



wwPDB EM Validation Summary Report ⓘ

Mar 14, 2026 – 03:49 AM UTC

PDB ID : 8IVQ / pdb_00008ivq
EMDB ID : EMD-35759
Title : Cryo-EM structure of mouse BIRC6, Global map
Authors : Liu, S.; Jiang, T.; Bu, F.; Zhao, J.; Wang, G.; Li, N.; Gao, N.; Qiu, X.
Deposited on : 2023-03-28
Resolution : 3.60 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>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

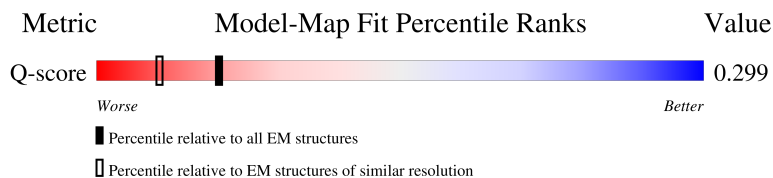
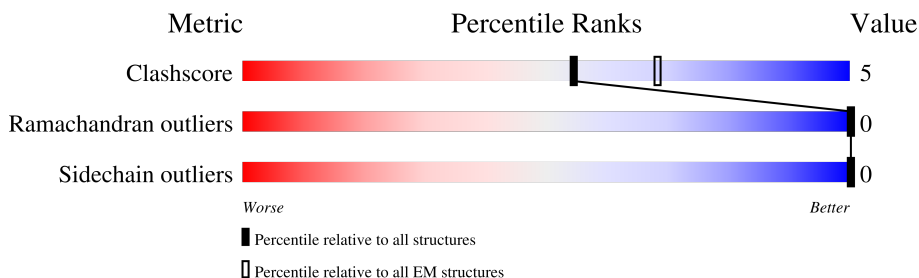
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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	12797 (3.10 - 4.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	4896	25% 52% 7% 40%
1	B	4896	25% 52% 8% 40%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 41900 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 Isoform 2 of Baculoviral IAP repeat-containing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2921	Total	C	N	O	S	0	0
			20950	13236	3680	3904	130		
1	B	2921	Total	C	N	O	S	0	0
			20950	13236	3680	3904	130		

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-50	MET	-	initiating methionine	UNP O88738
A	-49	ASP	-	expression tag	UNP O88738
A	-48	TYR	-	expression tag	UNP O88738
A	-47	LYS	-	expression tag	UNP O88738
A	-46	ASP	-	expression tag	UNP O88738
A	-45	HIS	-	expression tag	UNP O88738
A	-44	ASP	-	expression tag	UNP O88738
A	-43	GLY	-	expression tag	UNP O88738
A	-42	ASP	-	expression tag	UNP O88738
A	-41	TYR	-	expression tag	UNP O88738
A	-40	LYS	-	expression tag	UNP O88738
A	-39	ASP	-	expression tag	UNP O88738
A	-38	HIS	-	expression tag	UNP O88738
A	-37	ASP	-	expression tag	UNP O88738
A	-36	ILE	-	expression tag	UNP O88738
A	-35	ASP	-	expression tag	UNP O88738
A	-34	TYR	-	expression tag	UNP O88738
A	-33	LYS	-	expression tag	UNP O88738
A	-32	ASP	-	expression tag	UNP O88738
A	-31	ASP	-	expression tag	UNP O88738
A	-30	ASP	-	expression tag	UNP O88738
A	-29	ASP	-	expression tag	UNP O88738
A	-28	LYS	-	expression tag	UNP O88738
A	-27	ARG	-	expression tag	UNP O88738
A	-26	VAL	-	expression tag	UNP O88738
A	-25	VAL	-	expression tag	UNP O88738

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	PRO	-	expression tag	UNP O88738
A	-23	LEU	-	expression tag	UNP O88738
A	-22	GLU	-	expression tag	UNP O88738
A	-21	SER	-	expression tag	UNP O88738
A	-20	THR	-	expression tag	UNP O88738
A	-19	GLY	-	expression tag	UNP O88738
A	-18	LEU	-	expression tag	UNP O88738
A	-17	GLN	-	expression tag	UNP O88738
A	-16	GLU	-	expression tag	UNP O88738
A	-15	LEU	-	expression tag	UNP O88738
A	-14	ALA	-	expression tag	UNP O88738
A	-13	THR	-	expression tag	UNP O88738
A	-12	MET	-	expression tag	UNP O88738
A	-11	GLU	-	expression tag	UNP O88738
A	-10	GLN	-	expression tag	UNP O88738
A	-9	LYS	-	expression tag	UNP O88738
A	-8	LEU	-	expression tag	UNP O88738
A	-7	ILE	-	expression tag	UNP O88738
A	-6	SER	-	expression tag	UNP O88738
A	-5	GLU	-	expression tag	UNP O88738
A	-4	GLU	-	expression tag	UNP O88738
A	-3	ASP	-	expression tag	UNP O88738
A	-2	LEU	-	expression tag	UNP O88738
A	-1	GLU	-	expression tag	UNP O88738
A	0	PHE	-	expression tag	UNP O88738
A	178	ILE	THR	conflict	UNP O88738
A	690	THR	ALA	conflict	UNP O88738
A	2079	ARG	GLY	conflict	UNP O88738
A	2418	GLY	CYS	conflict	UNP O88738
A	2959	ILE	THR	conflict	UNP O88738
A	3226	THR	SER	conflict	UNP O88738
A	3914	VAL	MET	conflict	UNP O88738
A	3929	VAL	ILE	conflict	UNP O88738
A	4346	MET	VAL	conflict	UNP O88738
B	-50	MET	-	initiating methionine	UNP O88738
B	-49	ASP	-	expression tag	UNP O88738
B	-48	TYR	-	expression tag	UNP O88738
B	-47	LYS	-	expression tag	UNP O88738
B	-46	ASP	-	expression tag	UNP O88738
B	-45	HIS	-	expression tag	UNP O88738
B	-44	ASP	-	expression tag	UNP O88738
B	-43	GLY	-	expression tag	UNP O88738

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-42	ASP	-	expression tag	UNP O88738
B	-41	TYR	-	expression tag	UNP O88738
B	-40	LYS	-	expression tag	UNP O88738
B	-39	ASP	-	expression tag	UNP O88738
B	-38	HIS	-	expression tag	UNP O88738
B	-37	ASP	-	expression tag	UNP O88738
B	-36	ILE	-	expression tag	UNP O88738
B	-35	ASP	-	expression tag	UNP O88738
B	-34	TYR	-	expression tag	UNP O88738
B	-33	LYS	-	expression tag	UNP O88738
B	-32	ASP	-	expression tag	UNP O88738
B	-31	ASP	-	expression tag	UNP O88738
B	-30	ASP	-	expression tag	UNP O88738
B	-29	ASP	-	expression tag	UNP O88738
B	-28	LYS	-	expression tag	UNP O88738
B	-27	ARG	-	expression tag	UNP O88738
B	-26	VAL	-	expression tag	UNP O88738
B	-25	VAL	-	expression tag	UNP O88738
B	-24	PRO	-	expression tag	UNP O88738
B	-23	LEU	-	expression tag	UNP O88738
B	-22	GLU	-	expression tag	UNP O88738
B	-21	SER	-	expression tag	UNP O88738
B	-20	THR	-	expression tag	UNP O88738
B	-19	GLY	-	expression tag	UNP O88738
B	-18	LEU	-	expression tag	UNP O88738
B	-17	GLN	-	expression tag	UNP O88738
B	-16	GLU	-	expression tag	UNP O88738
B	-15	LEU	-	expression tag	UNP O88738
B	-14	ALA	-	expression tag	UNP O88738
B	-13	THR	-	expression tag	UNP O88738
B	-12	MET	-	expression tag	UNP O88738
B	-11	GLU	-	expression tag	UNP O88738
B	-10	GLN	-	expression tag	UNP O88738
B	-9	LYS	-	expression tag	UNP O88738
B	-8	LEU	-	expression tag	UNP O88738
B	-7	ILE	-	expression tag	UNP O88738
B	-6	SER	-	expression tag	UNP O88738
B	-5	GLU	-	expression tag	UNP O88738
B	-4	GLU	-	expression tag	UNP O88738
B	-3	ASP	-	expression tag	UNP O88738
B	-2	LEU	-	expression tag	UNP O88738
B	-1	GLU	-	expression tag	UNP O88738

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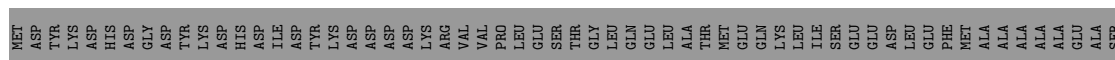
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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	PHE	-	expression tag	UNP O88738
B	178	ILE	THR	conflict	UNP O88738
B	690	THR	ALA	conflict	UNP O88738
B	2079	ARG	GLY	conflict	UNP O88738
B	2418	GLY	CYS	conflict	UNP O88738
B	2959	ILE	THR	conflict	UNP O88738
B	3226	THR	SER	conflict	UNP O88738
B	3914	VAL	MET	conflict	UNP O88738
B	3929	VAL	ILE	conflict	UNP O88738
B	4346	MET	VAL	conflict	UNP O88738

