



wwPDB EM Validation Summary Report ⓘ

Feb 24, 2025 – 05:02 PM JST

PDB ID : 8X4E
EMDB ID : EMD-38048
Title : Cryo-EM structure of Ryanodine receptor 1 (TM helix S0, 5 mM Ca2+)
Authors : Chen, Q.; Hu, H.
Deposited on : 2023-11-15
Resolution : 3.30 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.dev117
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.2

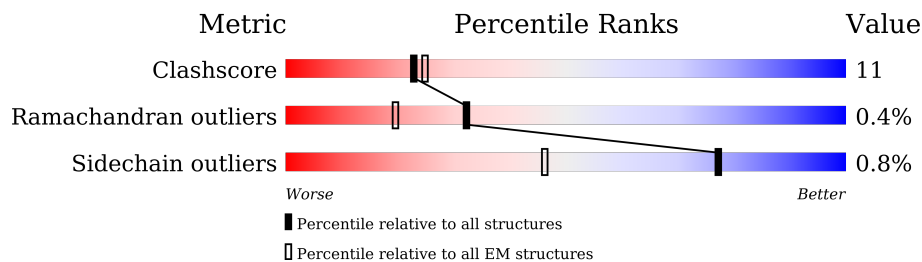
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	5037	 62% 17% 21%
1	B	5037	 61% 17% 21%
1	C	5037	 61% 17% 21%
1	D	5037	 61% 17% 21%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 118280 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 Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3982	Total	C	N	O	S	0	0
			29568	18816	5133	5431	188		
1	B	3982	Total	C	N	O	S	0	0
			29568	18816	5133	5431	188		
1	C	3982	Total	C	N	O	S	0	0
			29568	18816	5133	5431	188		
1	D	3982	Total	C	N	O	S	0	0
			29568	18816	5133	5431	188		

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Zn	0
			1	1	
2	B	1	Total	Zn	0
			1	1	
2	C	1	Total	Zn	0
			1	1	
2	D	1	Total	Zn	0
			1	1	

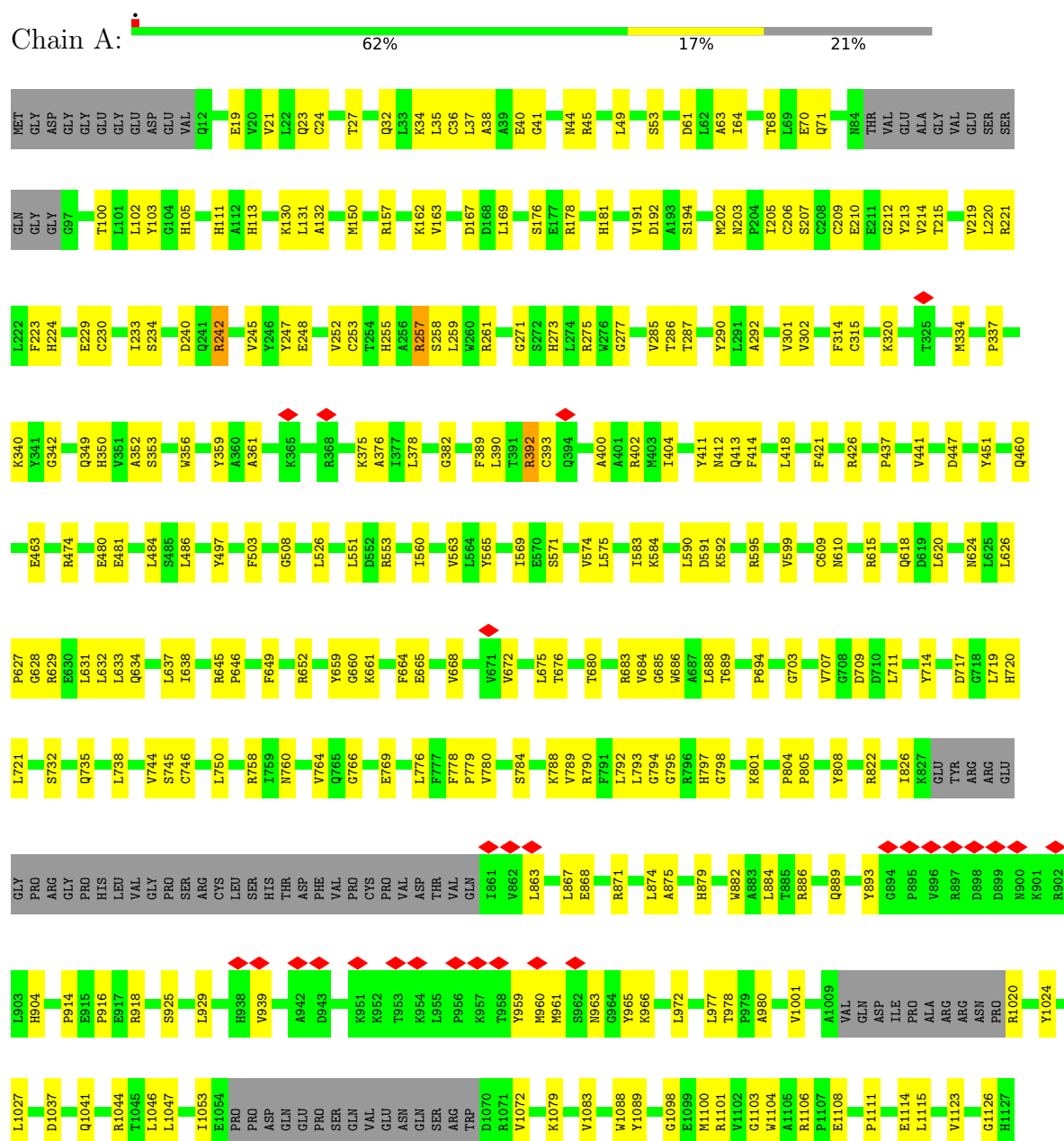
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Ca	0
			1	1	
3	B	1	Total	Ca	0
			1	1	
3	C	1	Total	Ca	0
			1	1	
3	D	1	Total	Ca	0
			1	1	

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.

