



Full wwPDB EM Validation Report ⓘ

Jan 5, 2023 – 02:39 PM JST

PDB ID : 8HGH
EMDB ID : EMD-34739
Title : Structure of 2:2 PAPP-A.STC2 complex
Authors : Zhong, Q.H.; Chu, H.L.; Wang, G.P.; Zhang, C.; Wei, Y.; Qiao, J.; Hang, J.
Deposited on : 2022-11-14
Resolution : 4.16 Å (reported)

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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:

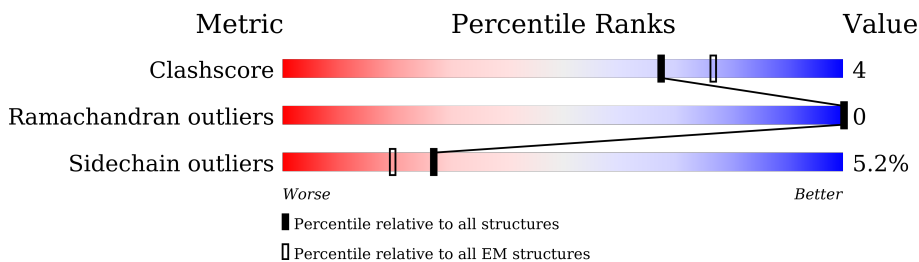
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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 4.16 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	1944	
1	B	1944	
2	C	302	
2	G	302	

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 25512 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 Maltose/maltodextrin-binding periplasmic protein,Pappalysin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1462	11420	7150	1974	2199	97	0	0
1	B	1462	11420	7150	1974	2199	97	0	0

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-396	ALA	-	expression tag	UNP P0AEX9
A	-395	ALA	-	expression tag	UNP P0AEX9
A	-394	SER	-	expression tag	UNP P0AEX9
A	-393	HIS	-	expression tag	UNP P0AEX9
A	-392	HIS	-	expression tag	UNP P0AEX9
A	-391	HIS	-	expression tag	UNP P0AEX9
A	-390	HIS	-	expression tag	UNP P0AEX9
A	-389	HIS	-	expression tag	UNP P0AEX9
A	-388	HIS	-	expression tag	UNP P0AEX9
A	-387	HIS	-	expression tag	UNP P0AEX9
A	-386	HIS	-	expression tag	UNP P0AEX9
A	-385	HIS	-	expression tag	UNP P0AEX9
A	-384	HIS	-	expression tag	UNP P0AEX9
A	-383	SER	-	expression tag	UNP P0AEX9
A	-382	GLY	-	expression tag	UNP P0AEX9
A	-15	ASP	-	linker	UNP P0AEX9
A	-14	TYR	-	linker	UNP P0AEX9
A	-13	ASP	-	linker	UNP P0AEX9
A	-12	ILE	-	linker	UNP P0AEX9
A	-11	PRO	-	linker	UNP P0AEX9
A	-10	THR	-	linker	UNP P0AEX9
A	-9	THR	-	linker	UNP P0AEX9
A	-8	GLU	-	linker	UNP P0AEX9
A	-7	ASN	-	linker	UNP P0AEX9
A	-6	LEU	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	TYR	-	linker	UNP P0AEX9
A	-4	PHE	-	linker	UNP P0AEX9
A	-3	GLN	-	linker	UNP P0AEX9
A	-2	GLY	-	linker	UNP P0AEX9
A	-1	GLU	-	linker	UNP P0AEX9
A	0	PHE	-	linker	UNP P0AEX9
B	-396	ALA	-	expression tag	UNP P0AEX9
B	-395	ALA	-	expression tag	UNP P0AEX9
B	-394	SER	-	expression tag	UNP P0AEX9
B	-393	HIS	-	expression tag	UNP P0AEX9
B	-392	HIS	-	expression tag	UNP P0AEX9
B	-391	HIS	-	expression tag	UNP P0AEX9
B	-390	HIS	-	expression tag	UNP P0AEX9
B	-389	HIS	-	expression tag	UNP P0AEX9
B	-388	HIS	-	expression tag	UNP P0AEX9
B	-387	HIS	-	expression tag	UNP P0AEX9
B	-386	HIS	-	expression tag	UNP P0AEX9
B	-385	HIS	-	expression tag	UNP P0AEX9
B	-384	HIS	-	expression tag	UNP P0AEX9
B	-383	SER	-	expression tag	UNP P0AEX9
B	-382	GLY	-	expression tag	UNP P0AEX9
B	-15	ASP	-	linker	UNP P0AEX9
B	-14	TYR	-	linker	UNP P0AEX9
B	-13	ASP	-	linker	UNP P0AEX9
B	-12	ILE	-	linker	UNP P0AEX9
B	-11	PRO	-	linker	UNP P0AEX9
B	-10	THR	-	linker	UNP P0AEX9
B	-9	THR	-	linker	UNP P0AEX9
B	-8	GLU	-	linker	UNP P0AEX9
B	-7	ASN	-	linker	UNP P0AEX9
B	-6	LEU	-	linker	UNP P0AEX9
B	-5	TYR	-	linker	UNP P0AEX9
B	-4	PHE	-	linker	UNP P0AEX9
B	-3	GLN	-	linker	UNP P0AEX9
B	-2	GLY	-	linker	UNP P0AEX9
B	-1	GLU	-	linker	UNP P0AEX9
B	0	PHE	-	linker	UNP P0AEX9

- Molecule 2 is a protein called Stanniocalcin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	171	1335	834	241	243	17	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	171	Total	C	N	O	S	0	0
			1335	834	241	243	17		

