



wwPDB EM Validation Summary Report ⓘ

Sep 28, 2026 – 12:38 PM EDT

PDB ID : 11IM / pdb_000011im
EMDB ID : EMD-75718
Title : Focused Cryo-EM map of a half-region of the human ZNFX1 tetramer
Authors : Wang, F.; He, Q.; Li, H.
Deposited on : 2026-02-25
Resolution : 3.71 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.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.2
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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) : 2.51

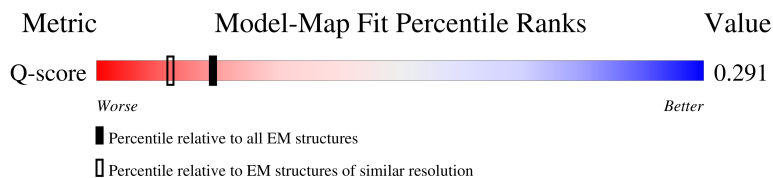
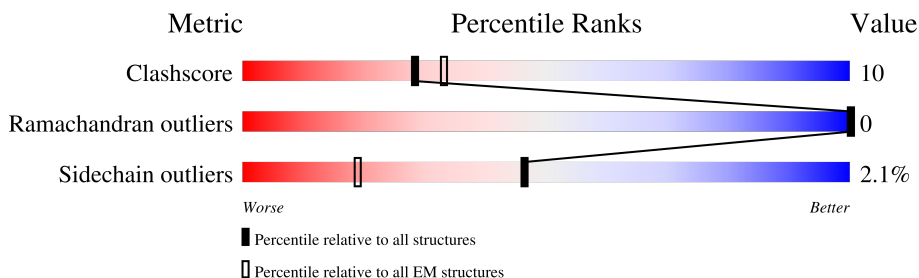
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.71 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	10534 (3.21 - 4.21)

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	1918	10% 53% 14% 33%
1	B	1918	19% 50% 16% 33%
1	C	1918	7% 6% 91%

2 Entry composition [i](#)

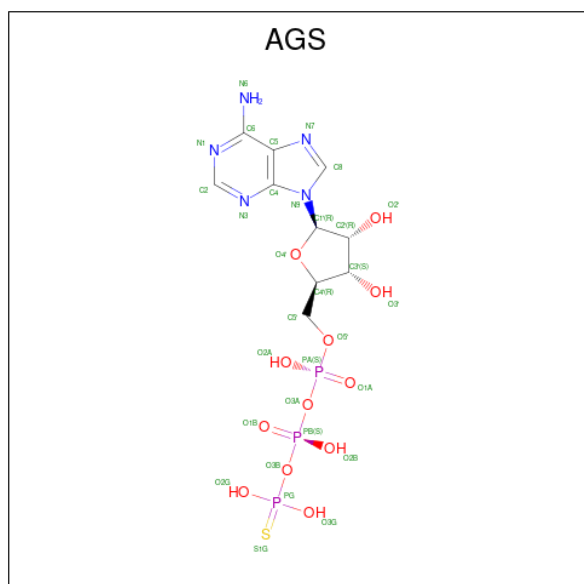
There are 2 unique types of molecules in this entry. The entry contains 22020 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NFX1-type zinc finger-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1282	Total	C	N	O	S	0	0
			10307	6503	1814	1909	81		
1	B	1282	Total	C	N	O	S	0	0
			10307	6503	1814	1909	81		
1	C	172	Total	C	N	O	S	0	0
			1344	855	226	256	7		

- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	B	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