R1281	R1282	F1283	K1284	K1285	K1286	S1287	I1288	C1289	K1290	E1291	R1292	V1293	Q1294	R1295	C1296	A1297	M1298	L1299	Q1300	F1301	S1302	H1305	E1306	L1309	R1314	R1315	S1316	D1317	D1318	G1319	Q1320	L1328	A1332	L1336	A1337	G1338	S1341	N1342	G1343	S1344	G1345	S1346	S1347	K1348	E1349	G1350	N1351	E1352	C1353	L1354	K1357								
VAL	ARG	LEU	PRO	SER	LEU	LEU	GLN	GLY	HIS	GLY	TYR	SER	LEU	ALA	SER	ALA	VAL	VAL	ALA	ALA	GLY	LYS	LYS	SER	ASN	ASN	VAL	VAL	ASN	GLU	ASN	ALA	GLY	GLY	THR	ARG	LYS	SER	ASP	ASP	GLY	ALA	ALA	ASP	GLU	GLY	CYS	SER	GLY	ARG	PRO	VAL							
E1155	D1156	I1157	L1158	C1159	G1160	P1161	V1162	W1163	K1164	A1165	S1166	G1167	L1168	D1169	L1170	H1173	A1174	G1175	M1176	K1183	L1184	V1185	K1186	L1187	M1188	A1189	G1190	G1191	K1192	Y1193	R1194	S1195	F1196	L1197	I1198	H1199	V1200	K1201	A1202	V1203	S1204	ASP	ARG	GLY	ALA	ALA	ASP	GLU	MET	CYS	SER	GLY	ARG	PRO	VAL				
Q1095	I1096	Q1097	V1098	T1099	L1100	L1101	K1102	M1103	K1104	A1105	P1106	GLY	LEU	GLY	LYS	ALA	ASN	ALA	LEU	ASN	ILE	GLU	VAL	GLY	HIS	ASN	GLY	ASN	GLU	GLY	THR	MET	HIS	F1196	L1197	I1198	H1199	V1200	K1201	A1202	V1203	S1204	ASP	ARG	GLY	ALA	ALA	ASP	GLU	MET	CYS	SER	GLY	ARG	PRO	VAL			
P1035	Q1036	H1037	L1038	H1039	Q1040	Q1041	H1042	H1043	G1044	D1045	A1046	A1047	Q1048	H1049	T1050	R1051	T1052	W1053	K1054	L1055	Q1056	T1057	D1058	S1059	N1060	S1061	W1062	D1063	E1064	H1065	V1066	F1067	E1068	L1069	V1070	L1071	P1072	K1073	A1074	C1075	M1076	V1077	G1078	H1079	V1080	D1081	F1082	K1083	F1084	V1085	L1086	S1087	S1088	L1089	I1090	T1091	S1092	V1093	P1094
GLY	SER	ARG	PRO	LEU	ASN	PRO	SER	PRO	GLY	SER	G984	V985	E986	L987	L988	V989	D990	Q991	P992	F993	1997	L998	E1003	L1004	T1005	R1006	F1007	E1008	T1009	L1010	T1011	P1012	R1013	F1014	S1015	A1016	T1017	V1018	P1019	P1020	C1021	W1022	V1023	E1024	V1025	Q1026	Q1027	E1028	Q1029	Q1030	Q1031	R1032	R1033	H1034					
THR	GLU	E912	Q913	T914	F916	F917	S918	V919	L920	Y921	C922	S923	G924	T925	D926	R927	L928	C929	A930	C931	T932	K933	G934	G935	E936	L937	H938	F939	L940	Q941	I942	G943	THR	CYS	ASP	ASP	ILE	ASP	ALA	ASP	ILE	LEU	VAL	ASP	GLY	SER	LYS	GLY	ILE	PRO	ALA	LEU	GLU						
CYS	GLU	PRO	GLU	GLU	MET	GLN	ALA	SER	LYS	ASN	GLY	ILE	ARG	GLU	LYS	LYS	SER	ASP	ILE	SER	T875	L876	G877	H878	L879	V880	H881	T882	T883	Q884	G885	G886	Y887	V888	K889	V890	D892	L893	S894	N895	F896	E897	T898	L899	A900	R901	V902	E903	P904	P905	K906	K907	E908	GLY					
PRO	GLU	GLN	ARG	ASN	VAL	V796	S797	G798	T799	Y800	L801	W802	L803	Y804	K805	M806	N807	Y808	T809	T810	R811	I812	V813	T814	L815	E816	E817	E818	P819	W820	K821	I822	Q823	H824	I825	K826	D827	P828	Q829	D830	T831	I832	T833	S834	L835	I836	L837	L838	P839	P840	D841	I842	L843	D844	N845	ARG	GLU	ASP	ASP
ALA	ALA	SER	LEU	THR	SER	PRO	ASP	GLU	LYS	TRP	ASN	S683	V684	F685	P686	K687	P688	G689	T690	L691	V692	Q693	C694	L695	R696	L697	P698	ILE	ILE	GLU	MET	A701	E702	E703	E704	T705	L706	C707	I708	D709	S710	I711	T712	P713	C714	A715	D716	G717	I718	H719	L720	L721	G723	L724	R725	T726	C727	SER	VAL
GLU	SER	LEU	SER	ALA	ILE	ASN	GLN	VAL	ALA	LEU	ASN	ASN	LEU	LYS	ASN	SER	ALA	CYS	ASN	ARG	ARG	LYS	GLY	ASP	GLU	SER	ASN	VAL	VAL	ASN	GLY	ALA	ASN	ILE	SER	VAL	ILE	GLN	HIS	LEU	ILE	ARG																	
Y550	K551	S552	PRO	ALA	THR	THR	PRO	PRO	GLY	SER	ASN	HIS	ARG	SER	GLY	LEU	SER	ARG	THR	GLN	GLY	GLU	ASP	PHE	THR	VAL	GLN	GLY	ILE	ASP	ASN	GLU	SER	THR	ASN	PRO	PRO	VAL	R599	R600	T601	L602	P603	V604	L605	L606	L607	Y608	S609										
I610	K611	E612	S613	ASP	GLU	THR	ALA	LYS	ILE	PHE	SER	MET	ASN	ASN	ILE	MET	SER	LEU	THR	HIS	GLN	ASP	PHE	THR	VAL	GLN	GLY	ILE	ASP	ASN	GLU	SER	THR	ASN	PRO	PRO	VAL	R599	R600	T601	L602	P603	V604	L605	L606	L607	Y608	S609											
Q490	P491	E492	LYS	LEU	GLN	TRP	GLU	ILE	VAL	ALA	ASN	VAL	LEU	THR	VAL	ASP	LEU	GLY	ALA	ASN	GLY	ALA	ASN	PRO	ILE	THR	GLN	ASN	THR	LYS	GLY	THR	GLU	HIS	GLN	GLY	ASN	GLN	H535	N536	I537	P538	F539	P540	C541	L542	L543	A544	G545	L546	L548	T549							