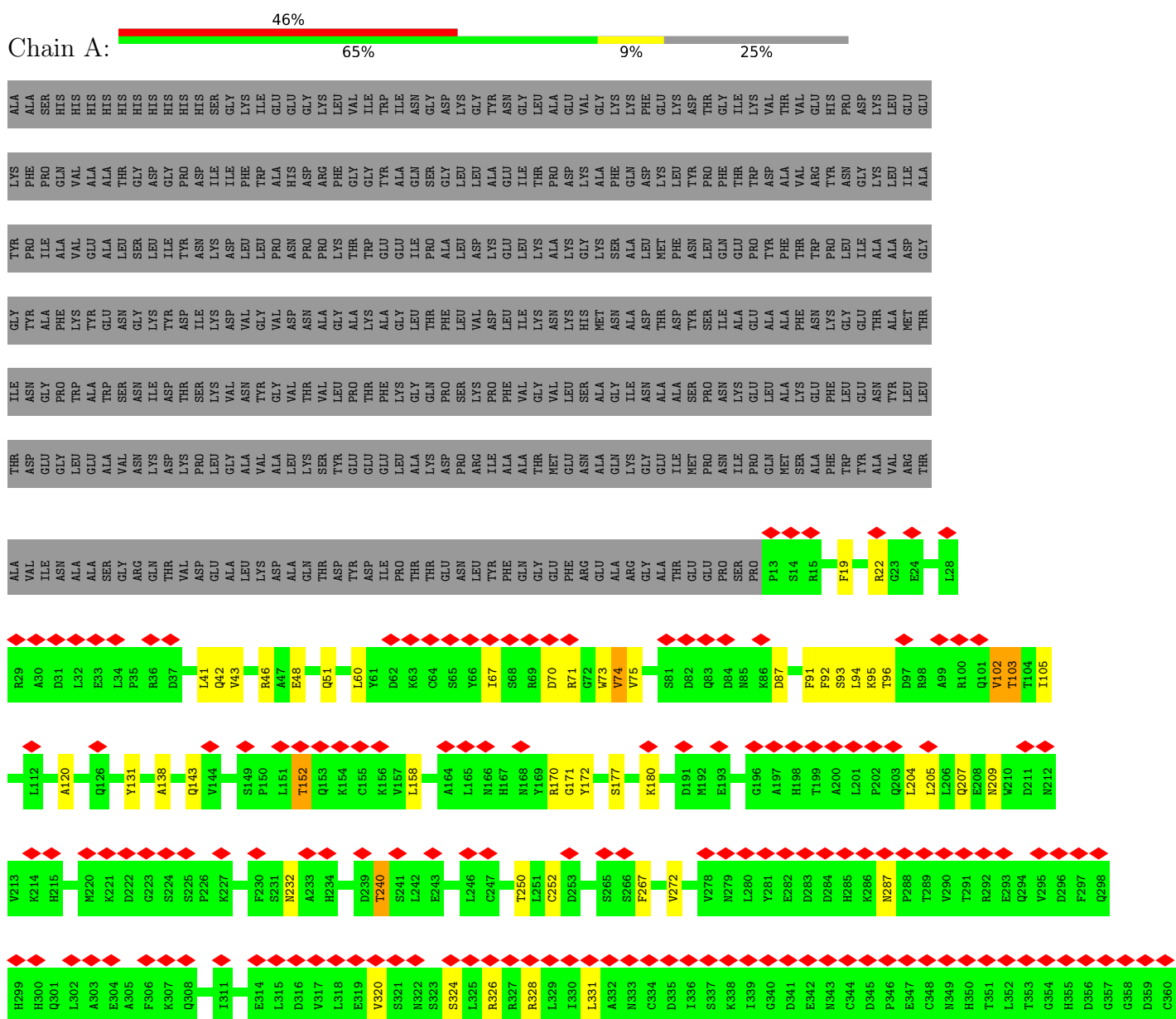
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

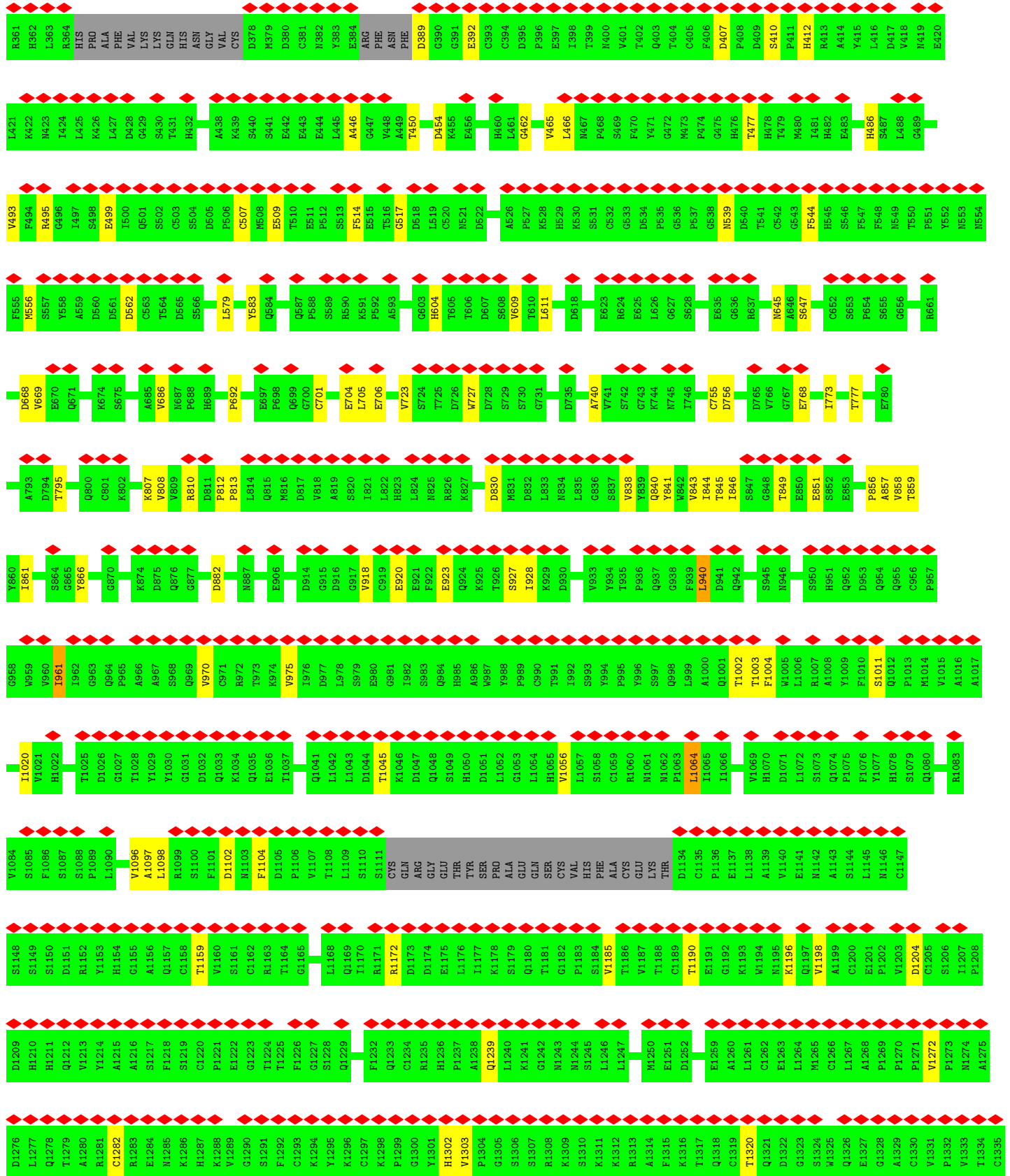
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	

