



Full wwPDB EM Validation Report ⓘ

Dec 12, 2023 – 06:14 PM JST

PDB ID : 8IEN
EMDB ID : EMD-35387
Title : Cryo-EM structure of ATP13A2 in the E2-Pi state
Authors : Liu, Z.M.; Mu, J.Q.; Xue, C.Y.
Deposited on : 2023-02-15
Resolution : 3.25 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.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

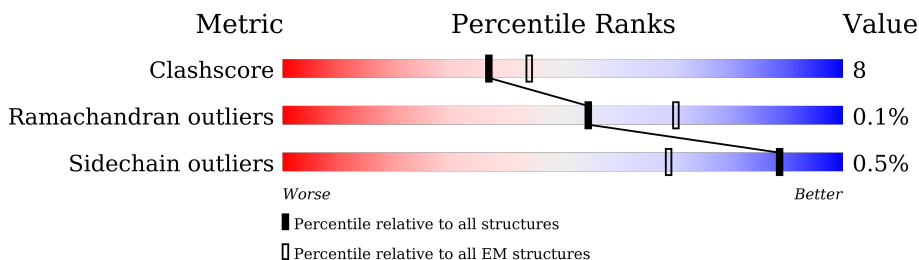
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.25 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	P	1180	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SPM	P	1203	-	-	X	-
4	SPM	P	1204	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7730 atoms, of which 52 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.

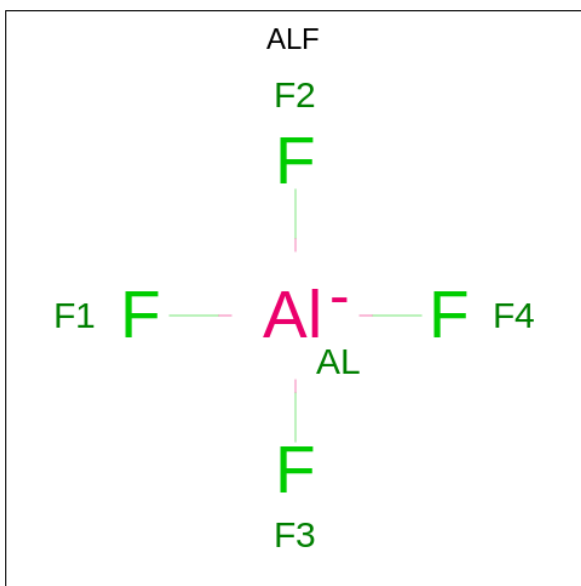
- Molecule 1 is a protein called Polyamine-transporting ATPase 13A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	P	991	7644	4939	1312	1340	53	0	0

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

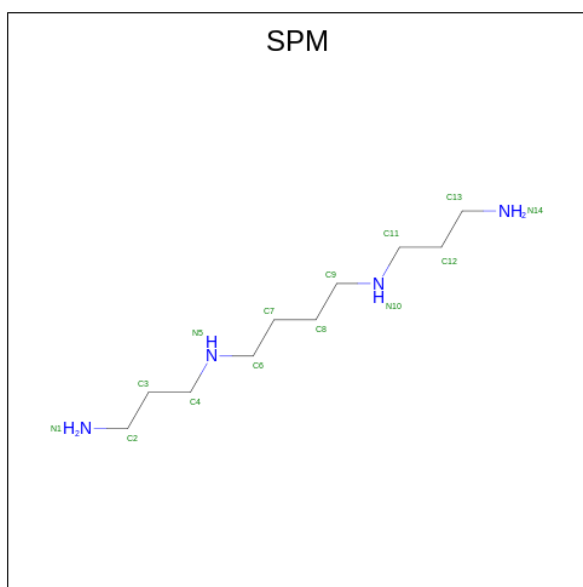
Mol	Chain	Residues	Atoms		AltConf
2	P	1	Total	Mg	0
			1	1	

- Molecule 3 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF_4).



Mol	Chain	Residues	Atoms			AltConf
3	P	1	Total	Al	F	0
			5	1	4	

- Molecule 4 is SPERMINE (three-letter code: SPM) (formula: $\text{C}_{10}\text{H}_{26}\text{N}_4$).

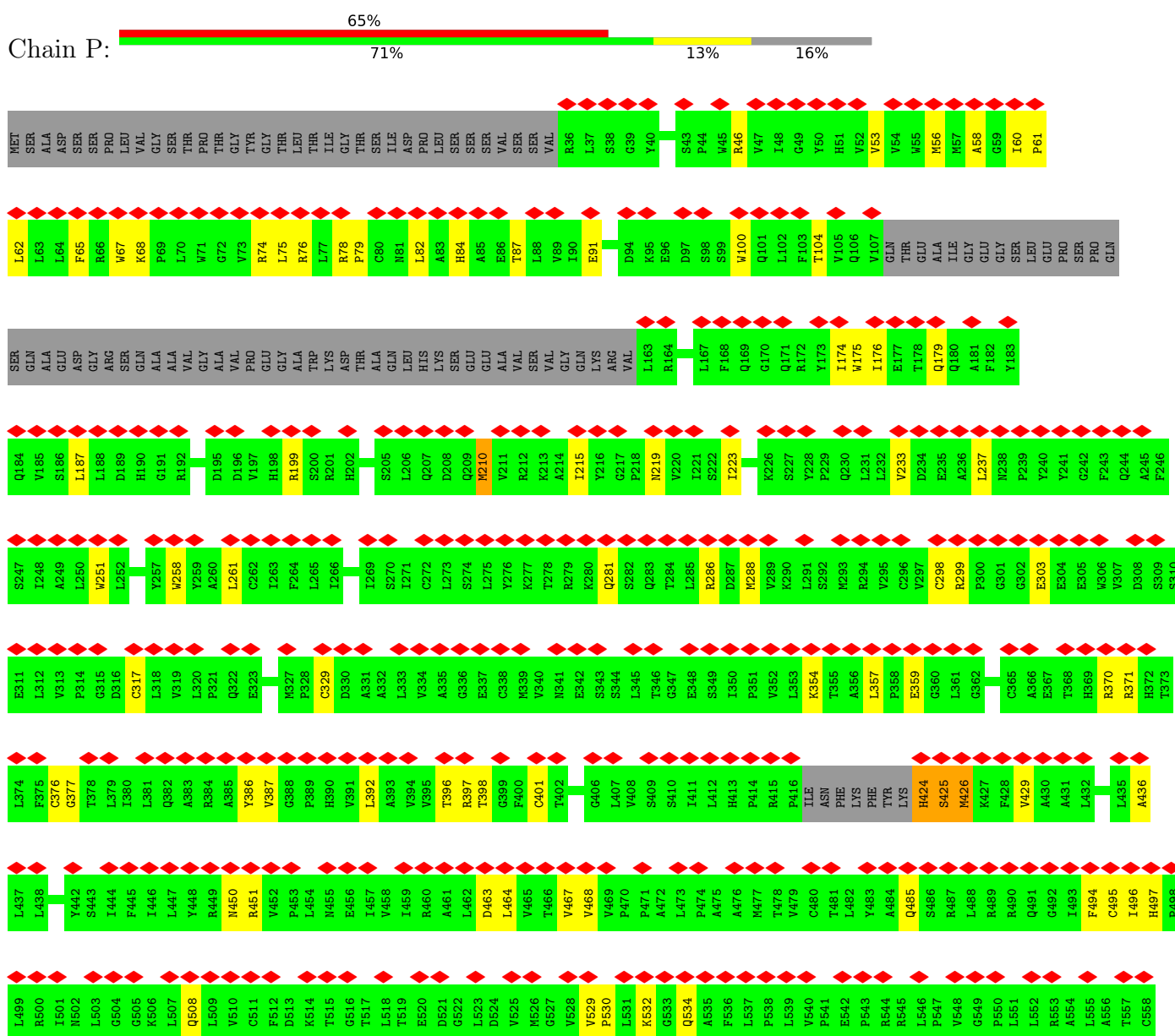


Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	N	
4	P	1	40	10	26	4	0
4	P	1	40	10	26	4	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Polyamine-transporting ATPase 13A2



