



wwPDB EM Validation Summary Report ⓘ

Mar 27, 2026 – 03:30 AM UTC

PDB ID : 8OTX / pdb_00008otx
EMDB ID : EMD-17186
Title : Cryo-EM structure of Strongylocentrotus purpuratus sperm-specific Na⁺/H⁺ exchanger SLC9C1 in nanodisc
Authors : Yeo, H.; Mehta, V.; Gulati, A.; Drew, D.
Deposited on : 2023-04-21
Resolution : 3.08 Å(reported)

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

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A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
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) : 2.49

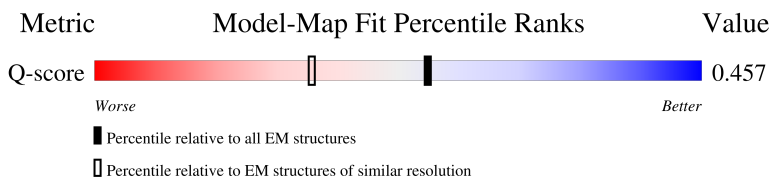
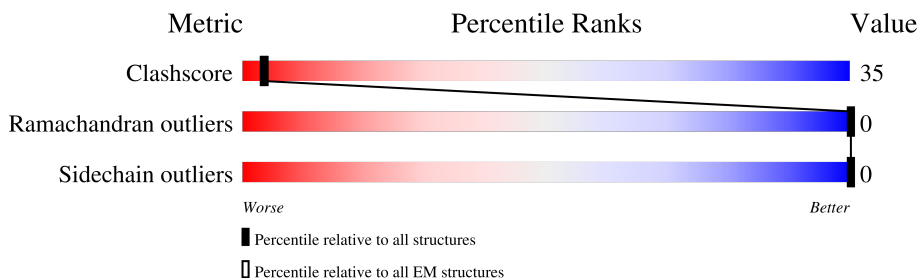
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.08 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	14000 (2.58 - 3.58)

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	1331	10% 44% 35% 21%
1	B	1331	10% 45% 34% 21%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16116 atoms, of which 150 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.

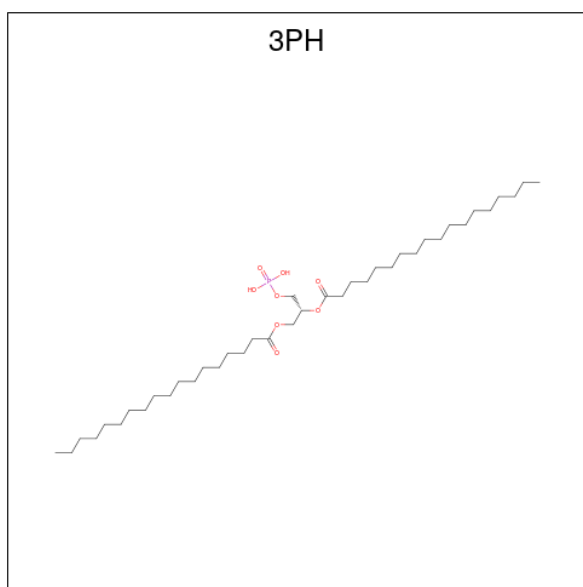
- Molecule 1 is a protein called Sperm-specific sodium proton exchanger.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	1054	Total	C	N	O	S	1	0
			7889	5097	1334	1421	37		
1	A	1054	Total	C	N	O	S	1	0
			7889	5097	1334	1421	37		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1326	GLU	-	expression tag	UNP A3RL54
B	1327	ASN	-	expression tag	UNP A3RL54
B	1328	LEU	-	expression tag	UNP A3RL54
B	1329	TYR	-	expression tag	UNP A3RL54
B	1330	PHE	-	expression tag	UNP A3RL54
B	1331	GLN	-	expression tag	UNP A3RL54
A	1326	GLU	-	expression tag	UNP A3RL54
A	1327	ASN	-	expression tag	UNP A3RL54
A	1328	LEU	-	expression tag	UNP A3RL54
A	1329	TYR	-	expression tag	UNP A3RL54
A	1330	PHE	-	expression tag	UNP A3RL54
A	1331	GLN	-	expression tag	UNP A3RL54

- Molecule 2 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	H	O	P	0
			123	39	75	8	1	
2	B	1	Total	C	O	P		0
			45	36	8	1		
2	A	1	Total	C	H	O	P	0
			123	39	75	8	1	
2	A	1	Total	C	O	P		0
			45	36	8	1		

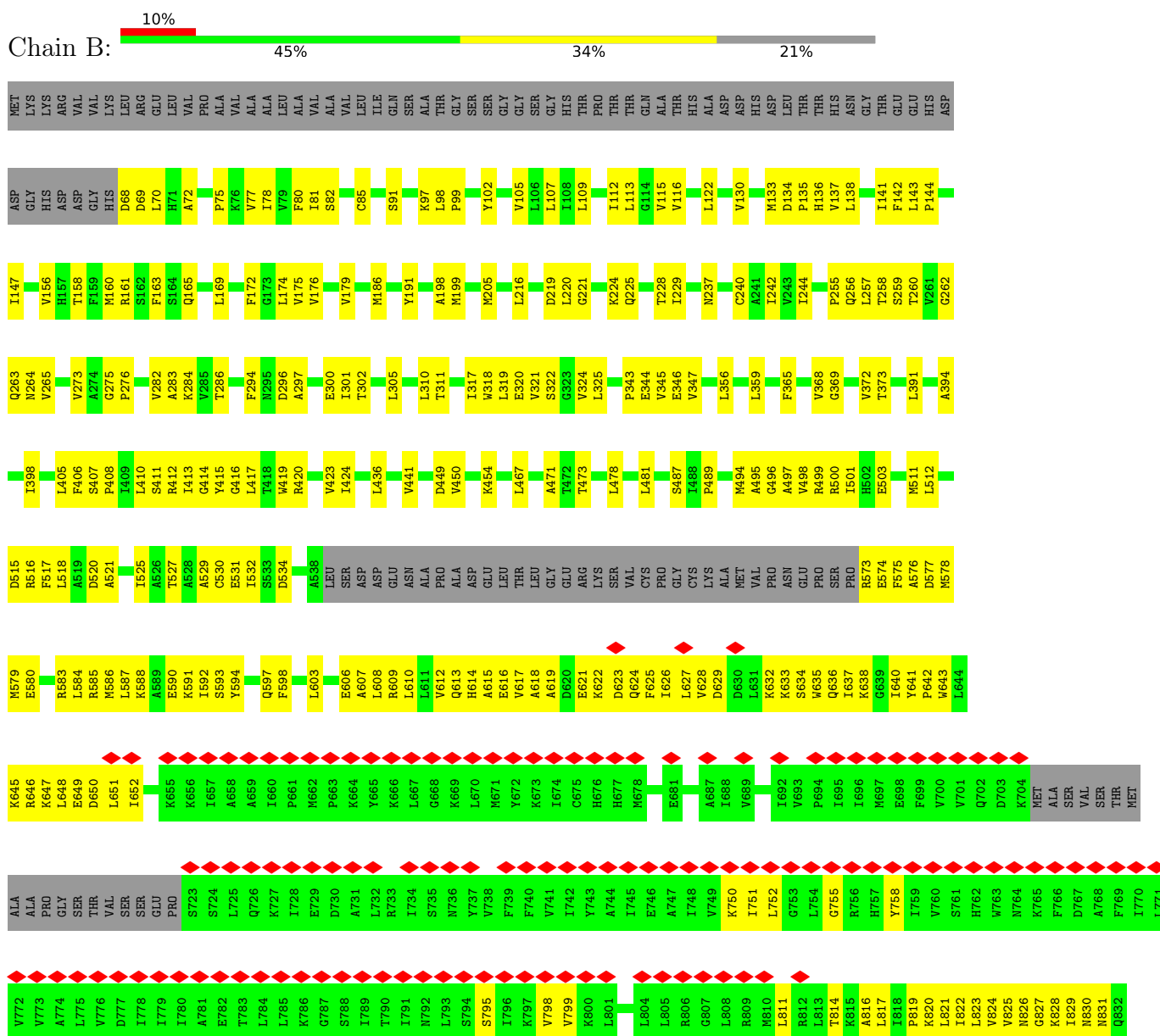
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		AltConf
3	B	1	Total	O	0
			1	1	
3	A	1	Total	O	0
			1	1	

3 Residue-property plots

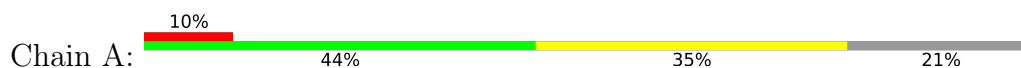
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Sperm-specific sodium proton exchanger