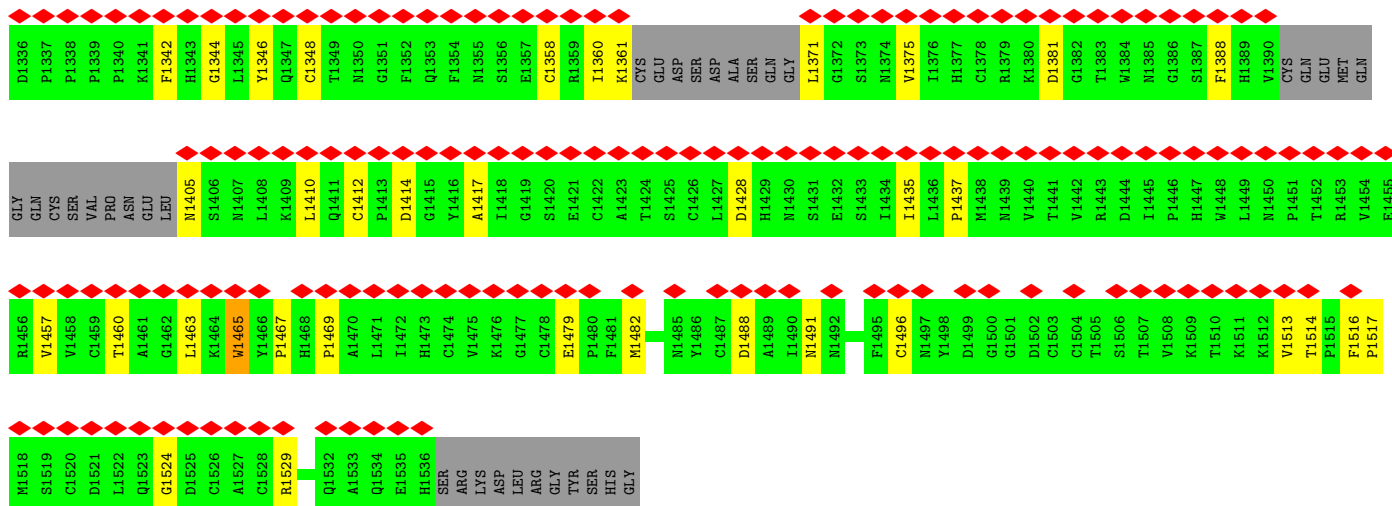
3 Residue-property plots

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.

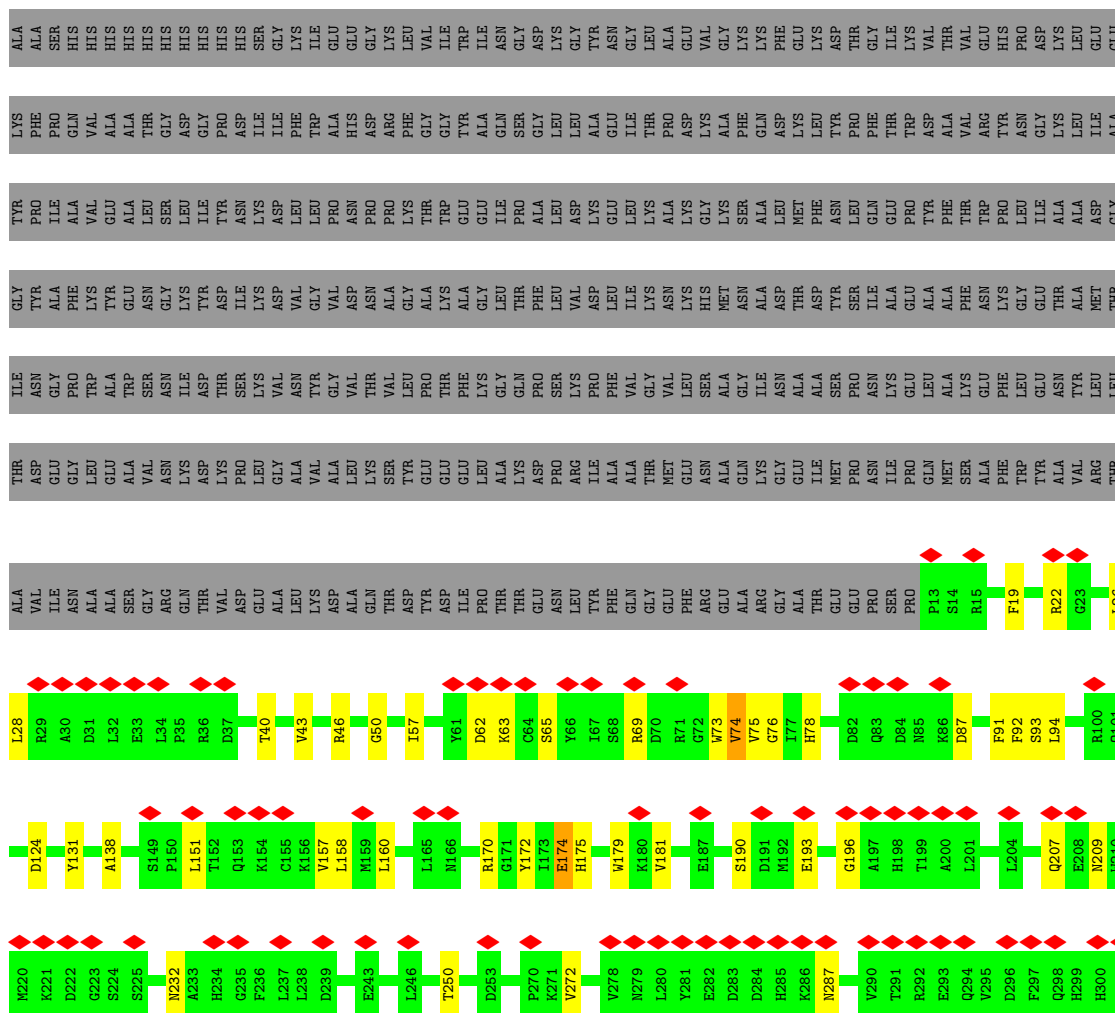
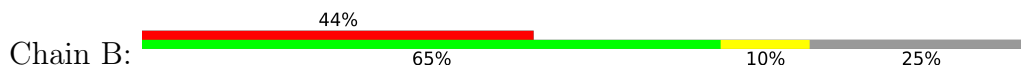
- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, Pappalysin-1