CYS	R1354	G1227	M1228	M130	V1005	L908	E838	V766	R701	I616	V543	I410	Y319	L254
PRO	C1372	C1230	H132	E1007	E1006	N909	E839	Q767	E702	P620	Y548	Y411	T320	V255
GLY	S1378	L1237	A1134	L1020	L1020	A913	V843	W771	R704	G623	L549	I416	L321	S256
HIS	K1379	V1240	V1138	L1028	E1008	A914	V844	W708	R707	G624	L550	I417	V322	P259
SER	L1380	W1243	L1140	L1029	A1009	E915	V845	W709	R708	Y627	M551	M420	P324	A260
PHE	V1395	H1246	Y1143	L1030	L1029	A916	V846	L710	L707	V628	R554	S422	E325	E265
ARG	Q1396	R1251	F1144	Q1036	E1007	E918	Q847	L711	W708	Y627	F557	S423	A326	T266
HIS	C1398	E1252	L1145	L1037	E1008	E919	Q848	L712	R709	G624	F557	S423	E327	S267
ARG	S1399	L1256	Q1147	L1038	E1009	E920	R849	W716	R713	K631	L560	I426	D328	M268
CYS	E1400	L1260	E1148	L1039	E1010	E921	R850	Y715	R714	I632	I561	I427	H329	L269
GLN	M1401	L1261	Y1149	L1040	E1011	E922	R851	Y716	R715	V633	E562	Y428	V330	V270
PRO	V1402	L1262	L1150	L1041	E1012	E923	R852	Y717	R716	Q634	N563	K429	E331	S271
CYS	T1403	C1263	P1151	L1042	E1013	E924	R853	Y718	Y717	Q635	P564	K435	S332	L272
ARG	K1405	L1264	Q1153	L1043	E1014	E925	R854	Y719	Y718	L636	S565	K438	R334	L273
LEU	L1406	H1267	L1157	L1044	E1015	E926	R855	Y720	Y719	S641	A566	K438	P274	P274
LEU	L1407	T1270	T1158	L1045	E1016	E927	R856	Y721	Y720	G641	T567	N444	S276	S276
ILE	C1408	H1271	Q1163	L1046	E1017	E928	R857	Y722	Y721	I645	G568	S445	L277	N278
SER	H1409	T1272	L1167	L1047	E1018	E929	R858	Y723	Y722	I646	E569	K446	D347	A279
HIS	H1410	L1273	L1168	L1048	E1019	E930	R859	Y724	Y723	Q648	F570	N445	L347	L280
CYS	S1411	K1276	C1166	L1049	E1020	E931	R860	Y725	Y724	K649	L571	C455	A279	A279
GLN	Q1412	A1277	L1167	L1050	E1021	E932	R861	Y726	Y725	F650	L572	M456	P351	R281
GLU	P1413	S1278	L1168	L1051	E1022	E933	R862	Y727	Y726	L653	N573	S457	F352	A282
PRO	V1414	D1279	G1178	L1052	E1023	E934	R863	Y728	Y727	V654	V574	F461	L353	S283
ILE	K1415	K1282	V1181	L1053	E1024	E935	R864	Y729	Y728	V655	E575	L465	I357	Q284
GLY	C1416	V1283	Q1188	L1054	E1025	E936	R865	Y730	Y729	H660	E576	L477	G360	V285
GLY	G1417	L1283	Q1189	L1055	E1026	E937	R866	Y731	Y730	G668	E577	L481	D363	D286
CYS	H1418	S1289	E1190	L1056	E1027	E938	R867	Y732	Y731	I669	E578	E488	I367	E288
PRO	V1419	L1290	E1191	L1057	E1028	E939	R868	Y733	Y732	Y670	R581	Q491	E378	E290
CYS	E1420	E1293	I1195	L1058	E1029	E940	R869	Y734	Y733	N671	N582	Q492	D379	T291
ARG	G1421	G1297	S1198	L1059	E1030	E941	R870	Y735	Y734	K674	N583	A495	F380	E292
THR	L1422	L1297	L1199	L1060	E1031	E942	R871	Y736	Y735	V678	N584	E496	V381	K293
CYS	L1423	K1314	V1200	L1061	E1032	E943	R872	Y737	Y736	R679	V585	L384	L385	N294
ASN	Y1424	E1315	N1203	L1062	E1033	E944	R873	Y738	Y737	V680	L586	D501	K385	L295
ARG	G1425	E1315	Q1204	L1063	E1034	E945	R874	Y739	Y738	G681	L587	S502	V298	Q299
CYS	G1426	G1323	E1205	L1064	E1035	E946	R875	Y740	Y739	V681	L588	F503	Q299	T300
VAL	L1427	K1324	E1206	L1065	E1036	E947	R876	Y741	Y740	S884	L589	L504	I302	I302
HIS	L1428	Q1328	K1207	L1066	E1037	E948	R877	Y742	Y741	E687	L590	M505	E303	E303
SER	V1429	E1329	I1213	L1067	E1038	E949	R878	Y743	Y742	I688	L591	V506	H304	H304
GLN	K1430	G1330	Y1213	L1068	E1039	E950	R879	Y744	Y743	K690	L592	T508	D397	Q398
CYS	C1431	V1348	N1215	L1069	E1040	E951	R880	Y745	Y744	K691	L593	R516	Q398	Q398
LYS	T1432	P1349	A1224	L1070	E1041	E952	R881	Y746	Y745	L694	L594	H517	G399	G399
CYS	L1433	K1350	K1225	L1071	E1042	E953	R882	Y747	Y746	R695	L595	L522	L400	R310
GLY	K1434	T1351	K1226	L1072	E1043	E954	R883	Y748	Y747	E696	L596	L522	R401	E311
	C1435	I1352	L1226	L1073	E1044	E955	R884	Y749	Y748	L697	L597	H542	K402	G312
	G1436	P1353	L1226	L1074	E1045	E956	R885	Y750	Y749	R698	L598	H542	R403	T313
	T1437	L1438	L1226	L1075	E1046	E957	R886	Y751	Y750	K699	L599	H542	K404	L314
	L1439	D1440	L1226	L1076	E1047	E958	R887	Y752	Y751	M603	L600	H542	D407	R315
CYS				L1077	E1048	E959	R888	Y753	Y752	A609	L601	H542	I408	D317
GLY				L1078	E1049	E960	R889	Y754	Y753	L610	L602	H542	I409	T318
				L1079	E1050	E961	R890	Y755	Y754	L611	L603	H542	I410	
				L1080	E1051	E962	R891	Y756	Y755	L612	L604	H542	I411	
				L1081	E1052	E963	R892	Y757	Y756	L613	L605	H542	I412	
				L1082	E1053	E964	R893	Y758	Y757	L614	L606	H542	I413	
				L1083	E1054	E965	R894	Y759	Y758	L615	L607	H542	I414	
				L1084	E1055	E966	R895	Y760	Y759	L616	L608	H542	I415	
				L1085	E1056	E967	R896	Y761	Y760	L617	L609	H542	I416	
				L1086	E1057	E968	R897	Y762	Y761	L618	L610	H542	I417	
				L1087	E1058	E969	R898	Y763	Y762	L619	L611	H542	I418	
				L1088	E1059	E970	R899	Y764	Y763	L620	L612	H542	I419	
				L1089	E1060	E971	R900	Y765	Y764	L621	L613	H542	I420	
				L1090	E1061	E972	R901	Y766	Y765	L622	L614	H542	I421	
				L1091	E1062	E973	R902	Y767	Y766	L623	L615	H542	I422	
				L1092	E1063	E974	R903	Y768	Y767	L624	L616	H542	I423	
				L1093	E1064	E975	R904	Y769	Y768	L625	L617	H542	I424	
				L1094	E1065	E976	R905	Y770	Y769	L626	L618	H542	I425	
				L1095	E1066	E977	R906	Y771	Y770	L627	L619	H542	I426	
				L1096	E1067	E978	R907	Y772	Y771	L628	L620	H542	I427	
				L1097	E1068	E979	R908	Y773	Y772	L629	L621	H542	I428	
				L1098	E1069	E980	R909	Y774	Y773	L630	L622	H542	I429	
				L1099	E1070	E981	R910	Y775	Y774	L631	L623	H542	I430	
				L1100	E1071	E982	R911	Y776	Y775	L632	L624	H542	I431	
				L1101	E1072	E983	R912	Y777	Y776	L633	L625	H542	I432	
				L1102	E1073	E984	R913	Y778	Y777	L634	L626	H542	I433	
				L1103	E1074	E985	R914	Y779	Y778	L635	L627	H542	I434	
				L1104	E1075	E986	R915	Y780	Y779	L636	L628	H542	I435	
				L1105	E1076	E987	R916	Y781	Y780	L637	L629	H542	I436	
				L1106	E1077	E988	R917	Y782	Y781	L638	L630	H542	I437	
				L1107	E1078	E989	R918	Y783	Y782	L639	L631	H542	I438	
				L1108	E1079	E990	R919	Y784	Y783	L640	L632	H542	I439	
				L1109	E1080	E991	R920	Y785	Y784	L641	L633	H542	I440	
				L1110	E1081	E992	R921	Y786	Y785	L642	L634	H542	I441	
				L1111	E1082	E993	R922	Y787	Y786	L643	L635	H542	I442	
				L1112	E1083	E994	R923	Y788	Y787	L644	L636	H542	I443	
				L1113	E1084	E995	R924	Y789	Y788	L645	L637	H542	I444	
				L1114	E1085	E996	R925	Y790	Y789	L646	L638	H542	I445	
				L1115	E1086	E997	R926	Y791	Y790	L647	L639	H542	I446	
				L1116	E1087	E998	R927	Y792	Y791	L648	L640	H542	I447	
				L1117	E1088	E999	R928	Y793	Y792	L649	L641	H542	I448	
				L1118	E1089	E1000	R929	Y794	Y793	L650	L642	H542	I449	
				L1119	E1090	E1001	R930	Y795	Y794	L651	L643	H542	I450	
				L1120	E1091	E1002	R931	Y796	Y795	L652	L644	H542	I451	
				L1121	E1092	E1003	R932	Y797	Y796	L653	L645	H542	I452	
				L1122	E1093	E1004	R933	Y798	Y797	L654	L646	H542	I453	
				L1123	E1094	E1005	R934	Y799	Y798	L655	L647	H542	I454	
				L1124	E1095	E1006	R935	Y800	Y799	L656	L648	H542	I455	
				L1125	E1096	E1007	R936	Y801	Y800	L657	L649	H542	I456	
				L1126	E1097	E1008	R937	Y802	Y801	L658	L650	H542	I457	
				L1127	E1098	E1009	R938	Y803	Y802	L659	L651	H542	I458	
				L1128	E1099	E1010	R939	Y804	Y803	L660	L652	H542	I459	
				L1129	E1100	E1011	R940	Y805	Y804	L661	L653	H542	I460	
				L1130	E1101	E1012	R941	Y806	Y805	L662	L654	H542	I461	
				L1131	E1102	E1013	R942	Y807	Y806	L663	L655	H542	I46	

[illegible]

- Molecule 1: NFX1-type zinc finger-containing protein 1



LEU	GLN	LYS	LEU	R309	T244	F183	ASN	ALA	MET
LEU	GLN	VAL	ASP	R310	T247	L184	ASP	ALA	GLU
GLY	GLN	GLN	THR	E311	T248	L185	ASN	TYR	GLU
GLY	GLN	PHE	PHE	G312	T249	L186	PHE	TRP	ARG
ARG	LEU	THR	ARG	THR	T250	L187	GLN	ARG	PRO
TYR	ALA	LYS	LEU	LEU	T251	C188	TRP	GLU	LEU
ASP	GLU	PRO	LEU	ARG	T252	C188	ARG	GLU	HIS
VAL	VAL	LEU	ARG	VAL	Q252	Q189	ASP	ARG	ASP
THR	GLN	LYS	GLU	ASP	D253	V190	PRO	PHE	ALA
PRO	PHE	VAL	ASP	THR	T254	L191	HIS	ARG	ARG
SER	VAL	VAL	PHE	TYR	T255	L192	GLN	ALA	PRO
ASP	ARG	ARG	VAL	THR	T256	R192	LYS	MET	ARG
GLU	THR	ARG	ARG	LEU	V257	L193	PRO	GLY	ASN
ASN	PHE	GLN	PRO	VAL	F258	A194	THR	ARG	ASN
PRO	LEU	ASN	LEU	GLN	LEU	C195	GLU	ASN	HIS
SER	MET	ARG	ARG	PRO	T259	S196	GLN	THR	ASN
ALA	VAL	LYS	GLU	GLU	A260	S197	PRO	HIS	ASN
THR	GLU	ARG	GLY	ALA	T261	S197	GLN	GLN	HIS
GLY	THR	LEU	ILE	GLU	T262	C198	GLN	GLY	ASN
THR	THR	LEU	LEU	ASP	V263	M199	GLN	ARG	GLY
PHE	ALA	TYR	GLU	HIS	T264	D200	VAL	ARG	PRO
LEU	TYR	GLY	LEU	VAL	Q264	R201	ASN	GLN	ASP
ARG	PHE	SER	LEU	GLU	E265	Q202	GLY	GLU	GLY
ASN	GLU	LEU	GLN	SER	T266	S203	GLY	HIS	LEU
VAL	VAL	VAL	SER	TYR	E267	Y204	VAL	LEU	LEU
GLU	TYR	CYS	PHE	ARG	T268	T205	GLY	ALA	PRO
GLY	ARG	MET	GLU	THR	S267	H206	ASP	SER	PRO
HIS	SER	SER	ASP	MET	N268	V207	K147	GLY	ARG
VAL	LYS	LYS	GLN	PRO	L269	L208	F148	ASP	ARG
LEU	ASP	ASP	GLY	ILE	S271	L208	E150	GLU	ALA
PRO	GLU	ASN	LEU	TYR	T270	V207	L149	ALA	ARG
GLY	GLY	PHE	ARG	PRO	S271	L208	ASP	ASN	GLN
ILE	LEU	GLU	LYS	THR	T276	G209	S151	GLN	ALA
GLN	GLN	THR	ARG	TYR	L277	T210	L152	ARG	ASN
VAL	GLU	PHE	LYS	ASN	T277	L211	L153	HIS	ASN
LEU	LEU	PHE	PHE	GLU	N278	K212	Q154	ASP	PRO
ASP	GLN	PHE	VAL	VAL	A279	K212	GLN	PRO	PRO
PRO	GLU	ALA	ASP	HIS	L280	N213	K155	GLU	ALA
GLY	GLU	THR	ILE	LEU	R281	D156	D156	ASN	ASN
ASN	VAL	VAL	ARG	ASP	T281	S214	P157	ASN	ALA
TRP	VAL	SER	ILE	GLU	A292	K215	ASP	ASP	ALA
PRO	PRO	ASN	THR	ARG	S283	F216	S158	THR	LEU
SER	PHE	ARG	PHE	PRO	G294	L217	E159	ARG	LEU
LYS	GLN	GLU	PHE	THR	T297	K215	V160	TRP	GLY
GLU	ARG	GLN	THR	LEU	D296	V219	V161	GLY	GLY
ALA	ASN	GLU	ARG	ARG	T298	C220	T162	ASN	ALA
LEU	ILE	ASP	ILE	PRO	T297	L221	T163	GLY	SER
LYS	VAL	LEU	ILE	ASN	E298	P222	L164	ASN	HIS
LEU	GLU	CYS	THR	ILE	T299	A223	A165	ASP	GLY
ASP	CYS	ARG	PRO	ILE	E299	Y224	T166	CYS	ARG
ASP	ASN	GLY	MET	SER	E299	A223	T166	ARG	HIS
SER	SER	ILE	CYS	GLY	T291	G227	S167	ASN	PRO
SER	LYS	VAL	SER	LYS	E292	K228	L168	ARG	ALA
GLN	VAL	GLN	SER	TYR	E292	T229	G169	ARG	ALA
MET	VAL	LEU	SER	ASP	K293	T230	L170	PRO	ASN
GLY	LYS	GLY	SER	GLY	N294	T230	L170	PRO	ASN
ALA	GLU	PHE	ILE	THR	T295	E231	K171	TRP	HIS