L833	L904	L980	L1048	K1116	V1188	LYS	GLN
S834	I905	H981	T1049	L1119	V1189	GLU	GLY
L836	L906	F982	K1050	L1122	ASN	GLU	GLU
Y837	I913	D983	K1051	E1127	ALA	THR	GLU
D838	H914	Y984	P1052	V1127	GLY	PRO	GLU
V839	E915	E985	R1053	D1128	TYR	ILE	THR
G840	L916	E986	V1057	L1129	ASN	PRO	GLU
K841	L922	T1058	T1059	A1130	GLY	ASN	GLU
I844	D923	Y989	T1061	E1131	THR	ASN	GLU
I845	D924	E991	T1062	S1132	ILE	THR	GLU
E849	M925	G992	V1063	F1133	LEU	ALA	GLU
V850	E926	D993	Q1064	Q1135	ASP	VAL	PRO
G851	K929	E994	Y1066	Q1136	GLY	GLN	ALA
K852	L930	D996	F1067	N1137	ARG	VAL	VAL
I853	E931	D997	I1068	I1138	ASP	ALA	VAL
I854	I932	L998	T1069	D1139	VAL	GLY	GLU
D855	T933	F999	A1070	A1140	SER	SER	ASN
R856	K937	I1000	I1071	T1141	PRO	PRO	LEU
M857	M938	I1001	D1072	E1142	ARG	VAL	TYR
V858	V1002	V1002	M1073	E1143	SER	VAL	PHE
D859	K939	N1074	N1074	D1144	PRO	PRO	GLN
N860	R940	I1075	I1075	Y1145	LEU	ILE	
K861	L941	A1076	A1076	I1146	SER	THR	
K862	Y1009	I1077	I1077	L1147	LYS	LYS	
I863	G1010	D1078	D1078	T1148	THR	THR	
L864	K1011	I1082	L1082	G1150	GLU	PRO	
R865	S1012	ALA	LYS	Y1153	LYS	LYS	
E866	PHE	PHE	Y1083	N1154	SER	PRO	
L867	LEU	LEU	P1084	A1155	ASN	LYS	
K868	ASP	ASP	S1085	A1156	MET	SER	
S871	HIS	HIS	L1086	R1158	CYS	LEU	
G874	ASN	ASN	R1089	E1159	LEU	PRO	
Q877	PRO	PRO	L1090	E1160	LYS	LEU	
V878	VAL	VAL	R1092	I1161	HIS	GLY	
V879	THR	THR	V1093	S1162	ALA	LEU	
K880	ALA	ALA	V1094	S1163	GLY	MET	
E881	GLY	GLY	A1095	L1166	LEU	SER	
L885	SER	SER	I1096	I1167	ARG	LYS	
Q886	GLU	GLU	R1097	S1168	GLY	GLU	
R887	ASN	ASN	I1098	T1170	ASN	ARG	
I892	E1030	E1030	P1101	V1171	LYS	ASN	
A893	E1033	E1033	M1104	H1172	VAL	VAL	
V894	D1034	D1034	E1105	K1173	GLY	GLY	
S895	Y1035	Y1035	Q1106	L1174	ALA	ALA	
V896	L1036	L1036	M1107	T1175	VAL	VAL	
K897	T1037	T1037	A1108	F1176	GLU	GLU	
T898	V1038	V1038	F1109	Q1177	LYS	GLY	
Q900	V1041	V1041	Q1110	P1178	SER	SER	
A901	I1042	I1042	G1111	P1184	PRO	VAL	
R903	I1043	I1043	T1112	R1185	GLY	GLU	
			T1113	L1186	ALA	GLU	
			Q1114	F1187	THR	THR	
			E1115		LYS	LYS	

• Molecule 1: Sperm-specific sodium proton exchanger



MET	ASP	I147	S259	L391	E503	R573
LYS	GLY	V156	T260	A394	M511	E574
LYS	HIS	V157	V261	L392	L512	F575
ARG	ASP	T158	Q262	L393	D515	A576
VAL	ASP	T159	N263	L405	R516	D577
VAL	GLY	F159	Q264	P406	F517	M578
LYS	HIS	M160	V265	S407	L518	E580
ILE	THR	R161	V273	P408	A519	R583
PRO	VAL	F162	A274	I409	D520	L584
ASN	LEU	S164	G275	L410	A521	R585
ASN	VAL	Q165	P276	S411	I525	M586
GLN	ALA	L169	V282	R412	A526	L587
VAL	VAL	F172	A283	I413	T527	K588
ALA	ALA	I778	K284	G414	A528	E589
LEU	LEU	V779	V285	Y415	A529	K590
ALA	ALA	F80	T286	G416	C530	I592
VAL	VAL	L174		L417	E531	S593
VAL	VAL	V176	F294	T418	L532	Y594
ALA	VAL	V179	N295	W419	S533	W595
LEU	VAL	D296	D296	R420	D534	K596
ILE	ILE	C85	A297	V423	P535	Q597
THR	GLN	S91	E300	I424	A538	F598
LYS	SER	M186	E301	M425	LEU	E599
THR	ALA	R187	T302	L436	SER	L603
THR	THR	F189	L305	V441	ASP	E606
GLY	GLY	N190	L310	D449	GLU	A607
LYS	SER	Y191	T311	V450	ASN	L608
PRO	GLY	Y102	W318	K454	ALA	R609
LYS	THR	V105	L319	L467	ASP	L610
SER	THR	L106	E320	A471	GLU	L611
LEU	THR	L107	V321	T472	LEU	V612
PRO	PRO	L108	S322	T473	THR	Q613
LYS	GLY	L109	G323	L478	LEU	H614
HIS	THR	L216	V324	L481	GLY	A615
PRO	THR	D219	L325	S487	GLY	E616
THR	THR	L220	ALA	I488	GLU	V617
THR	GLN	G221	V115	P489	ARG	A618
ALA	ALA	K224	V116	M494	LYS	A619
GLY	THR	Q225	L122	A495	SER	D620
THR	HIS	T228	V130	E344	VAL	E621
ASP	ASP	I229	A131	V345	VAL	K622
ASP	HIS	N237	H132	E346	PRO	D623
LEU	LEU	C240	M133	V347	GLY	Q624
THR	THR	I242	D134	L359	CYS	F625
THR	THR	I244	P135	A241	LYS	L626
VAL	VAL	P255	H136	G496	ALA	L627
ASN	ASN	Q256	V243	A497	MET	V628
GLY	GLY	T258	L138	V498	VAL	D629
THR	THR		I141	R499	PRO	D630
GLU	GLU		F142	R500	ASN	L631
GLU	GLU		L143	I501	GLU	K632
HIS	HIS		P144	S502	PRO	K633
ASP	ASP			T373	SER	S634
					PRO	W635
						Q636

GLY	VAL	K1173	M104	E1033	K968	V894	V824	H762	Q702	I637
GLU	MET	L1174	E105	D1034	L969	S895	V825	V763	D703	K638
ALA	LEU	T1175	Q1106	Y1035	S896	K897	N826	N764	K704	G839
VAL	SER	F1176	M107	L1036	D971	K897	G827	K765	MET	I640
GLU	ARG	Q1177	A1108	T1037	F972	T898	K828	F766	ALA	Y641
GLU	LYS	Y1178	F1109	V1038	K974	R899	I829	D767	SER	W643
SER	SER		Q1110			Q900	N830		VAL	L644
PRO	SER	E1183	G1111	V1041	A975	A901	N831		SER	K645
VAL	GLY	P1184	G1112	I1042	A976	I902	Q832	A768	THR	R646
LYS	ALA	R1185	T1113	G1043	A977	R903	L833	F769	MET	K647
THR	ALA	L1186	Q1114			T904	S834	I770	ALA	L648
LYS	ALA	F1187		L1048	L980	I905	L835	I771	ALA	E649
GLN	LYS	V1188	L1119	T1049	R981	L906	G836	V772	PRO	D850
GLY	GLU	V1189		K1050	F982		Y837	I773	GLY	L651
GLU	GLU			P1051	D983	I913	V838	A774	SER	I652
THR	ASP	ASN	E1122	R1053	G985	E915	G840	L775	VAL	S953
PRO	CYS	ALA	V1127	T1056	E986	L916	K941	V776	SER	E654
GLU	ILE	TYR	D1128	V1057	V987			D777	SER	K655
THR	PRO	ASN	L1129	T1058	I988	L921	I844	I778	GLU	K656
GLU	ASN	GLY	A1130		V989	L922	I845	I779	PRO	I657
GLY	THR	ILE	S1132	T1061	R990	E924	E849	I780		A658
ALA	ASP	LEU	H1133	T1062	E991	M925	V850	I781		A659
VAL	ASP	ASP	F1134	V1063	G992	E926	G851	I782		I660
GLU	VAL	GLY	Q1135	Q1064	D993		K852	I783		P661
ARG	GLN	GLY	F1136	V1065	E994	K929	I853	I784		M662
VAL	ALA	LEU	M1137	Y1066	S995	L830	I854	I785		P663
ASN	ALA	ASP	T1138	F1067	D996	L932	D855	E729		Y665
VAL	GLY	VAL	D1139	I1068	G997	L933	R856	D730		K666
ASN	VAL	ASP	A1140	T1069	F999	T933	M857	I734		G667
GLU	SER	SER	T1141	A1070	L1000		V858	I735		K669
LEU	PRO	LYS	E1143	E1071	I1001	K937	D859	S736		L670
TYR	SER	ARG	D1144	D1072	V1002	M938	N860	N737		M671
PHE	SER	SER	L1145	M1073		K939	K861	I738		Y672
GLN	THR	ILE	T1146	N1074	L1005	R940	I862	I739		K673
	PRO	GLU	L1147	I1075		L941	L864	F740		I674
LYS	PRO	LYS	A1076		Y1009	A944	E865	I741		C675
THR	THR	THR	I1077	D1078	G1010	P945	E866	I742		H676
LYS	PRO	GLU	L1082		S1012		L867	A743		H677
PRO	PRO	LYS	Y1083	Y1082	ALA	I948	K968	A744		M678
LYS	LYS	SER	P1084	P1083	PHE	P949		I745		E681
SER	SER	SER	S1085	S1084	LEU	P950	S871	A746		M685
ASN	ASN	ASN	L1086	L1086	ASP	P951	G874	A747		I686
PHE	MET	LYS			HIS	P952	R876	I748		A687
LEU	LEU	CYS	R1089	R1089	ASN	E954	Q877	V749		I688
PRO	PRO	LEU	V1091	V1090	PRO	N955	V878	K750		V689
SER	LYS	LYS	A1092	A1091	PRO	L956	V879	I751		L690
ILE	HIS	HIS	R1093	R1092	VAL	K957	K880	L752		M691
GLY	ALA	ALA	V1094	V1093	THR	N959	E881	G753		N691
LEU	GLU	GLY	A1095	A1094	ALA	V960		L754		I692
SER	GLU	LEU	I1096	I1095	GLY	P961	L885	G755		V693
MET	SER	LEU	T1097	T1096	SER	S961	Q886	H756		P694
LYS	GLN	ARG	R1097	R1096	GLU	W862	R887	I757		E598
GLY	LYS	LYS	I1098	I1097	GLU	L863		Y758		F699
ARG	ASN	ASN	T1101	T1100	ASN	A964	I892	I759		V700
VAL	SER	LYS			E1030	M967	A893	V760		V701
ASN			H1172					L821		
								L822		
								L823		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1737146	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 ($e^-/\text{\AA}^2$)	58.45	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.655	Depositor
Minimum map value	-0.333	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.11	Depositor
Map size (Å)	365.47998, 365.47998, 365.47998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9136999, 0.9136999, 0.9136999	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: 3PH