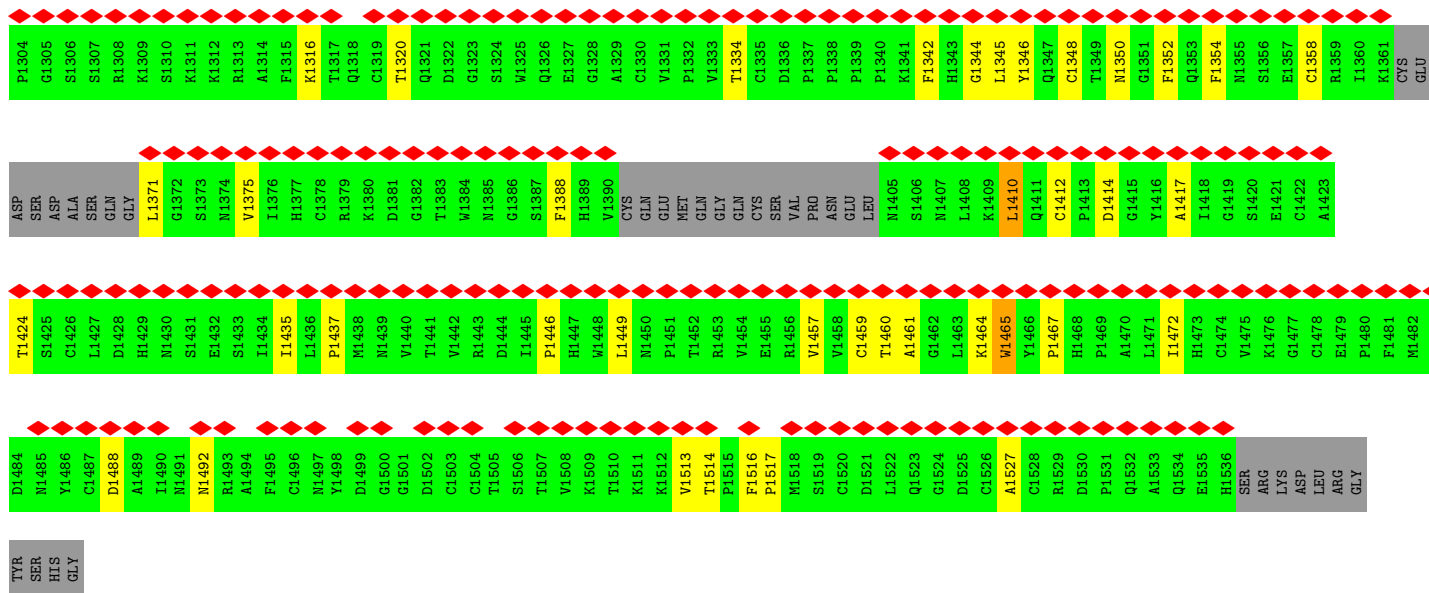




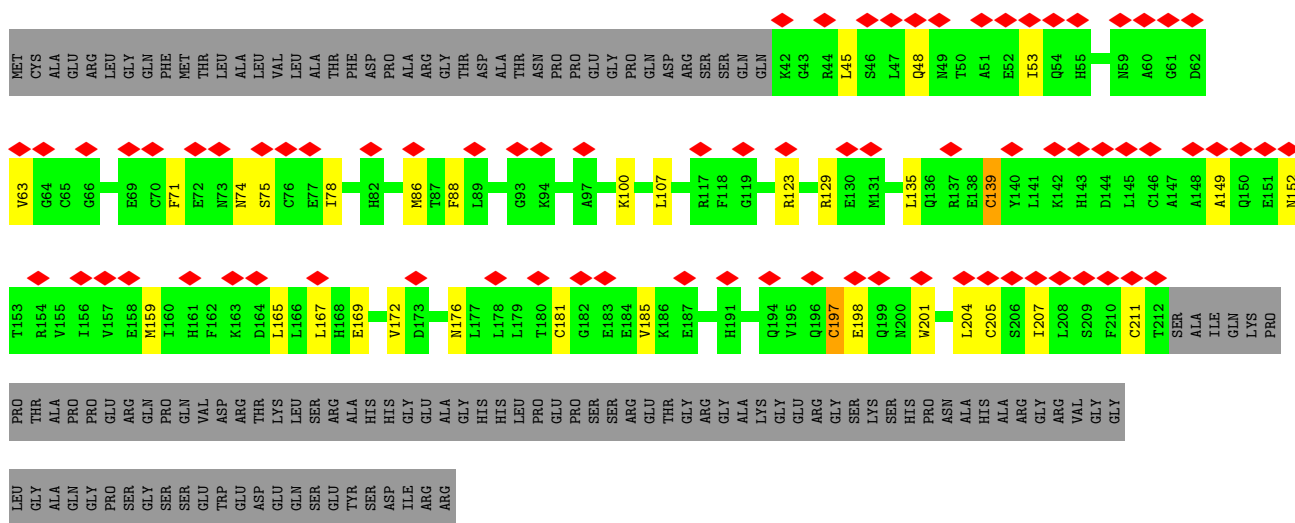
● Molecule 1: Maltose/maltodextrin-binding periplasmic protein, Pappalysin-1