A2552	L2553	D2554	A2555	L2557	E2558	E2562	Q2563	Q2564	A2565	E2566	L2567	E2578	L2584	T2585	N2586	T2587	S2588	PRO	THR	PHE	SER	GLN	GLY	SER	PRO	THR	THR	GLY	THR	ASP	SER	LEU	LEU	GLY	ASN	ASN	LEU	GLN	PRO	ALA	ASN	ASN	GLN	SER	GLN	VAL	ILE	Q2618	L2632	V2638	V2641	L2649
N2656	S2657	S2658	SER	SER	GLY	ASN	LYS	GLY	ALA	ASP	F2669	A2674	N2675	L2701	L2702	R2703	C2706	N2717	N2721	GLY	SER	ALA	GLY	SER	SER	PRO	THR	THR	ILE	GLY	ILE	Q2731	V2739	T2755	S2756	N2761	Q2762	H2763	V2767	A2771	R2781	L2782	Q2783	GLU	GLY	HIS	GLY	L2909	S2795	E2796	L2797	
L2798	R2809	G2817	P2818	T2829	Q2832	Q2833	F2834	V2837	L2842	V2853	D2861	K2862	S2865	R2866	S2867	GLY	SER	ASP	SER	SER	ALA	GLY	ALA	ARG	ALA	ALA	CYS	PHE	GLY	GLY	PHE	ALA	ASN	LEU	ILE	ARG	PRO	GLY	ASP	GLY	VAL	CYS	GLY	GLU	HIS	PHE	HIS	GLY	L2909	S2795	E2796	L2797
L2915	R2929	V2930	SER	VAL	THR	THR	THR	ASN	THR	THR	VAL	VAL	GLY	GLY	LYS	VAL	ASN	GLY	SER	SER	ALA	ILE	PRO	GLY	SER	THR	THR	SER	P2963	S2990	A2993	M2994	I2995	ILE	GLY	ALA	SER	GLY	LEU	HIS	THR	LYS	HIS	ASN	PHE	HIS	GLY	L2909	S2795	E2796	L2797	
LEU	ASP	A3015	Y3051	M3052	Q3055	G3056	T3060	V3112	S3113	T3114	F3118	L3119	D3120	SER	PRO	GLY	LYS	ALA	VAL	ASP	THR	THR	LYS	THR	THR	ILE	ARG	LEU	ALA	SER	GLU	PRO	ASN	ALA	G3145	I3146	H3147	P3174	H3175	R3176	R3177	A3178	R3179	F3187	E3190	L3206						
T3209	H3210	L3218	P3222	E3228	N3235	P3238	L3239	S3240	T3241	L3255	C3265	L3268	L3277	S3280	K3283	L3284	L3285	T3293	A3295	THR	VAL	ASN	PRO	PHE	LEU	PRO	PRO	SER	GLU	D3307	R3318	H3322	H3326	L3330	M3334	L3345	Q3346	L3352	M3353													
M3359	I3364	L3382	N3389	S3395	D3396	P3397	T3398	L3399	L3400	N3401	L3405	R3408	N3410	G3411	L3412	D3415	S3416	T3417	I3418	K3433	G3456	R3457	MET	ASN	TYR	MET	CYS	PRO	SER	SER	ALA	V3468	A3485	L3502	L3503	D3504	S3515	C3520	N3521	K3525	M3550											
G3551	I3552	T3553	PRO	PRO	VAL	GLN	CYS	HIS	HIS	ARG	LEU	SER	MET	THR	ASP	ASP	LYS	GLN	ASP	SER	SER	LEU	THR	ASP	SER	LYS	ASN	ALA	GLN	PRO	LEU	S3590	E3593	L3599	Q3604	L3617	L3621	V3622	C3629	F3630	S3631	H3632	ILE	SER	TYR	SER						
GLU	SER	ILE	ALA	GLN	SER	VAL	ASP	ASN	GLN	ASP	LYS	GLN	CYS	N3660	K3661	M3662	D3667	I3672	E3678	L3697	L3701	L3702	F3703	L3704	S3708	GLY	SER	THR	ALA	GLY	GLY	HIS	ASN	LEU	GLY	ALA	ALA	GLN	SER	THR	ARG	SER	ALA									
SER	HIS	SER	ALA	THR	THR	THR	V3736	T3739	T3749	I3757	H3760	M3767	L3774	F3775	Q3776	T3777	ALA	PRO	GLN	ARG	GLY	SER	LEU	LEU	PRO	THR	SER	G3788	L3797	F3798	L3799	Q3800	L3801	M3802	L3803	E3804	K3807	L3812	Q3813	S3814	R3822	T3823	H3824	A3825	G3836	L3844	H3845					
L3846	P3847	V3848	S3849	T3850	S3853	D3854	R3858	V3859	S3860	D3861	T3862	P3863	SER	ILE	THR	ALA	LYS	LYS	LEU	ILE	SER	GLN	ASP	LYS	GLY	SER	ALA	ALA	ALA	HIS	GLU	GLY	LYS	VAL	ASN	GLY	GLN	ASP	ASN	TYR	SER	VAL	VAL	VAL	ALA	SER	GLY	LYS	SER			
GLN	SER	LYS	ARG	VAL	ALA	SER	THR	PRO	PRO	ARG	PRO	PRO	PRO	ARG	ARG	GLY	THR	VAL	ASP	PRO	LYS	ILE	GLY	SER	ALA	ALA	ALA	LYS	ILE	THR	THR	V3949	R3957	L3958	L3959	A3960	A3966	L3970	K3981	G3985	V3993	G3996	SER	LYS								
VAL	ILE	THR	ASP	PRO	LEU	SER	LYS	THR	ASP	PHE	LYS	ARG	HIS	PRO	GLY	GLU	LYS	ASP	VAL	GLY	SER	GLY	SER	ALA	ALA	ALA	LEU	THR	PRO	SER	ASP	ILE	GLU	CYS	MET	ASP	GLY	VAL	L4044	D4045	E4046	S4047	L4048	L4049	E4050	L4058	Q4059	A4062	I4070			











SER	HIS	GLN	TRP	ILE	PHE	A4481	V4421	S4361
	ALA	ALA	HIS	THR	LYS	M4482	G4422	S4362
	ALA	THR	GLY	GLY	VAL	M4483	G4423	S4363
	LEU	VAL	ARG	PRO	ASN	R4484	T4423	L4364
LEU	LYS	LYS	PRO	ALA	TYR	R4485	L4424	ARG
	TRP	GLU	GLU	THR	HIS	Q4485	L4425	ASN
	ALA	GLU	GLU	THR	TYR	ALA	L4426	
	ARG	MET	LYS	PRO	MET	ASN	A4426	D4367
THR	HIS	LEU	TRP	TYR	GLN	GLN	K4427	S4368
	ALA	GLU	ASN	ALA	GLN	GLU	M4428	V4369
	GLN	GLN	PRO	ASN	VAL	LYS	K4429	L4370
	ILE	ILE	GLN	CYS	LYS	LEU	T4430	D4371
ARG	ARG	ARG	THR	CYS	ASN	GLY	C4431	M4372
	ASN	ASN	SER	PHE	ALA	GLU	V4432	A4373
	PRO	PRO	SER	PHE	ASP	GLU	D4433	A4374
	LEU	PRO	PHE	PHE	ASP	TYR	T4434	R4375
LYS	CYS	CYS	GLN	VAL	ASN	SER	Y4435	V4376
	PHE	PHE	VAL	TYR	SER	LYS	T4436	P4377
	LYS	LYS	LEU	PHE	ALA	VAL	M4437	L4378
	GLU	GLU	VAL	PRO	ALA	VAL	R4438	Y4379
PRO	VAL	VAL	SER	GLN	ARG	MET	L4439	R4380
	ILE	ILE	VAL	TYR	ARG	LYS	R4440	A4381
	GLY	HIS	SER	PRO	ARG	PRO	S4441	L4382
	LEU	LYS	LEU	SER	LEU	LEU	K4442	L4383
PRO	ASP	HIS	ILE	SER	ALA	LEU	ARG	E4384
	PRO	THR	ILE	PRO	GLN	VAL	GLU	L4385
	ILE	THR	VAL	PRO	ALA	LEU	ASN	L4386
	GLU	ILE	GLU	PRO	VAL	VAL	VAL	R4387
ASP	ALA	LEU	PHE	GLU	LEU	GLU	LYS	A4388
	VAL	MET	ASN	THR	SER	GLU	ALA	L4389
	CYS	ALA	GLU	THR	SER	LYS	GLY	A4390
	ARG	GLN	PRO	GLY	LEU	LYS	VAL	S4391
ALA	ALA	GLY	GLY	GLY	PRO	TYR	PRO	C4392
	THR	GLU	TYR	HIS	LEU	VAL	ASP	T4393
	GLY	GLU	ARG	SER	LEU	ALA	ALA	S4394
	TRP	TRP	ARG	VAL	SER	MET	LYS	M4395
ILE	ALA	ILE	SER	VAL	SER	LYS	GLN	V4396
	ALA	ASP	GLY	ASN	SER	LEU	PRO	P4397
	GLU	THR	ARG	ASN	PHE	GLN	GLU	L4398
	THR	THR	SER	PRO	VAL	GLN	GLY	L4399
HIS	THR	TYR	GLY	TYR	ARG	THR	LEU	LEU
	ASP	SER	THR	ASN	CYS	PHE	A4463	PRO
	HIS	SER	GLN	ASN	ASP	GLU	L4464	LEU
	VAL	ASP	SER	GLY	GLU	MET	L4465	SER
ASN	ASN	LYS	SER	LYS	GLU	VAL	V4466	THR
	PRO	ARG	ARG	CYS	LEU	SER	P4467	GLU
	VAL	VAL	GLU	VAL	ASP	GLU	D4468	ASN
	SER	GLY	TYR	LEU	ASP	ILE	T4469	GLY
SER	ARG	ARG	ASP	SER	ILE	ASP	L4470	GLU
	THR	THR	GLY	THR	MET	ASP	Q4471	GLU
	LEU	MET	ASN	LEU	LYS	GLY	R4472	GLU
	ASP	SER	ILE	ASN	VAL	LYS	T4473	ASP
LEU	LEU	SER	ILE	ASN	VAL	LEU	A4474	GLN
	PRO	HIS	ARG	THR	LEU	GLY	E4475	SER
							I4476	GLU
							H4477	CYS
							A4478	GLN
							A4479	THR
							S4420	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	154000	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 ($e^-/\text{\AA}^2$)	68.4	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.180	Depositor
Minimum map value	-0.086	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	438.4, 438.4, 438.4	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.37, 1.37, 1.37	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	A	0.24	0/21276	0.54	5/28980 (0.0%)
1	B	0.24	0/21276	0.54	4/28980 (0.0%)
All	All	0.24	0/42552	0.54	9/57960 (0.0%)