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	0.14	0/8033	0.29	2/10927 (0.0%)
1	B	0.10	0/8033	0.24	0/10927
All	All	0.12	0/16066	0.27	2/21854 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1184	PRO	CA-N-CD	-14.79	91.29	112.00
1	A	1184	PRO	N-CD-CG	-6.65	93.22	103.20

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	7889	0	7744	584	0
1	B	7889	0	7744	590	0
2	A	93	75	141	11	0
2	B	93	75	141	9	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	15966	150	15770	1117	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 35.

The worst 5 of 1117 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:A:1184:PRO:HD2	1:A:1184:PRO:O	1.54	1.06
1:B:1138:ILE:HA	1:B:1142:LEU:HD21	1.37	1.06
1:A:1142:LEU:HA	1:A:1190:ARG:HA	1.38	1.05
1:A:1138:ILE:HA	1:A:1142:LEU:HD21	1.39	1.03
1:B:1142:LEU:HA	1:B:1190:ARG:HA	1.37	1.02

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	1047/1331 (79%)	982 (94%)	65 (6%)	0	100	100
1	B	1047/1331 (79%)	985 (94%)	62 (6%)	0	100	100
All	All	2094/2662 (79%)	1967 (94%)	127 (6%)	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	781/1138 (69%)	781 (100%)	0	100	100
1	B	781/1138 (69%)	781 (100%)	0	100	100
All	All	1562/2276 (69%)	1562 (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 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	510	ASN
1	A	1149	ASN
1	A	614	HIS
1	A	1172	HIS
1	A	1040	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](#)

4 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	3PH	B	1402	-	44,44,47	0.65	1 (2%)	47,49,52	0.61	1 (2%)
2	3PH	B	1401	-	47,47,47	0.62	1 (2%)	50,52,52	0.61	1 (2%)
2	3PH	A	1401	-	47,47,47	0.63	1 (2%)	50,52,52	0.62	1 (2%)
2	3PH	A	1402	-	44,44,47	0.65	1 (2%)	47,49,52	0.61	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	3PH	B	1402	-	-	16/46/46/49	-
2	3PH	B	1401	-	-	22/49/49/49	-
2	3PH	A	1401	-	-	22/49/49/49	-
2	3PH	A	1402	-	-	16/46/46/49	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1401	3PH	P-O11	3.33	1.70	1.60
2	A	1402	3PH	P-O11	3.30	1.70	1.60
2	B	1401	3PH	P-O11	3.29	1.70	1.60
2	B	1402	3PH	P-O11	3.29	1.70	1.60

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1401	3PH	O13-P-O11	-2.18	100.99	106.67
2	A	1402	3PH	O13-P-O11	-2.18	100.99	106.67
2	A	1401	3PH	O13-P-O11	-2.17	101.00	106.67
2	B	1402	3PH	O13-P-O11	-2.16	101.04	106.67

There are no chirality outliers.

5 of 76 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1401	3PH	C1-O11-P-O13
2	B	1401	3PH	C1-O11-P-O14
2	B	1401	3PH	O11-C1-C2-O21

Continued on next page...

Continued from previous page...

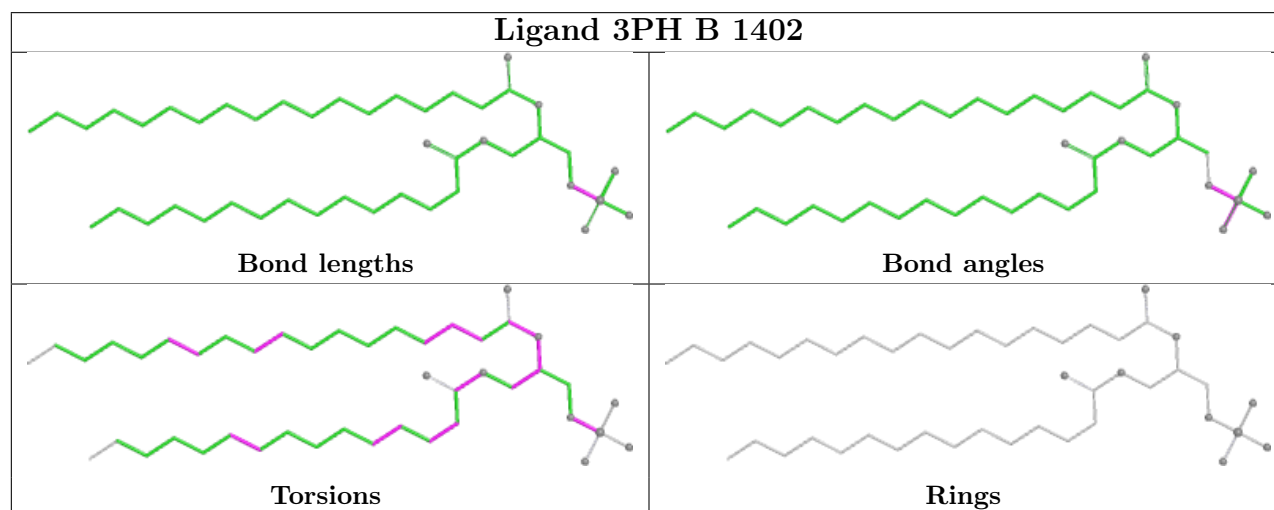
Mol	Chain	Res	Type	Atoms
2	B	1401	3PH	O22-C21-O21-C2
2	B	1402	3PH	C1-O11-P-O13