ALA	GLY	PRO	LEU	ARG	H559	A560	L561	SER	ARG	LEU	GLN	ASP	THR	PRO	VAL	G570	D571	P572	M573	D574	L575	K576	M577	V578	E579	S580	T581	G582	V583	V584	LEU	GLU	GLU	GLU	PRO	ALA	ALA	ASP	SER	SER	ALA	PHE	GLY	THR	GLN	VAL	LEU	ALA	VAL	MET	ARG	PRO	PRO	LEU	TRP	GLU	PRO	GLN	LEU	Q613	A614	M615	E616	E617	P618
					P619	V620	P621	S622	S623	V624	L625	H626	R627	F628	S631	S632	A633	L634	Q635	R636	M637	S638	V639	V640	V641	A642	M643	P644	G645	A646	T647	Q648	P649	E650	A651	V652	V653	K654	G655	S656	P657	E658	L659	V660	A661	G662	L663	C664	M665	P666	E667	T668	V669	P670	T671	D672	F673	A674	Q675	M676	L677	Q678	S679		
					Y680	T681	A682	G683	G684	Y685	R686	V687	V688	A689	L690	A691	S692	K693	P694	L695	R696	THR	VAL	SER	LEU	GLU	ALA	ALA	GLN	LEU	THR	ARG	ARG	THR	VAL	E713	G714	D715	L716	S717	L718	L719	G720	L721	L722	V723	M724	R725	L727	L728	K729	P730	Q731	T732	T733	F734	V735	L736	Q737	R740					
					R741	T742	R743	T744	R745	V746	V747	M748	V749	T750	G751	D752	M753	L754	Q755	T756	A757	V758	T759	V760	A761	R762	G763	C764	G765	M766	V767	A768	F769	Q770	E771	H772	L773	T774	I775	V776	H777	T779	H780	P781	E782	R783	G784	Q785	P786	A787	S788	L789	E790	PHE	LEU	PRO	MET	GLU	SER	THR	ALA	VAL			
					ASN	GLY	VAL	LYS	ASP	PRO	ASP	GLN	ALA	ALA	TYR	THR	VAL	GLU	PRO	PRO	ARG	S820	R821	H822	L823	A824	L825	S826	G827	P828	T829	F830	G831	I832	I833	H836	F837	P838	K839	L840	L841	P842	K843	V844	L845	V846	Q847	G848	T849	V850	F851	A852	R853	M854	A855	P856	E857	Q858	K859	E861					
					L862	V863	C864	E865	L866	Q867	K868	L869	Q870	V871	C872	V873	G874	M875	C876	G877	D878	G879	A880	N881	D882	C883	G884	A885	L886	K887	A888	A889	D890	V891	G892	I893	S894	S895	L896	S896	Q897	A898	E899	A900	S901	V902	V903	S904	P905	F906	T907	S908	S909	N910	A911	S912	T913	E914	C915	V916	P917	N918	V919	I920	R921
					E922	G923	R924	C925	S926	L927	D928	T929	S930	F931	S932	V933	F934	K935	Y936	M937	A938	L939	Y940	S941	L942	T943	Q944	F945	I946	L949	I950	L951	Y952	T953	I954	N955	T956	N957	L958	G959	D960	L961	Q962	F963	L964	A965	I966	D967	L968	Y969	I970	S971	A1038	P1039	D1040	N1041	L1042	Y1045	E1046	N978	S979	R980	P983		
					A984	L985	V986	L987	G988	R989	V990	P991	P992	P993	G994	A995	L996	S997	V998	P1000	V1001	L1002	S1003	S1004	L1007	Q1008	L1011	Y1012	V1015	Q1016	G1019	Y1020	F1021	L1022	A1025	Q1026	P1027	W1028	F1029	V1030	P1031	L1032	N1033	R1034	T1035	V1036	A1037	A1038	G1100	L1101	L1102	Q1103	G1104	L1105	L1106	A1107	L1108	R1109	N1110	I1111					
					V1050	F1051	S1052	L1053	S1054	S1055	F1056	Q1057	Y1058	L1059	L1060	L1061	A1062	A1063	A1064	V1065	S1066	K1067	G1068	A1069	P1070	F1071	R1072	R1073	P1074	L1075	Y1076	T1077	N1078	V1079	P1080	F1081	L1082	V1083	A1084	L1085	A1086	L1087	L1088	S1089	V1093	G1094	L1095	V1096	L1097	L1098	V1099	G1100	L1101	L1102	Q1103	G1104	L1105	L1106	A1107	L1108	R1109	N1110	I1111		
					T1114	K1117	L1118	L1119	L1120	L1121	G1122	L1123	V1124	T1125	L1126	N1127	F1128	V1129	F1132	M1133	L1134	E1135	S1136	V1137	L1138	D1139	Q1140	C1141	L1142	P1143	A1144	C1145	L1146	R1147	R1149	R1150	P1151	K1152	R1153	A1154	K1157	R1158	F1159	K1160	Q1161	L1162	E1163	R1164	E1165	L1166	A1167	E1168	Q1169	PRO	TRP	PRO	PRO	LEU	PRO						

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	290927	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.559	Depositor
Minimum map value	-2.596	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.075	Depositor
Recommended contour level	0.576	Depositor
Map size (\AA)	328.5, 328.5, 328.5	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.095, 1.095, 1.095	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: SPM, MG, ALF

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	P	0.24	0/7812	0.43	0/10639

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	P	7644	0	7925	129	0
2	P	1	0	0	0	0
3	P	5	0	0	0	0
4	P	28	52	51	41	0
All	All	7678	52	7976	130	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 8.