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	258760	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.060	Depositor
Minimum map value	-0.676	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.07	Depositor
Map size ($\text{\AA}$)	331.2, 331.2, 331.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.828, 0.828, 0.828	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: AGS

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	0.18	0/10508	0.47	0/14189
1	B	0.23	0/10508	0.51	0/14189
1	C	0.19	0/1361	0.53	0/1836
All	All	0.21	0/22377	0.49	0/30214

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10307	0	10368	171	0
1	B	10307	0	10368	220	0
1	C	1344	0	1417	36	0
2	A	31	0	12	2	0
2	B	31	0	12	8	0
All	All	22020	0	22177	421	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.

The worst 5 of 421 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:621:PRO:HG3	1:B:1035:GLN:HE21	1.28	0.94
1:B:621:PRO:HG3	1:B:1035:GLN:NE2	1.93	0.84
1:A:1068:ARG:HH22	1:A:1090:ASP:H	1.27	0.82
1:B:1068:ARG:HH22	1:B:1089:GLN:H	1.27	0.81
1:A:554:ARG:HD2	1:A:581:ARG:HB3	1.65	0.78

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	1278/1918 (67%)	1221 (96%)	57 (4%)	0	100	100
1	B	1278/1918 (67%)	1232 (96%)	46 (4%)	0	100	100
1	C	170/1918 (9%)	163 (96%)	7 (4%)	0	100	100
All	All	2726/5754 (47%)	2616 (96%)	110 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1162/1726 (67%)	1139 (98%)	23 (2%)	48	64

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	1162/1726 (67%)	1134 (98%)	28 (2%)	43	62
1	C	159/1726 (9%)	157 (99%)	2 (1%)	61	71
All	All	2483/5178 (48%)	2430 (98%)	53 (2%)	46	64

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	427	VAL
1	B	744	LEU
1	B	1260	LEU
1	B	477	LEU
1	B	543	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1235	GLN
1	B	1147	GLN
1	A	1345	GLN
1	B	1317	GLN
1	B	685	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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	AGS	B	2000	-	32,33,33	0.68	1 (3%)	45,52,52	0.56	0
2	AGS	A	2000	-	32,33,33	0.64	0	45,52,52	0.76	1 (2%)

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	AGS	B	2000	-	-	2/21/38/38	0/3/3/3
2	AGS	A	2000	-	-	5/21/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2000	AGS	PG-S1G	2.01	1.95	1.90

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2000	AGS	PB-O3B-PG	-2.75	123.12	133.17

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

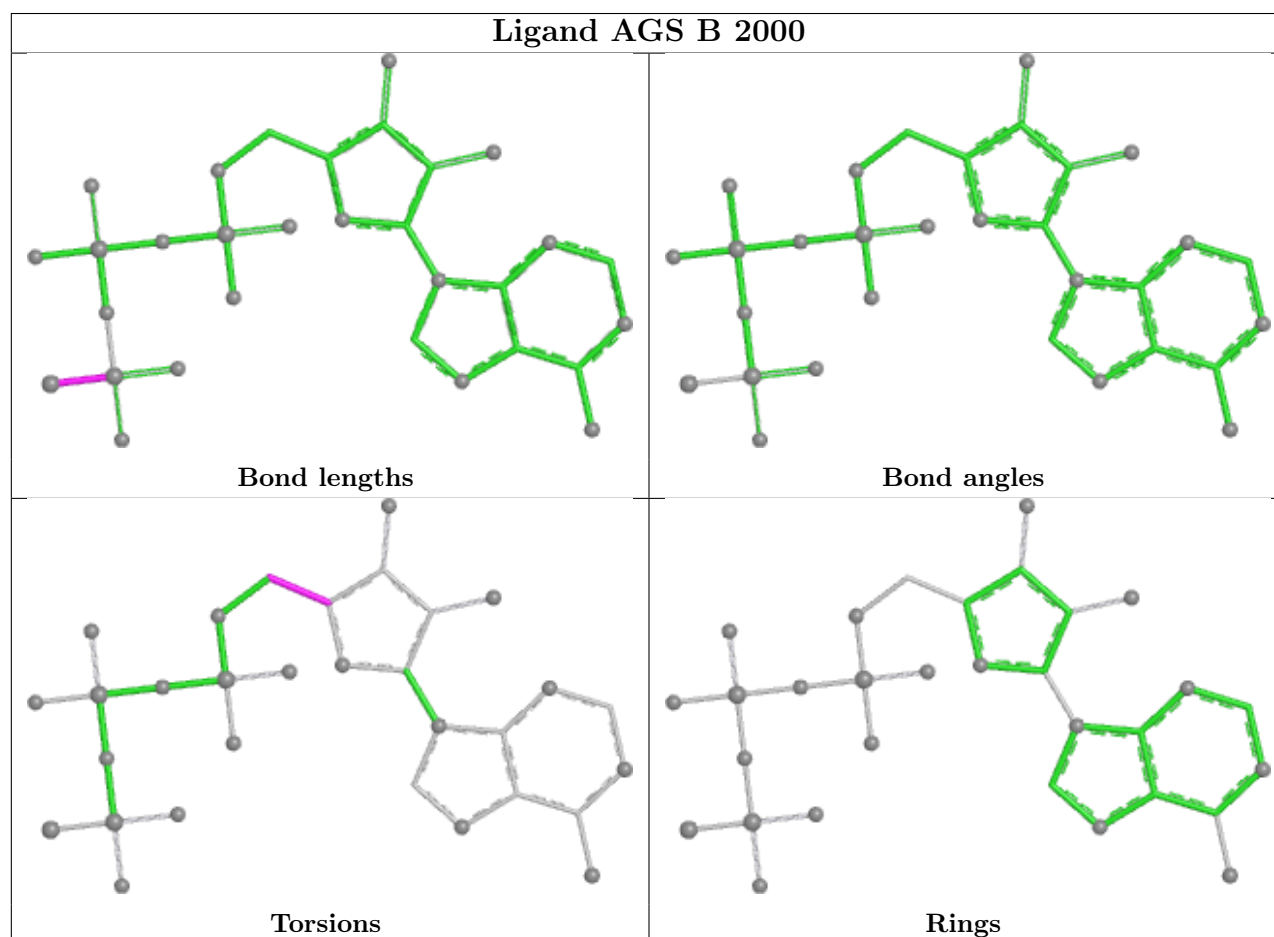
Mol	Chain	Res	Type	Atoms
2	A	2000	AGS	C5'-O5'-PA-O2A
2	A	2000	AGS	C5'-O5'-PA-O3A
2	A	2000	AGS	C4'-C5'-O5'-PA
2	A	2000	AGS	C3'-C4'-C5'-O5'
2	A	2000	AGS	O4'-C4'-C5'-O5'