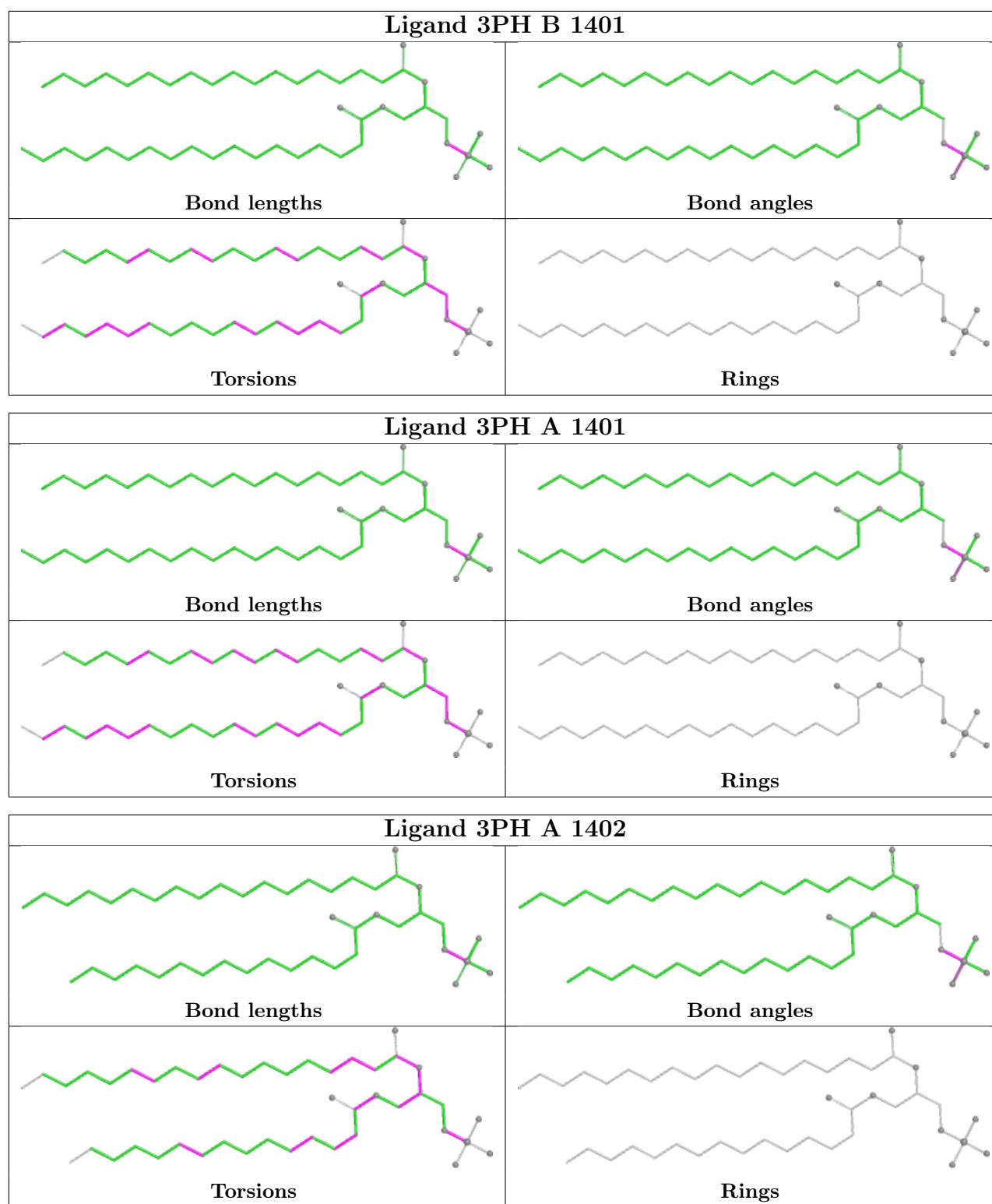
There are no ring outliers.

4 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1402	3PH	5	0
2	B	1401	3PH	4	0
2	A	1401	3PH	5	0
2	A	1402	3PH	6	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 ⓘ

There are no chain breaks in this entry.

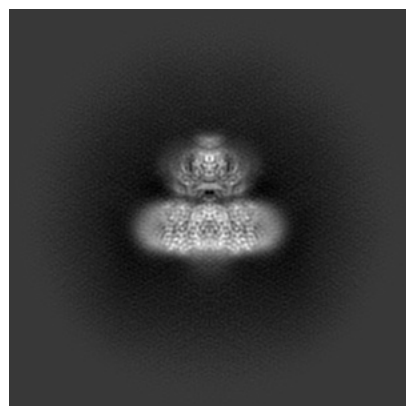
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17186. These allow visual inspection of the internal detail of the map and identification of artifacts.

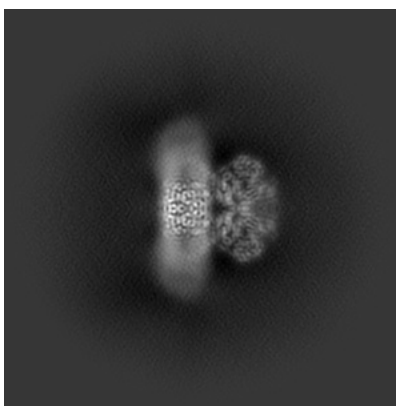
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

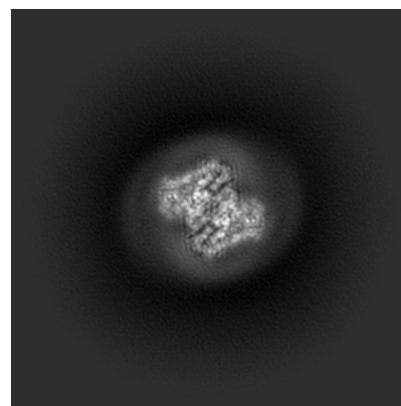
6.1.1 Primary map



X

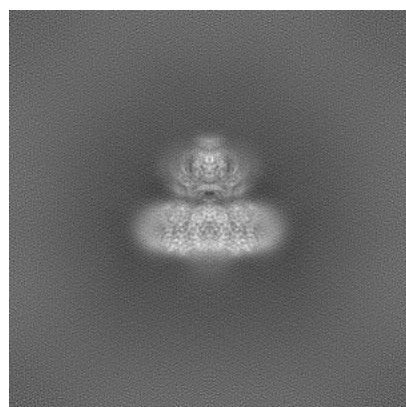


Y

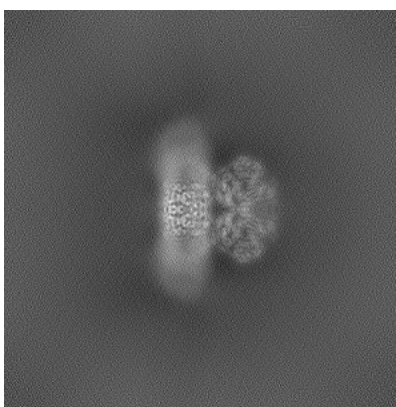


Z

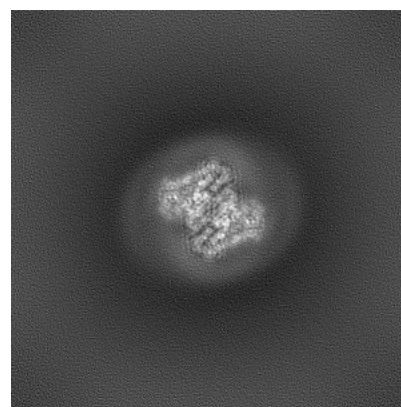
6.1.2 Raw map



X



Y

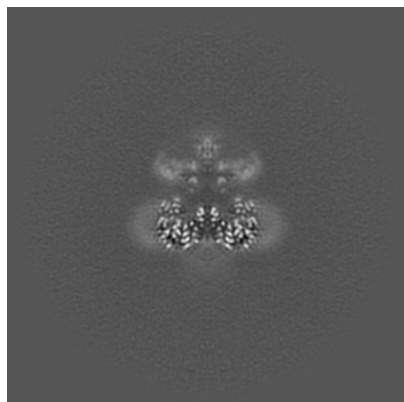


Z

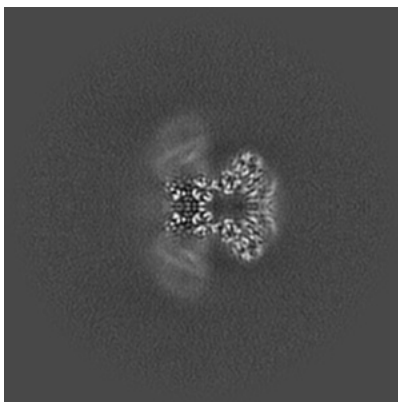
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

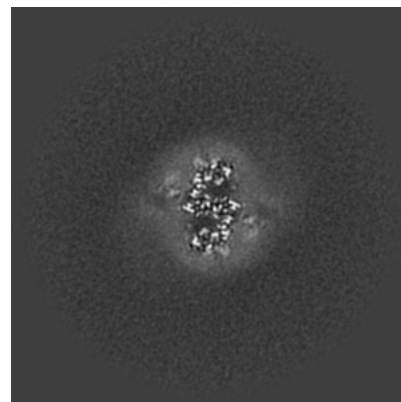
6.2.1 Primary map



X Index: 200

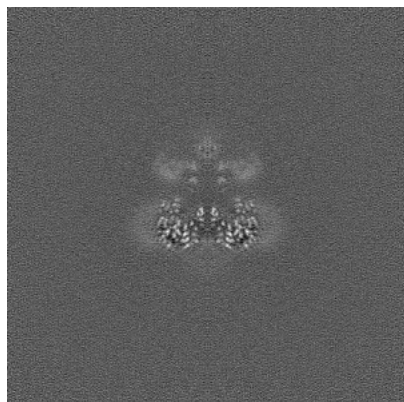


Y Index: 200

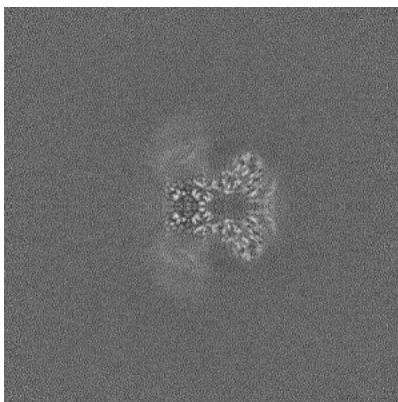


Z Index: 200

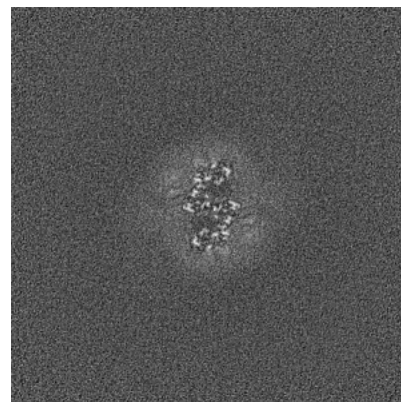
6.2.2 Raw map



X Index: 200



Y Index: 200

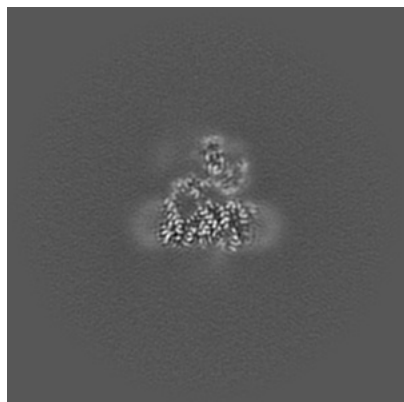


Z Index: 200

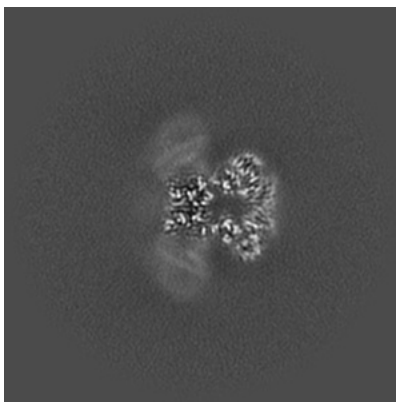
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