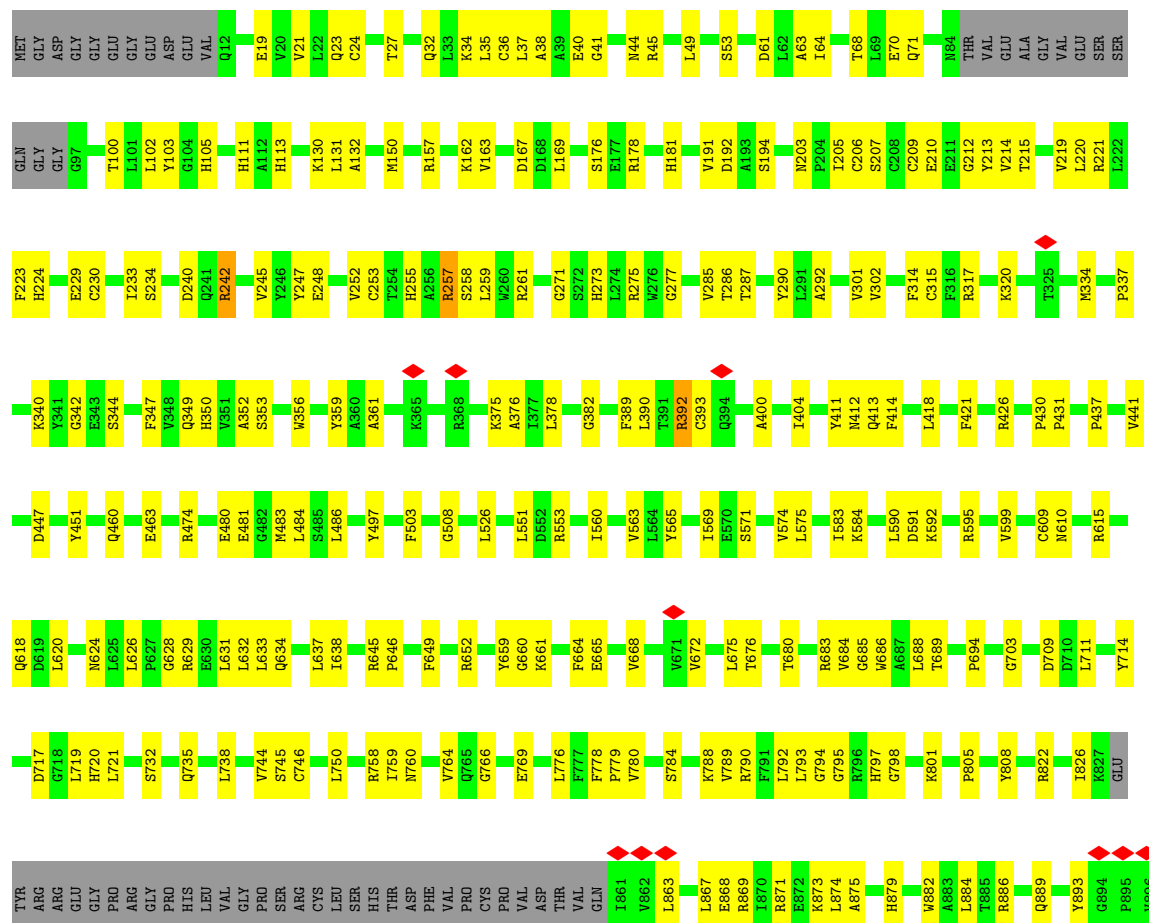
• Molecule 1: Ryanodine receptor 1





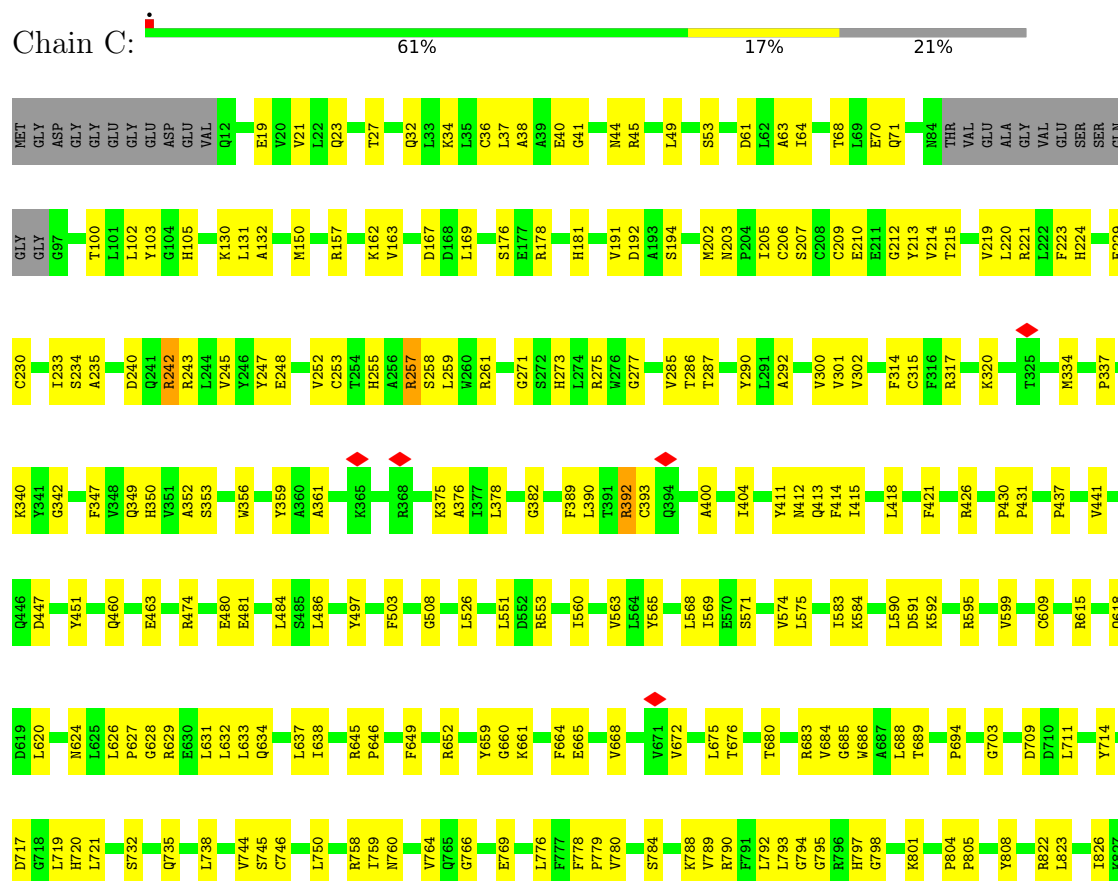


- Molecule 1: Ryanodine receptor 1



S2459	L2460	L2463	D2464	L2474	L2479	L2487	F2494	V2495	P2496	D2497	F2505	Y2510	G2511	L2512	T2538	A2539	L2548	R2552	L2556	A2557	L2558	L2559	A2570	H2574	V2586	Y2587	S2590	R2591	K2597	L2603	A2637	P2640	L2644																		
V2149	W2323	W2324	P2325	L2331	L2332	F2340	T2368	E2174	E2175	S2181	I2182	L2185	H2194	L2197	V2207	V2210	L2215	T2220	I2223	P2226	K2227	M2228	V2229	C2240	S2243	N2246	Q2247	D2252	S2279	E2286	V2299	S2300	Y2301	L2302	K2316	G2317	Y2318														
GLU	GLU	GLU	GLU	GLU	GLU	GLU	THR	SER	SER	SER	LEU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU														
R1808	D1809	K1810	M1814	A1826	P1829	G1832	S1833	V1834	F1835	F1836	Q1837	F1838	V1839	P1840	V1841	L1842	V1859	K1860	I1861	L1862	L1863	M1864	E1865	I1866	E1867	P1868	F1871	E1874	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	ASP														
Q1660	H1663	T1666	T1666	R1671	A1675	L1676	G1677	R1680	H1683	L1694	E1699	G1705	P1706	L1707	R1708	Y1712	L1715	I1716	S1717	M1730	I1735	P1750	G1765	V1765	G1766	S1770	L1771	R1772	A1788	ALA	VAL	E1793	A1796	R1797	P1800	E1805															
LYS	ASN	ILE	P1574	L1575	S1576	A1577	A1578	M1579	F1580	R1584	C1591	R1594	L1600	M1601	P1602	W1605	S1606	R1607	M1608	P1609	N1610	V1615	GLU	THR	ARG	ALA	GLY	E1622	W1626	Q1629	P1633	M1637	A1638	L1639	C1647	M1648	D1649	I1650	L1651	E1652	L1653	S1654	E1655	D1658	L1659						
Y1457	H1458	Q1459	H1460	N1463	V1469	T1473	G1481	N1482	V1483	K1488	C1492	V1495	W1496	G1497	S1501	S1502	P1503	G1507	R1508	V1515	C1518	L1526	M1532	G1533	K1534	S1536	N1537	T1538	F1539	F1540	Q1541	V1542	E1543	P1544	V1554	L1555	P1556	F1564	GLU	LEU	GLY	LYS	GLN								
LYS	LYS	ARG	GLY	PHE	LEU	PHE	LYS	LYS	LYS	LYS	ALA	ALA	MET	THR	GLN	PRO	PRO	ALA	LEU	PRO	HIS	ASP	ALA	ASP	ASN	GLY	ILE	ILE	LEU	ASN	T1430	Y1434	V1437	R1438	V1439	W1449	W1452	V1453	T1454	P1455	D1456										
ALA	ALA	GLU	PRO	ASP	PRO	ASP	TYR	GLU	ASN	LEU	ARG	ARG	SER	ALA	GLY	THR	PRO	GLY	GLY	GLY	THR	PRO	GLY	THR	PRO	GLY	VAL	GLU	ALA	GLM	PRO	LEU	ALA	VAL	ARG	ALA	GLU	ASN	GLU	LYS	THR	GLU	LYS	ASN							
Q1220	E1221	G1222	F1223	E1224	T1228	N1229	F1238	S1239	K1240	P1243	H1252	P1253	H1254	Y1255	R1259	C1269	H1274	L1287	L1293	P1294	V1295	Q1296	F1297	HIS	GLN	HIS	PHE	ARG	CYS	THR	ALA	GLY	VAL	GLU	ALA	THR	PRO	LEU	ALA	PRO	GLY	ASN	GLU	LEU	GLN	PRO	GLY	ASP	GLU	ALA	ARG
E1114	L1115	V1123	G1126	H1127	H1128	F1139	G1140	R1141	P1142	W1143	Q1144	D1147	V1148	C1151	M1152	T1153	D1154	L1155	N1158	T1161	N1165	D1172	E1176	T1177	R1180	E1183	F1188	L1189	P1190	G1195	Q1198	G1205	Q1206	D1207	V1208	R1212	A1215	G1218	L1219												
ASN	PRO	R1020	Y1024	L1027	D1028	D1037	Q1041	R1044	T1045	L1046	L1047	G1048	I1053	E1054	PRO	PRO	T1153	D1154	L1155	N1158	T1161	N1165	D1172	E1176	T1177	R1180	E1183	F1188	L1189	P1190	G1195	Q1198	G1205	Q1206	D1207	V1208	R1212	A1215	G1218	L1219											
R897	D898	D899	H900	K901	R902	L903	H904	P914	E915	P916	E917	R918	S925	L929	H938	V939	A942	D943	K951	K952	T953	K954	L955	P956	K957	T958	Y959	H960	H961	S962	G964	Y965	K966	L972	L977	T978	P979	A980	V1001	L1009	VAL	GLN	ASP	ILE	PRO	ALA	ARG				