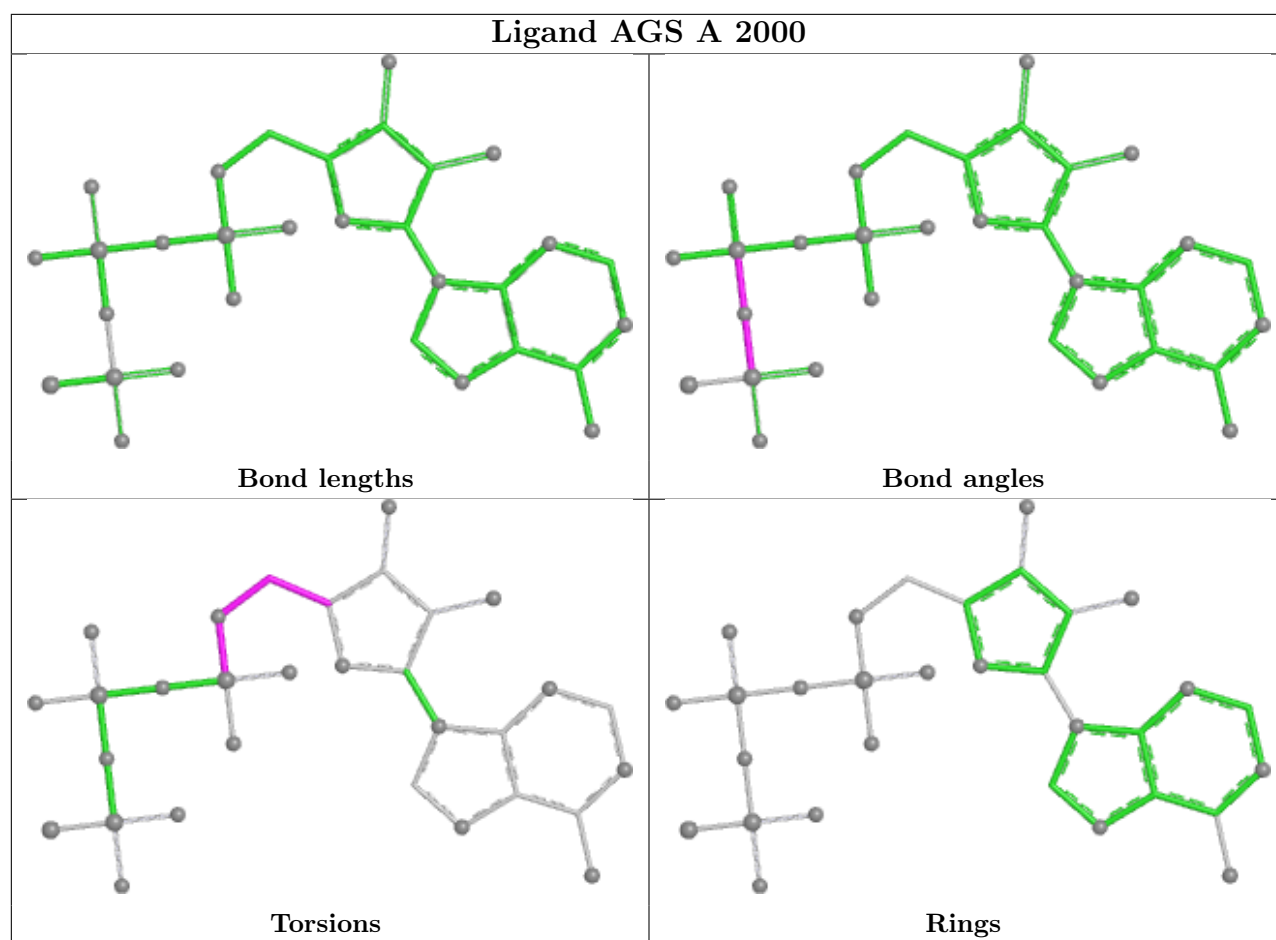
There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2000	AGS	8	0
2	A	2000	AGS	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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.

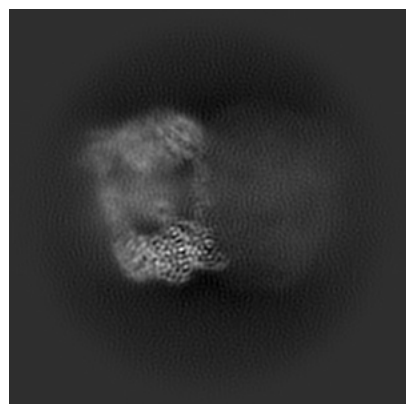
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-75718. These allow visual inspection of the internal detail of the map and identification of artifacts.

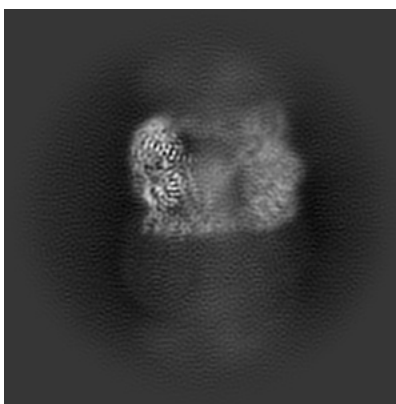
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

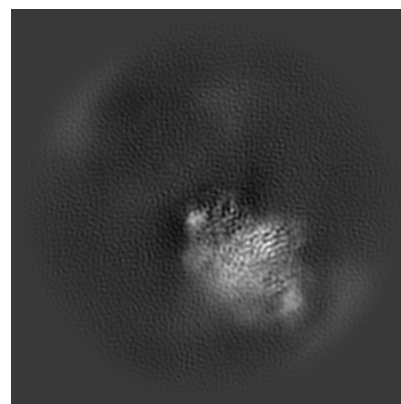
6.1.1 Primary map



X

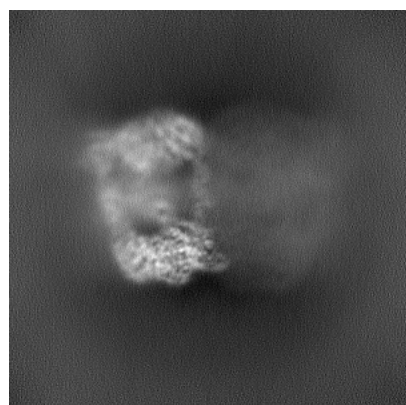


Y

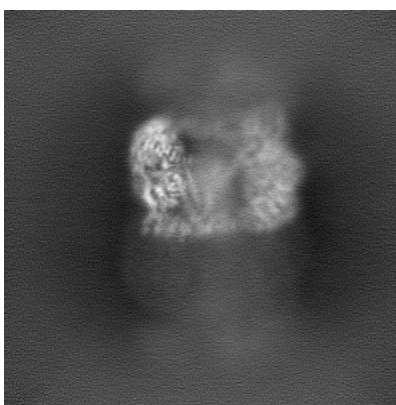


Z

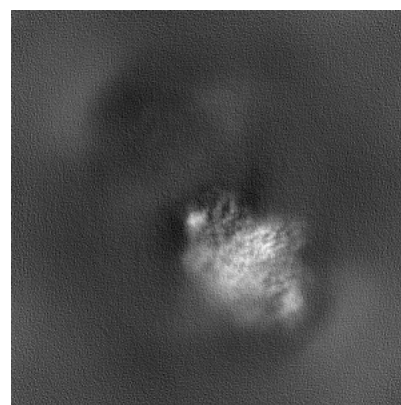
6.1.2 Raw map



X



Y

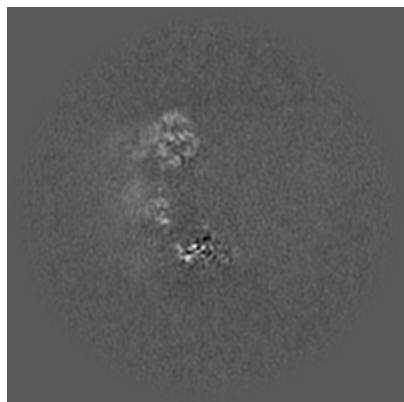


Z

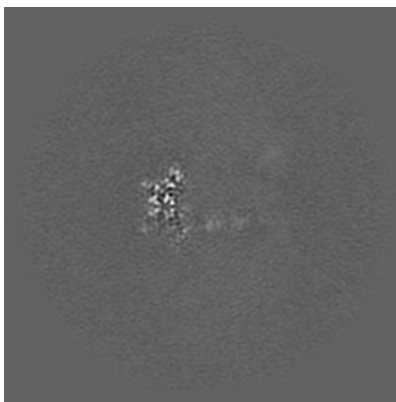
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