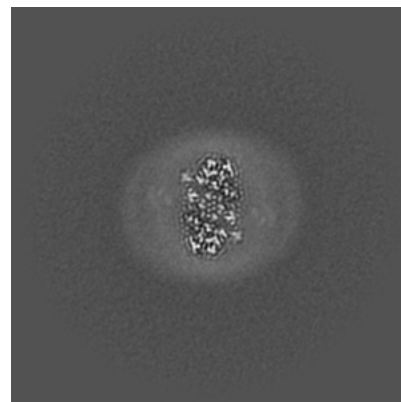
6.3.1 Primary map



X Index: 187

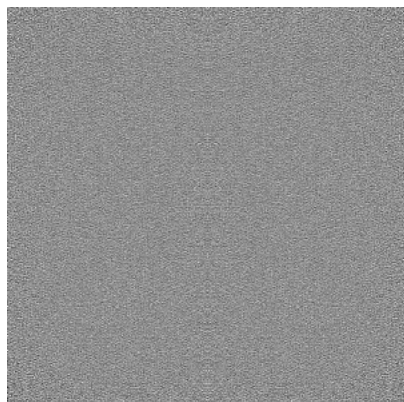


Y Index: 198

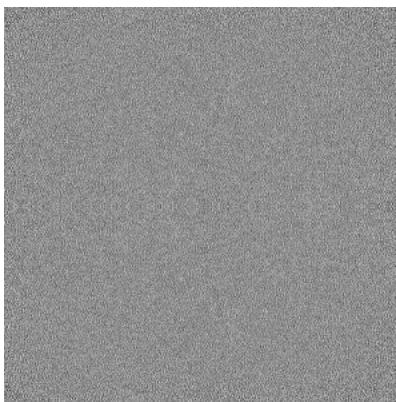


Z Index: 170

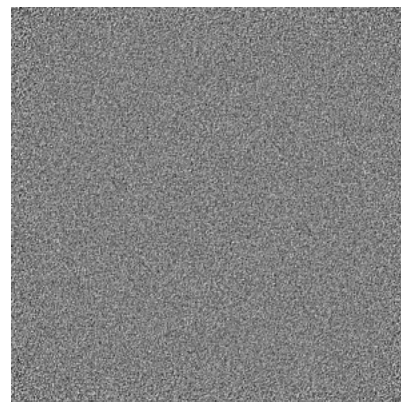
6.3.2 Raw map



X Index: 0



Y Index: 0

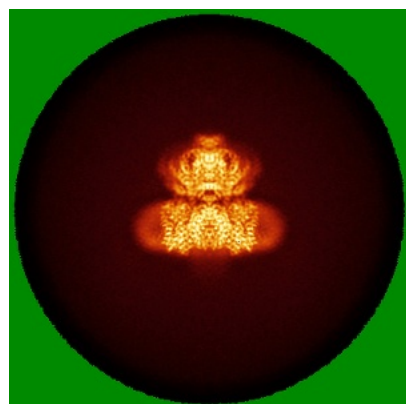


Z Index: 399

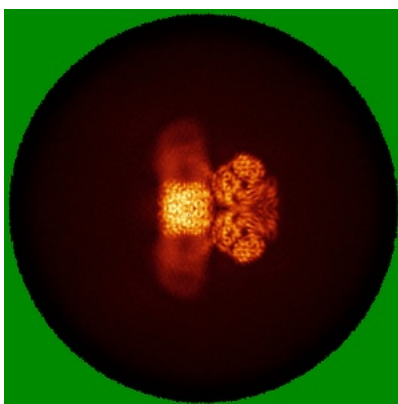
The images above show the largest variance slices of the map in three orthogonal directions.

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

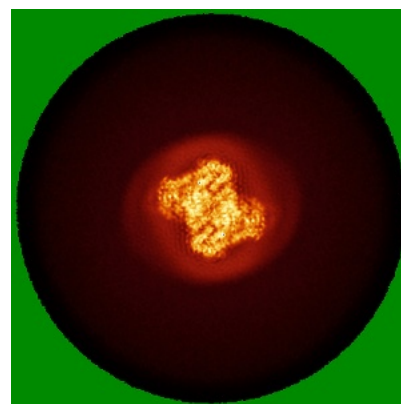
6.4.1 Primary map



X

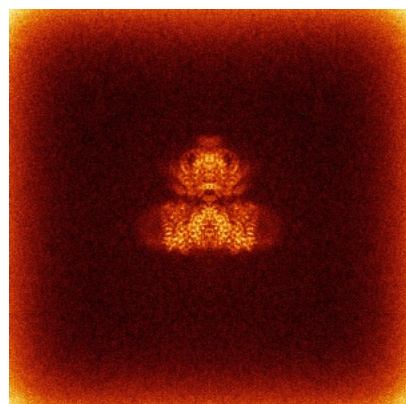


Y

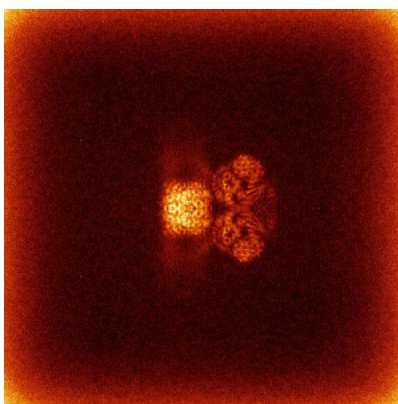


Z

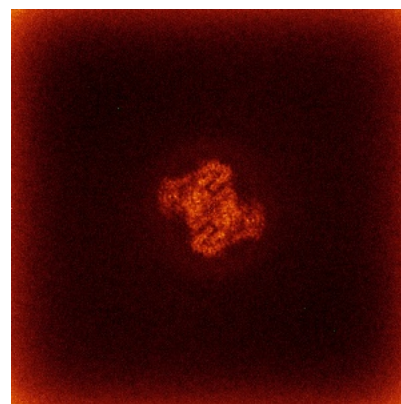
6.4.2 Raw map



X



Y

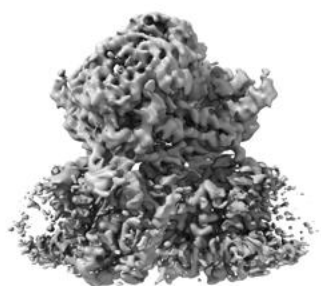


Z

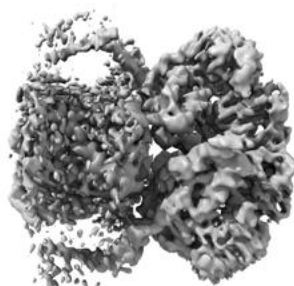
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

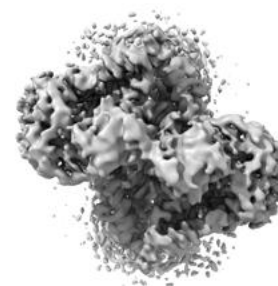
6.5.1 Primary map



X



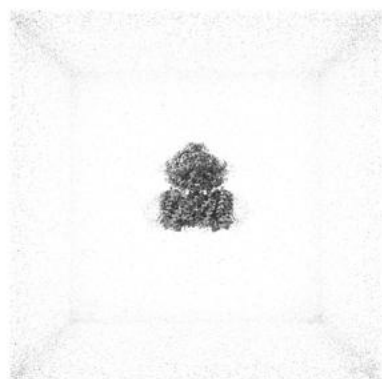
Y



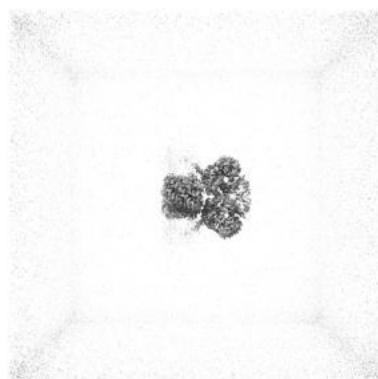
Z

The images above show the 3D surface view of the map at the recommended contour level 0.11. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

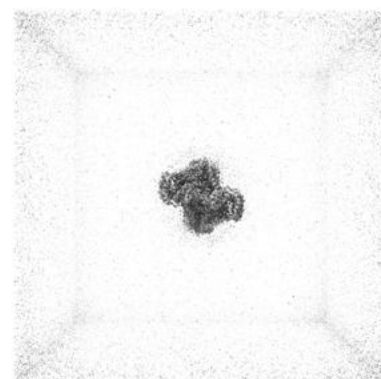
6.5.2 Raw map



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.

