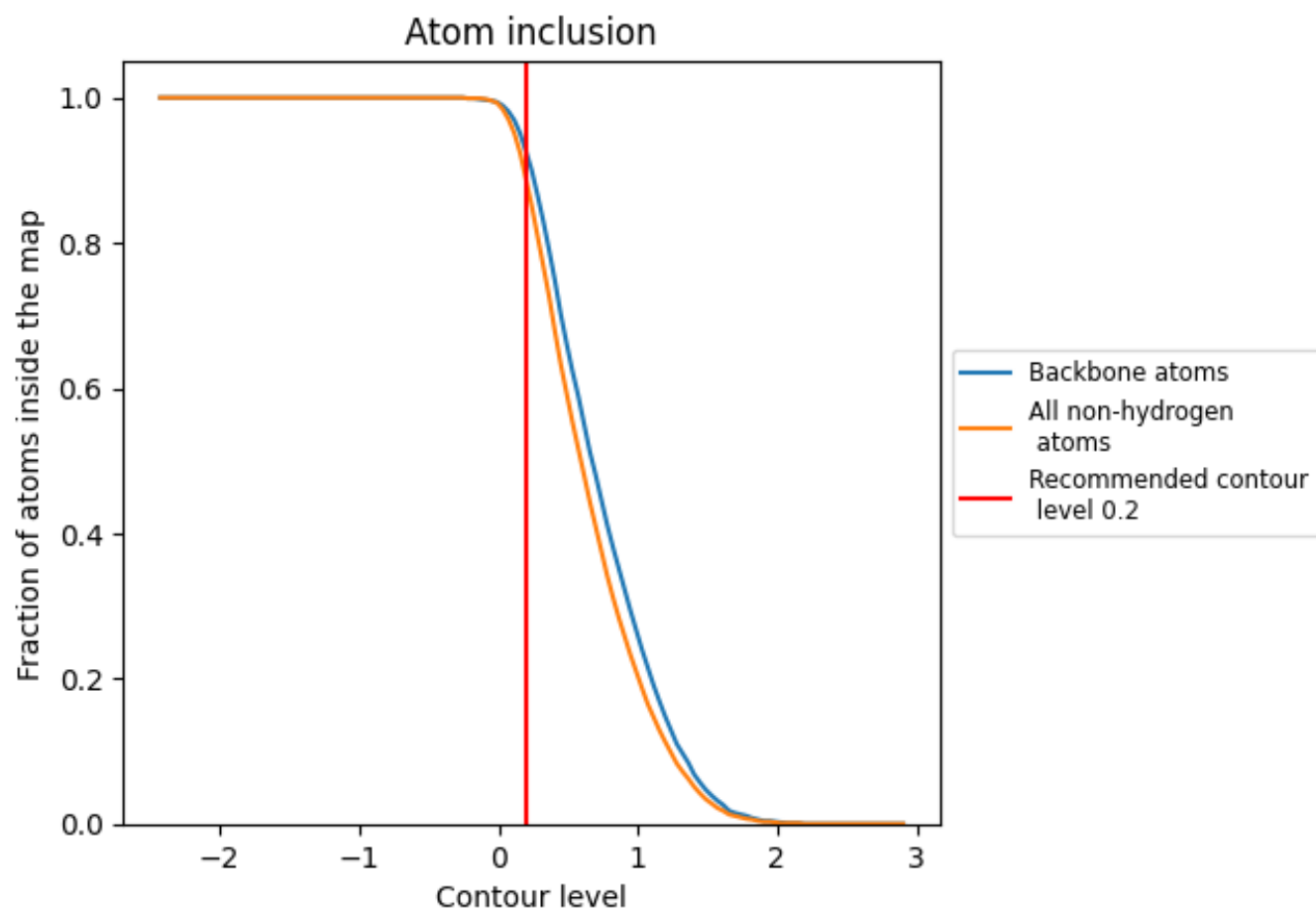
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 92% of all backbone atoms, 89% 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	0.8860	0.5290
D	0.8730	0.5140
E	0.8630	0.5160
F	0.9210	0.5570