K2316	P2139	G2043	LYS	E1805	D1658	ASN	Q1459	ARG	GLU	F1223	E1114	PRO	D899	GLU	D899	
G2317	Y2142	I2044	GLU	R1808	L1659	ILE	H1460	GLY	PRO	E1224	L1115	R1020	D899	TTR		
Y2318	Y2149	G2048	ASP	D1809	Q1660	P1573	M1463	PHE	ASP	I1228	V1123	Y1024	D899	ARG		
W2323	W2152	GLU	GLU	K1810	H1663	L1575	V1469	PHE	ASP	N1229	G1126	L1027	D901	GLU		
W2324	T2182	GLU	GLU	M1814	T1666	S1576	T1473	ALA	TVR	F1238	H1127	D1028	D902	PRO		
P2325	L2155	GLU	GLU	A1826	R1671	A1577	GLY	LYS	ASN	S1239	R1128	D1037	L903	ARG		
Y2331	R2163	GLU	LYS	P1829	A1675	A1578	G1481	LYS	LEU	K1240	F1139	Q1041	P914	GLY		
L2332	S2164	GLU	GLU	P1832	L1676	F1580	N1482	ALA	ARG	S1241	G1140	Q1041	E915	HIS		
F2340	L2167	THR	ALA	G1832	G1677	R1584	V1483	MET	SER	P1243	P1141	R1044	P916	LEU		
I2359	W2168	SER	GLU	S1833	R1680	C1591	K1488	THR	GLY	H1282	W1143	T1045	E917	VAL		
L2368	E2174	GLU	LYS	W1834	H1683	R1594	C1492	GLN	GLY	P1253	Q1144	L1046	R918	GLY		
L2376	E2175	GLU	GLU	F1836	G1677	F1580	V1484	PRO	TRP	H1254	Q1144	L1047	S925	PRO		
A2383	S2181	ARG	ALA	W1837	E1699	L1600	V1495	ALA	GLY	Y1255	D1147	G1048	S925	ARG		
L2386	L2182	GLU	GLU	F1838	H1694	M1601	V1496	THR	ALA	R1269	C1151	T1063	L929	CYS		
P2395	P1840	THR	LYS	W1839	R1708	P1602	W1497	PRO	GLU	C1269	M1152	E1064	H938	LEU		
GLY	L1842	VAL	GLU	L1849	R1708	W1605	V1496	PRO	GLU	H1274	D1154	PRO	H939	SER		
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ARG	K1860	LEU	ASP	K1860	L1715	R1607	S1502	ASP	LYS	G1296	F1156	PRO	D943	ASP		
ARG	Q1861	VAL	LYS	I1862	L1716	R1607	S1502	VAL	GLY	F1297	T1155	GLN	A942	PHE		
ARG	I1863	LYS	LYS	L1863	S1717	M1608	P1503	VAL	GLY	HIS	T1156	PRO	D943	VAL		
GLU	K1864	LYS	LYS	L1864	W1717	M1608	P1503	ALA	THR	L1293	I1161	SER	K951	PRO		
GLU	M1865	GLU	GLU	M1865	M1730	R1607	S1502	GLY	GLY	P1294	M1152	GLN	K951	CYS		
LYS	E1867	LYS	LYS	E1867	M1730	R1607	S1502	GLY	GLY	V1295	T1153	VAL	K952	PRO		
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PRO	GLU	GLU	GLU	Q1629	E1535	W1626	G1532	ILE	GLY	THR	V1072	ASP	K957	GLN		
ALA	GLU	ALA	ALA	E1535	M1537	W1626	G1532	ILE	VAL	ALA	K1079	ALA	K960	CYS		
GLU	GLU	GLU	GLU	M1537	T1538	W1626	G1532	LEU	GLU	THR	N961	ALA	K960	PRO		
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GLU	GLU	GLU	GLU	E1643	F1564	W1626	G1532	W1449	THR	GLU	L1219	E1108	A1009	GLN		
GLU	GLU	GLU	GLU	E1643	F1564	W1626	G1532	W1449	THR	GLU	Q1220	E1108	A1009	GLN		
GLU	GLU	GLU	GLU	E1643	F1564	W1626	G1532	W1449	THR	GLU	L1219	E1108	A1009	GLN		
GLU	GLU	GLU	GLU	E1643	F1564	W1626	G1532	W1449	THR	GLU	Q1220	E1108	A1009	GLN		
GLU	GLU	GLU	GLU	E1643	F1564	W1626	G1532	W1449	THR	GLU	L1219	E1108	A1009	GLN		
GLU	GLU	GLU	GLU	E1643	F1564	W1626	G1532	W1449	THR	GLU	Q1220	E1108	A1009	GLN		
GLU	GLU	GLU	GLU	E1643	F1564	W1626	G1532	W1449	THR	GLU	L1219	E1108	A1009	GLN		
GLU	GLU	GLU	GLU	E1643	F1564	W1626	G1532	W1449	THR	GLU	Q1220	E1108	A1009	GLN		
GLU	GLU	GLU	GLU	E1643	F1564	W1626	G1532	W1449	THR	GLU	L1219	E1108	A1009	GLN		
GLU	GLU	GLU	GLU	E1643	F1564	W1626	G1532	W1449	THR	GLU	Q1220	E1108	A1009	GLN		
GLU	GLU	GLU	GLU	E1643	F1564	W1626	G1532	W1449	THR	GLU	L1219	E1108	A1009	GLN		
GLU	GLU	GLU	GLU	E1643	F1564	W1626	G1532	W1449	THR	GLU	Q1220	E1108	A1009	GLN		
GLU	GLU	GLU	GLU	E1643	F1564	W1626	G1532	W1449	THR	GLU	L1219	E1108	A1009	GLN		
GLU																







C4958	H4812	L4646	L4577	GLU	VAL	ALA	R4192
F4969	L4813		L4578	PRO	THR	ALA	F4193
I4960	L4814	V4666	F4579	GLU	VAL	ALA	Y4194
	D4815	P4667	Y4580	PRO	THR	ARG	
F4968	I4816	L4668	K4581	VAL	GLU	ALA	F4219
	A4817	V4669		PRO	LEU	LEU	
F4975	M4818		F4687	VAL	LEU	ARG	E4227
H4978	G4819	K4672	GLY	LYS	ALA	GLY	A4228
	V4520		GLU	ALA	ALA	LEU	E4229
H4983	T4825	A4678	GLU	ASP	GLY	TYR	D4240
N4984	R4679	R4679	ASP	GLU	PRO	ARG	
L4985	S4828	K4680	MET	GLU	PRO	ARG	T4247
		L4681	GLY	ASN	PRO	LEU	
Y4988	H4832	E4682	GLY	GLY	THR	ARG	E4253
		F4683	SER	GLU	SER	ARG	PRO
L4992	L4837	D4684	ALA	LYS	ASP	ARG	
M4993		G4685	ALA	GLU	GLY	ARG	GLY
Y4994	L4850	Y4687	GLY	VAL	VAL	GLY	GLU
L4995		I4688	ASP	PRO	HIS	PRO	GLU
I4996	Y4863	T4689	LEU	GLY	GLY	PRO	PRO
	D4878	E4690	ALA	GLY	GLN	ALA	ALA
D4999	M4879	Q4691	ALA	PRO	ASP	ASP	ASP
		P4692	GLY	PRO	MET	ALA	GLU
Y5009			SER	GLY	GLY	T4323	ASP
V5010	Y4888	D4696	GLY	PRO	ASP		GLU
W5011		V4697	GLY	THR	THR	V4339	GLY
	R4892	K4698	GLY	PRO	THR	A4340	MET
C5027		G4699	SER	LYS	GLY	R4341	GLY
F5028	G4895		TRP	ALA	ALA	A4342	GLU
R5029	G4896	D4702	GLY	PRO	ASP	G4343	ALA
	I4897		GLY	PRO	GLY	A4344	ALA
		P4712	SER	SER	PRO	A4345	ALA
	E4900		GLY	PRO	ALA		GLY
	E4901	Y4715	ALA	PRO	GLY	ALA	GLY
E4902	D4903		GLY	ALA	GLY	ALA	ALA
P4904	P4904	K4718	GLU	LYS	GLY	ALA	GLU
A4905	A4905	F4719	GLU	LYS	SER	ALA	GLU
G4906	D4907	V4720	ALA	GLU	PRO	GLY	GLY
D4907		V4724	GLY	ALA	ILE	GLY	ALA
E4908	Y4909		ASP	GLY	LYS	ASP	ALA
E4910		G4763	GLY	ARG	GLU	LEU	GLY
L4911	E4910		ASP	LYS	ALA	LEU	GLU
Y4912		W4767	GLU	GLY	GLY	LEU	GLY
	I4918	L4790	MET	GLY	ASP	TRP	ALA
			F4540	ASP	GLY	ALA	ALA
	F4923	M4796	L4631	GLY	GLY	LEU	THR
		V4797	L4632	GLY	GLU	PHE	VAL
		M4798	E4633	GLY	VAL	GLY	ALA
L4928	L4928	S4799	S4634	GLU	GLY	GLY	ALA
L4929	A4930		T4636	GLU	GLY	GLY	GLY
A4930	I4931	G4802	C4637	VAL	HIS	LEU	ALA
I4932			Y4638	PRO	GLU	VAL	THR
Q4933		F4807	M4639	GLY	ALA	GLY	ALA
		F4808	E4640	PRO	GLY	GLY	ARG
		F4809	P4641	GLU	PRO	ALA	LEU
		A4810		PRO	GLY	LYS	ALA
		A4811		PRO	GLY	LYS	ALA