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
1	A	0	2
1	B	0	2
All	All	0	4

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1396	PRO	CA-N-CD	-5.95	103.67	112.00
1	A	1396	PRO	CA-N-CD	-5.93	103.70	112.00
1	A	4321	MET	CA-CB-CG	5.34	124.79	114.10
1	B	4321	MET	CA-CB-CG	5.32	124.75	114.10
1	A	4305	GLU	CA-CB-CG	5.23	124.57	114.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1396	PRO	Peptide
1	A	1834	ILE	Peptide
1	B	1396	PRO	Peptide
1	B	1834	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	A	20950	0	19684	215	0
1	B	20950	0	19684	224	0
All	All	41900	0	39368	413	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 413 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:B:3798:PHE:O	1:B:3802:MET:HB3	1.81	0.81
1:A:3798:PHE:O	1:A:3802:MET:HB3	1.81	0.80
1:B:1383:ARG:HH21	1:B:2562:GLU:HB2	1.52	0.74
1:A:1383:ARG:HH21	1:A:2562:GLU:HB2	1.52	0.73
1:A:2375:GLY:HA2	1:A:2641:VAL:HA	1.76	0.68

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2841/4896 (58%)	2786 (98%)	55 (2%)	0	100	100
1	B	2841/4896 (58%)	2787 (98%)	54 (2%)	0	100	100
All	All	5682/9792 (58%)	5573 (98%)	109 (2%)	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	A	2046/4236 (48%)	2046 (100%)	0	100	100
1	B	2046/4236 (48%)	2046 (100%)	0	100	100
All	All	4092/8472 (48%)	4092 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3962	GLN
1	B	3513	ASN
1	B	1056	GLN
1	B	4169	GLN
1	B	3095	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

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.

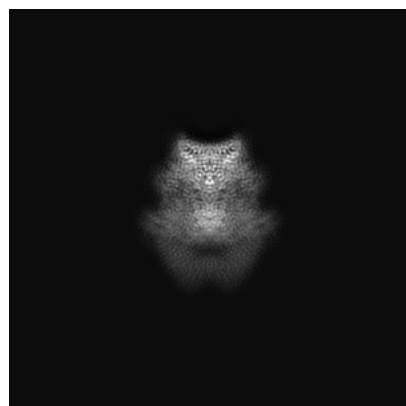
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35759. These allow visual inspection of the internal detail of the map and identification of artifacts.

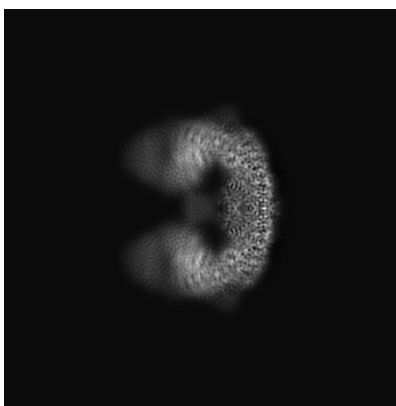
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

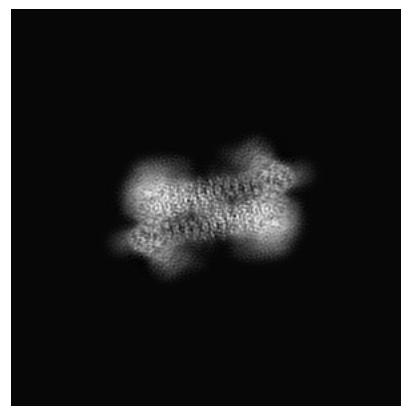
6.1.1 Primary map



X

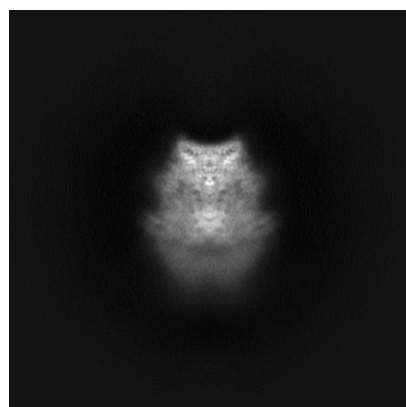


Y

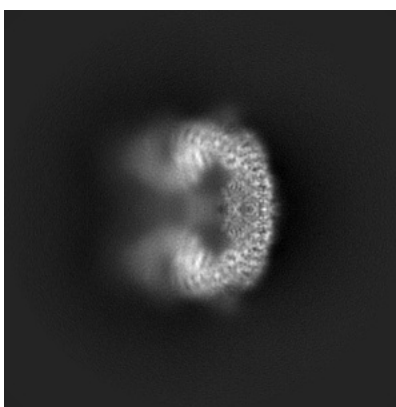


Z

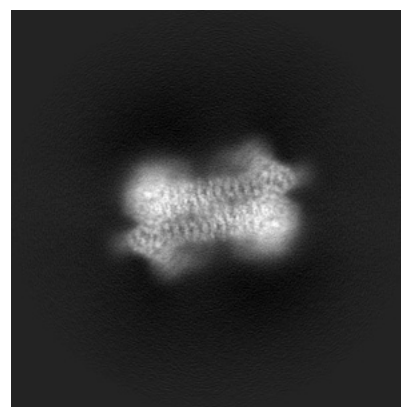
6.1.2 Raw map



X



Y



Z

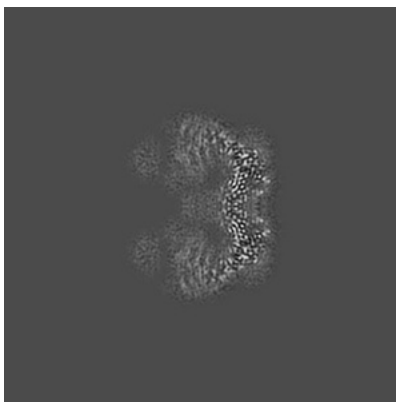
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

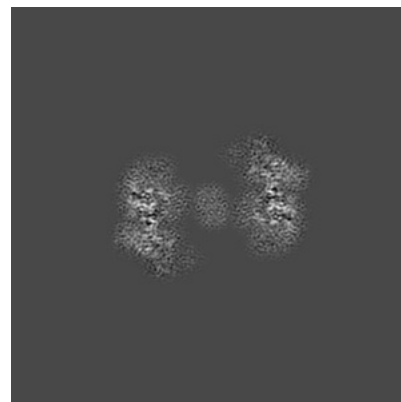
6.2.1 Primary map



X Index: 160

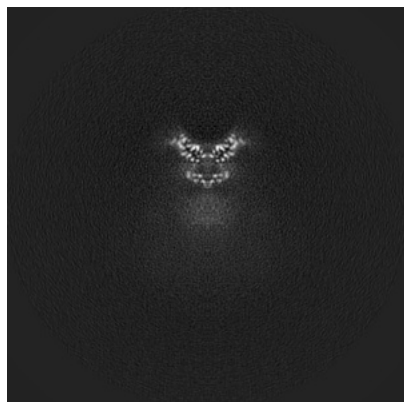


Y Index: 160

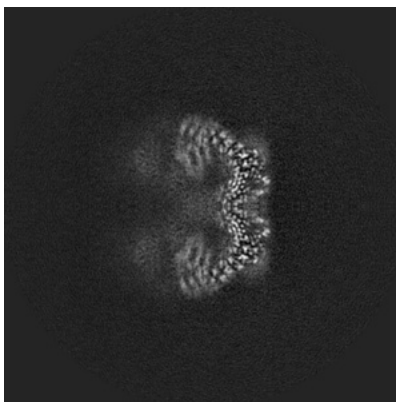


Z Index: 160

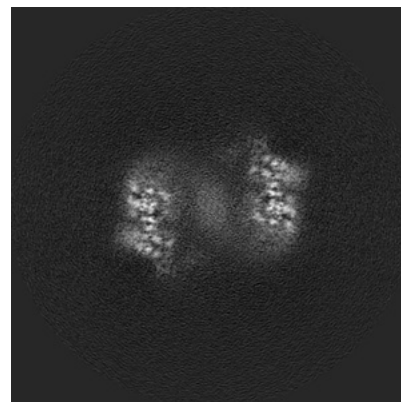
6.2.2 Raw map



X Index: 160



Y Index: 160

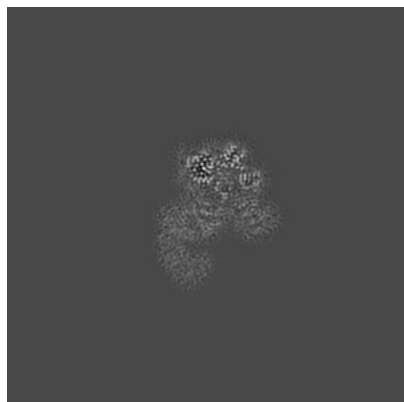


Z Index: 160

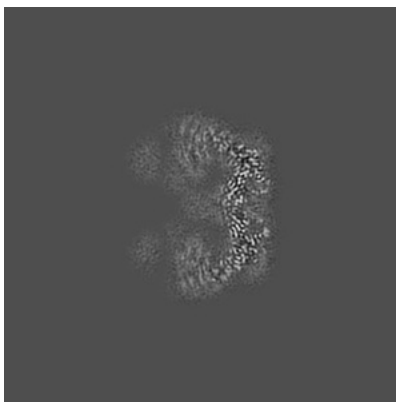
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