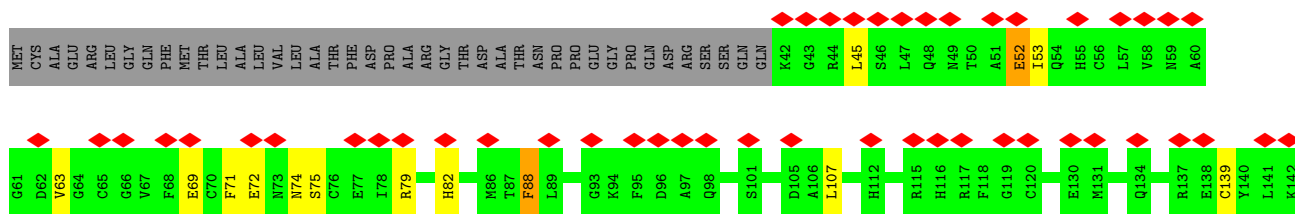
V317	L318	E319	V320	N321	N322	S323	S324	L325	R326	R327	R328	L329	I330	L331	A332	N333	C334	D335	I336	S337	K338	I339	G340	D341	E342	N343	C344	D345	P346	E347	C348	N349	H350	T351	L352	T353	G354	H355	D356	G357	G358	D359	C360	R361	H362	L363	R364	HIS	PRO	ALA	PHE	VAL	LYS	LYS	GLN	HIS	ASN	GLY		
VAL	CYS	D378	M379	D380	C381	N382	I383	E384	ARG	PHE	ASN	PHE	D389	G390	G391	E392	C393	C394	D395	P396	E397	I398	T399	M400	V401	T402	Q403	T404	C405	F406	D407	P408	D409	S410	P411	H412	R413	A414	Y415	L416	D417	V418	M419	E420	L421	K422	M423	I424	L427	D428	G429	F436	F437	A438	K439	S440	S441			
E442	E443	E444	L445	A446	G447	V448	A449	E384	D454	K455	E456	H460	L461	G462	V465	L466	M467	P468	S469	F470	Y471	G472	M473	P474	G475	H476	T477	H478	I481	H482	E483	I484	G485	H486	V493	F494	R495	G496	I497	S498	E499	I500	Q501	S502	C503	S504	D505	P506	C507	M508	E509	T510	E511	P512						
S513	F514	E515	T516	G517	D518	L519	N524	P525	A526	P527	K528	H529	K530	S531	C532	G533	D534	P535	G536	P537	G538	N539	D540	T541	C542	G543	F544	H545	S546	F547	F548	N549	T550	P551	Y552	N553	N554	F555	M556	S557	Y558	A559	D560	D561	D562	C563	T564	D565	L579	Y583	Q584	Q587	P588	S589	R590					
K591	P592	A593	T605	T606	D607	S608	V609	T610	L611	D618	E623	R624	E625	L626	G627	S628	A629	G636	R637	S647	P651	C652	S653	P654	S655	G656	S659	P660	R661	D668	V669	E670	Q671	S675	N683	S684	A685	P688	H689	E697	P698	Q699	G700	C701	E704	L705														
E706	L711	E714	S715	T725	D726	W727	D728	S729	S730	G731	S742	G743	K744	C755	D765	V766	G767	E768	E780	S791	T792	A793	D794	T795	L799	Q800	C801	K802	K807	V808	V809	R810	D811	P812	P813	L814	Q815	M816	D817	V818	A819	S820	I821	L822	F828	V829	D830	M831												
D832	L833	M834	L835	G836	V838	T839	Y841	W842	V843	L844	T845	R846	S847	G848	T849	E850	E851	A857	V858	T859	I861	S864	G865	Y866	C867	G870	K874	D875	Q876	D877	D882	K885	I886	R887	G888	R896	D905	E906	D914	G915	D916	G917	Y918	C919	E920	E921	F922													
E923	S927	I928	R929	D930	C931	G932	V933	Y934	T935	P936	Q937	F938	L940	G941	Q942	Y943	Y946	A947	H951	Q952	D953	Q954	Q955	C956	P957	Y958	V960	I961	I962	G963	Q964	P965	A966	A967	S968	Q969	V970	C971	R972	T973	K974	I975	I976	D977	L978	D979	S979	E980	G981	I982	S983	Q984	H985	A986						
P989	C990	T991	I992	S993	Y994	P995	Y996	S997	Q998	L999	A1000	Q1001	T1002	T1003	F1004	R1007	A1008	Y1009	F1010	S1011	Q1012	Q1013	M1014	G1015	A1016	A1017	I1020	V1024	T1025	D1026	G1027	T1028	Y1029	Y1030	G1031	I1032	Q1033	K1034	Q1035	E1036	T1037	V1040	Q1041	S1111	CYS	GLN	ARG	GLY	GLU	THR	TYR	SER	PRO	ALA						
L1054	H1055	V1056	L1057	S1058	C1059	R1060	M1061	N1062	P1063	V1069	H1070	D1071	L1072	S1073	Q1074	P1075	F1076	Y1077	H1078	R1083	V1084	S1085	F1086	S1087	S1088	P1089	L1090	V1091	A1092	I1093	S1094	A1097	L1098	R1099	S1100	F1101	D1102	M1103	F1104	D1105	P1106	V1107	T1108	L1109	S1110	S1111	GLN	ARG	GLY	GLU	THR	TYR	SER	PRO	ALA					
GLU	GLN	SER	CYS	VAL	HIS	PHE	ALA	GLU	LYS	THR	D1134	C1135	P1136	E1137	L1138	A1139	V1140	E1141	M1142	A1143	S1144	L1145	M1146	C1147	S1148	S1149	S1150	D1151	R1152	Y1153	H1154	G1155	A1156	Q1157	C1158	T1159	V1160	S1161	C1162	R1163	T1164	G1165	V1166	V1167	L1168	Q1169	S1170	I1171	R1172	L1173	D1174	E1175	L1176	I1177	K1178	S1179	Q1180	T1181		
G1182	P1183	S1184	V1185	T1186	V1187	T1188	C1189	T1190	E1191	G1192	K1193	M1194	N1195	K1196	Q1197	V1198	A1199	C1200	E1201	V1202	V1203	D1204	C1205	S1206	I1207	P1208	D1209	H1210	H1211	Q1212	V1213	Y1214	A1215	A1216	S1217	F1218	S1219	C1220	P1221	E1222	G1223	T1224	L1225	F1226	G1227	S1228	Q1229	C1230	S1231	F1232	Q1233	R1234	H1235	P1236	P1237	A1238	G1300	H1301	L1240	K1241
G1242	N1243	M1244	S1245	L1246	L1247	M1250	E1251	D1252	G1253	L1254	F1257	P1258	E1259	A1260	L1261	C1262	E1263	L1264	M1265	C1266	L1267	A1268	P1269	P1270	P1271	V1272	P1273	M1274	A1275	D1276	L1277	Q1278	L1279	A1280	R1281	C1282	R1283	E1284	N1285	K1286	H1287	K1288	V1289	G1290	S1291	F1292	C1293	K1294	Y1295	K1296	C1297	K1298	P1299	G1300	H1301	L1302	V1303			

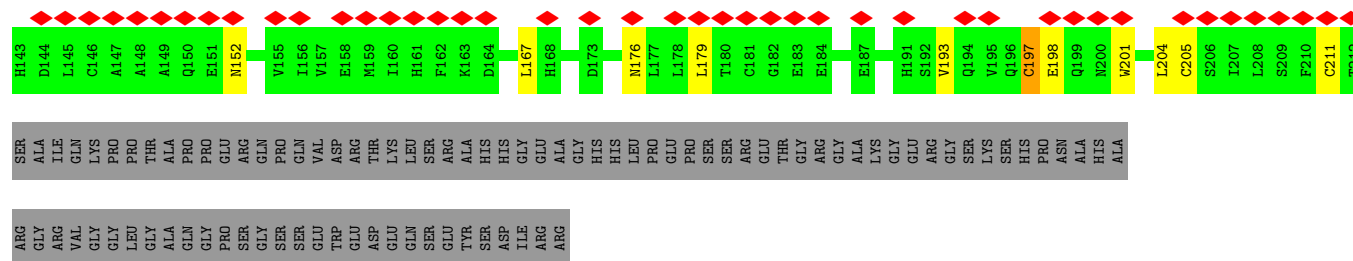


• Molecule 2: Stanniocalcin-2



• Molecule 2: Stanniocalcin-2





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	253671	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 ($e^-/\text{\AA}^2$)	59.8	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.082	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0217	Depositor
Map size (Å)	270.08, 270.08, 270.08	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.055, 1.055, 1.055	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

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	0.27	0/11725	0.50	0/15963
1	B	0.27	0/11725	0.50	0/15963
2	C	0.28	0/1357	0.52	0/1825
2	G	0.28	0/1357	0.52	0/1825
All	All	0.27	0/26164	0.50	0/35576

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	11420	0	10786	83	0
1	B	11420	0	10786	92	0
2	C	1335	0	1313	14	0
2	G	1335	0	1313	13	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	25512	0	24198	195	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 4.