All (130) 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:P:467:VAL:CG2	4:P:1204:SPM:H121	1.57	1.35
1:P:251:TRP:CZ3	4:P:1204:SPM:H91	1.61	1.33
1:P:251:TRP:HZ3	4:P:1204:SPM:C9	1.56	1.18
1:P:251:TRP:CZ2	4:P:1204:SPM:H131	1.80	1.17
1:P:467:VAL:CG2	4:P:1204:SPM:C12	2.24	1.15
1:P:251:TRP:CZ3	4:P:1204:SPM:C9	2.28	1.14
1:P:251:TRP:HH2	4:P:1204:SPM:C11	1.60	1.14
1:P:467:VAL:HG22	4:P:1204:SPM:C12	1.79	1.12
1:P:251:TRP:CH2	4:P:1204:SPM:C11	2.39	1.05
1:P:251:TRP:CH2	4:P:1204:SPM:H112	1.90	1.05
1:P:251:TRP:HH2	4:P:1204:SPM:N10	1.62	0.97
1:P:251:TRP:CH2	4:P:1204:SPM:H131	1.98	0.97
1:P:467:VAL:HG23	4:P:1204:SPM:H121	1.48	0.94
1:P:251:TRP:CH2	4:P:1204:SPM:N10	2.38	0.92
1:P:463:ASP:OD1	4:P:1204:SPM:N10	2.03	0.90
1:P:251:TRP:HZ3	4:P:1204:SPM:H91	1.01	0.84
1:P:467:VAL:HG22	4:P:1204:SPM:C13	2.07	0.84
1:P:467:VAL:HG21	4:P:1204:SPM:H121	1.63	0.81
1:P:251:TRP:CZ2	4:P:1204:SPM:C13	2.64	0.78
1:P:251:TRP:CH2	4:P:1204:SPM:C9	2.65	0.78
1:P:251:TRP:CH2	4:P:1204:SPM:H91	2.20	0.76
4:P:1203:SPM:H91	4:P:1203:SPM:H131	1.68	0.74
1:P:934:PHE:CE1	4:P:1203:SPM:H41	2.23	0.73
1:P:251:TRP:CH2	4:P:1204:SPM:C13	2.74	0.71
1:P:936:TYR:HB2	1:P:1065:VAL:HG21	1.75	0.69
1:P:251:TRP:HZ3	4:P:1204:SPM:H92	1.53	0.69
1:P:934:PHE:HE1	4:P:1203:SPM:H41	1.58	0.69
1:P:251:TRP:HZ2	4:P:1204:SPM:H131	1.51	0.68
1:P:467:VAL:HG22	4:P:1204:SPM:H132	1.76	0.68
1:P:1148:ARG:HG3	1:P:1151:PRO:HA	1.75	0.68
1:P:288:MET:HG3	1:P:899:GLU:HB2	1.76	0.67
1:P:251:TRP:HH2	4:P:1204:SPM:C12	2.08	0.66
1:P:467:VAL:CG2	4:P:1204:SPM:H122	2.27	0.62
1:P:467:VAL:HG21	4:P:1204:SPM:C12	2.24	0.62
1:P:939:LEU:HB3	1:P:1061:LEU:HD13	1.82	0.61
1:P:485:GLN:HG3	1:P:495:CYS:HB3	1.83	0.60
1:P:82:LEU:HD21	1:P:84:HIS:HD1	1.67	0.58
1:P:939:LEU:HD13	1:P:1061:LEU:HD22	1.84	0.58
1:P:966:ILE:HG23	1:P:970:ILE:HD12	1.84	0.58
1:P:396:THR:HG23	1:P:397:ARG:HG2	1.86	0.58
1:P:53:VAL:HA	1:P:56:MET:HG2	1.86	0.58
1:P:87:THR:HA	1:P:104:THR:HB	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:199:ARG:NH2	1:P:357:LEU:O	2.37	0.57
1:P:897:GLN:HE22	1:P:909:SER:HA	1.69	0.57
1:P:837:PHE:HD1	1:P:841:LEU:HD13	1.69	0.57
1:P:467:VAL:HG22	4:P:1204:SPM:H122	1.77	0.57
1:P:74:ARG:HA	1:P:78:ARG:HB2	1.86	0.56
1:P:376:CYS:SG	1:P:377:GLY:N	2.78	0.56
1:P:298:CYS:HB2	1:P:317:CYS:HB3	1.88	0.55
1:P:754:LEU:HD11	1:P:824:ALA:HB1	1.89	0.54
1:P:859:LYS:HB3	1:P:885:ALA:HB2	1.88	0.54
1:P:745:ARG:NH2	1:P:848:GLY:O	2.40	0.54
1:P:46:ARG:HG2	1:P:79:PRO:HG3	1.88	0.54
1:P:581:THR:HG23	1:P:583:TRP:H	1.73	0.54
1:P:176:ILE:HG22	1:P:179:GLN:H	1.73	0.54
1:P:463:ASP:CG	4:P:1204:SPM:HN0	2.10	0.54
1:P:251:TRP:HZ2	4:P:1204:SPM:C13	2.13	0.53
1:P:934:PHE:CE1	4:P:1203:SPM:H62	2.42	0.53
1:P:429:VAL:HB	4:P:1203:SPM:H32	1.91	0.53
1:P:1056:PHE:O	1:P:1060:ILE:HG12	2.09	0.53
1:P:1097:LEU:HA	1:P:1117:LYS:HD3	1.90	0.53
1:P:67:TRP:HD1	1:P:68:LYS:HE2	1.74	0.53
1:P:887:LYS:HE3	1:P:903:VAL:HB	1.91	0.53
1:P:329:CYS:HB2	1:P:398:THR:HG22	1.90	0.52
1:P:675:GLN:HG2	1:P:678:GLN:HE21	1.73	0.52
1:P:1012:VAL:HA	1:P:1015:VAL:HG12	1.91	0.52
1:P:281:GLN:HE22	1:P:497:HIS:HE1	1.56	0.52
1:P:826:SER:H	1:P:829:THR:HB	1.74	0.52
1:P:532:LYS:HE2	1:P:534:GLN:HB2	1.91	0.51
1:P:767:VAL:HG21	1:P:771:GLU:HB2	1.93	0.50
1:P:354:LYS:NZ	1:P:370:ARG:O	2.43	0.50
1:P:251:TRP:CH2	4:P:1204:SPM:C12	2.88	0.50
1:P:496:ILE:HG22	1:P:905:PRO:HA	1.93	0.50
1:P:1103:GLN:HG2	1:P:1108:LEU:HD12	1.93	0.49
1:P:219:ASN:HD21	1:P:329:CYS:HB3	1.78	0.49
1:P:613:GLN:NE2	1:P:623:SER:OG	2.45	0.49
1:P:425:SER:HA	4:P:1203:SPM:H72	1.95	0.49
1:P:725:ARG:HG3	1:P:727:LEU:H	1.78	0.48
1:P:934:PHE:HE1	4:P:1203:SPM:C4	2.24	0.48
1:P:299:ARG:HB2	1:P:303:GLU:HG2	1.96	0.48
1:P:529:VAL:HB	1:P:530:PRO:HD3	1.95	0.48
1:P:424:HIS:ND1	1:P:997:LEU:CB	2.77	0.48
1:P:210:MET:SD	1:P:210:MET:N	2.81	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:464:LEU:HD11	1:P:945:PHE:HD1	1.78	0.47
1:P:450:ASN:OD1	1:P:451:ARG:N	2.48	0.47
1:P:897:GLN:HE21	1:P:907:THR:HG22	1.79	0.47
1:P:187:LEU:HB2	1:P:397:ARG:HH21	1.80	0.47
1:P:425:SER:HB2	1:P:426:MET:CE	2.44	0.47
1:P:934:PHE:CZ	4:P:1203:SPM:H41	2.50	0.47
1:P:1160:LYS:O	1:P:1163:GLU:HG2	2.15	0.47
1:P:754:LEU:O	1:P:758:VAL:HG23	2.16	0.46
1:P:436:ALA:HB2	1:P:468:VAL:HG11	1.97	0.46
1:P:561:LEU:O	1:P:627:ARG:NH1	2.49	0.46
1:P:199:ARG:NH2	1:P:359:GLU:O	2.49	0.46
1:P:776:VAL:HG23	1:P:829:THR:HG23	1.99	0.45
1:P:485:GLN:NE2	1:P:495:CYS:O	2.49	0.45
1:P:943:THR:HA	1:P:946:ILE:HG12	1.98	0.45
1:P:663:LEU:HD23	1:P:716:LEU:HD12	1.99	0.45
1:P:62:LEU:HA	1:P:65:PHE:HB2	1.99	0.44
1:P:451:ARG:O	1:P:451:ARG:NH1	2.49	0.44
1:P:386:TYR:HD2	1:P:387:VAL:HG13	1.82	0.44
1:P:424:HIS:ND1	1:P:997:LEU:HB3	2.32	0.44
1:P:996:LEU:HD12	4:P:1203:SPM:H81	2.00	0.44
1:P:174:ILE:HG21	1:P:215:ILE:HG23	1.99	0.43
1:P:968:LEU:O	1:P:972:THR:OG1	2.31	0.43
1:P:60:ILE:HB	1:P:61:PRO:HD3	2.00	0.43
1:P:732:THR:HA	1:P:913:ILE:HG21	2.00	0.43
1:P:1068:GLY:HA2	1:P:1072:ARG:HB2	2.00	0.43
1:P:233:VAL:HA	1:P:237:LEU:HD12	2.01	0.43
1:P:386:TYR:CD2	1:P:387:VAL:HG13	2.53	0.43
1:P:508:GLN:HE21	1:P:872:CYS:H	1.66	0.43
1:P:58:ALA:HB3	1:P:76:ARG:HD3	2.01	0.42
1:P:84:HIS:CD2	1:P:175:TRP:HZ2	2.38	0.42
1:P:258:TRP:O	1:P:261:LEU:HG	2.18	0.42
1:P:392:LEU:HD23	1:P:392:LEU:HA	1.89	0.42
1:P:451:ARG:HA	1:P:451:ARG:HD2	1.71	0.42
1:P:1148:ARG:HH21	1:P:1152:LYS:HG3	1.84	0.42
1:P:75:LEU:HD23	1:P:75:LEU:HA	1.91	0.42
1:P:657:PRO:HG2	1:P:677:LEU:HD21	2.01	0.42
1:P:1074:PRO:O	1:P:1077:THR:OG1	2.37	0.42
1:P:223:ILE:HG13	1:P:286:ARG:HA	2.01	0.41
1:P:1063:ALA:O	1:P:1066:SER:OG	2.37	0.41
1:P:1011:LEU:HD13	1:P:1134:LEU:HD22	2.02	0.41
1:P:82:LEU:HD21	1:P:84:HIS:ND1	2.35	0.41

Continued on next page...

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:494:PHE:N	1:P:907:THR:O	2.49	0.41
1:P:693:LYS:HD2	1:P:694:PRO:HD2	2.02	0.41
1:P:91:GLU:HG3	1:P:100:TRP:HD1	1.85	0.40
1:P:397:ARG:HB2	1:P:401:CYS:HB2	2.03	0.40
1:P:58:ALA:O	1:P:61:PRO:HD2	2.22	0.40
1:P:965:ALA:O	1:P:969:VAL:HG22	2.22	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	P	977/1180 (83%)	927 (95%)	49 (5%)	1 (0%)	51 82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	425	SER

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	P	845/1002 (84%)	841 (100%)	4 (0%)	88 93

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	210	MET
1	P	371	ARG
1	P	424	HIS
1	P	426	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	198	HIS
1	P	219	ASN
1	P	281	GLN
1	P	508	GLN
1	P	613	GLN
1	P	897	GLN
1	P	1127	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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
3	ALF	P	1202	-	0,4,4	-	-	-		
4	SPM	P	1203	-	13,13,13	0.19	0	12,12,12	0.18	0
4	SPM	P	1204	1	13,13,13	1.14	2 (15%)	12,12,12	0.83	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
4	SPM	P	1203	-	-	8/11/11/11	-
4	SPM	P	1204	1	-	4/11/11/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	1204	SPM	C12-C11	-2.83	1.40	1.51
4	P	1204	SPM	C12-C13	-2.14	1.41	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	P	1204	SPM	N10-C11-C12-C13
4	P	1203	SPM	C7-C8-C9-N10
4	P	1203	SPM	C2-C3-C4-N5
4	P	1203	SPM	C8-C9-N10-C11
4	P	1204	SPM	C7-C6-N5-C4
4	P	1203	SPM	C6-C7-C8-C9
4	P	1204	SPM	C6-C7-C8-C9
4	P	1204	SPM	C11-C12-C13-N14
4	P	1203	SPM	N5-C6-C7-C8
4	P	1203	SPM	N10-C11-C12-C13
4	P	1203	SPM	N1-C2-C3-C4
4	P	1203	SPM	C7-C6-N5-C4

There are no ring outliers.