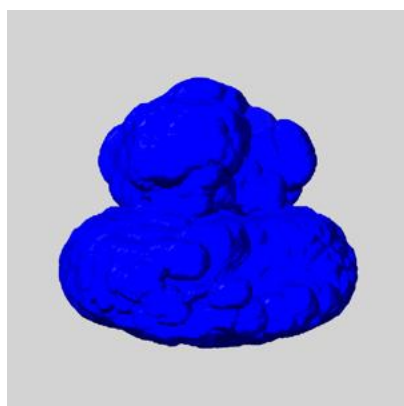
6.6 Mask visualisation [i](#)

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

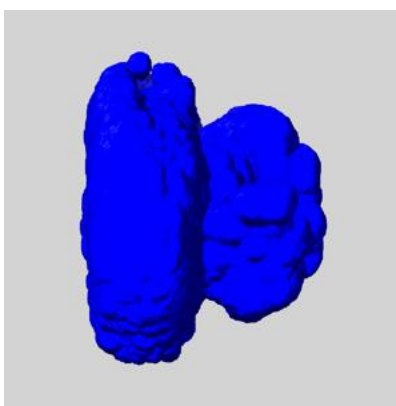
A mask typically either:

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

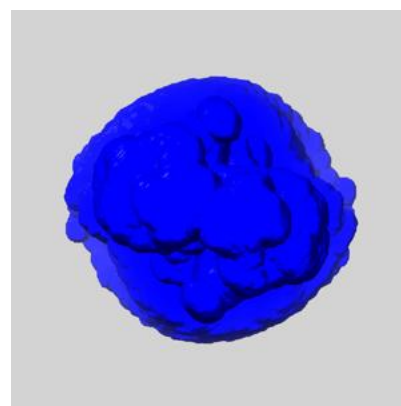
6.6.1 emd_17186_msk_1.map [i](#)



X



Y

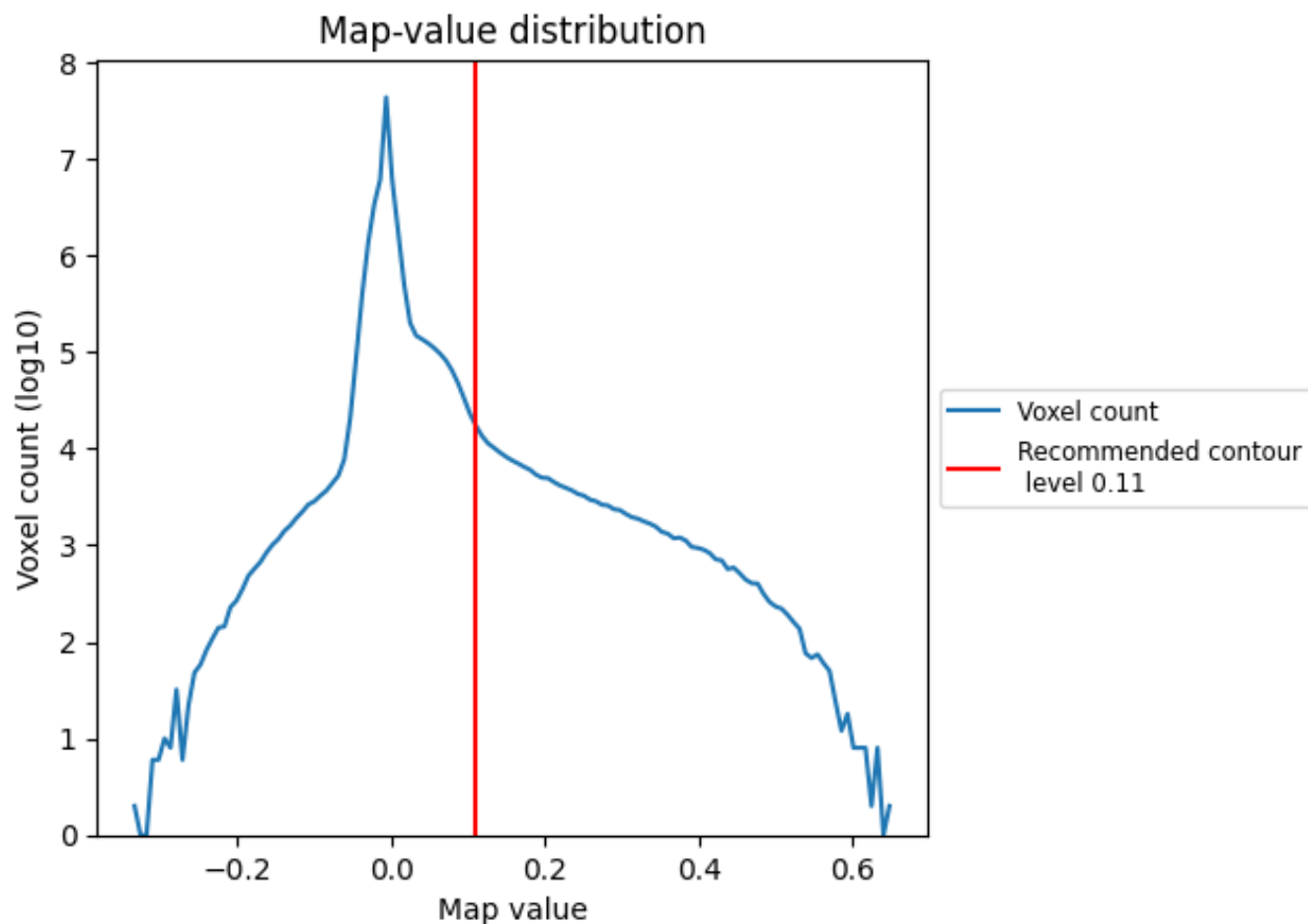


Z

7 Map analysis [i](#)

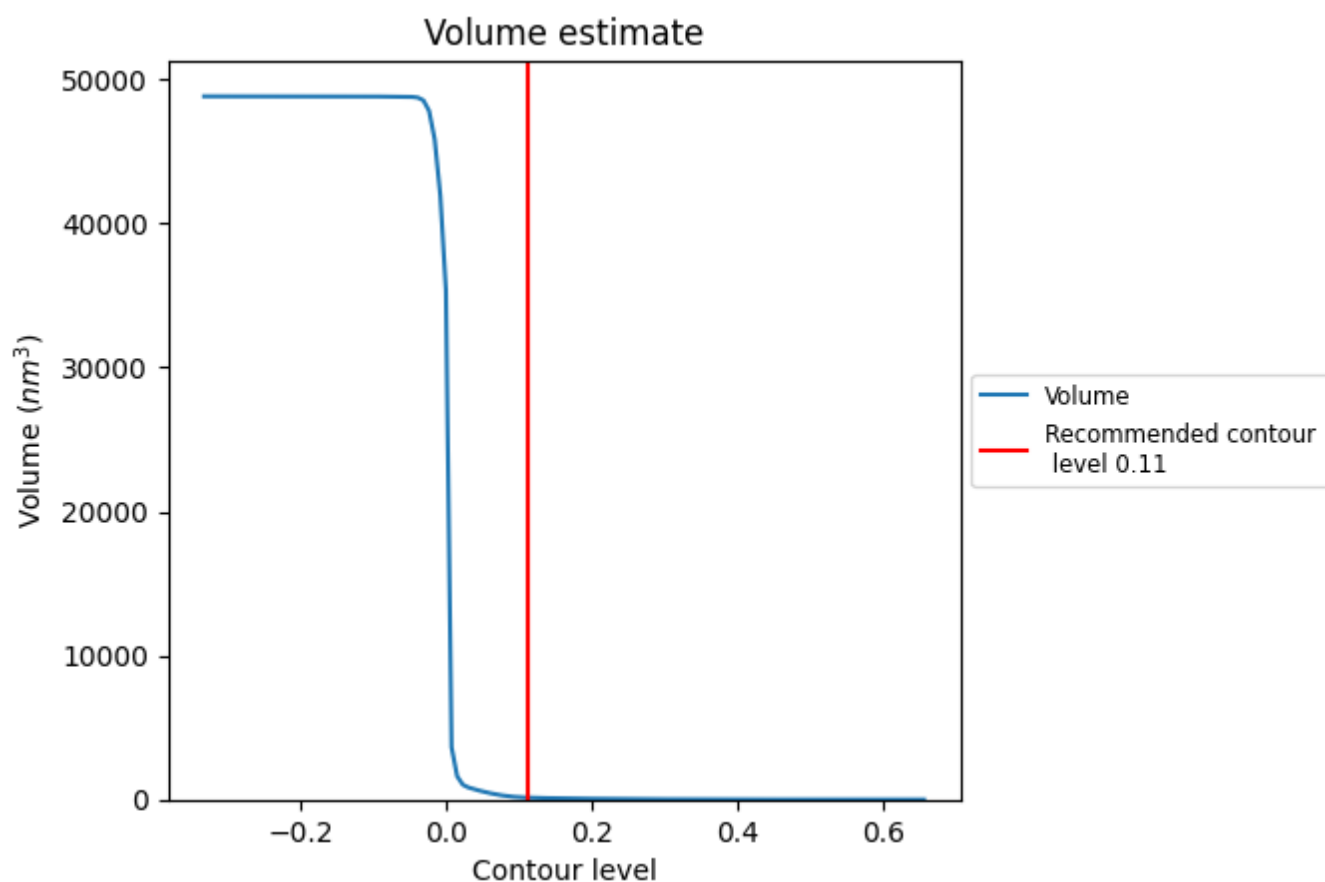
This section contains the results of statistical analysis of the map.