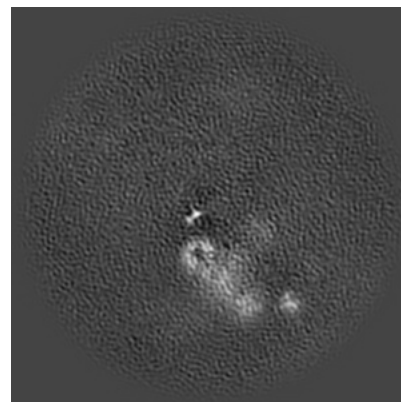
6.2.1 Primary map



X Index: 200



Y Index: 200



Z Index: 200

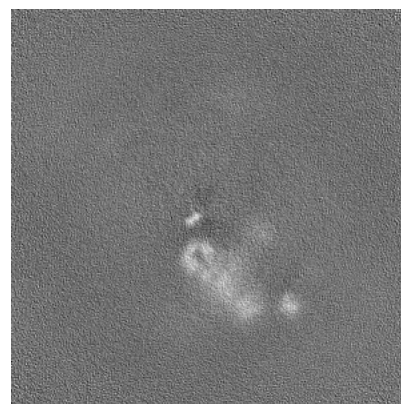
6.2.2 Raw map



X Index: 200



Y Index: 200

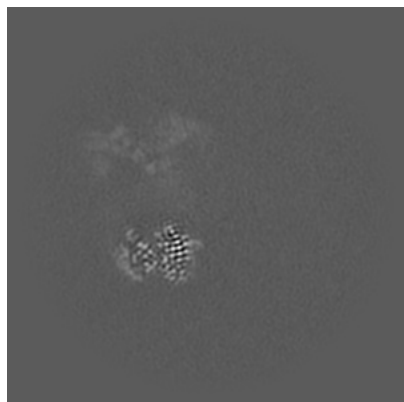


Z Index: 200

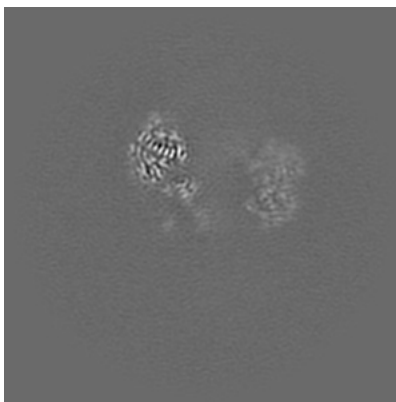
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

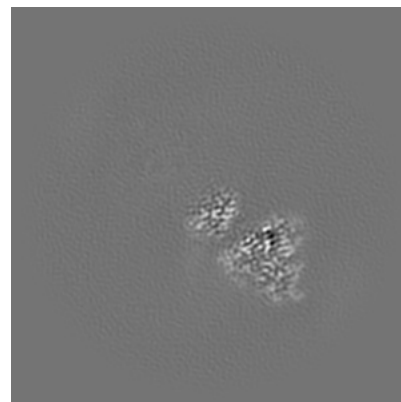
6.3.1 Primary map



X Index: 258

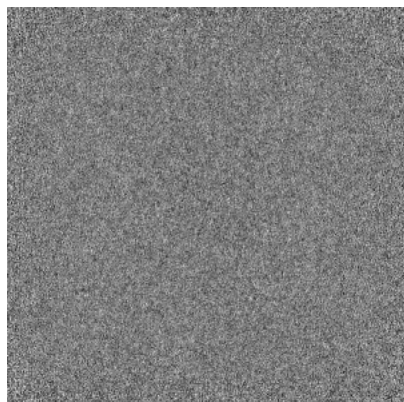


Y Index: 164

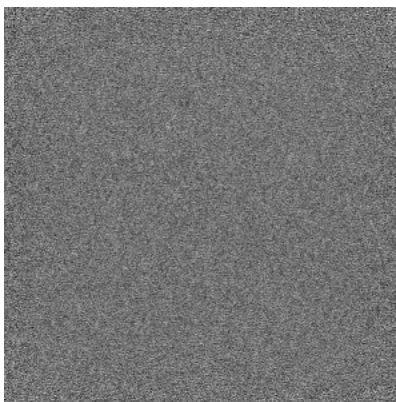


Z Index: 156

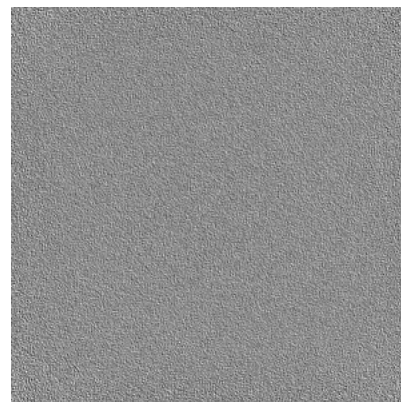
6.3.2 Raw map



X Index: 0



Y Index: 0

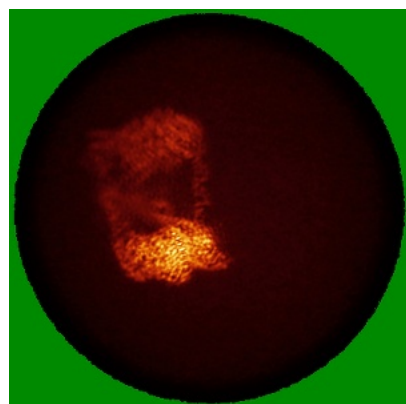


Z Index: 0

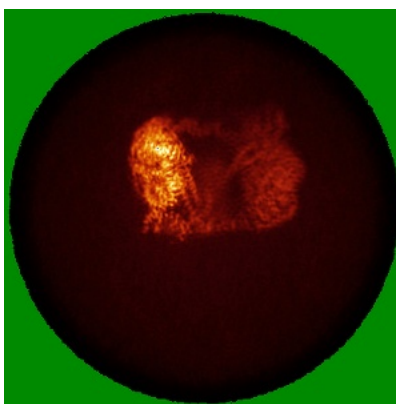
The images above show the largest variance slices of the map in three orthogonal directions.