2 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	P	1203	SPM	9	0
4	P	1204	SPM	32	0

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.

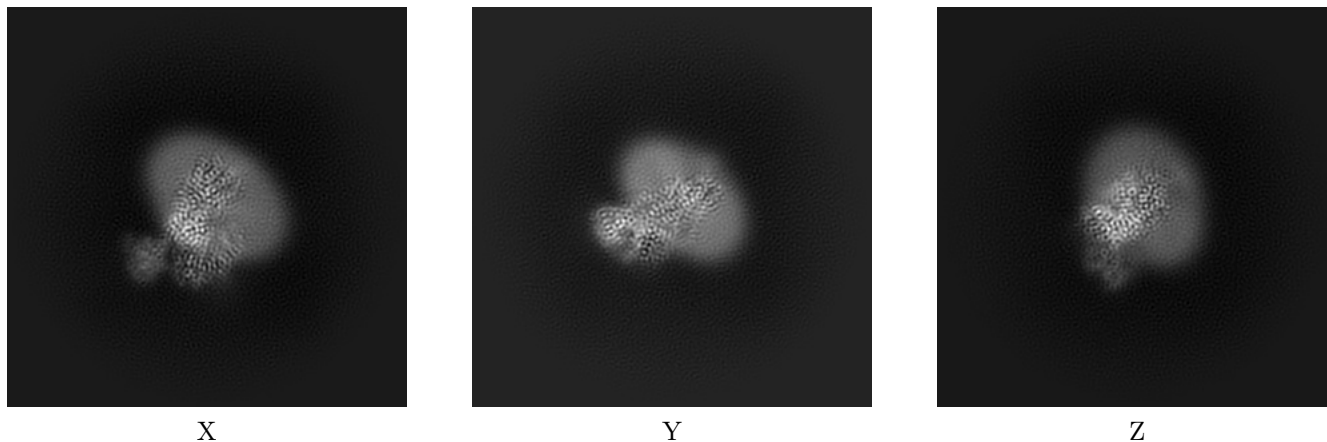
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35387. These allow visual inspection of the internal detail of the map and identification of artifacts.

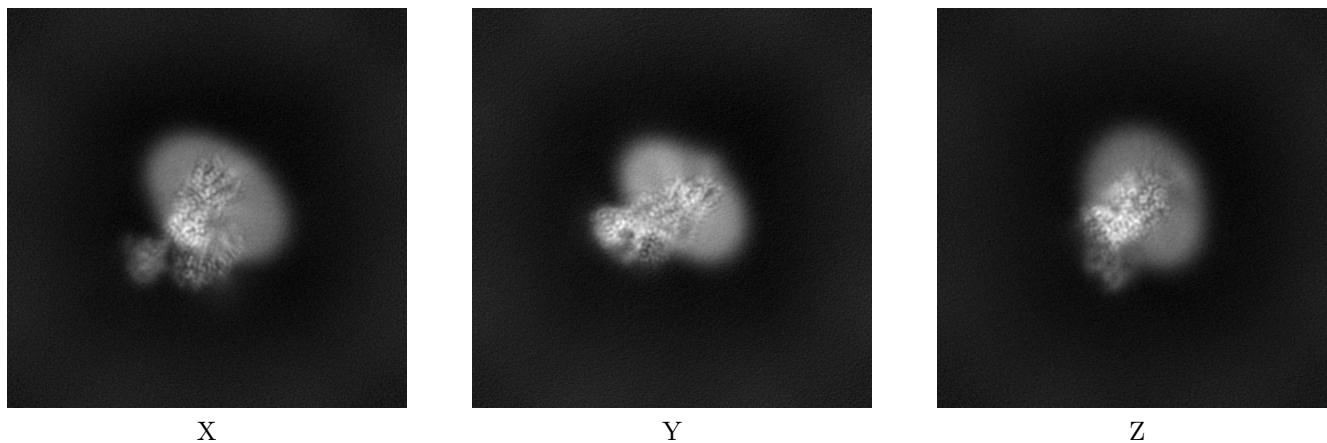
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



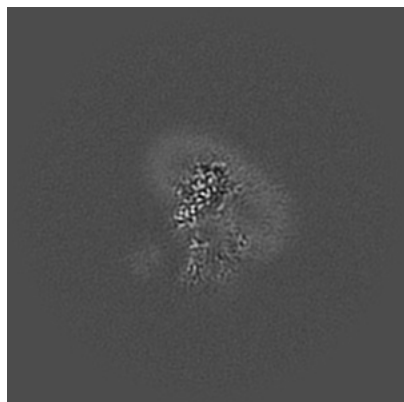
6.1.2 Raw map



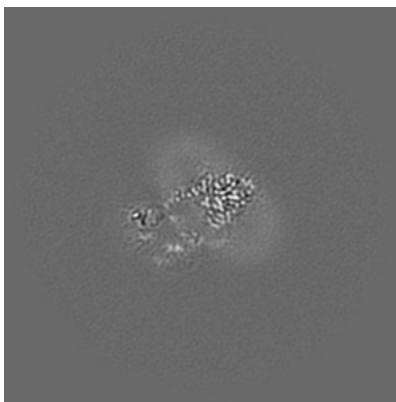
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

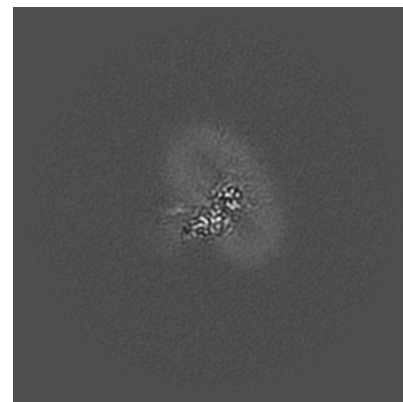
6.2.1 Primary map



X Index: 150

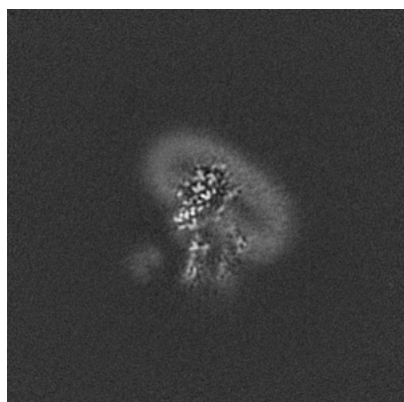


Y Index: 150

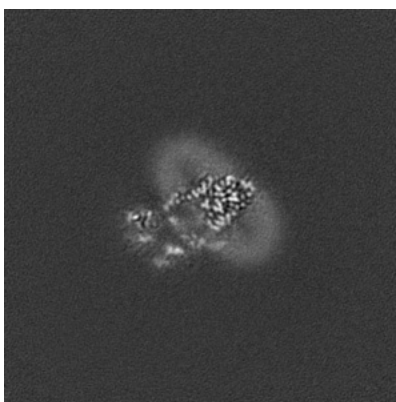


Z Index: 150

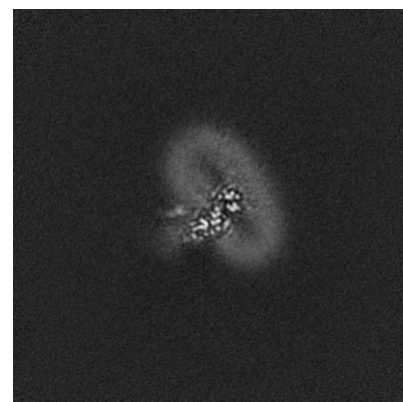
6.2.2 Raw map



X Index: 150



Y Index: 150

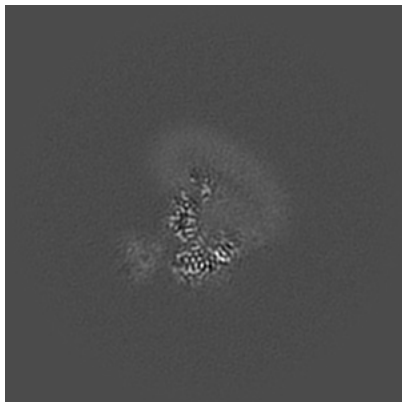


Z Index: 150

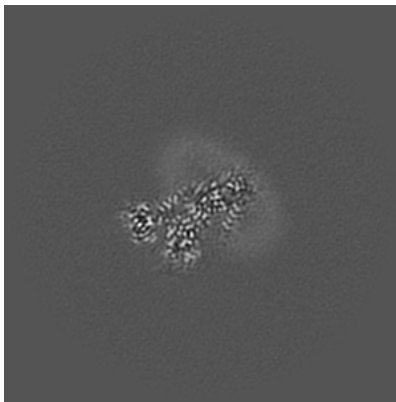
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