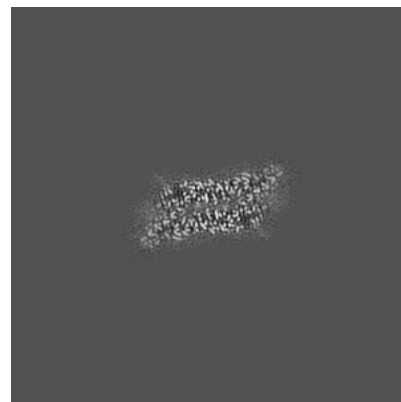
6.3.1 Primary map



X Index: 202

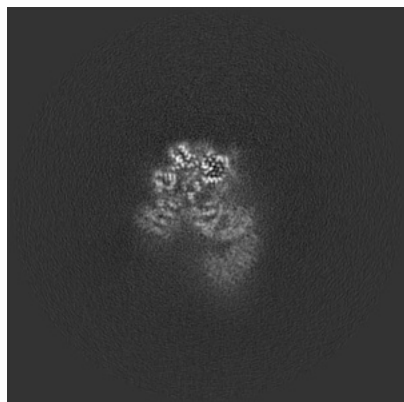


Y Index: 159

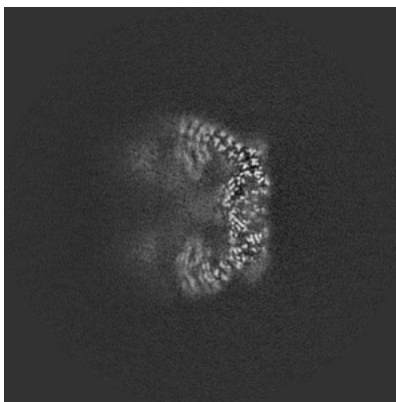


Z Index: 202

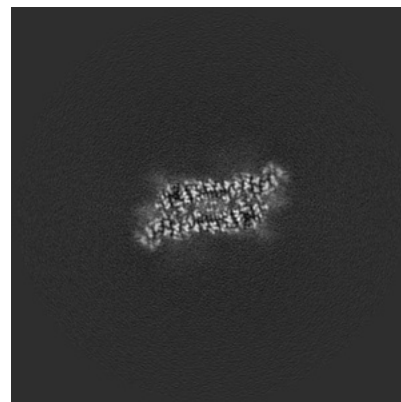
6.3.2 Raw map



X Index: 118



Y Index: 158

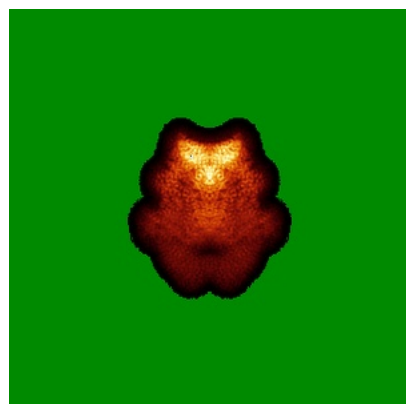


Z Index: 201

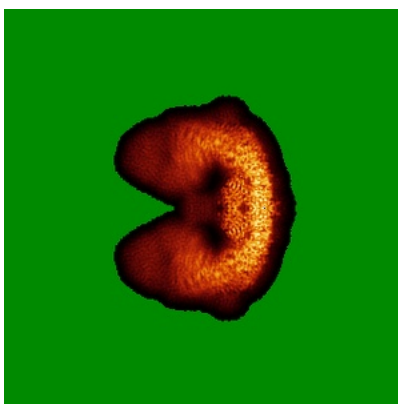
The images above show the largest variance slices of the map in three orthogonal directions.

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

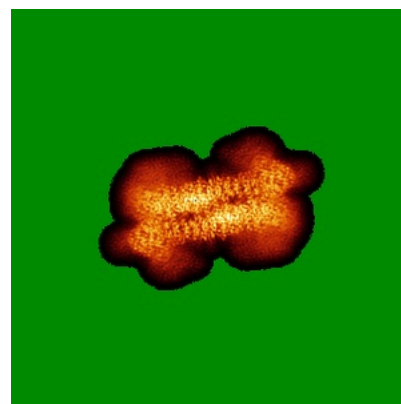
6.4.1 Primary map



X

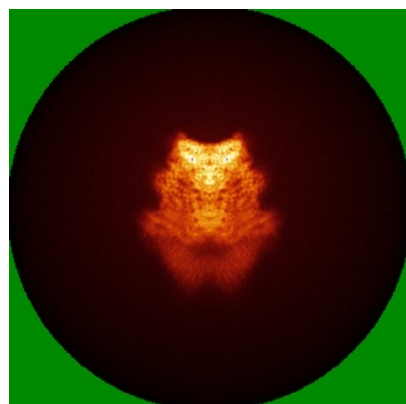


Y

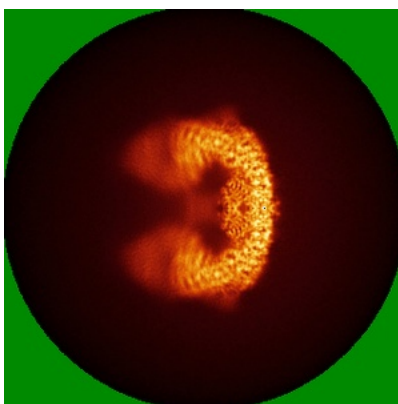


Z

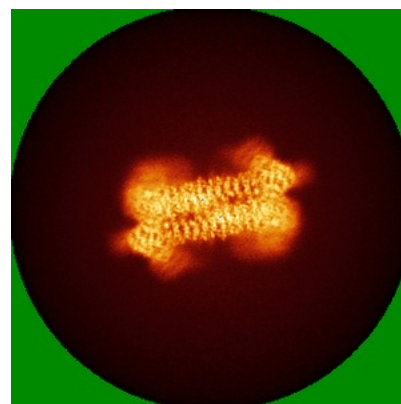
6.4.2 Raw map



X



Y

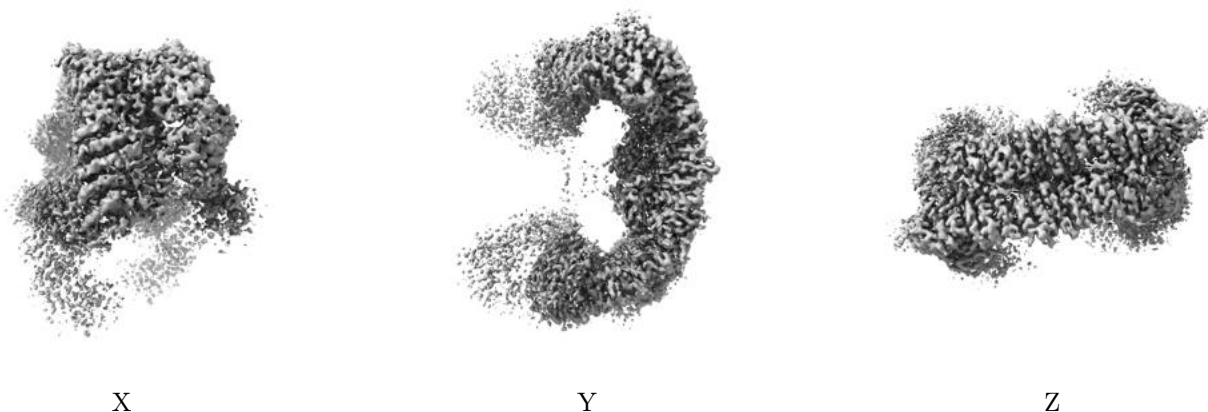


Z

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 0.03. 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.