All (195) 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:1405:ASN:HB2	1:A:1469:PRO:HB2	1.76	0.68
1:B:482:HIS:NE2	1:B:486:HIS:CE1	2.70	0.60
1:A:509:GLU:HB2	1:A:517:GLY:HA3	1.84	0.59
1:B:1020:ILE:HB	1:B:1097:ALA:HB3	1.85	0.58
1:A:1185:VAL:HG11	1:A:1198:VAL:HG11	1.85	0.58
1:B:1414:ASP:HB3	1:B:1417:ALA:HB3	1.85	0.58
1:B:19:PHE:O	1:B:170:ARG:HA	2.04	0.57
1:B:1281:ARG:HH12	1:B:1291:SER:HB3	1.69	0.57
2:C:211:CYS:N	2:G:211:CYS:SG	2.78	0.56
1:B:174:GLU:OE1	1:B:175:HIS:ND1	2.38	0.56
1:B:287:ASN:OD1	1:B:326:ARG:NH2	2.39	0.55
2:C:211:CYS:SG	2:G:211:CYS:N	2.80	0.55
1:A:209:ASN:OD1	1:A:209:ASN:N	2.40	0.55
1:A:1414:ASP:HB3	1:A:1417:ALA:HB3	1.90	0.54
1:A:46:ARG:HB3	1:A:172:TYR:HB2	1.90	0.54
1:A:1020:ILE:HB	1:A:1097:ALA:HB3	1.89	0.54
1:B:63:LYS:HA	1:B:69:ARG:HH22	1.72	0.54
1:B:509:GLU:HG2	1:B:525:PRO:HG3	1.90	0.53
2:C:207:ILE:HG21	2:G:193:VAL:HG21	1.91	0.53
1:B:65:SER:O	1:B:69:ARG:NH1	2.41	0.53
1:B:1204:ASP:OD1	1:B:1204:ASP:N	2.41	0.53
1:A:645:ASN:HB3	1:A:706:GLU:HB3	1.90	0.53
1:A:87:ASP:OD1	1:A:87:ASP:N	2.40	0.53
1:B:46:ARG:HB3	1:B:172:TYR:HB2	1.91	0.53
1:A:204:LEU:HD11	1:A:207:GLN:HB2	1.90	0.53
1:A:846:ILE:HG22	1:A:851:GLU:HA	1.91	0.53
1:A:1204:ASP:OD1	1:A:1204:ASP:N	2.41	0.53
1:B:50:GLY:O	1:B:170:ARG:NH1	2.42	0.53
1:B:1020:ILE:HD11	1:B:1099:ARG:HH21	1.74	0.53
1:A:668:ASP:N	1:A:668:ASP:OD1	2.42	0.52
1:A:1457:VAL:HG13	1:A:1467:PRO:HB2	1.89	0.52
1:B:668:ASP:OD1	1:B:668:ASP:N	2.43	0.52
1:B:815:GLN:NE2	1:B:832:ASP:OD2	2.42	0.52
1:B:1342:PHE:HD2	1:B:1388:PHE:HB3	1.74	0.52
1:A:73:TRP:HB3	1:A:94:LEU:HD13	1.91	0.52
1:A:19:PHE:O	1:A:170:ARG:HA	2.09	0.52
1:B:886:ILE:HG22	1:B:888:GLY:H	1.74	0.52
1:A:41:LEU:O	1:A:120:ALA:HA	2.11	0.51
1:B:1435:ILE:HG12	1:B:1472:ILE:HG12	1.92	0.51
1:B:1459:CYS:HA	1:B:1464:LYS:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ILE:HG23	1:A:138:ALA:HB3	1.93	0.51
2:G:45:LEU:HD11	2:G:74:ASN:HB2	1.92	0.51
1:B:838:VAL:HG12	1:B:861:ILE:HG12	1.91	0.51
1:A:71:ARG:NH1	1:A:96:THR:O	2.43	0.51
1:B:509:GLU:HB2	1:B:517:GLY:HA3	1.93	0.50
1:A:1516:PHE:HB2	2:C:100:LYS:HE2	1.92	0.50
2:C:45:LEU:HD11	2:C:74:ASN:HB2	1.93	0.50
1:A:51:GLN:NE2	1:A:170:ARG:O	2.44	0.50
1:B:1435:ILE:HG22	1:B:1437:PRO:HD3	1.93	0.50
1:A:120:ALA:HB3	1:A:131:TYR:HB2	1.94	0.50
1:A:882:ASP:OD1	1:A:882:ASP:N	2.44	0.50
1:A:287:ASN:OD1	1:A:326:ARG:NH2	2.44	0.50
1:B:882:ASP:OD1	1:B:882:ASP:N	2.43	0.49
1:B:807:LYS:HE2	1:B:844:ILE:HD11	1.94	0.49
1:A:1524:GLY:O	1:A:1529:ARG:NH2	2.46	0.49
1:B:579:LEU:HA	1:B:583:TYR:HB2	1.93	0.49
2:C:45:LEU:HA	2:C:75:SER:HB3	1.95	0.49
1:B:1350:ASN:ND2	1:B:1354:PHE:O	2.41	0.49
1:B:1460:THR:OG1	1:B:1461:ALA:N	2.45	0.49
2:C:53:ILE:HD11	2:C:71:PHE:HA	1.95	0.49
1:B:324:SER:O	1:B:328:ARG:NH1	2.46	0.49
1:A:42:GLN:HB2	1:A:177:SER:HB3	1.95	0.49
1:B:87:ASP:OD1	1:B:87:ASP:N	2.43	0.49
1:A:539:ASN:HA	1:B:1048:GLN:HE22	1.78	0.48
1:B:105:ILE:HG23	1:B:138:ALA:HB3	1.95	0.48
1:A:1002:THR:OG1	1:A:1003:THR:N	2.45	0.48
1:B:73:TRP:HB3	1:B:94:LEU:HD13	1.95	0.48
1:A:1348:CYS:HA	1:A:1358:CYS:HA	1.95	0.48
1:B:791:SER:OG	1:B:792:THR:N	2.47	0.48
2:G:72:GLU:OE1	2:G:79:ARG:NH2	2.46	0.48
1:A:807:LYS:HE2	1:A:844:ILE:HD11	1.95	0.48
1:B:501:GLN:NE2	1:B:505:ASP:OD1	2.47	0.48
1:A:180:LYS:HE2	1:A:205:LEU:HD13	1.94	0.48
1:A:562:ASP:OD1	1:A:562:ASP:N	2.43	0.48
1:B:196:GLY:O	1:B:207:GLN:NE2	2.47	0.47
2:C:172:VAL:O	2:C:176:ASN:ND2	2.47	0.47
1:B:62:ASP:O	1:B:69:ARG:NH2	2.47	0.47
1:A:940:LEU:HB2	1:A:1102:ASP:HB3	1.95	0.47
1:B:1185:VAL:HG11	1:B:1198:VAL:HG11	1.96	0.47
1:A:75:VAL:HG22	1:A:92:PHE:HD1	1.79	0.47
1:A:579:LEU:HA	1:A:583:TYR:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:810:ARG:HG2	1:B:812:PRO:HD2	1.97	0.47
2:C:149:ALA:HB1	2:C:185:VAL:HG21	1.96	0.47
2:G:74:ASN:N	2:G:74:ASN:OD1	2.46	0.47
1:A:1342:PHE:HD2	1:A:1388:PHE:HB3	1.79	0.47
1:B:1410:LEU:HB3	1:B:1424:THR:HG22	1.96	0.47
1:A:48:GLU:HG2	1:A:171:GLY:HA2	1.97	0.47
2:G:53:ILE:HD11	2:G:71:PHE:HA	1.96	0.47
1:A:1346:TYR:HA	1:A:1360:ILE:HG22	1.97	0.46
1:A:1435:ILE:HG22	1:A:1437:PRO:HD3	1.97	0.46
1:B:407:ASP:HB2	1:B:410:SER:HB2	1.97	0.46
1:A:152:THR:O	1:A:152:THR:OG1	2.34	0.46
1:B:209:ASN:OD1	1:B:209:ASN:N	2.49	0.46
1:B:345:ASP:N	1:B:345:ASP:OD1	2.48	0.46
1:B:120:ALA:HB3	1:B:131:TYR:HB2	1.97	0.46
1:A:232:ASN:OD1	1:A:232:ASN:N	2.49	0.46
1:B:378:ASP:N	1:B:393:CYS:HG	2.13	0.46
1:B:840:GLN:HG2	1:B:859:THR:HG22	1.97	0.46
1:A:838:VAL:HG12	1:A:861:ILE:HG12	1.98	0.45
1:B:1281:ARG:O	1:B:1287:HIS:NE2	2.49	0.45
2:G:45:LEU:HA	2:G:75:SER:HB3	1.98	0.45
1:A:407:ASP:HB2	1:A:410:SER:HB2	1.98	0.45
1:A:1361:LYS:HE2	1:A:1361:LYS:HB2	1.86	0.45
2:G:107:LEU:HD13	2:G:107:LEU:HA	1.83	0.45