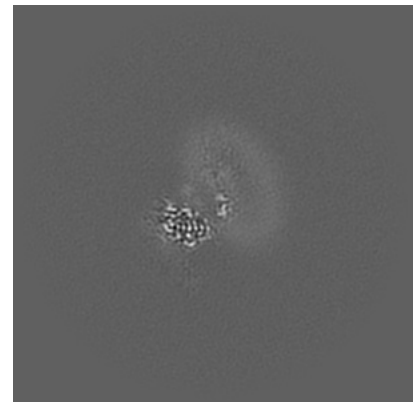
6.3.1 Primary map



X Index: 139

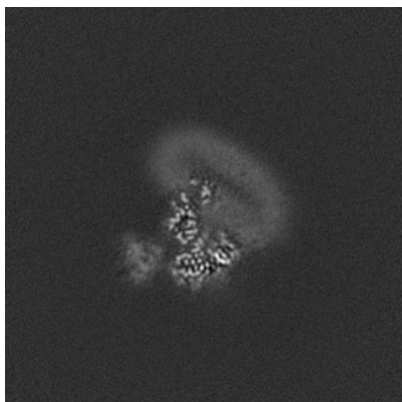


Y Index: 141

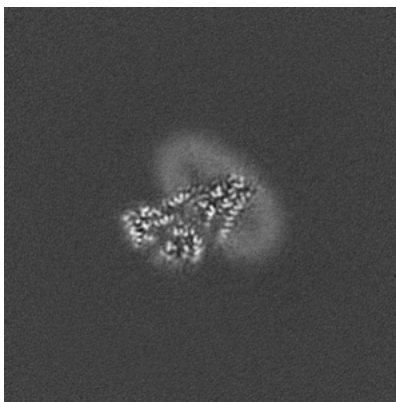


Z Index: 133

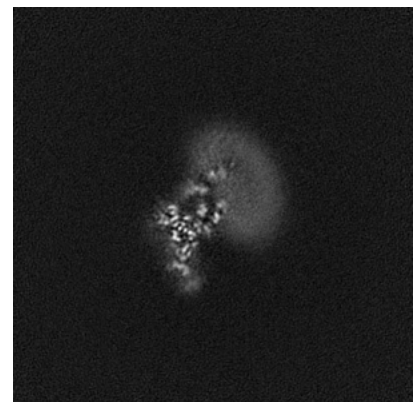
6.3.2 Raw map



X Index: 139



Y Index: 144

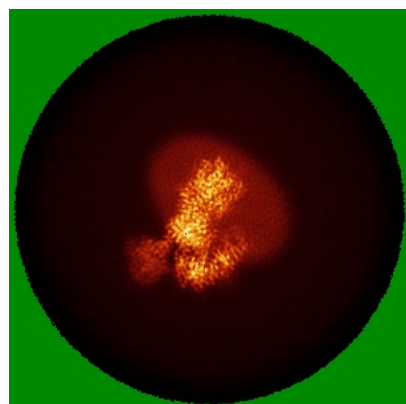


Z Index: 125

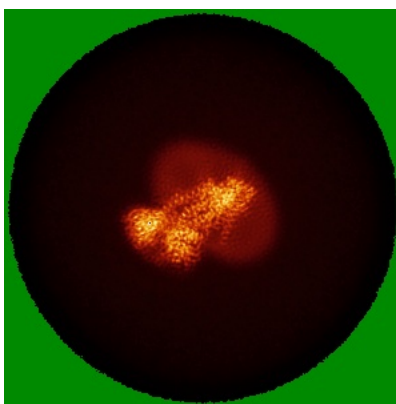
The images above show the largest variance slices of the map in three orthogonal directions.

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

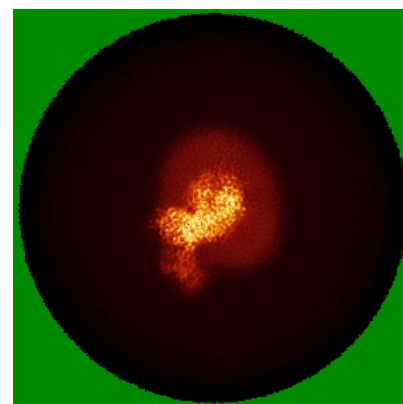
6.4.1 Primary map



X

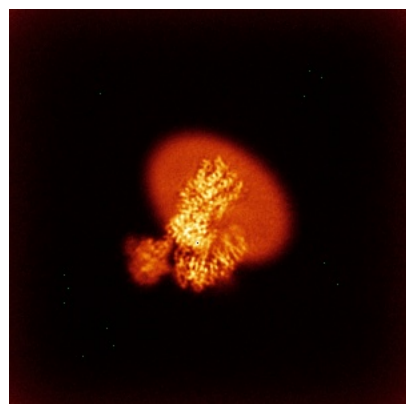


Y

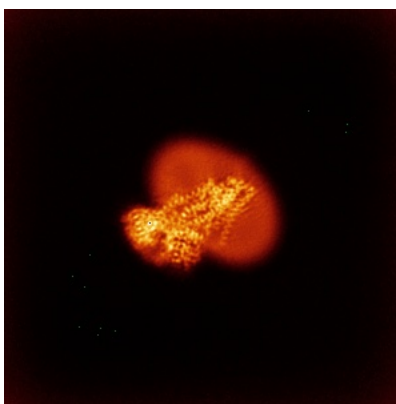


Z

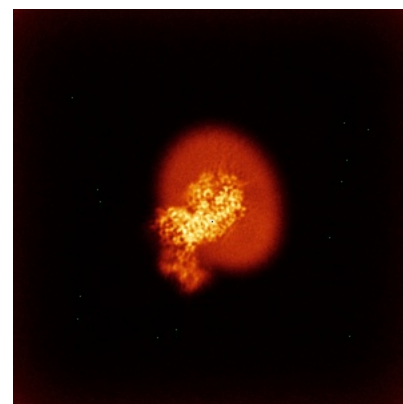
6.4.2 Raw map



X



Y

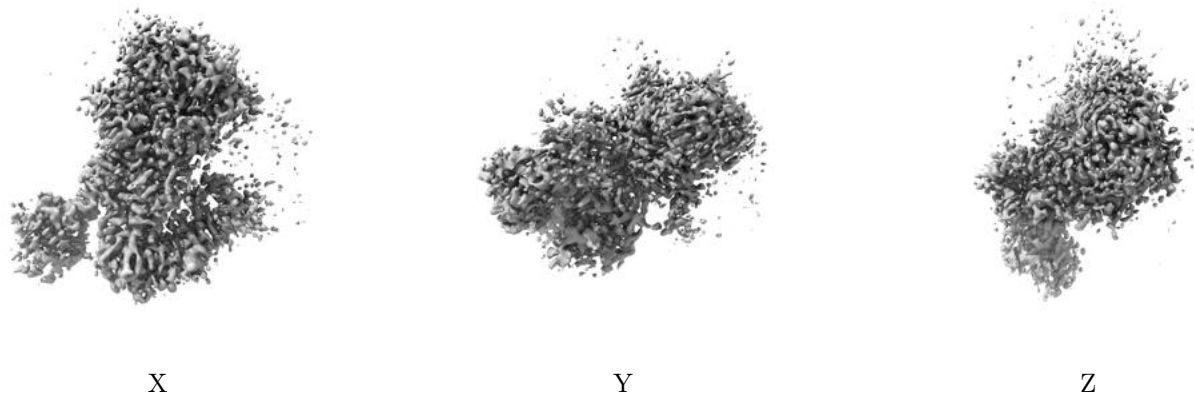


Z

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.