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.

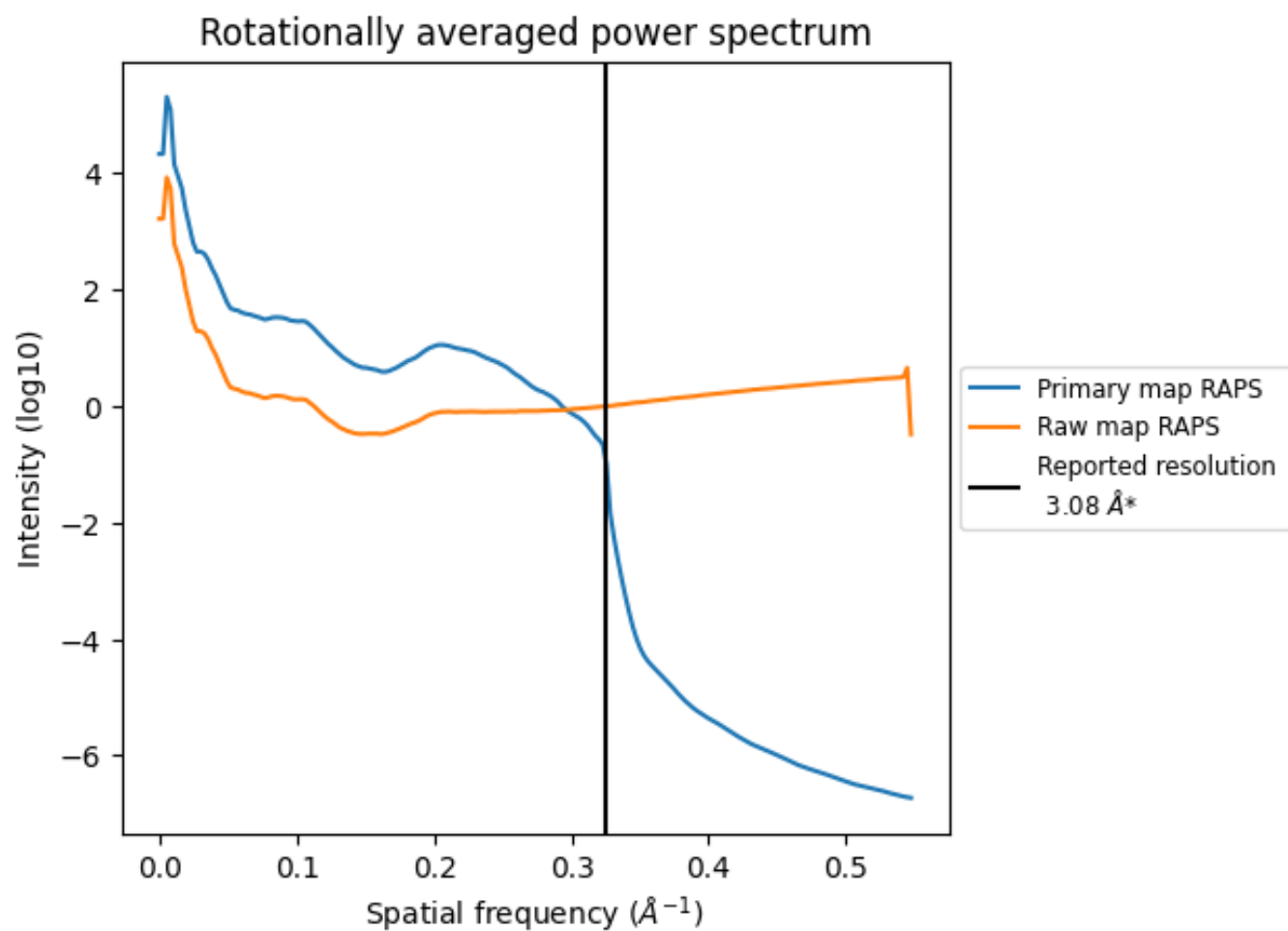
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 136 nm³; this corresponds to an approximate mass of 123 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 ⓘ

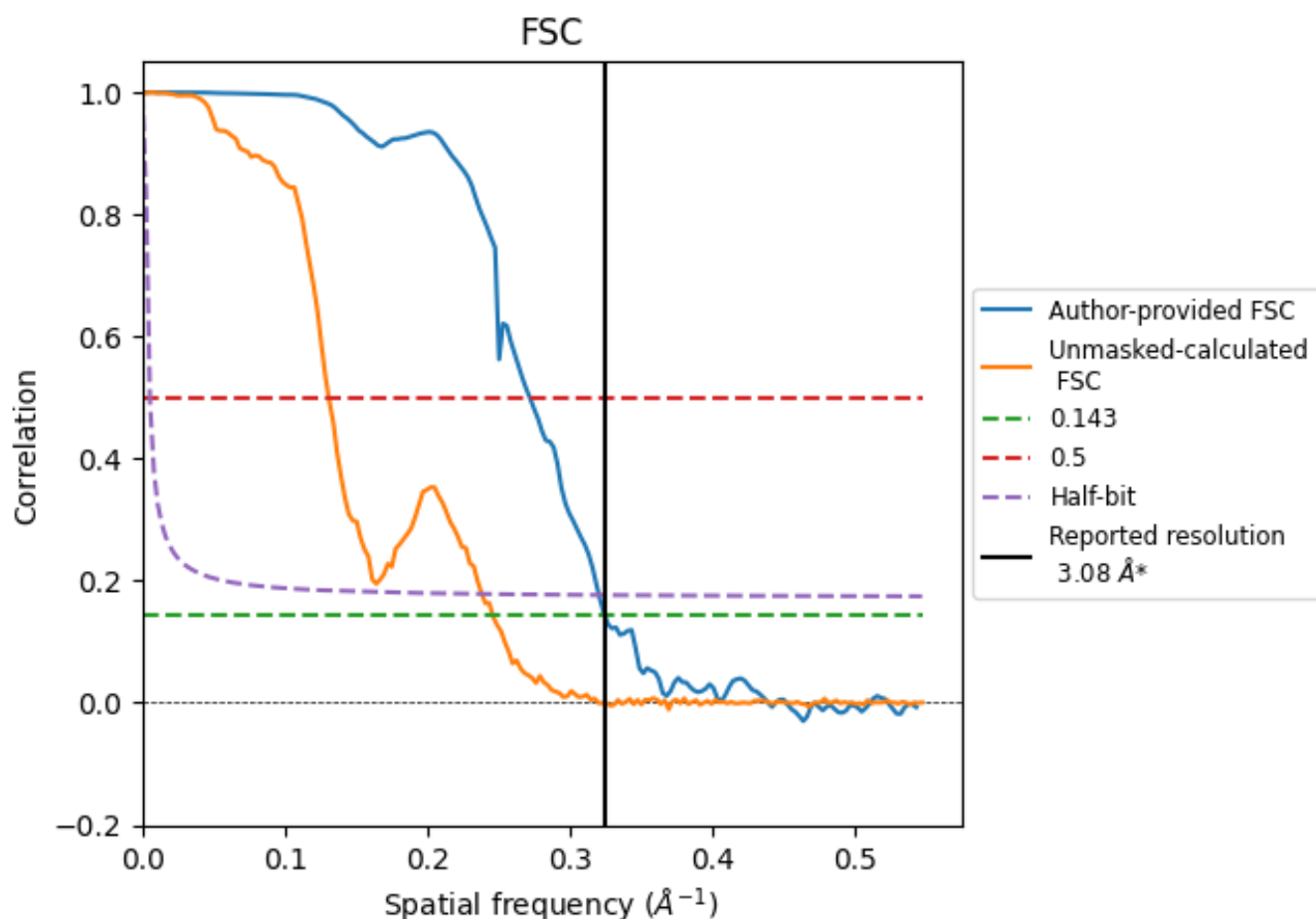


*Reported resolution corresponds to spatial frequency of 0.325 $\text{\AA}^{-1}$

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 0.325 Å⁻¹

8.2 Resolution estimates [i](#)

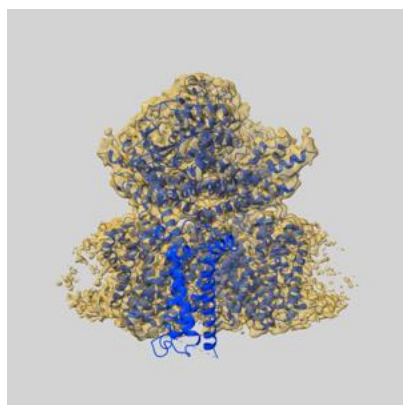
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.08	-	-
Author-provided FSC curve	3.08	3.68	3.12
Unmasked-calculated*	4.07	7.64	4.20