1:B:688:PRO:O	2:C:123:ARG:NH2	2.49	0.45
1:A:450:THR:HG21	1:A:462:GLY:HA2	1.99	0.45
1:A:647:SER:OG	1:A:704:GLU:OE1	2.31	0.45
1:A:1011:SER:HB3	1:B:1174:ASP:HA	1.98	0.45
1:B:57:ILE:HG13	1:B:76:GLY:HA2	1.99	0.45
1:B:1516:PHE:CG	1:B:1517:PRO:HD3	2.52	0.45
1:A:740:ALA:HB1	1:A:768:GLU:HG2	1.99	0.45
1:A:920:GLU:HB2	1:A:923:GLU:HB2	1.99	0.45
1:A:1064:LEU:HA	1:A:1064:LEU:HD13	1.85	0.45
2:C:197:CYS:SG	2:C:198:GLU:N	2.89	0.45
1:A:324:SER:O	1:A:328:ARG:NH1	2.50	0.45
1:B:190:SER:HA	1:B:193:GLU:HG2	1.97	0.45
1:B:40:THR:HB	1:B:179:TRP:HB2	1.98	0.44
1:B:1158:CYS:SG	1:B:1159:THR:N	2.90	0.44
1:A:1344:GLY:H	1:A:1346:TYR:HD1	1.64	0.44
1:A:1381:ASP:N	1:A:1381:ASP:OD1	2.49	0.44
1:B:841:TYR:O	1:B:857:ALA:HA	2.18	0.44
1:A:841:TYR:O	1:A:857:ALA:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:587:GLN:H	1:B:587:GLN:HG2	1.66	0.44
2:C:152:ASN:OD1	2:C:152:ASN:N	2.50	0.44
1:A:830:ASP:OD1	1:A:830:ASP:N	2.50	0.44
1:A:961:ILE:H	1:A:961:ILE:HG12	1.64	0.44
1:B:75:VAL:HG22	1:B:92:PHE:HD1	1.82	0.44
1:B:923:GLU:HG2	1:B:927:SER:HB3	2.00	0.44
2:G:197:CYS:SG	2:G:198:GLU:N	2.91	0.44
2:C:129:ARG:NH1	2:C:169:GLU:OE1	2.43	0.44
1:B:647:SER:OG	1:B:704:GLU:OE1	2.30	0.43
1:B:1492:ASN:ND2	1:B:1527:ALA:O	2.47	0.43
1:B:1294:LYS:HD3	1:B:1316:LYS:HZ1	1.82	0.43
1:B:1446:PRO:HG2	1:B:1449:LEU:HB2	2.00	0.43
1:A:95:LYS:HB2	1:A:102:VAL:HB	2.01	0.43
1:A:1479:GLU:H	1:A:1491:ASN:HD21	1.66	0.43
1:B:562:ASP:OD1	1:B:562:ASP:N	2.41	0.43
1:B:974:LYS:HB3	1:B:1030:TYR:HA	2.00	0.43
2:C:135:LEU:O	2:C:139:CYS:HB2	2.17	0.43
1:A:495:ARG:HA	1:A:499:GLU:HB2	2.01	0.43
1:A:1482:MET:HE1	1:A:1496:CYS:HB3	1.99	0.43
1:B:389:ASP:HB2	1:B:392:GLU:HB2	1.99	0.43
1:B:417:ASP:OD2	1:B:419:ASN:ND2	2.42	0.43
1:B:1348:CYS:HA	1:B:1358:CYS:HA	1.99	0.43
1:A:389:ASP:HB2	1:A:392:GLU:HB2	2.01	0.43
1:A:446:ALA:HB1	1:A:466:LEU:HA	2.01	0.43
1:B:846:ILE:HG22	1:B:851:GLU:HA	2.00	0.43
1:A:1172:ARG:HG3	1:A:1196:LYS:HG2	2.01	0.43
1:B:933:VAL:HG11	1:B:1020:ILE:HD13	2.01	0.43
1:B:1334:THR:HG23	1:B:1352:PHE:HB3	2.01	0.42
1:B:1457:VAL:HG13	1:B:1467:PRO:HG2	2.00	0.42
1:A:923:GLU:HG2	1:A:927:SER:HB3	2.00	0.42
1:B:726:ASP:N	1:B:726:ASP:OD1	2.51	0.42
1:B:1002:THR:OG1	1:B:1003:THR:N	2.52	0.42
1:A:103:THR:HG22	1:A:143:GLN:HE21	1.84	0.42
1:A:810:ARG:HG2	1:A:812:PRO:HD2	2.00	0.42
1:A:91:PHE:HA	1:A:105:ILE:O	2.19	0.42
1:A:1516:PHE:CD2	1:A:1517:PRO:HD3	2.54	0.42
1:B:74:VAL:HG13	1:B:93:SER:HB2	2.00	0.42
1:B:550:THR:HA	1:B:551:PRO:HD3	1.95	0.42
1:A:705:LEU:HD12	1:A:773:ILE:HD11	2.02	0.42
1:B:28:LEU:HD22	1:B:158:LEU:HD22	2.02	0.42
1:A:604:HIS:ND1	1:A:866:TYR:OH	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1463:LEU:HG	1:A:1465:TRP:H	1.85	0.42
1:A:686:VAL:HG11	1:A:692:PRO:HA	2.01	0.42
2:G:69:GLU:OE1	2:G:82:HIS:NE2	2.53	0.42
1:B:1344:GLY:H	1:B:1346:TYR:HD1	1.68	0.42
1:A:812:PRO:HA	1:A:813:PRO:HD3	1.92	0.41
1:B:26:LEU:HD12	1:B:160:LEU:HD23	2.01	0.41
1:A:1488:ASP:HA	1:A:1516:PHE:HD2	1.85	0.41
1:B:1345:LEU:HG	1:B:1465:TRP:CH2	2.54	0.41
1:A:74:VAL:HG13	1:A:93:SER:HB2	2.02	0.41
1:B:91:PHE:HA	1:B:105:ILE:O	2.21	0.41
1:B:493:VAL:HG13	1:B:556:MET:HB2	2.01	0.41
1:A:70:ASP:OD1	1:A:70:ASP:N	2.47	0.41
1:A:840:GLN:HG2	1:A:859:THR:HG22	2.02	0.41
1:B:1024:VAL:HG13	1:B:1094:SER:HB2	2.01	0.41
1:B:605:THR:OG1	1:B:606:THR:N	2.52	0.41
1:B:947:ALA:H	1:B:962:ILE:HD11	1.85	0.41
1:A:1428:ASP:OD1	1:A:1428:ASP:N	2.51	0.41
1:B:943:TRP:CD1	1:B:964:GLN:HG2	2.56	0.41
1:A:493:VAL:HG13	1:A:556:MET:HB2	2.01	0.41
1:A:830:ASP:OD2	1:A:841:TYR:OH	2.36	0.41
1:B:507:CYS:HB2	1:B:516:THR:HG23	2.03	0.41
1:B:1457:VAL:HG22	1:B:1467:PRO:HB2	2.02	0.41
1:A:240:THR:O	1:A:240:THR:OG1	2.39	0.41
1:A:267:PHE:HZ	1:A:856:PRO:HD3	1.86	0.40
1:A:1302:HIS:ND1	1:A:1303:VAL:O	2.53	0.40
1:B:450:THR:HG21	1:B:462:GLY:HA2	2.02	0.40
2:G:88:PHE:HD1	2:G:88:PHE:HA	1.71	0.40
1:B:446:ALA:HB1	1:B:466:LEU:HA	2.03	0.40
1:B:1294:LYS:HB2	1:B:1316:LYS:HZ3	1.86	0.40
1:B:481:ILE:O	1:B:484:ILE:HB	2.21	0.40
1:B:151:LEU:HD13	1:B:151:LEU:HA	1.98	0.40
2:G:52:GLU:H	2:G:52:GLU:HG3	1.76	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1450/1944 (75%)	1405 (97%)	45 (3%)	0	100	100
1	B	1450/1944 (75%)	1399 (96%)	51 (4%)	0	100	100
2	C	169/302 (56%)	162 (96%)	7 (4%)	0	100	100
2	G	169/302 (56%)	163 (96%)	6 (4%)	0	100	100
All	All	3238/4492 (72%)	3129 (97%)	109 (3%)	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	1284/1676 (77%)	1219 (95%)	65 (5%)	24	51
1	B	1284/1676 (77%)	1228 (96%)	56 (4%)	28	54
2	C	148/251 (59%)	133 (90%)	15 (10%)	7	28
2	G	148/251 (59%)	136 (92%)	12 (8%)	11	37
All	All	2864/3854 (74%)	2716 (95%)	148 (5%)	27	50