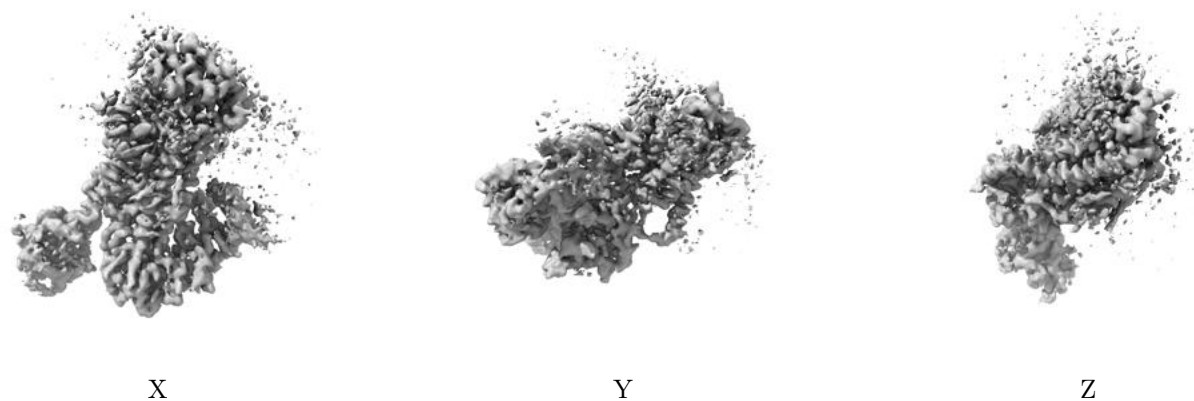
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.576. 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.

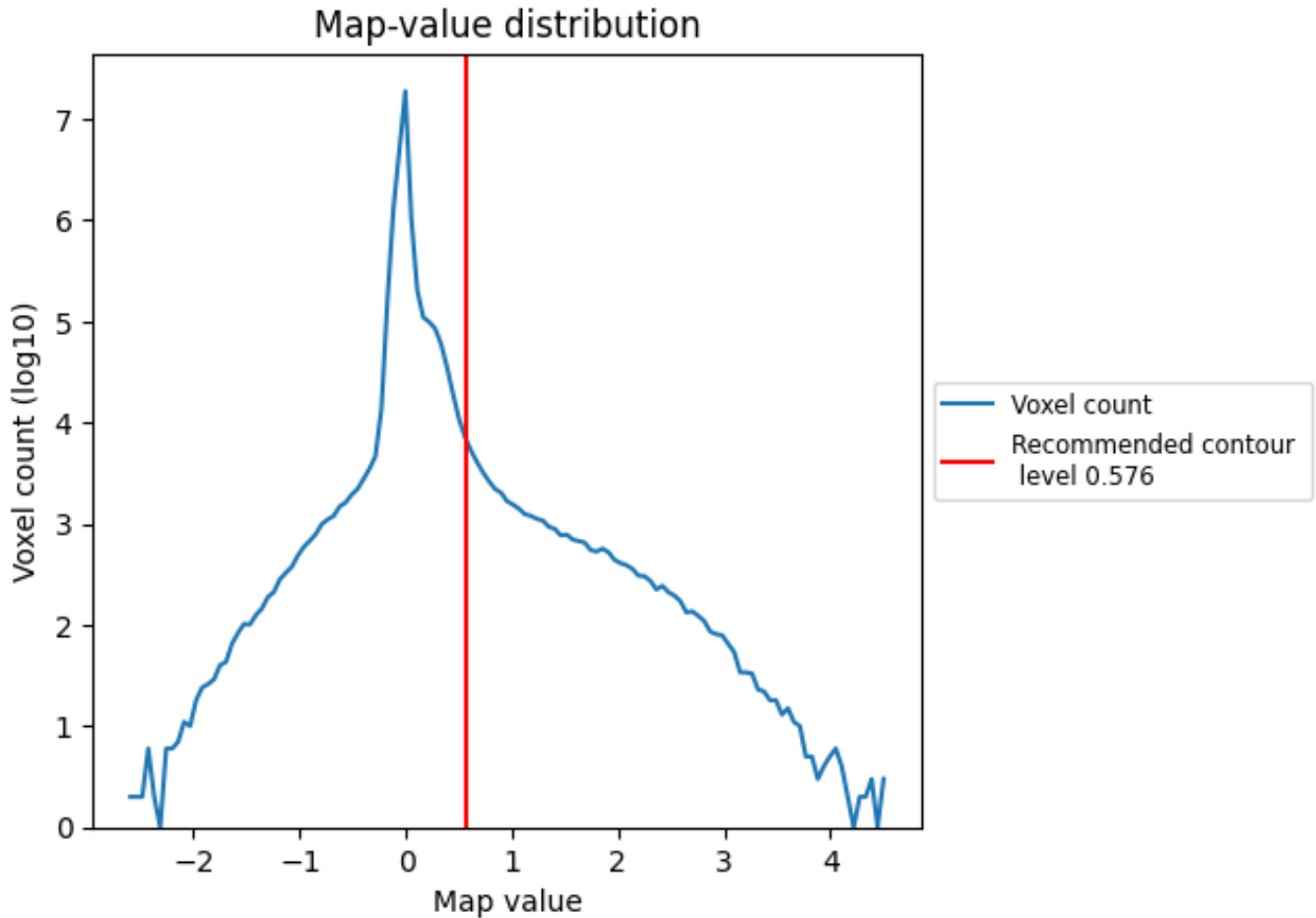
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

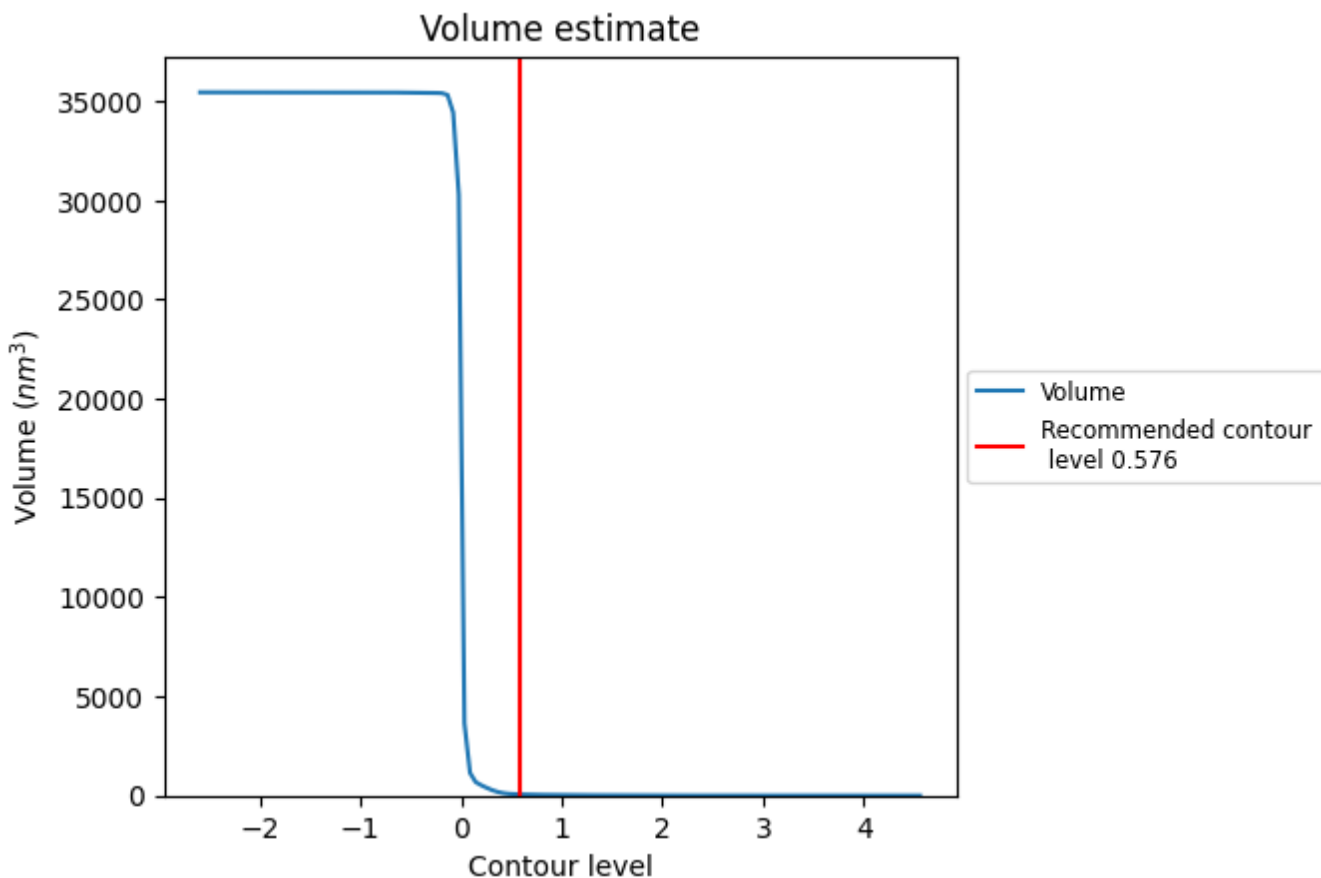
This section contains the results of statistical analysis of the map.

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.