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	279704	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)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	3.162	Depositor
Minimum map value	-1.419	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.061	Depositor
Recommended contour level	0.182	Depositor
Map size (Å)	643.2, 643.2, 643.2	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.072, 1.072, 1.072	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: ZN, CA

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	0.32	0/30188	0.46	0/41084
1	B	0.32	0/30188	0.46	0/41084
1	C	0.32	0/30188	0.46	0/41084
1	D	0.32	0/30188	0.46	0/41084
All	All	0.32	0/120752	0.46	0/164336

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	29568	0	27784	634	0
1	B	29568	0	27784	641	0
1	C	29568	0	27784	643	0
1	D	29568	0	27784	647	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	118280	0	111136	2512	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 11.

The worst 5 of 2512 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:4634:GLU:HG3	1:B:4636:THR:HG22	1.46	0.97
1:C:4634:GLU:HG3	1:C:4636:THR:HG22	1.46	0.97
1:A:4634:GLU:HG3	1:A:4636:THR:HG22	1.46	0.94
1:D:4634:GLU:HG3	1:D:4636:THR:HG22	1.46	0.94
1:D:4069:LYS:HB2	1:D:4133:GLN:HE22	1.41	0.85

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	3934/5037 (78%)	3496 (89%)	423 (11%)	15 (0%)	30	61
1	B	3934/5037 (78%)	3496 (89%)	423 (11%)	15 (0%)	30	61
1	C	3934/5037 (78%)	3496 (89%)	423 (11%)	15 (0%)	30	61
1	D	3934/5037 (78%)	3496 (89%)	423 (11%)	15 (0%)	30	61
All	All	15736/20148 (78%)	13984 (89%)	1692 (11%)	60 (0%)	32	61

5 of 60 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4808	PHE
1	B	4808	PHE
1	C	4808	PHE
1	D	4808	PHE
1	A	1835	GLU

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	2905/4276 (68%)	2882 (99%)	23 (1%)	79	87
1	B	2905/4276 (68%)	2882 (99%)	23 (1%)	79	87
1	C	2905/4276 (68%)	2882 (99%)	23 (1%)	79	87
1	D	2905/4276 (68%)	2882 (99%)	23 (1%)	79	87
All	All	11620/17104 (68%)	11528 (99%)	92 (1%)	77	87

5 of 92 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	4633	GLU
1	D	392	ARG
1	C	4635	SER
1	C	4901	ILE
1	D	4120	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1041	GLN
1	C	3976	ASN
1	D	3976	ASN
1	C	1165	ASN
1	C	3146	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

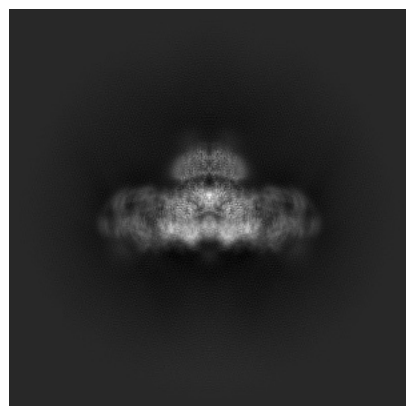
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38048. These allow visual inspection of the internal detail of the map and identification of artifacts.

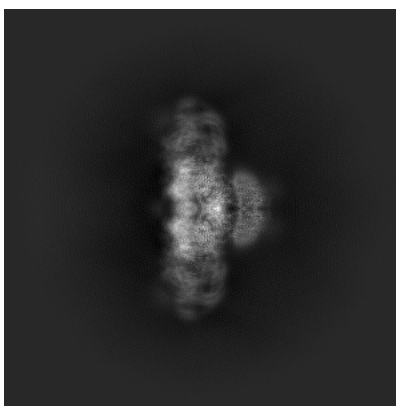
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

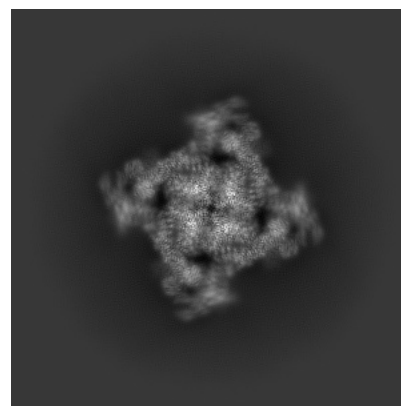
6.1.1 Primary map



X

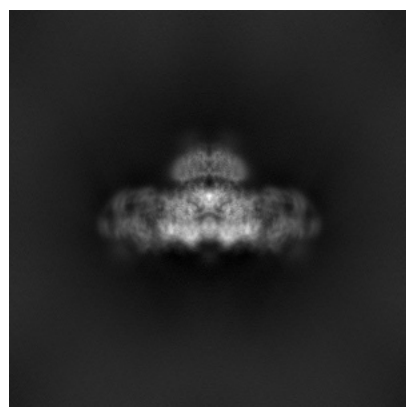


Y

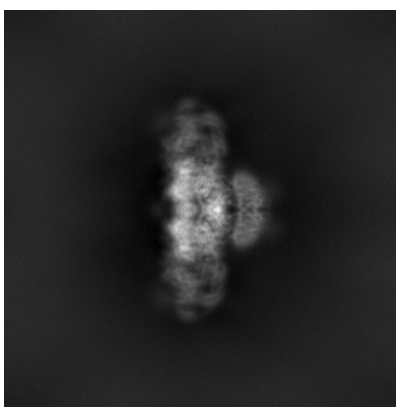


Z

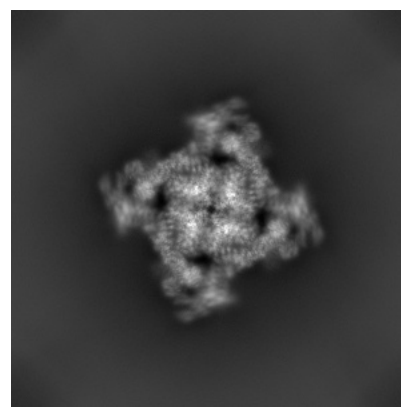
6.1.2 Raw map



X



Y

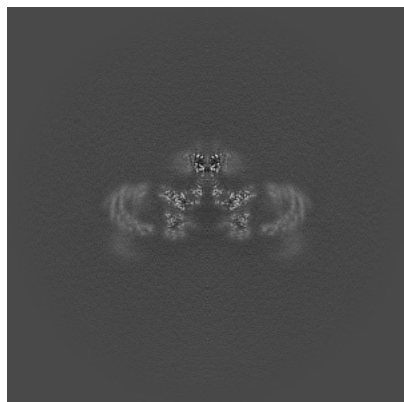


Z

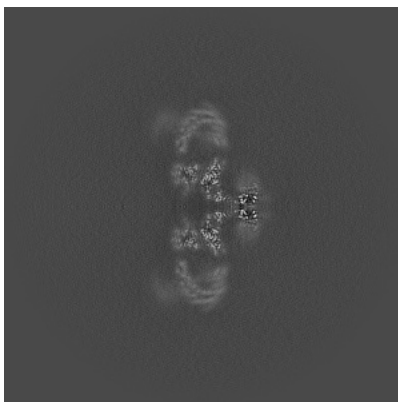
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