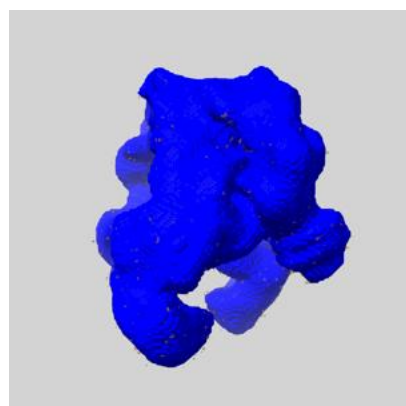
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

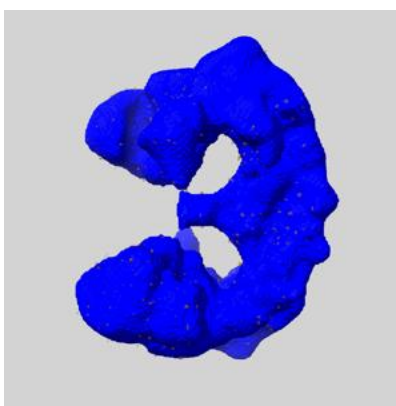
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

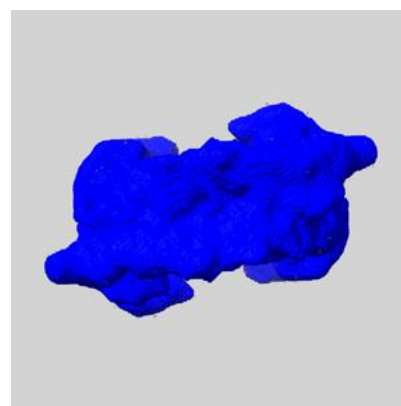
6.6.1 emd_35759_msk_1.map [i](#)



X



Y

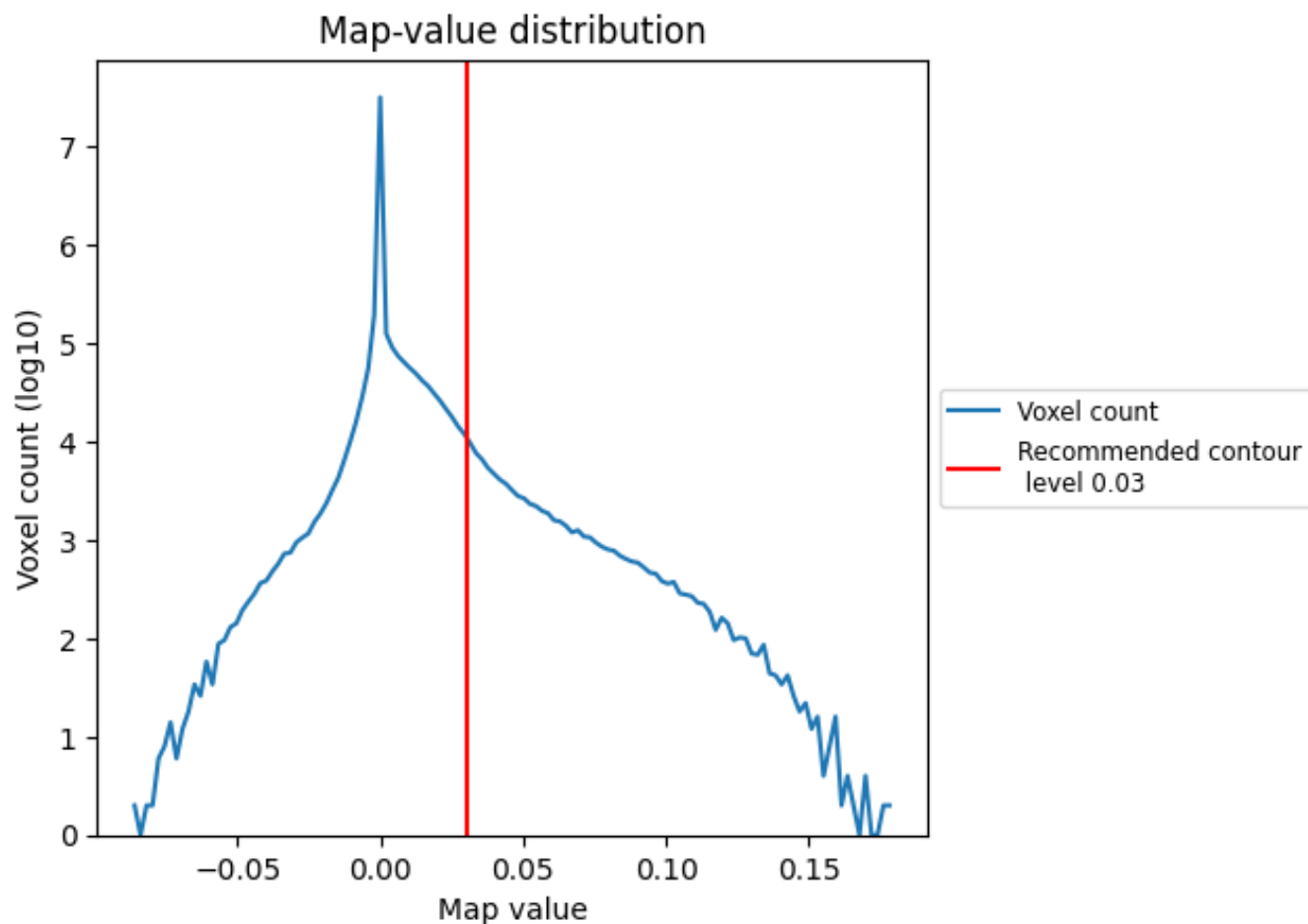


Z

7 Map analysis [i](#)

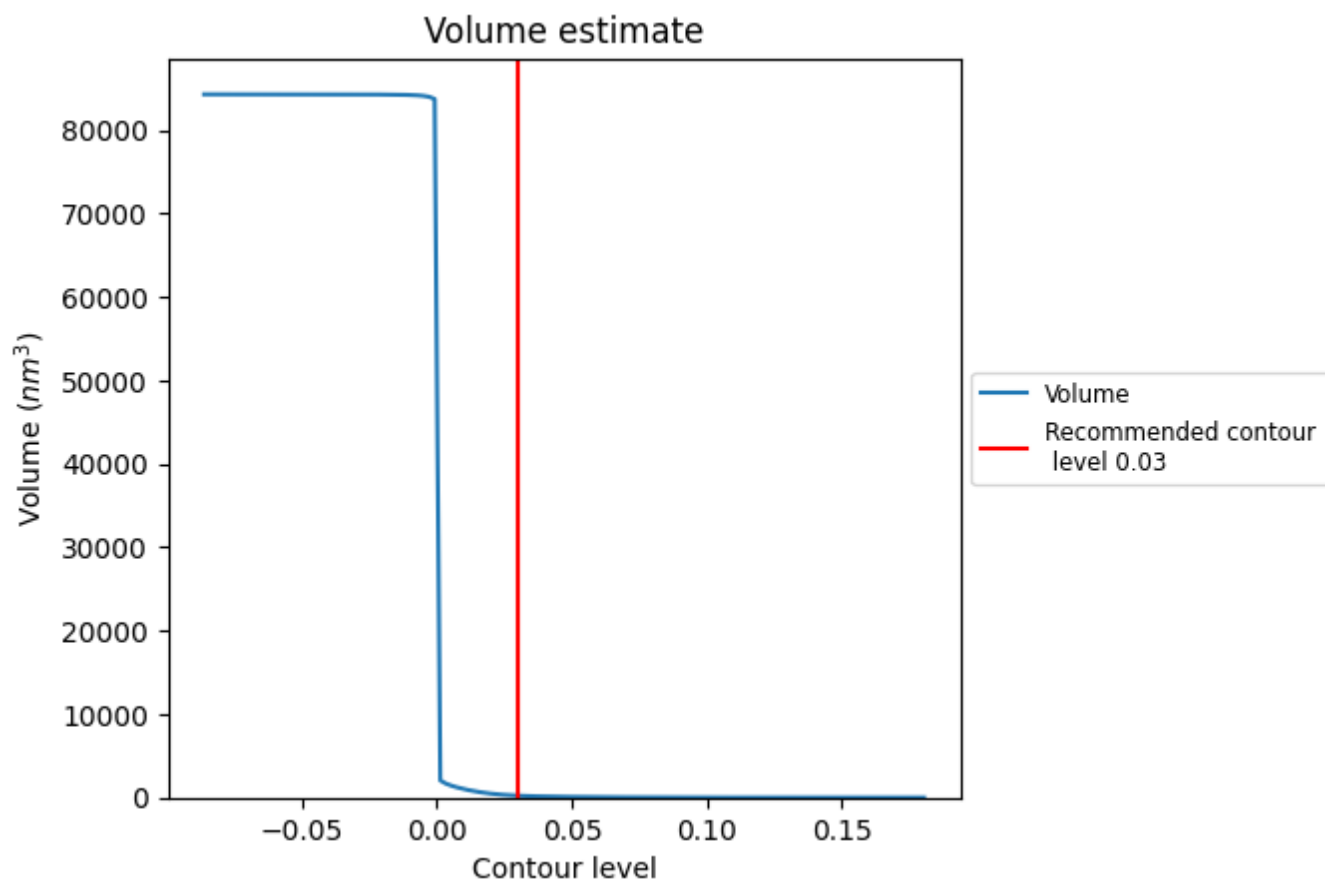
This section contains the results of statistical analysis of the map.