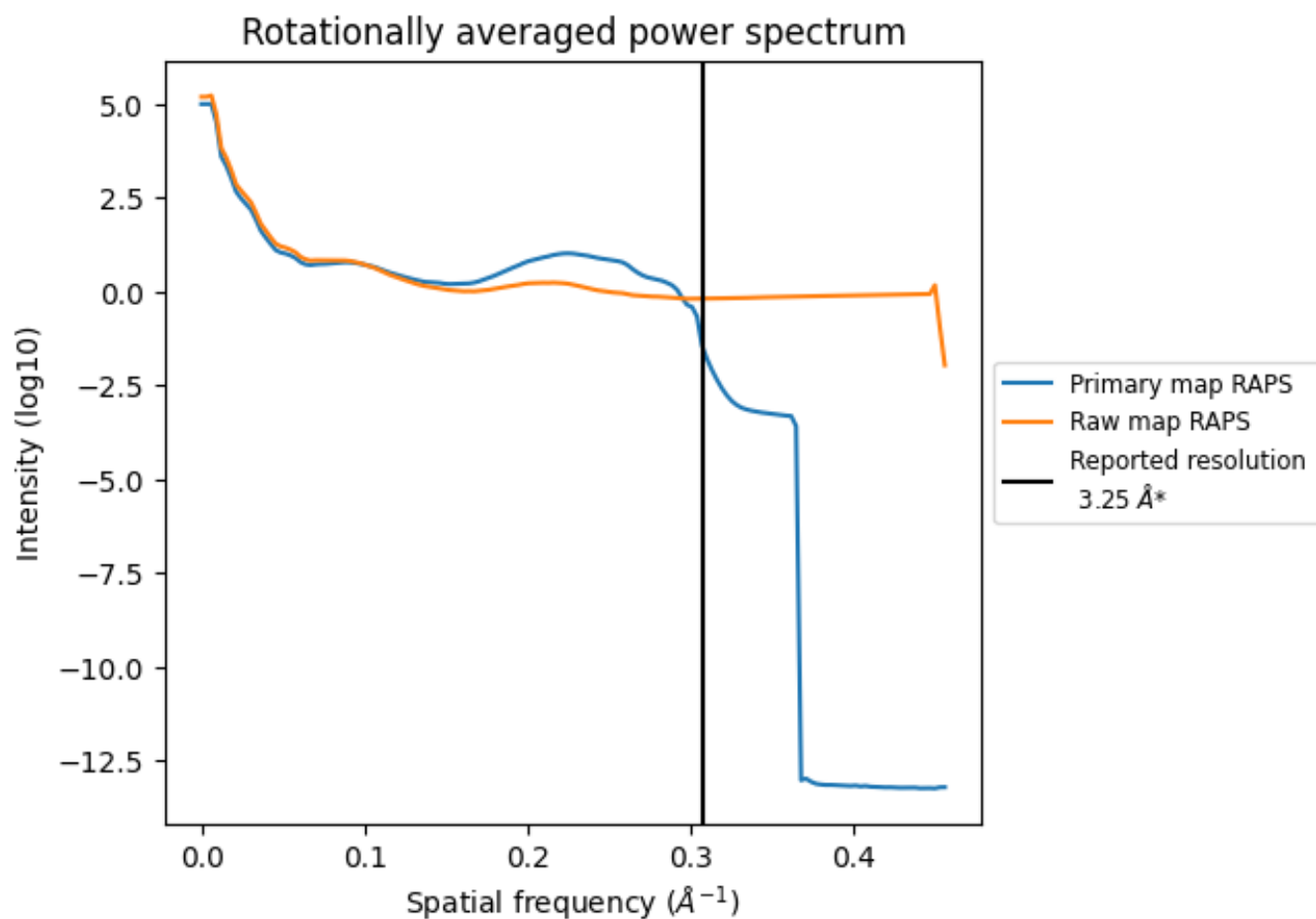
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 60 nm^3 ; this corresponds to an approximate mass of 54 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 i

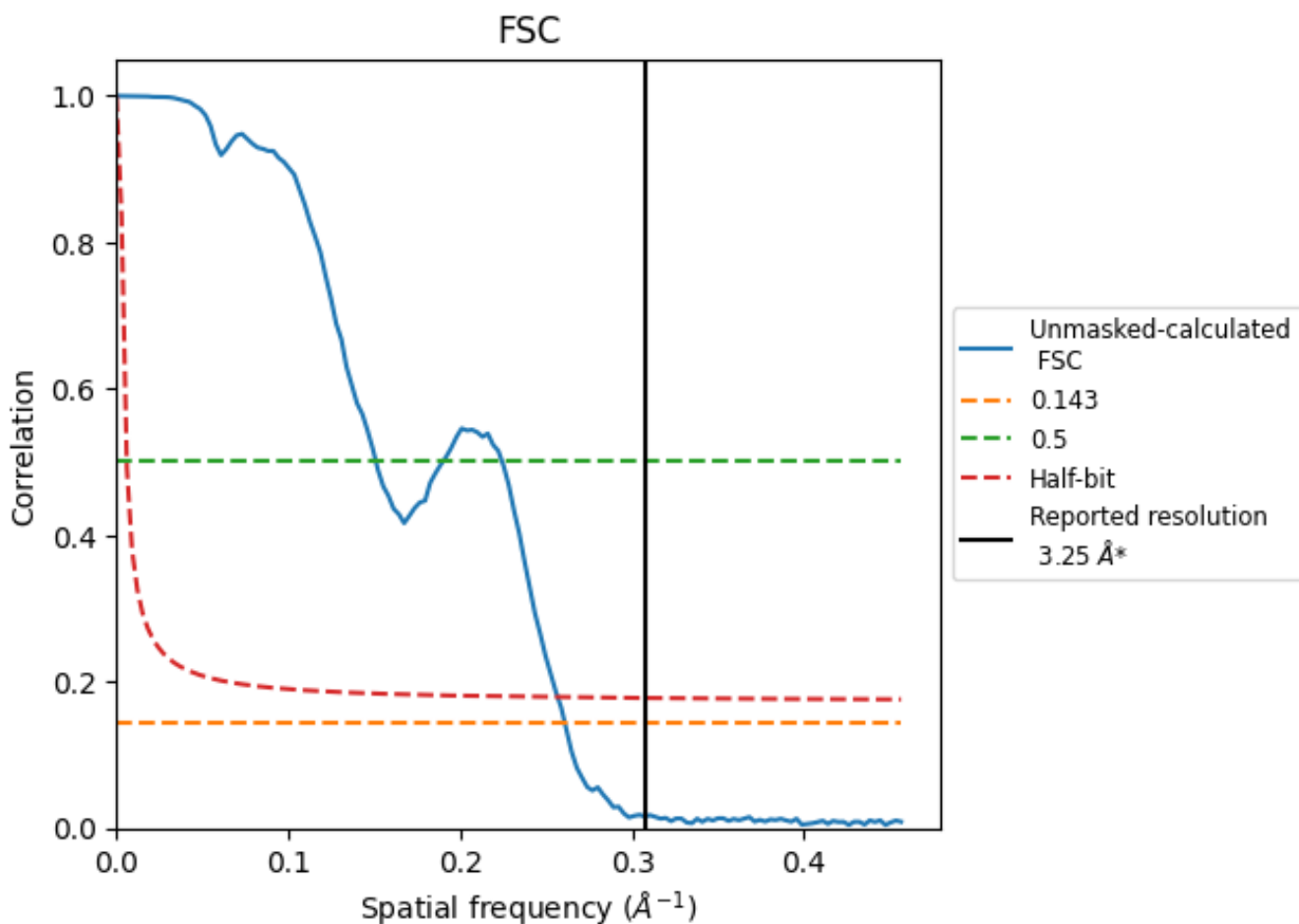


*Reported resolution corresponds to spatial frequency of 0.308 Å⁻¹

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 0.308 Å⁻¹

8.2 Resolution estimates [i](#)

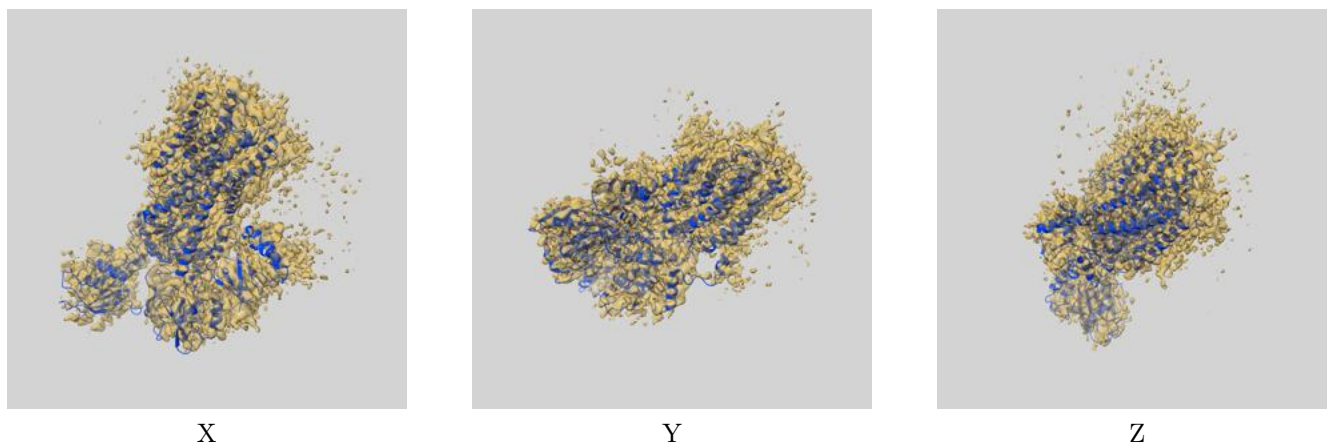
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.25	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.83	6.62	3.89