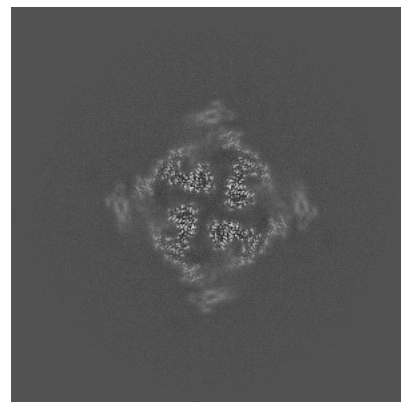
6.2.1 Primary map



X Index: 300

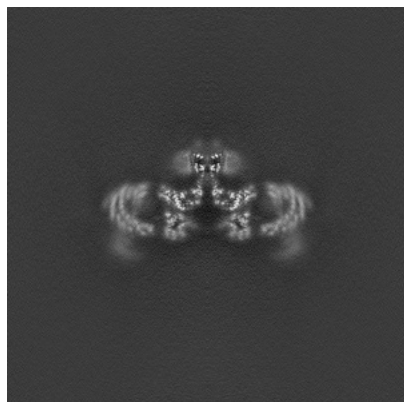


Y Index: 300

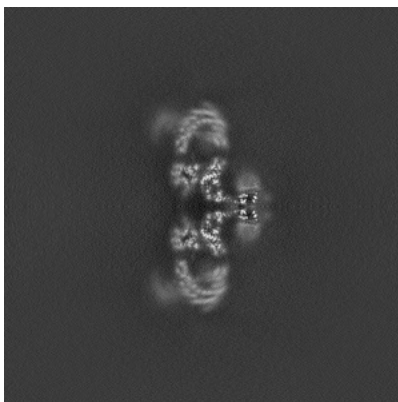


Z Index: 300

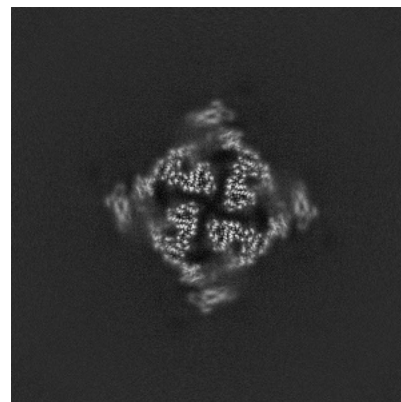
6.2.2 Raw map



X Index: 300



Y Index: 300

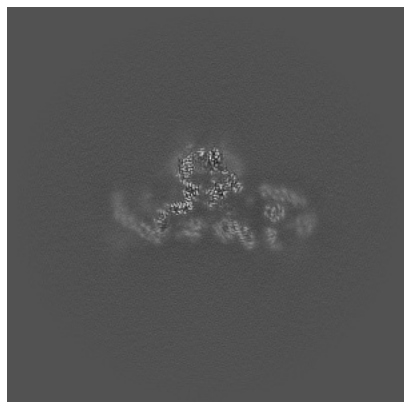


Z Index: 300

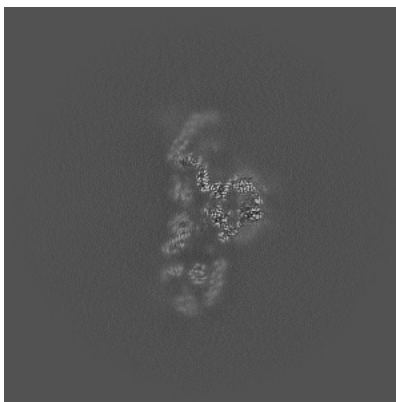
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

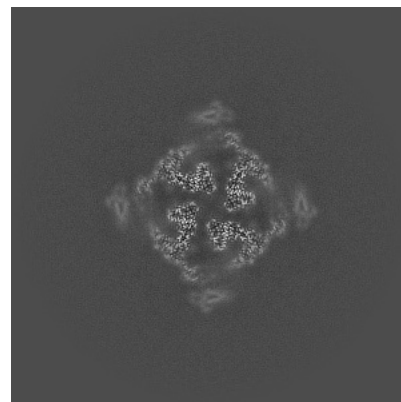
6.3.1 Primary map



X Index: 321

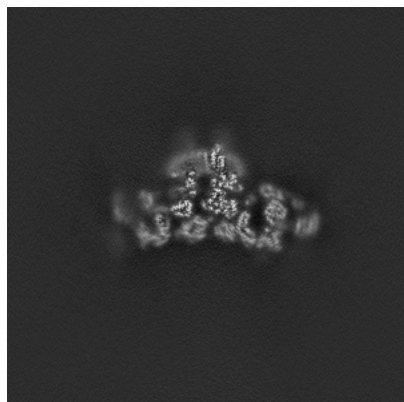


Y Index: 321

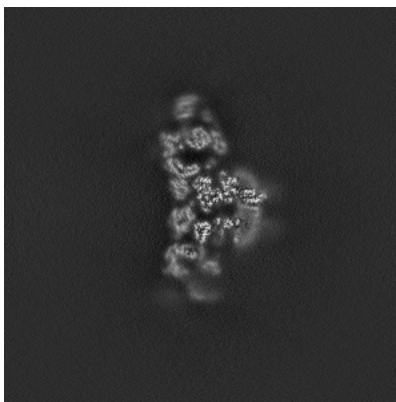


Z Index: 302

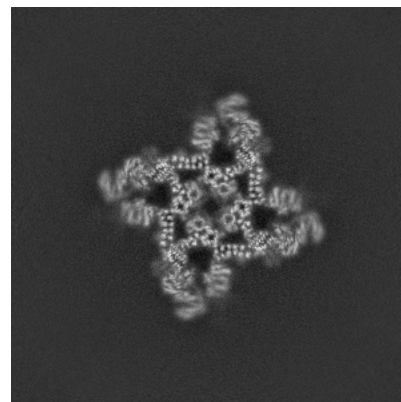
6.3.2 Raw map



X Index: 329



Y Index: 271

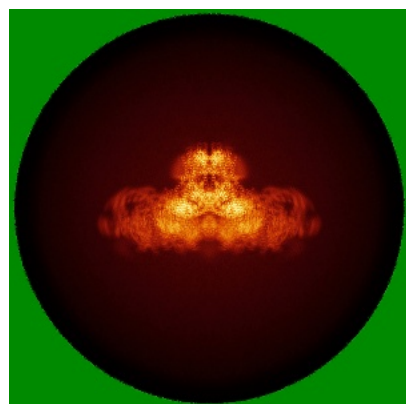


Z Index: 273

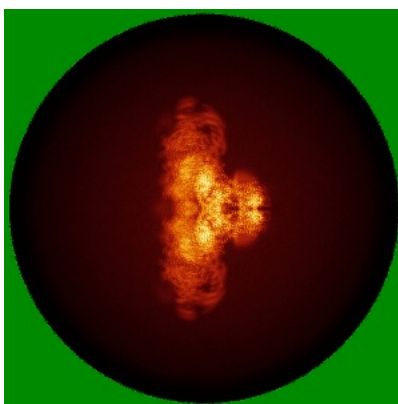
The images above show the largest variance slices of the map in three orthogonal directions.

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

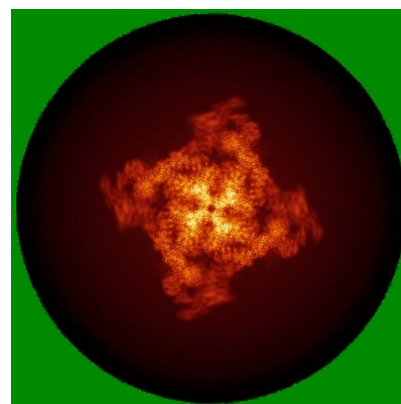
6.4.1 Primary map



X

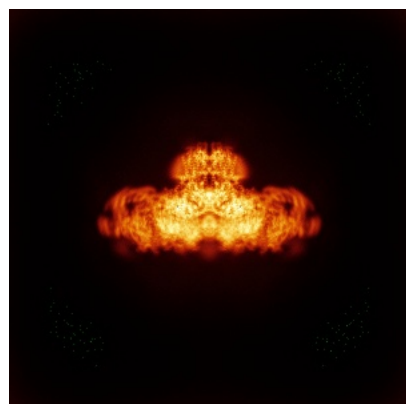


Y

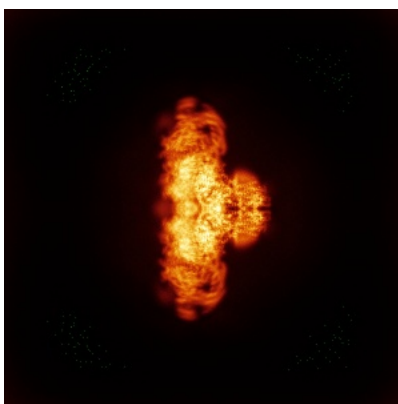


Z

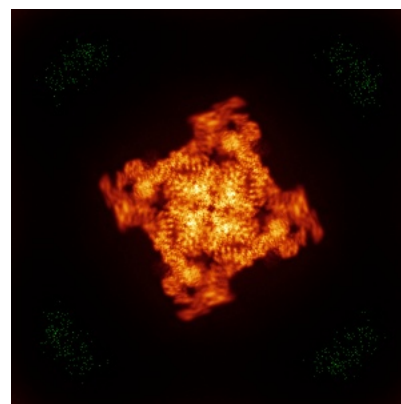
6.4.2 Raw map



X



Y

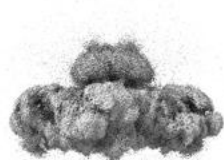


Z

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](#)

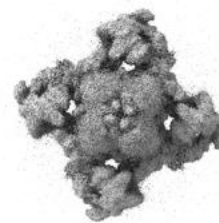
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.182. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

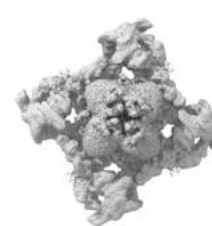
6.5.2 Raw map



X



Y



Z

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.