*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 4.07 differs from the reported value 3.08 by more than 10 %

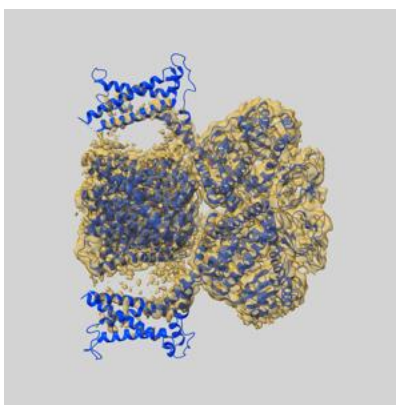
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-17186 and PDB model 8OTX. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

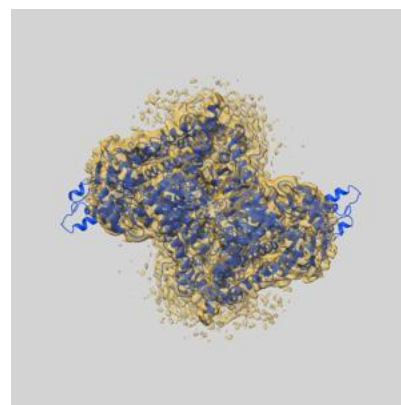
9.1 Map-model overlay [i](#)



X



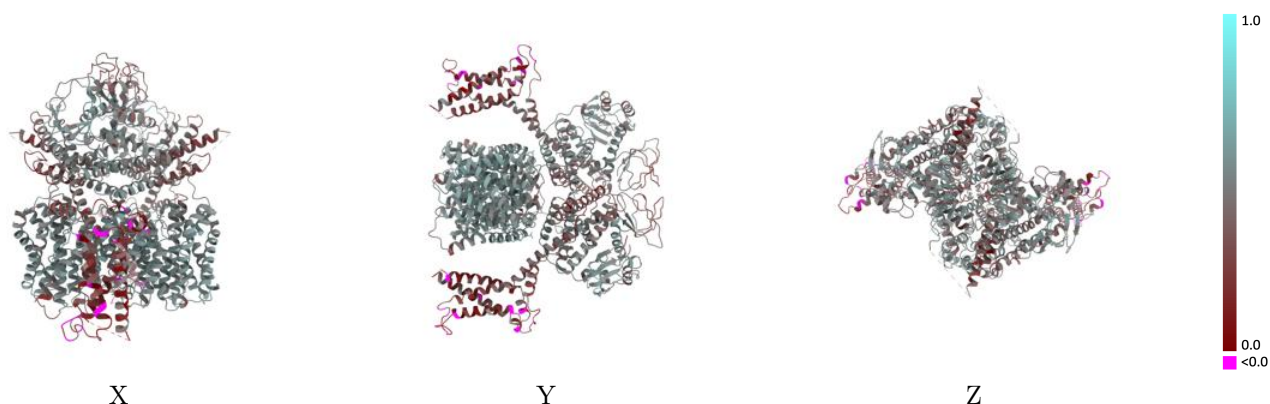
Y



Z

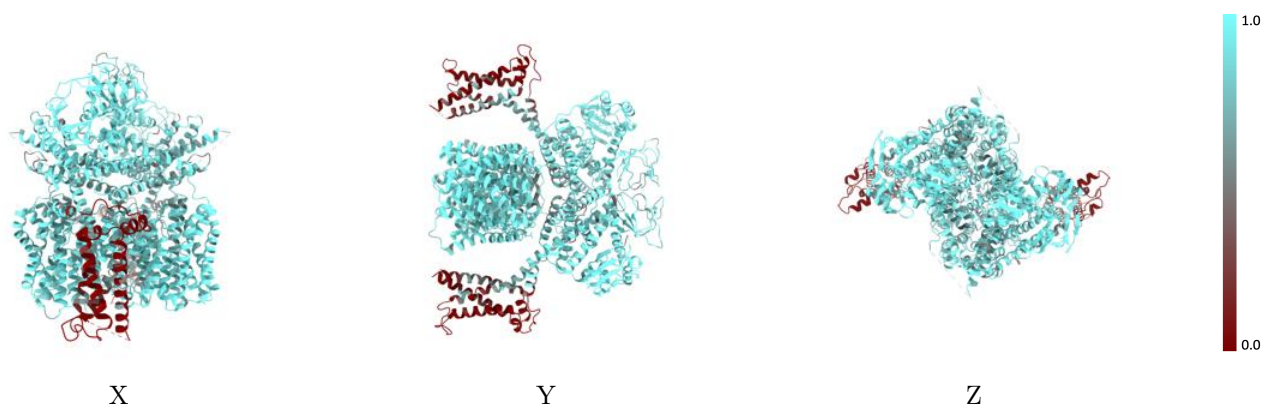
The images above show the 3D surface view of the map at the recommended contour level 0.11 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



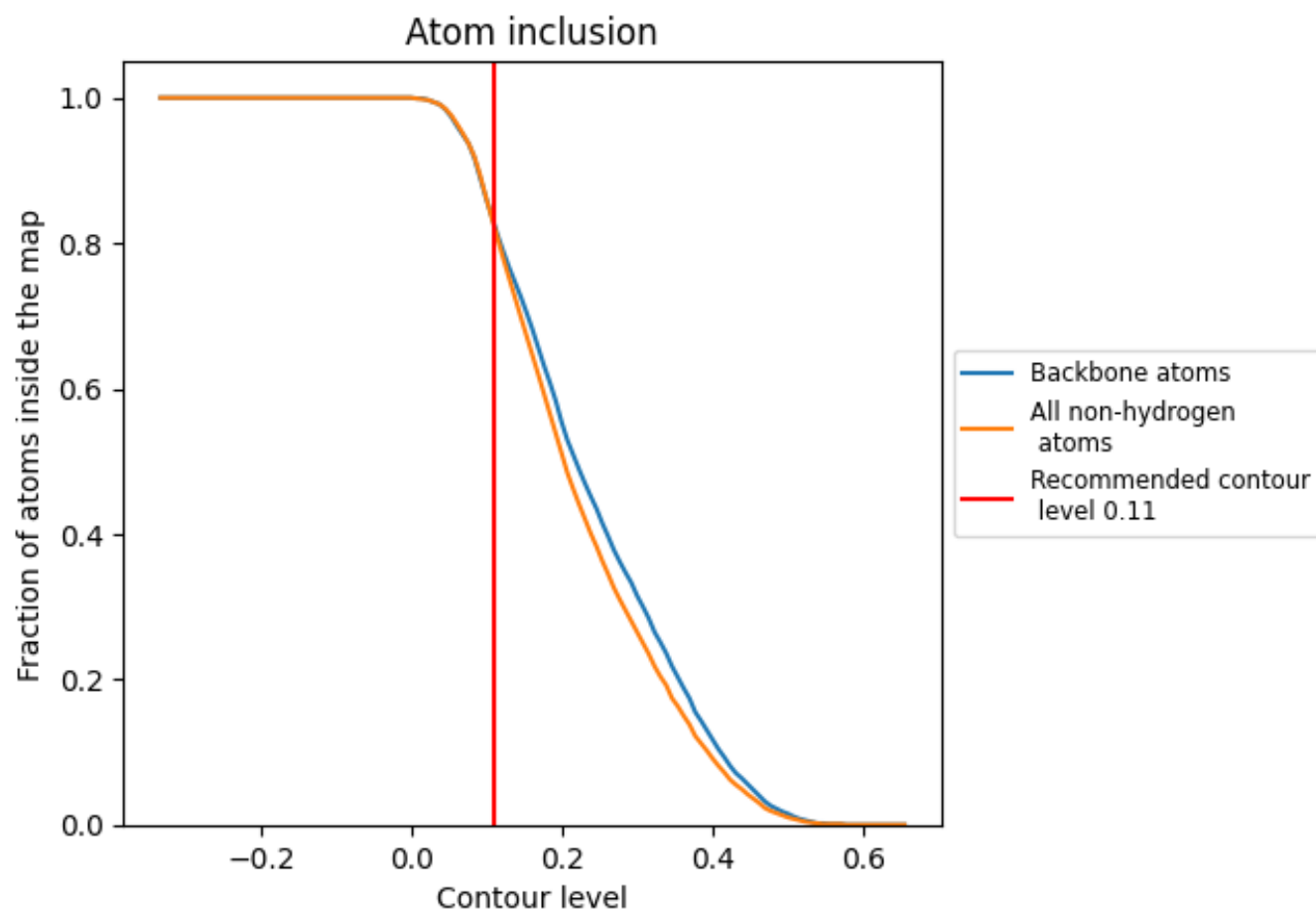
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.11).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 82% 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 (0.11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8230	0.4570
A	0.8250	0.4570
B	0.8250	0.4570