*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 3.83 differs from the reported value 3.25 by more than 10 %

9 Map-model fit [i](#)

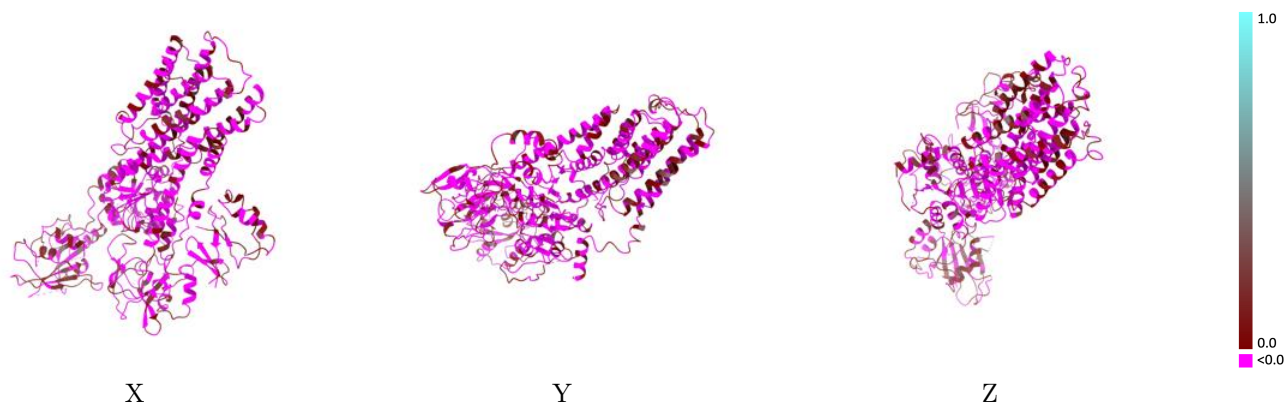
This section contains information regarding the fit between EMDB map EMD-35387 and PDB model 8IEN. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



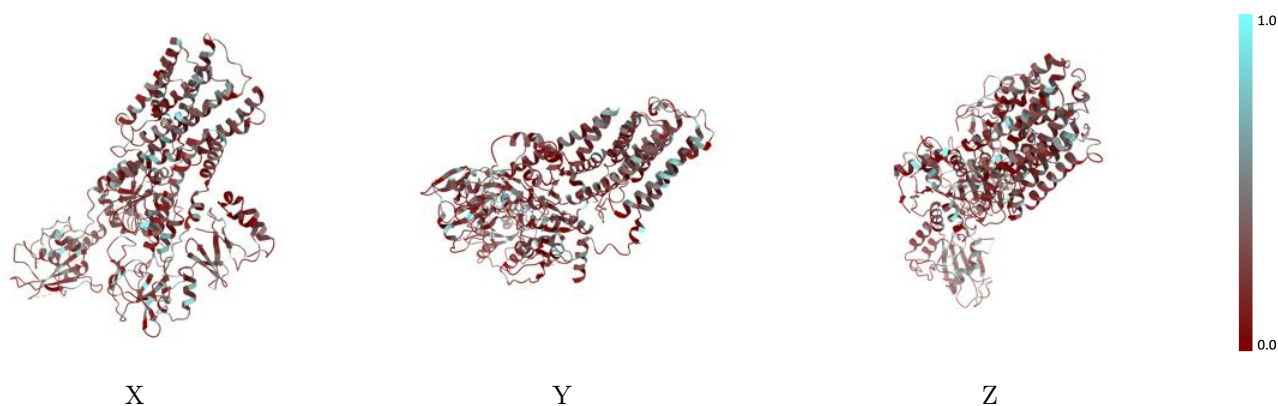
The images above show the 3D surface view of the map at the recommended contour level 0.576 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



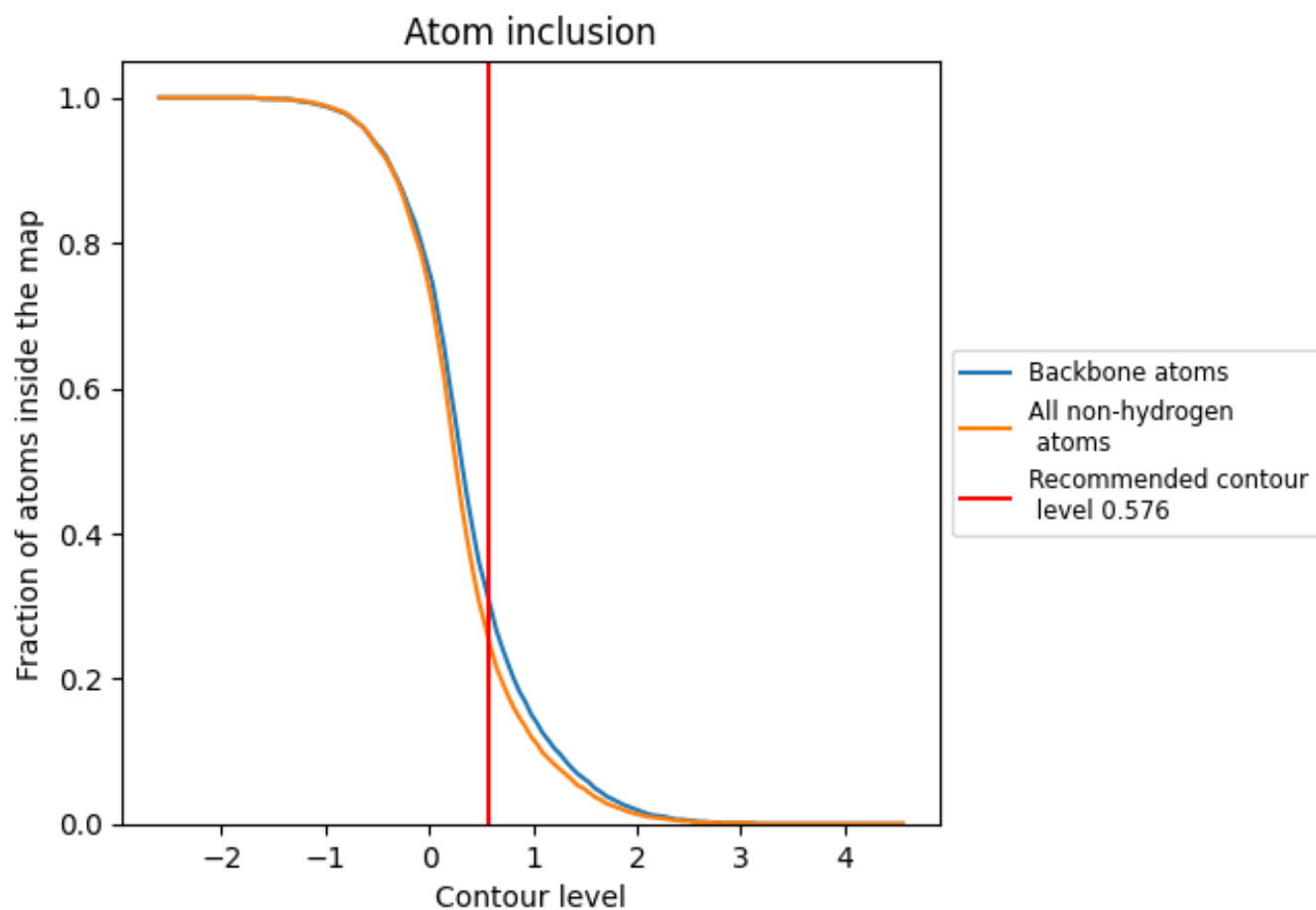
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.576).





9.4 Atom inclusion [i](#)



At the recommended contour level, 31% of all backbone atoms, 25% 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 (0.576) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.2530	 -0.0470
P	 0.2540	 -0.0470