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.

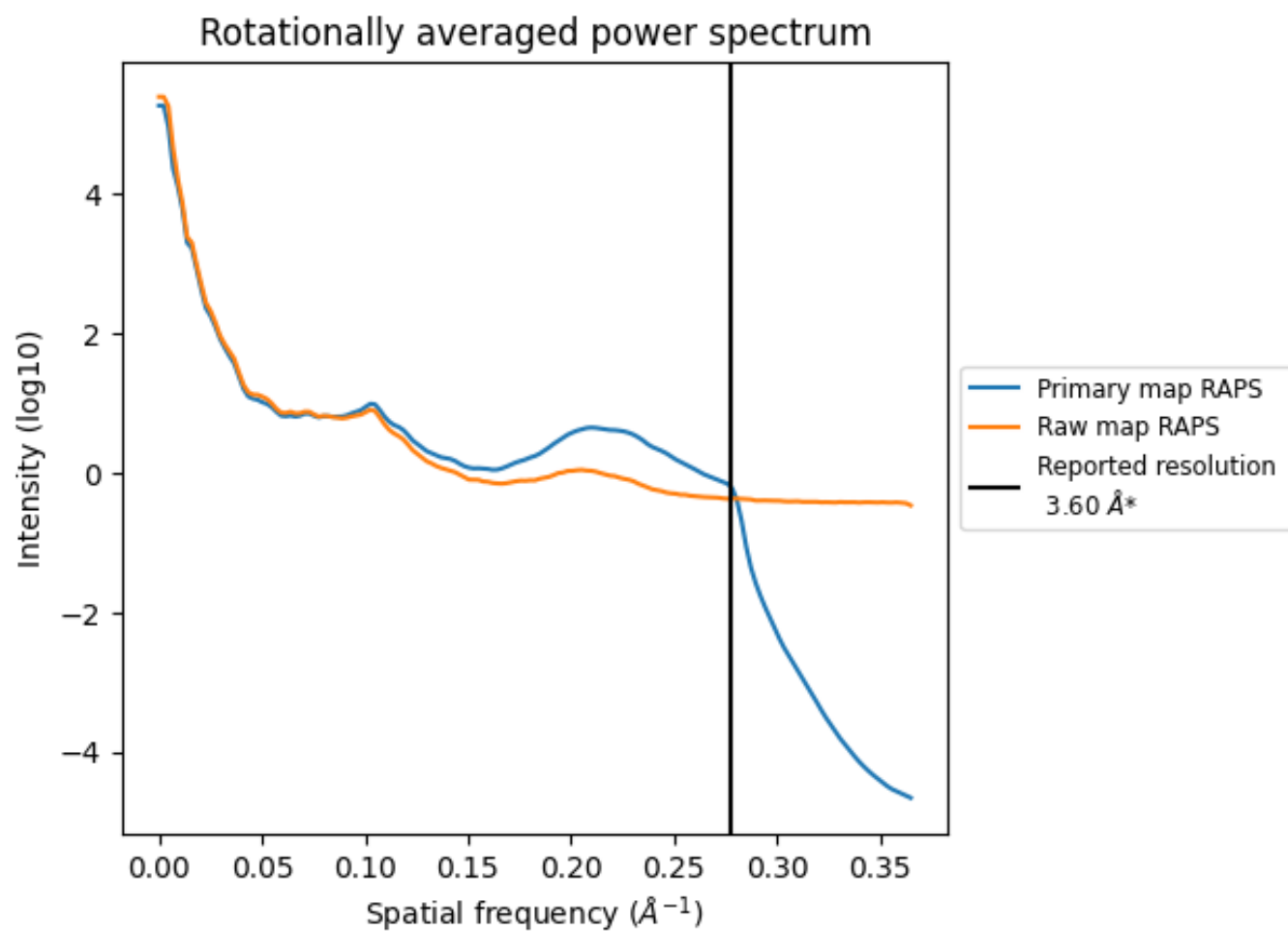
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 224 nm^3 ; this corresponds to an approximate mass of 203 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 ⓘ

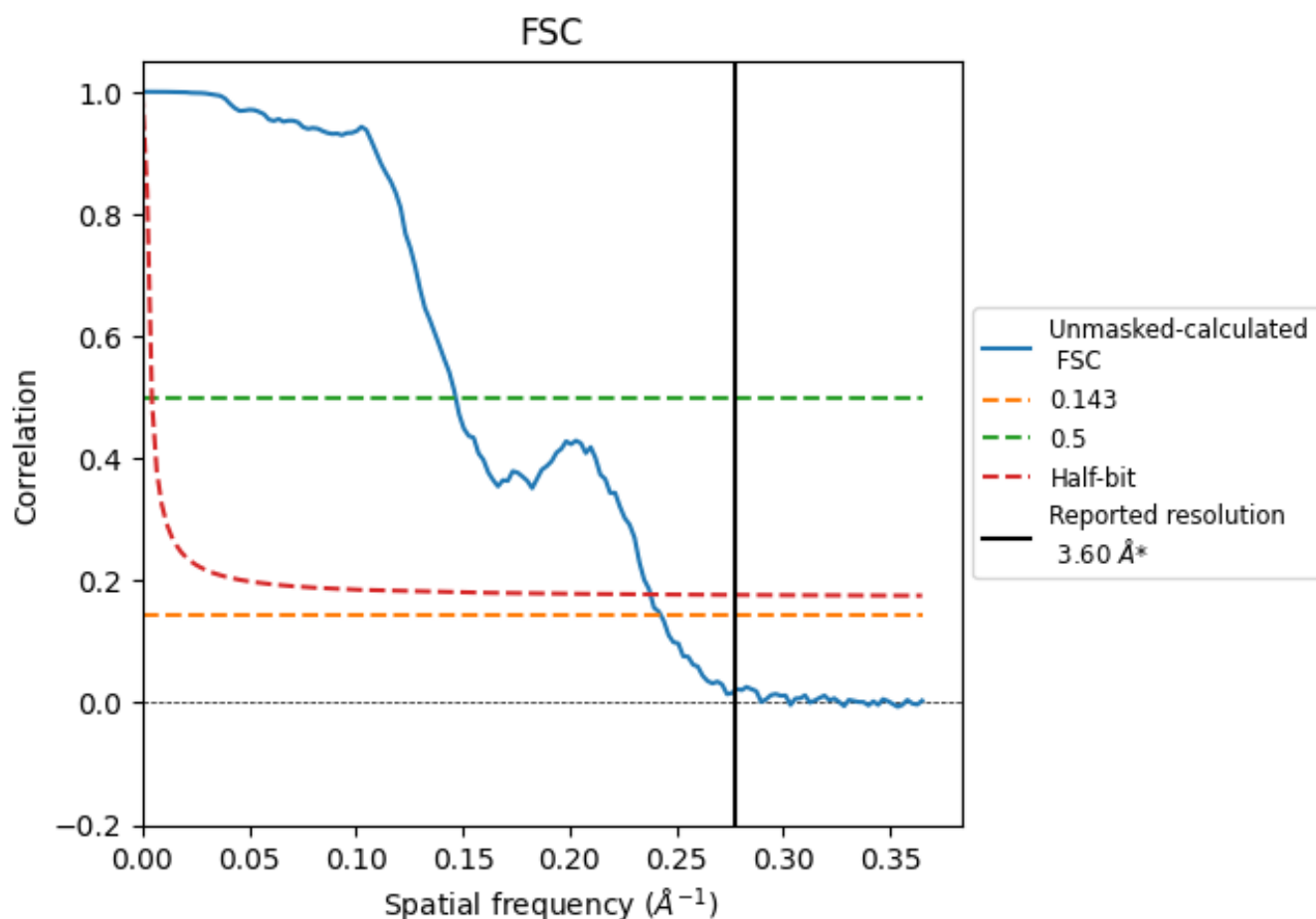


*Reported resolution corresponds to spatial frequency of 0.278 $\text{\AA}^{-1}$

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 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

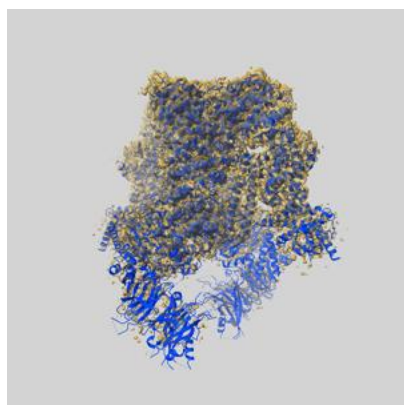
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.12	6.82	4.20

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.12 differs from the reported value 3.6 by more than 10 %

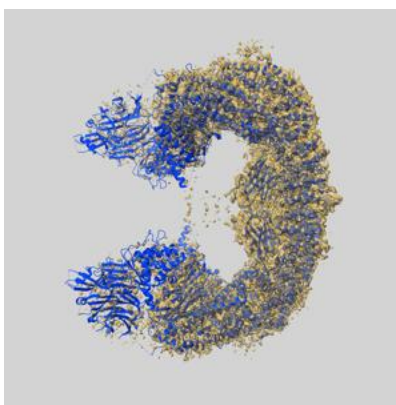
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-35759 and PDB model 8IVQ. Per-residue inclusion information can be found in section [3](#) on page [7](#).