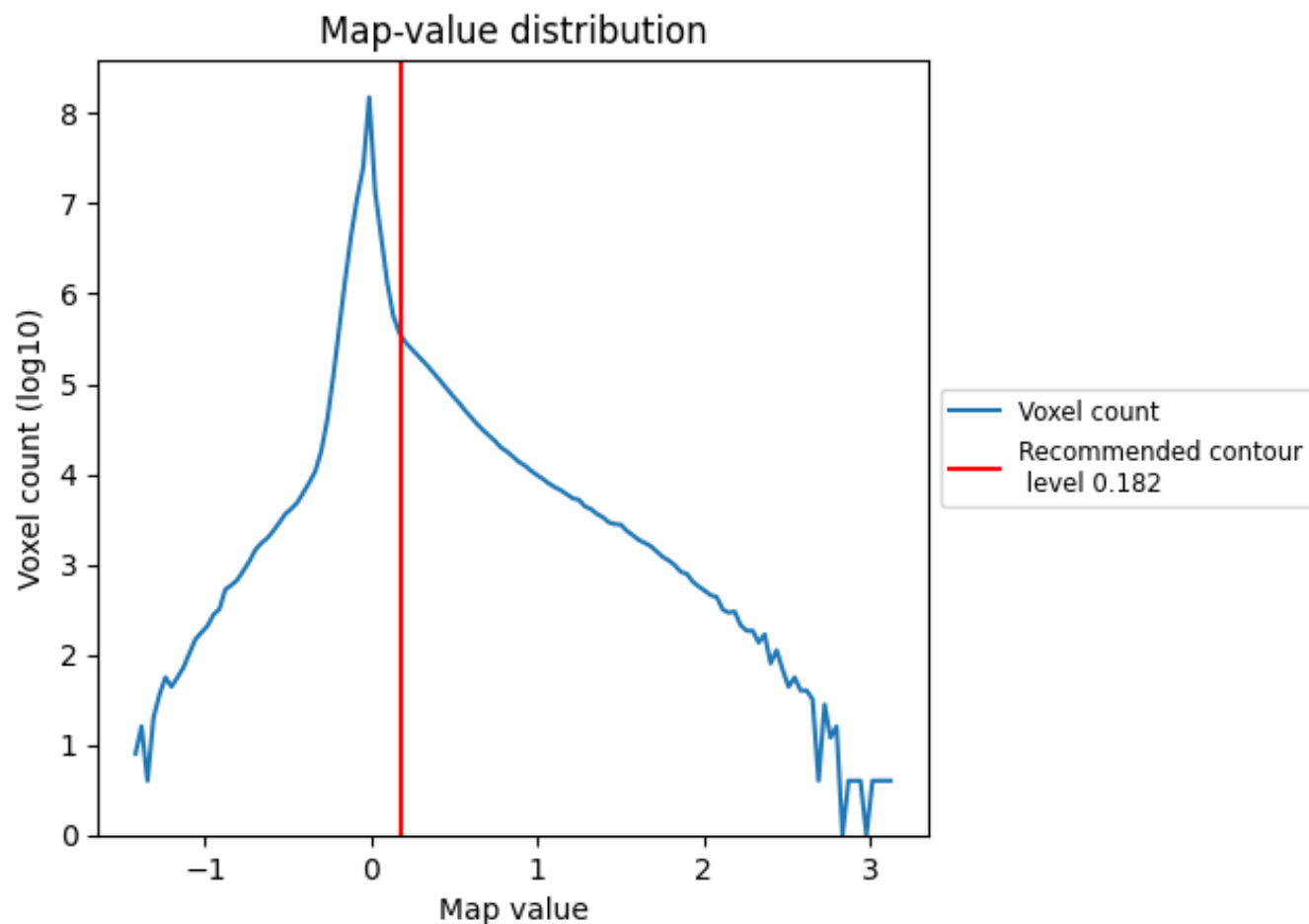
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

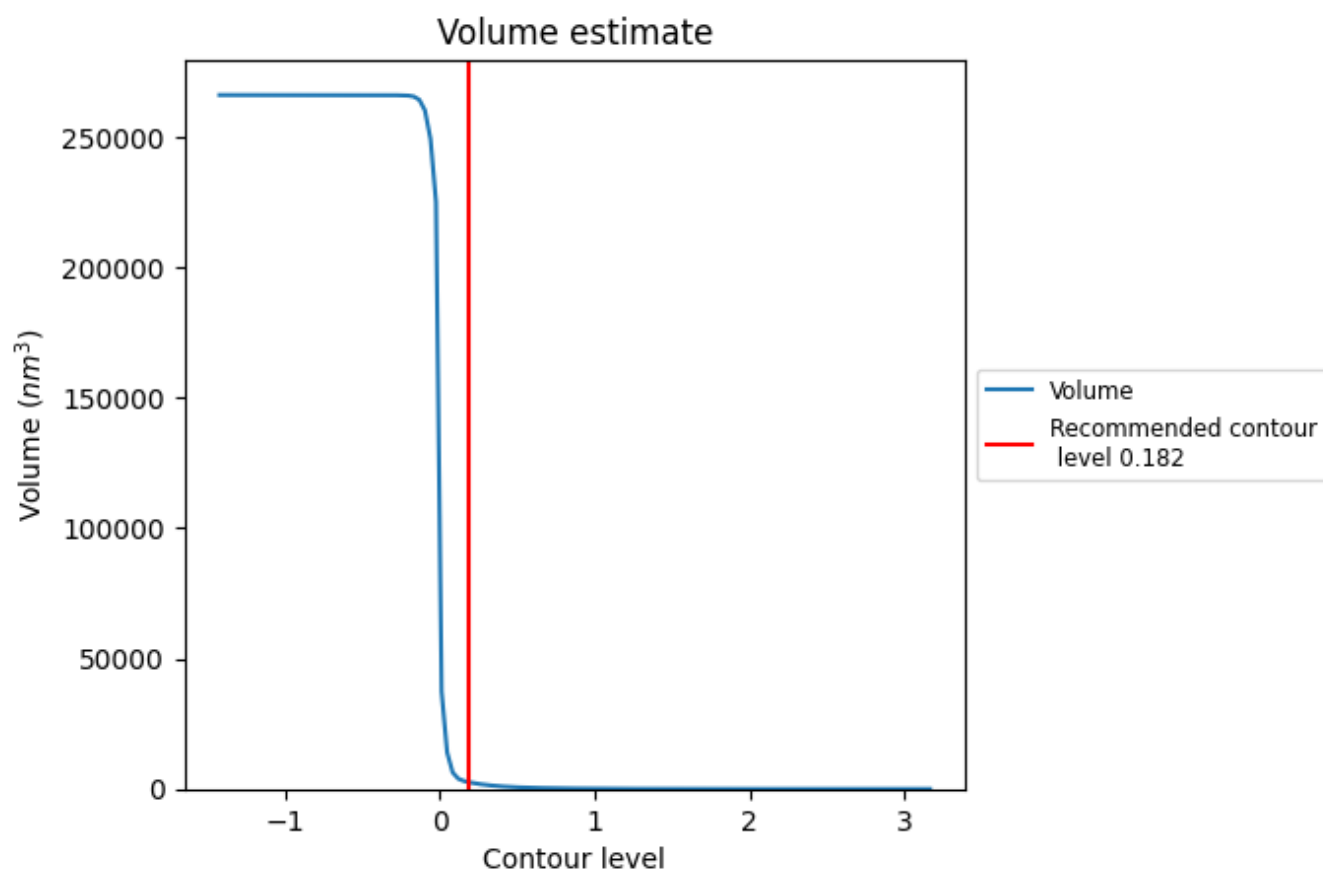
This section contains the results of statistical analysis of the map.

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.