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

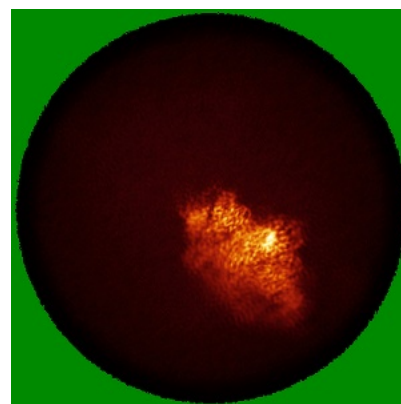
6.4.1 Primary map



X

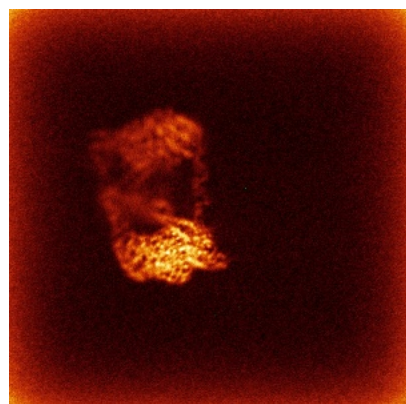


Y

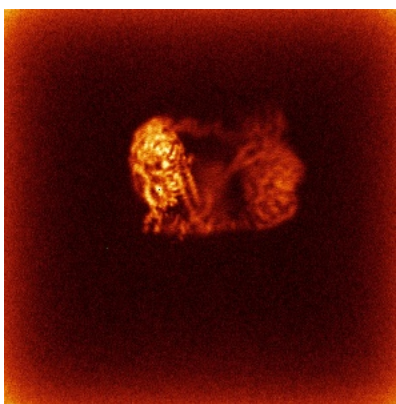


Z

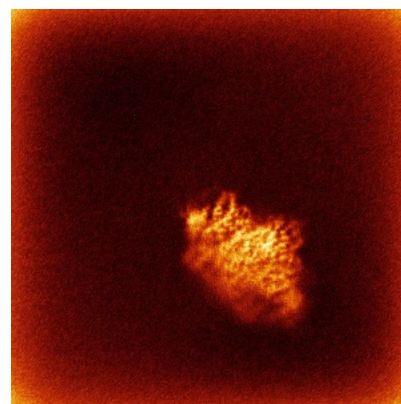
6.4.2 Raw map



X



Y

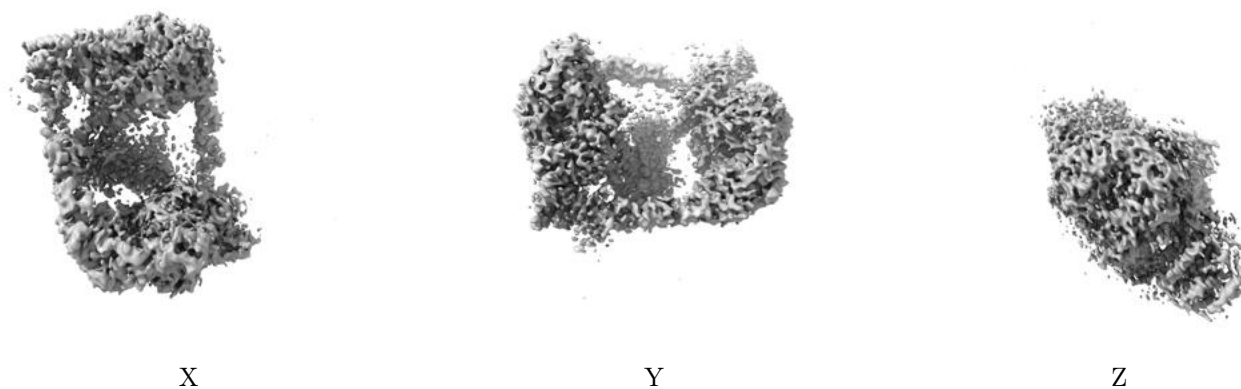


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

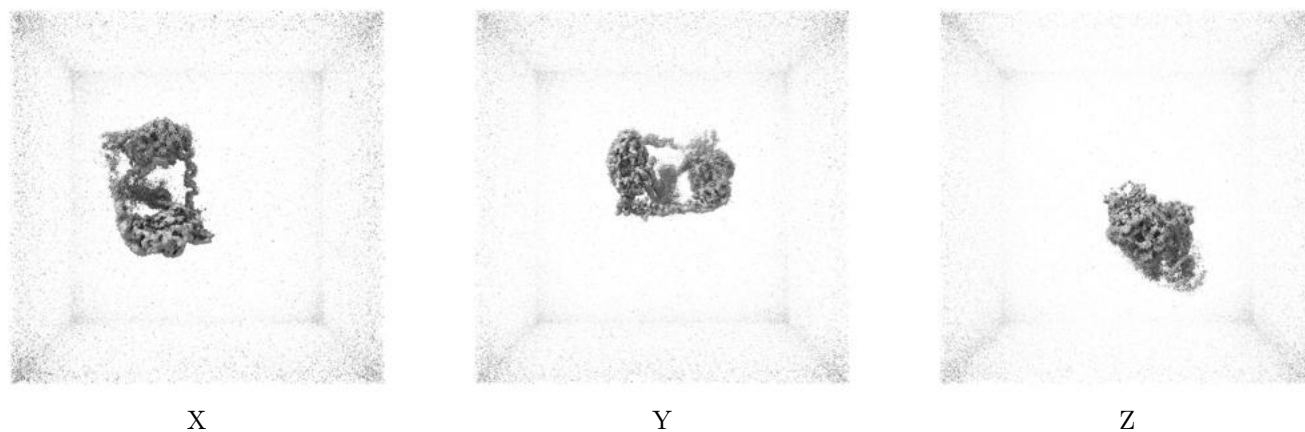
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.07. 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.

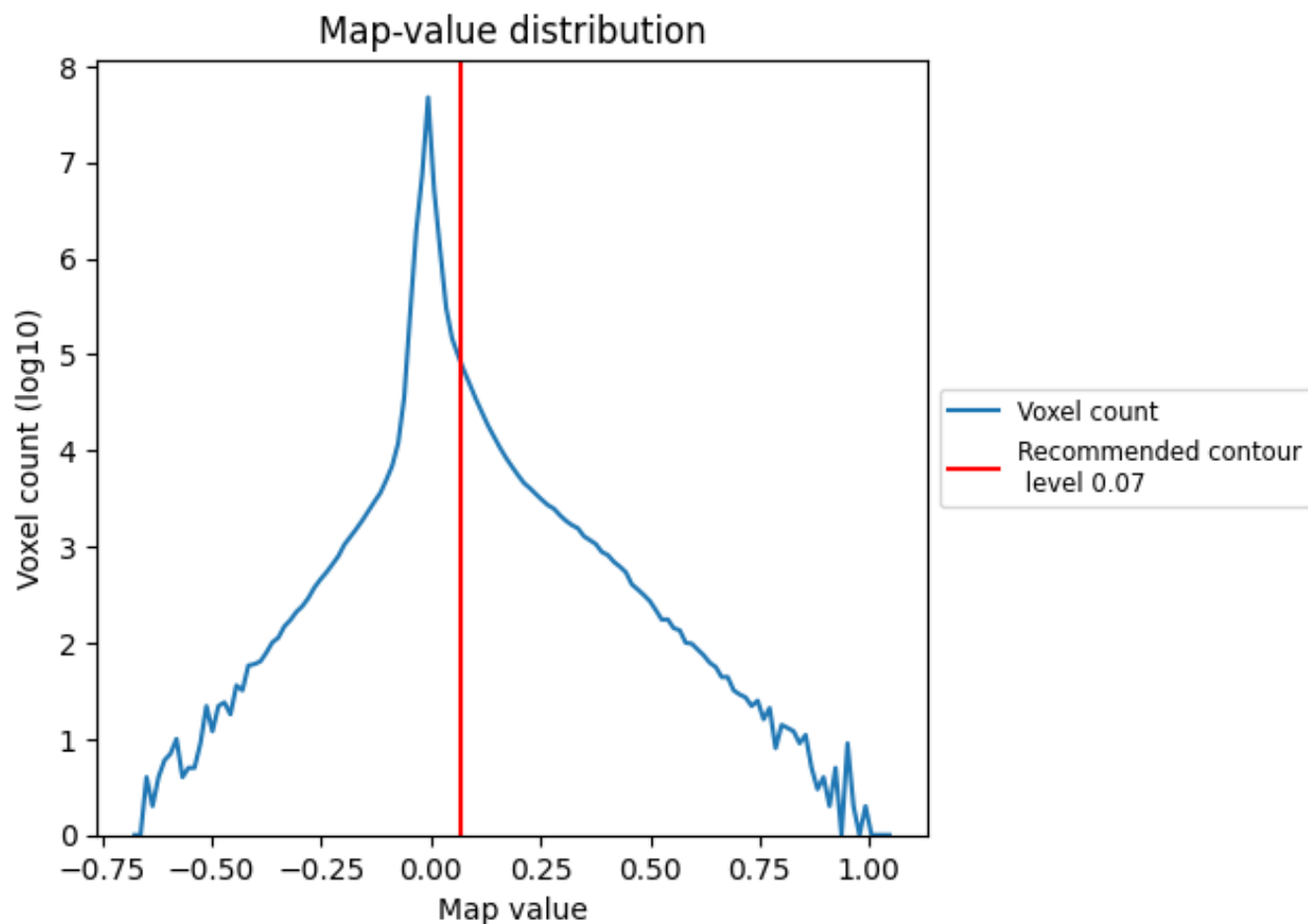
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

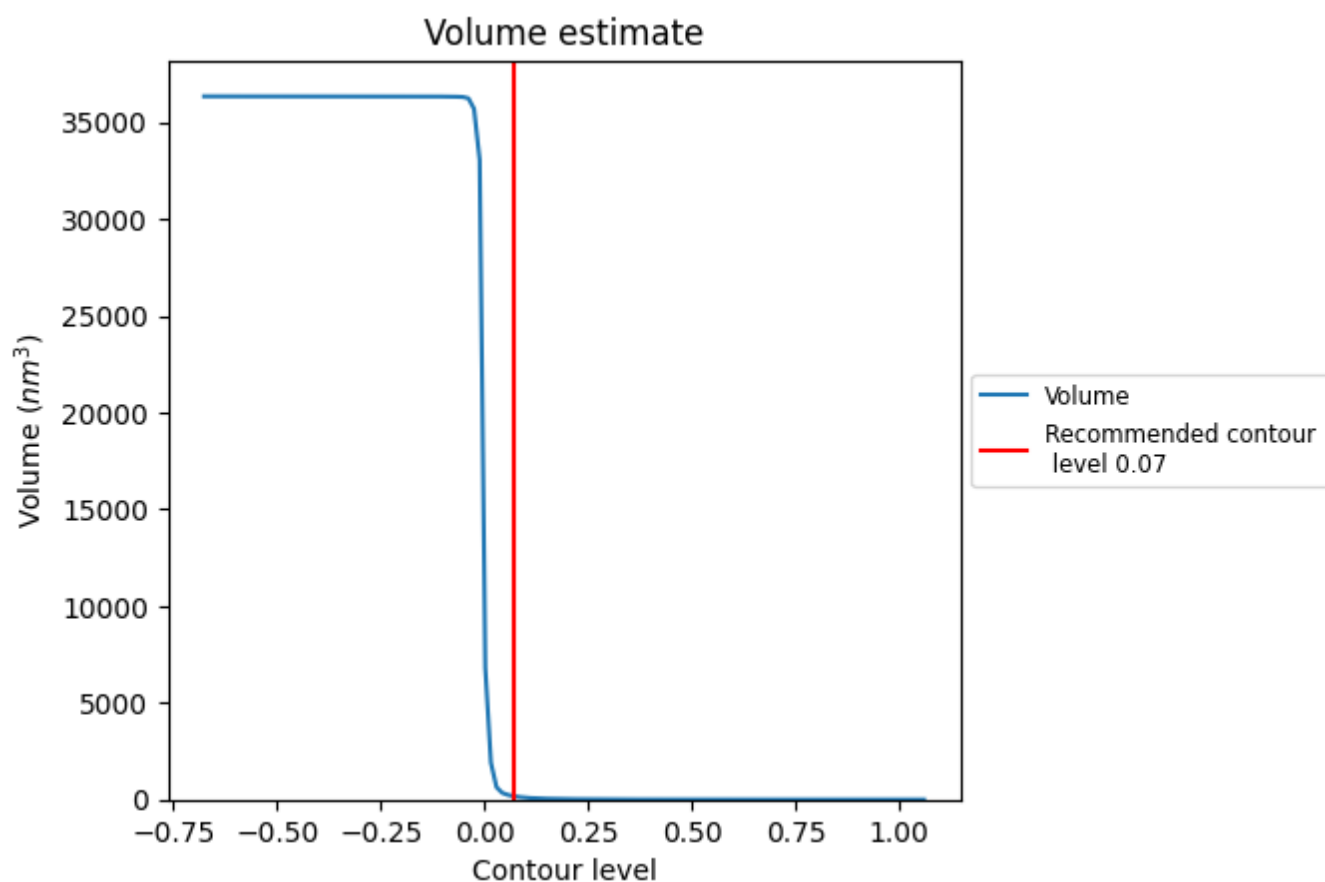
This section contains the results of statistical analysis of the map.