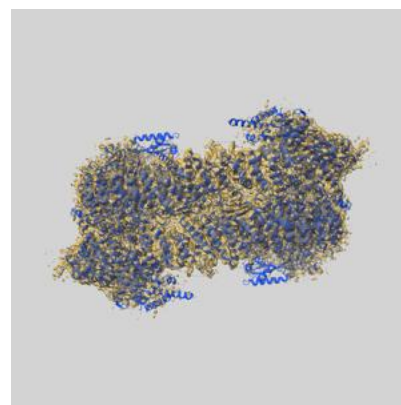
9.1 Map-model overlay [i](#)



X



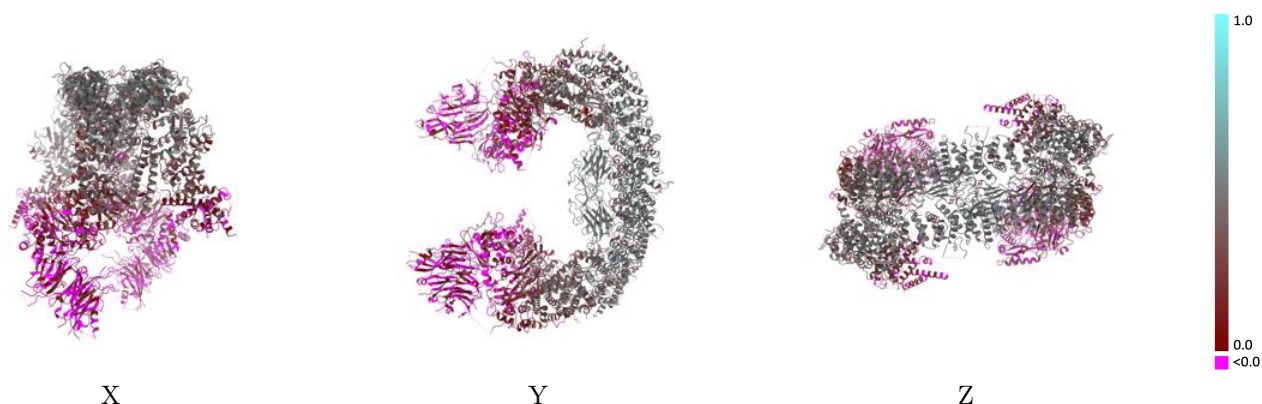
Y



Z

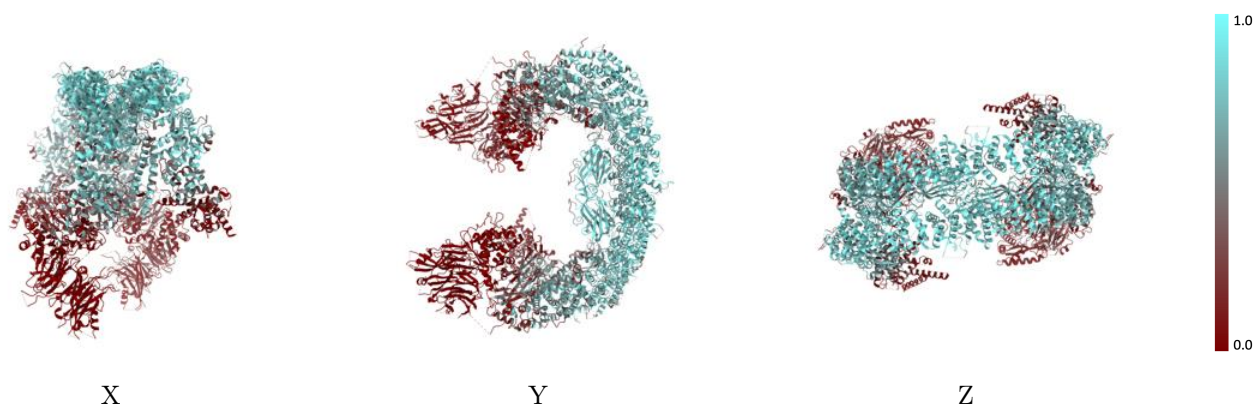
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



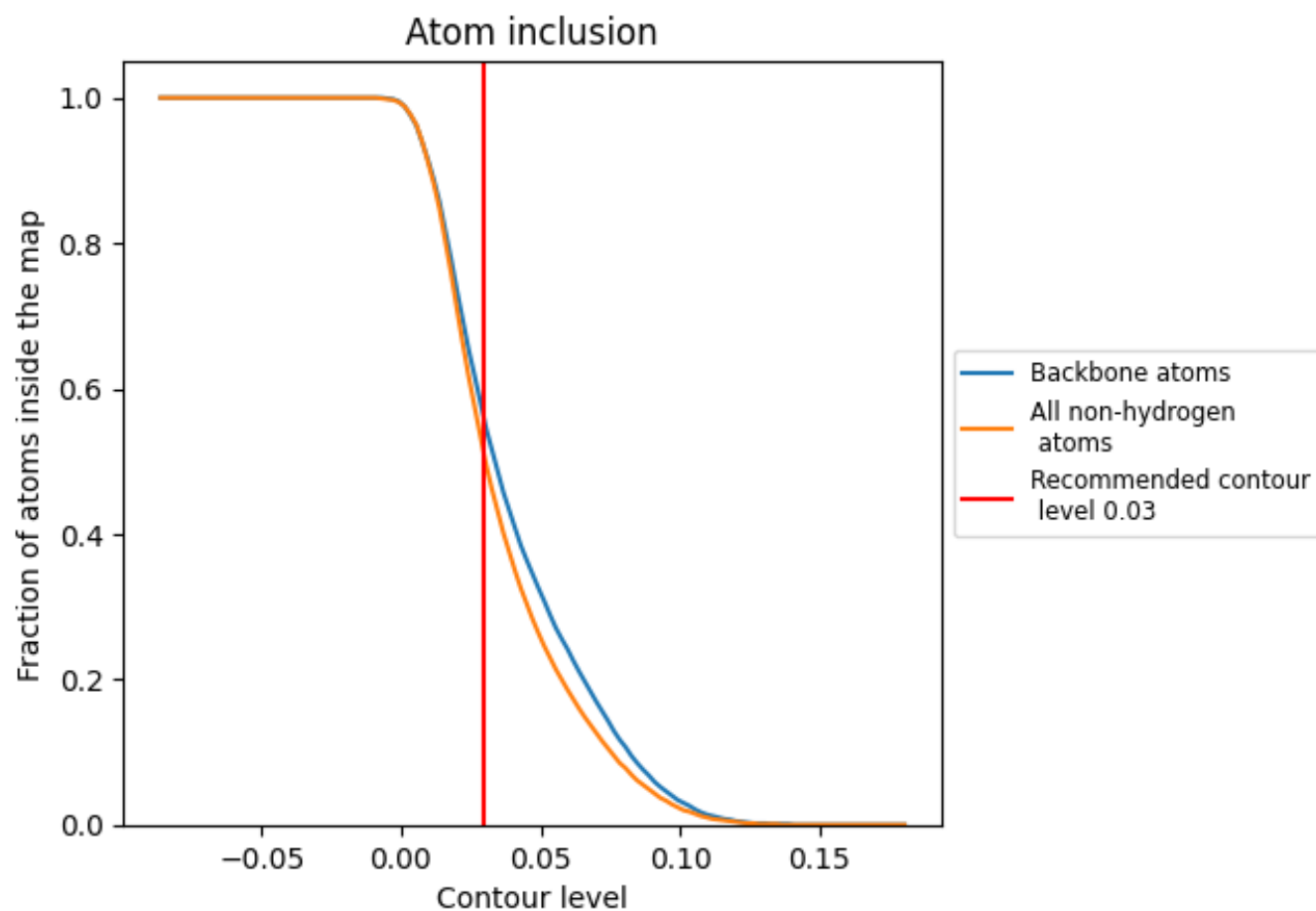
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 55% of all backbone atoms, 50% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5050	0.2990
A	0.5050	0.2990
B	0.5050	0.2990