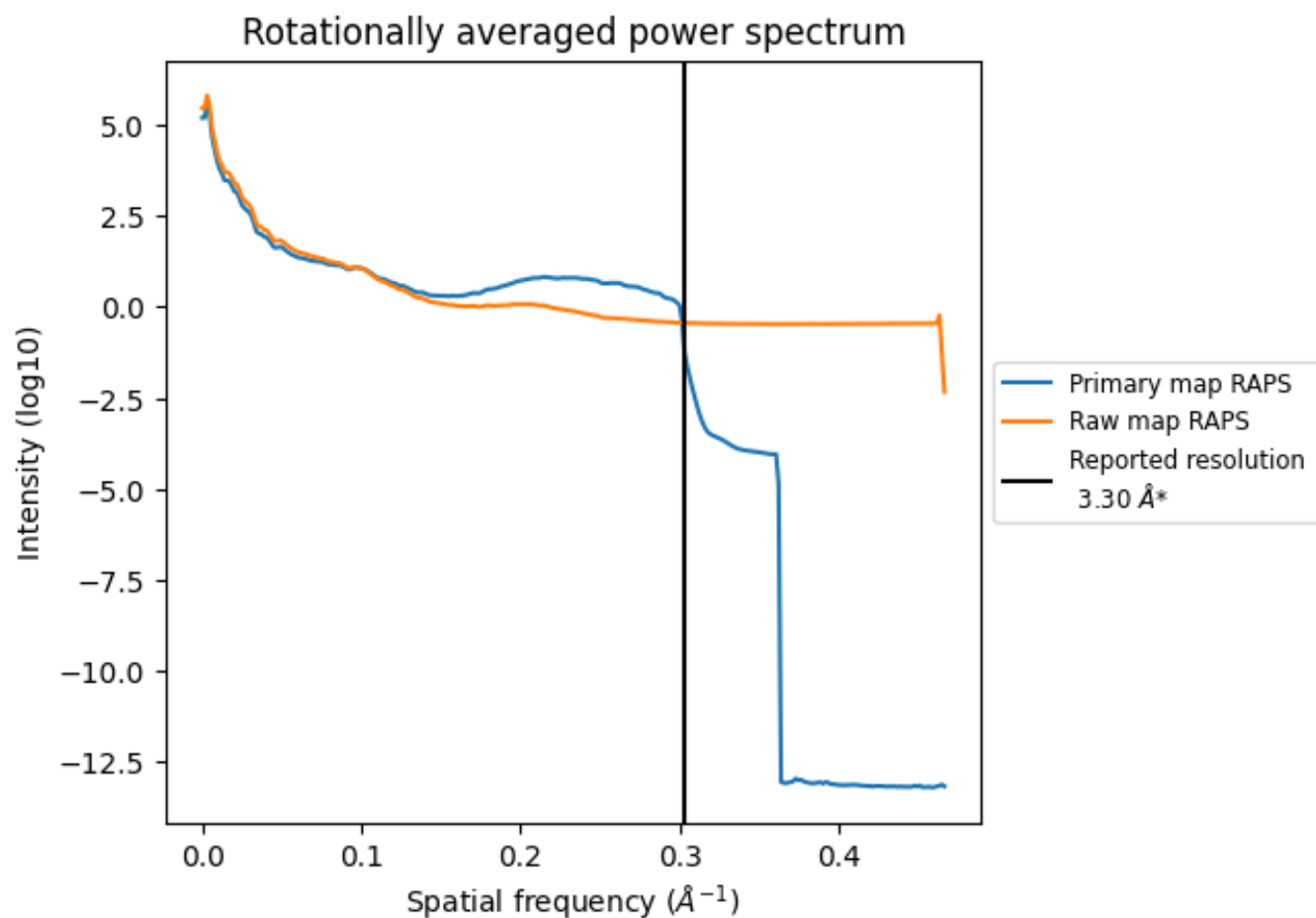
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2676 nm^3 ; this corresponds to an approximate mass of 2418 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 ⓘ

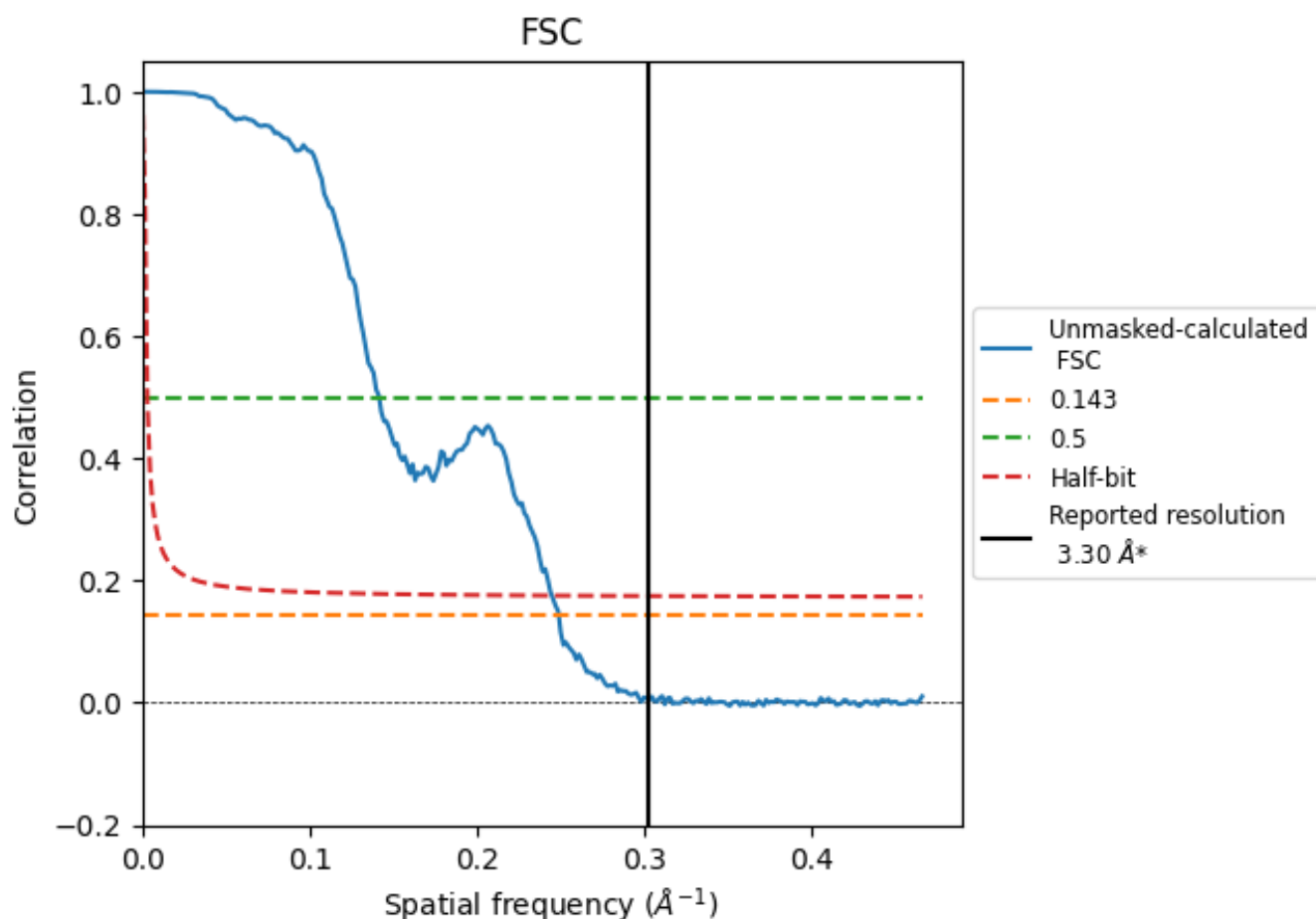


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

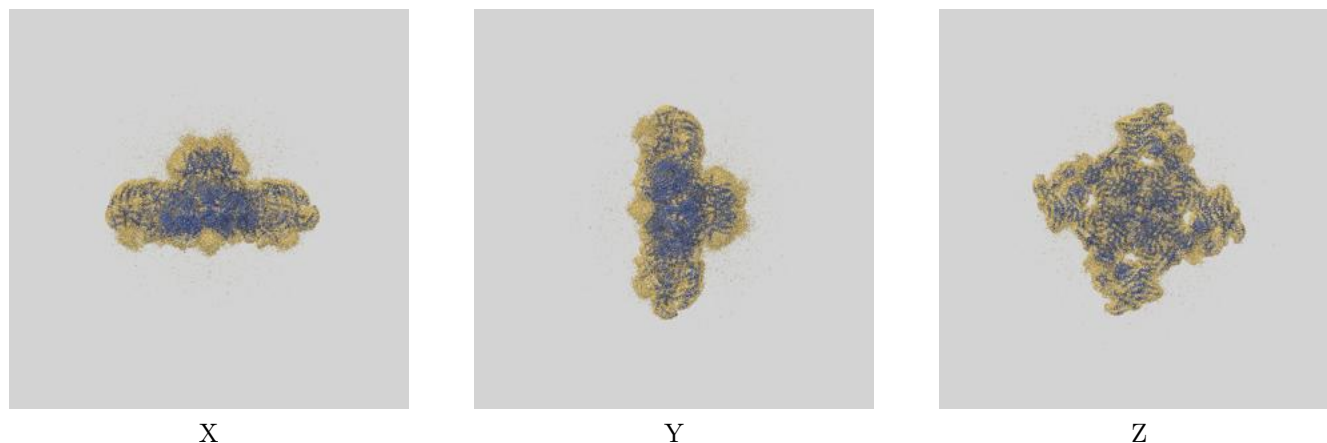
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.02	7.06	4.08