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.

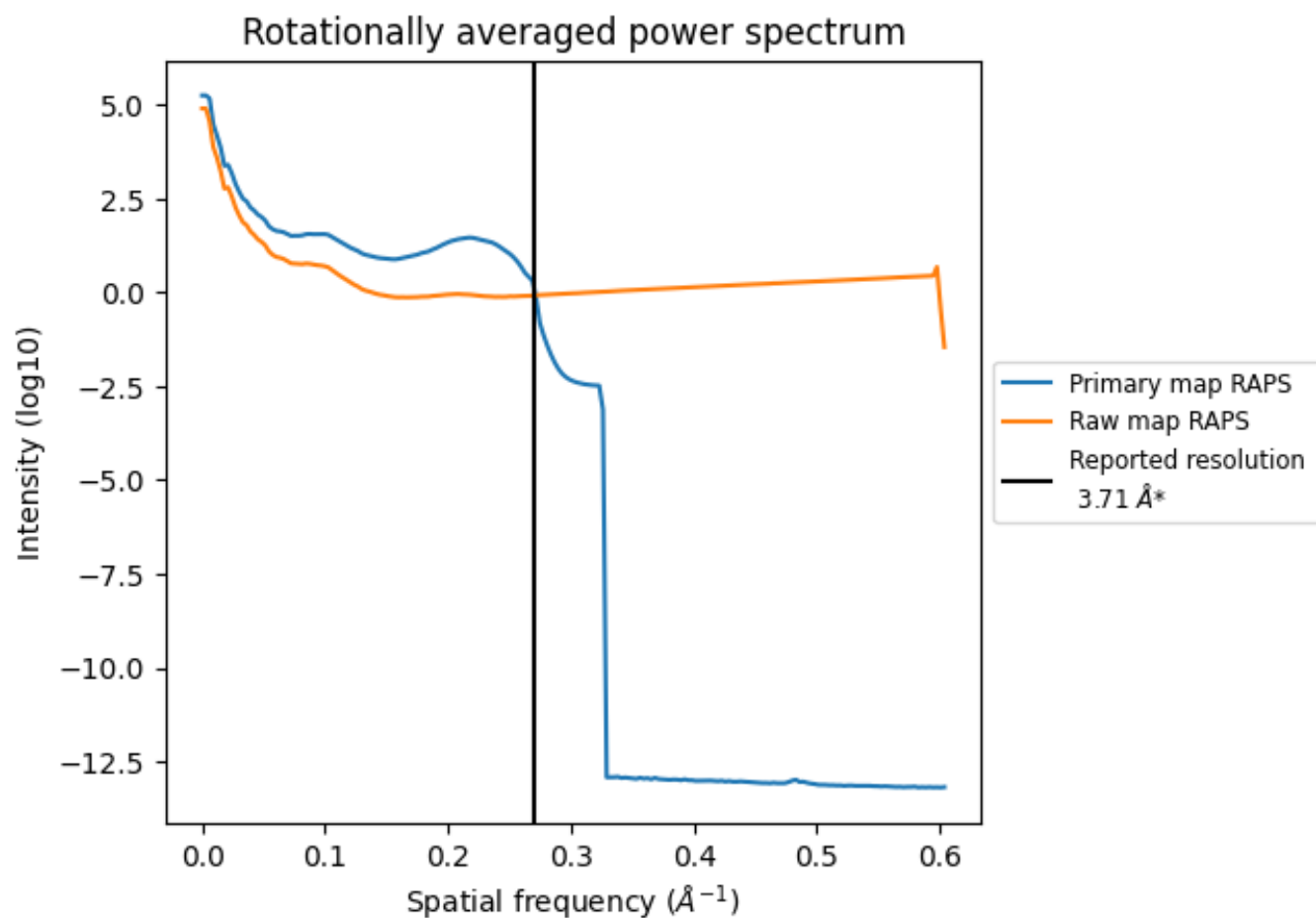
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 177 nm^3 ; this corresponds to an approximate mass of 160 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 ⓘ

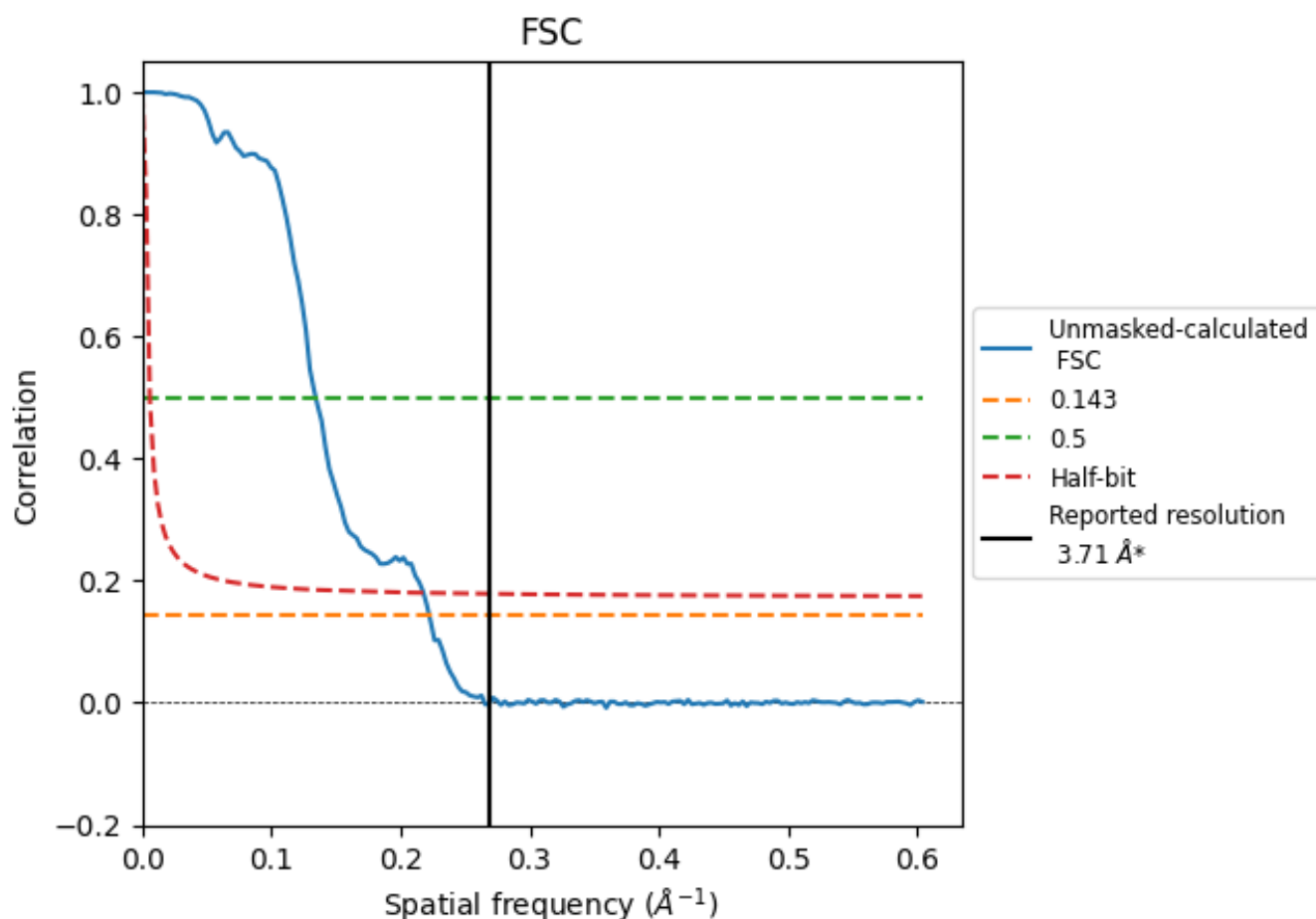


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

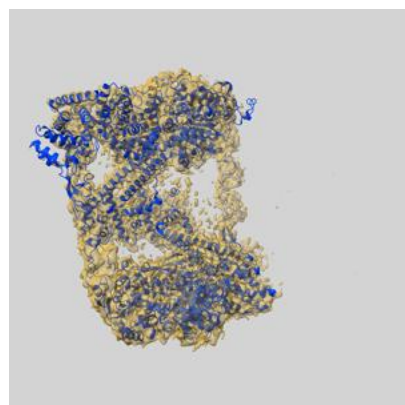
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.71	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.50	7.45	4.59

*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 4.50 differs from the reported value 3.71 by more than 10 %

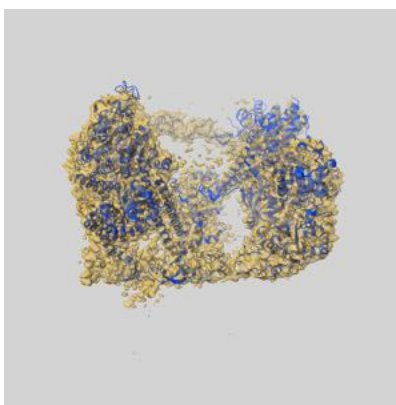
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-75718 and PDB model 11IM. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

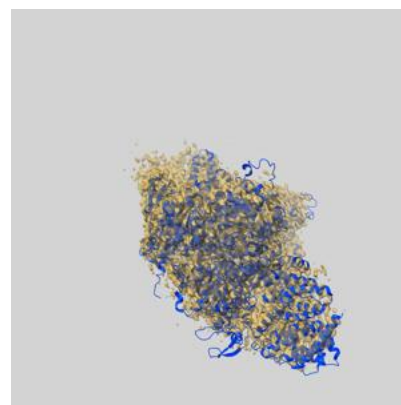
9.1 Map-model overlay [i](#)



X



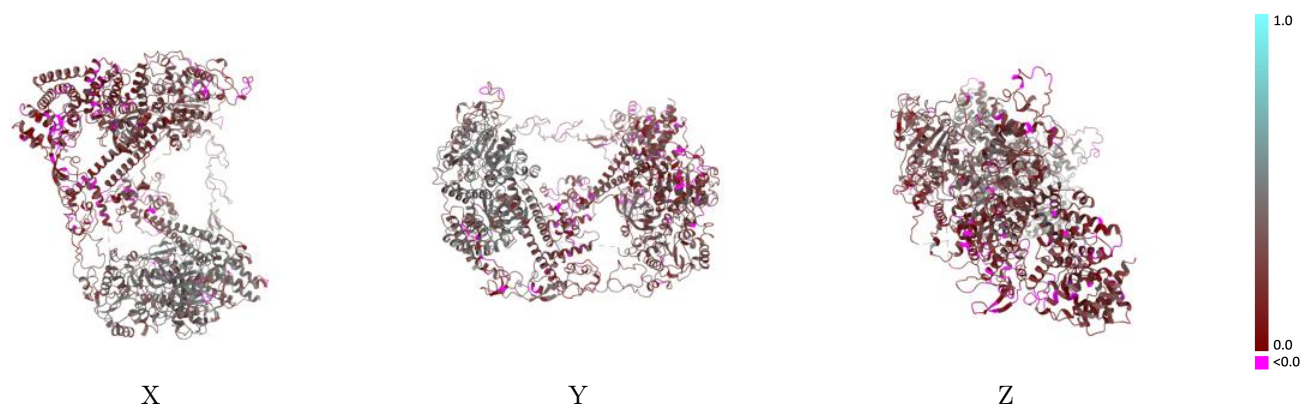
Y



Z

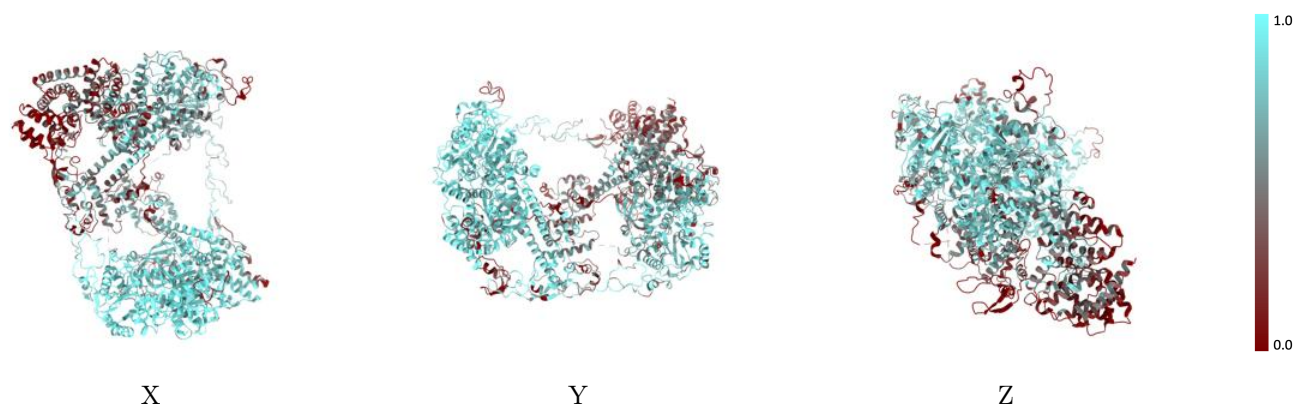
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



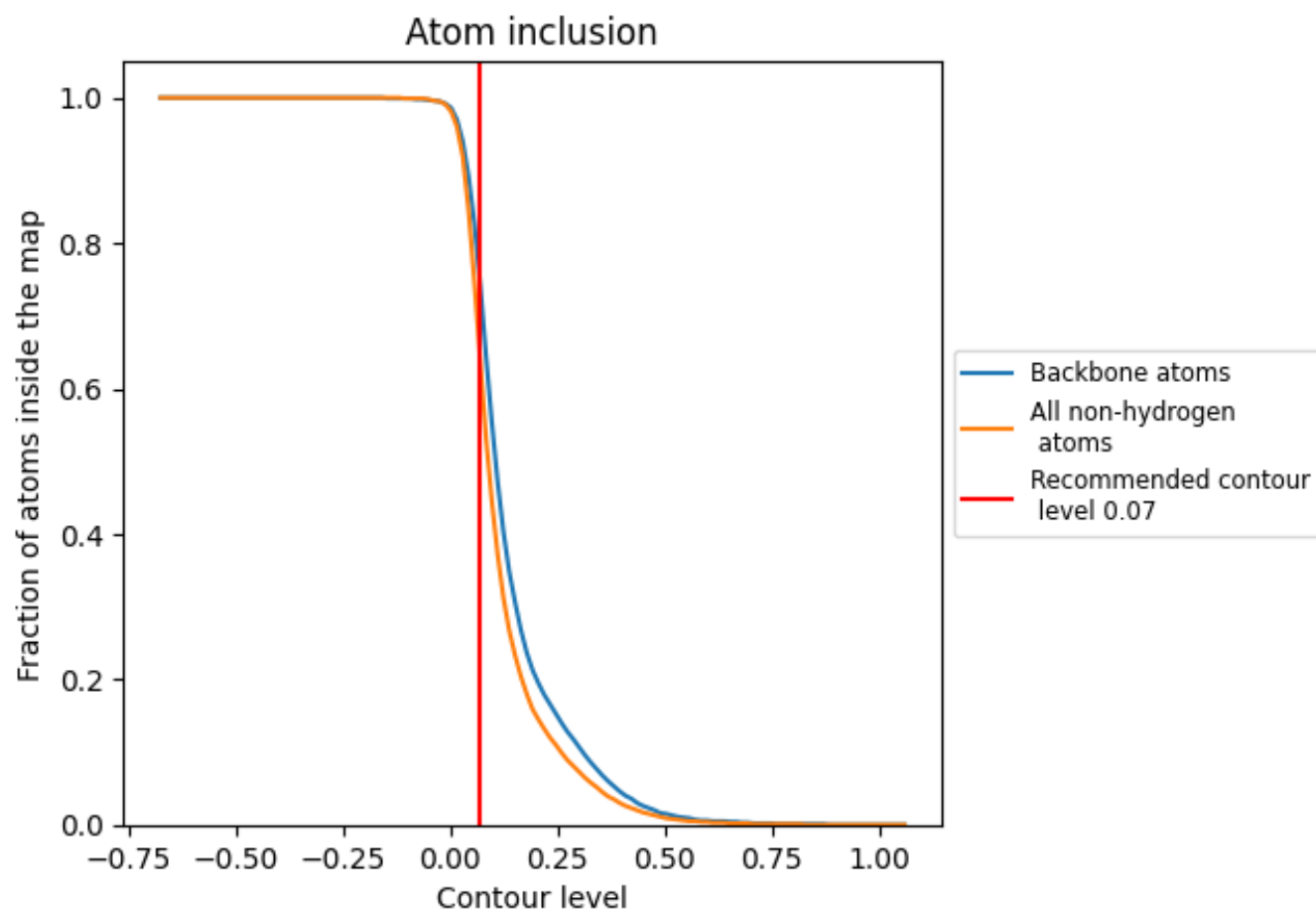
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 64% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6350	0.2910
A	0.7510	0.3560
B	0.5710	0.2380
C	0.2280	0.2000