*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 4.02 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

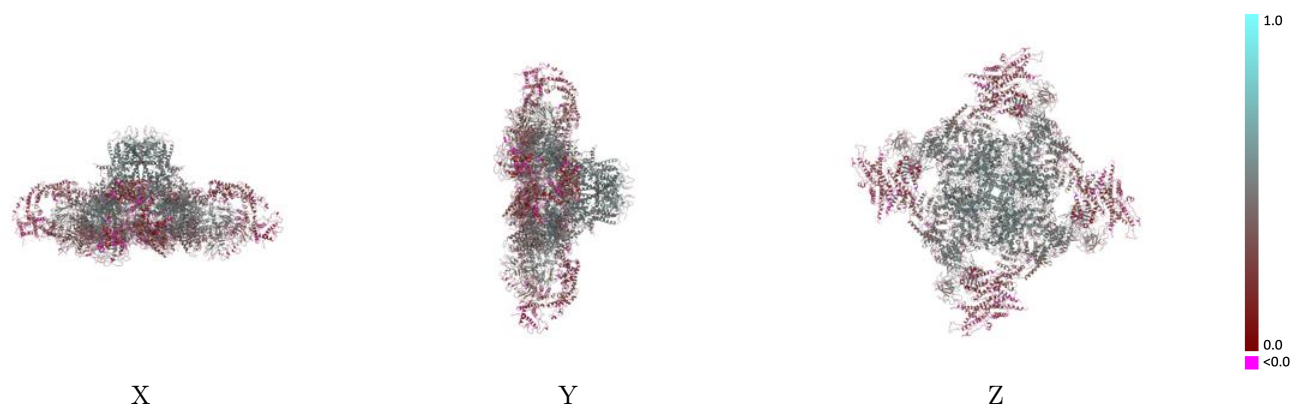
This section contains information regarding the fit between EMDB map EMD-38048 and PDB model 8X4E. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



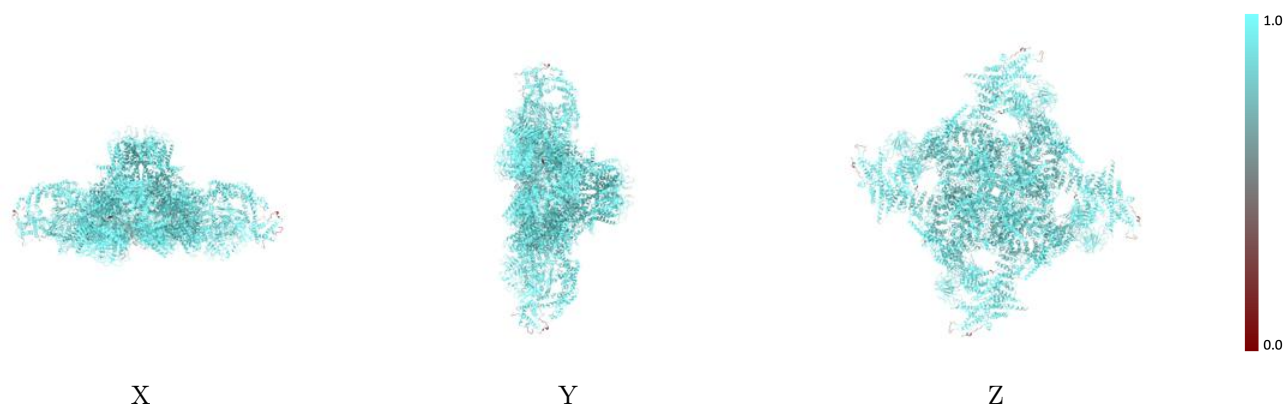
The images above show the 3D surface view of the map at the recommended contour level 0.182 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



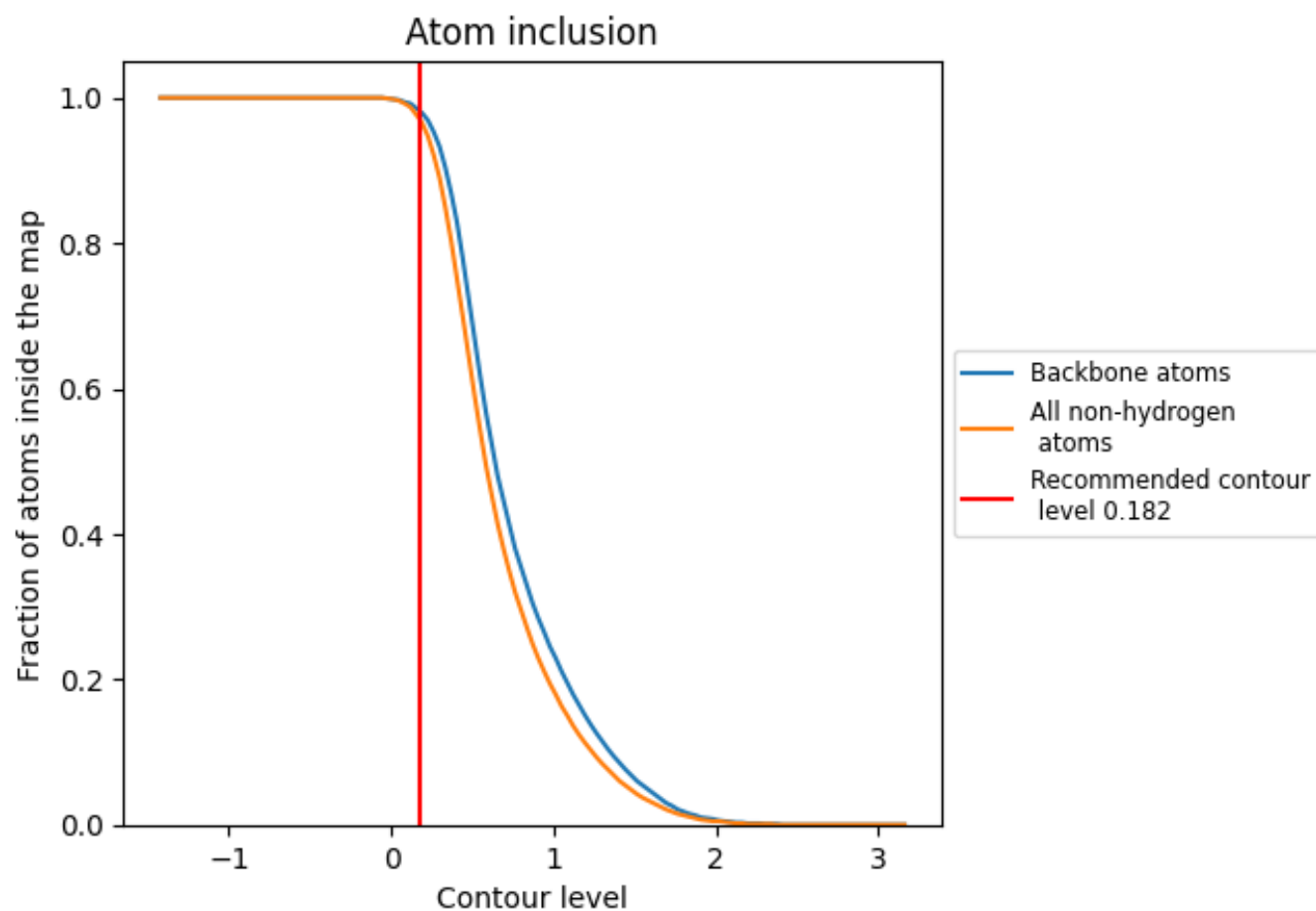
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.182).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 97% 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 (0.182) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9690	<div></div> 0.3850
A	<div></div> 0.9690	<div></div> 0.3840
B	<div></div> 0.9690	<div></div> 0.3850
C	<div></div> 0.9690	<div></div> 0.3850
D	<div></div> 0.9690	<div></div> 0.3850