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ARG
1	A	43	VAL
1	A	60	LEU
1	A	67	ILE
1	A	74	VAL
1	A	102	VAL
1	A	103	THR
1	A	152	THR

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Mol	Chain	Res	Type
1	A	158	LEU
1	A	240	THR
1	A	250	THR
1	A	252	CYS
1	A	272	VAL
1	A	320	VAL
1	A	331	LEU
1	A	412	HIS
1	A	454	ASP
1	A	465	VAL
1	A	477	THR
1	A	486	HIS
1	A	507	CYS
1	A	514	PHE
1	A	544	PHE
1	A	609	VAL
1	A	611	LEU
1	A	669	VAL
1	A	701	CYS
1	A	723	VAL
1	A	727	TRP
1	A	755	CYS
1	A	756	ASP
1	A	777	THR
1	A	795	THR
1	A	808	VAL
1	A	843	VAL
1	A	845	THR
1	A	849	THR
1	A	858	VAL
1	A	918	VAL
1	A	928	ILE
1	A	940	LEU
1	A	961	ILE
1	A	970	VAL
1	A	975	VAL
1	A	1004	PHE
1	A	1045	THR
1	A	1056	VAL
1	A	1064	LEU
1	A	1096	VAL
1	A	1098	LEU

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Mol	Chain	Res	Type
1	A	1104	PHE
1	A	1159	THR
1	A	1190	THR
1	A	1239	GLN
1	A	1272	VAL
1	A	1282	CYS
1	A	1320	THR
1	A	1371	LEU
1	A	1375	VAL
1	A	1410	LEU
1	A	1412	CYS
1	A	1460	THR
1	A	1465	TRP
1	A	1513	VAL
1	A	1514	THR
1	B	22	ARG
1	B	43	VAL
1	B	74	VAL
1	B	78	HIS
1	B	102	VAL
1	B	103	THR
1	B	124	ASP
1	B	157	VAL
1	B	174	GLU
1	B	181	VAL
1	B	232	ASN
1	B	250	THR
1	B	272	VAL
1	B	320	VAL
1	B	331	LEU
1	B	412	HIS
1	B	445	LEU
1	B	465	VAL
1	B	507	CYS
1	B	544	PHE
1	B	609	VAL
1	B	611	LEU
1	B	669	VAL
1	B	701	CYS
1	B	711	LEU
1	B	715	SER
1	B	727	TRP

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Mol	Chain	Res	Type
1	B	755	CYS
1	B	795	THR
1	B	808	VAL
1	B	843	VAL
1	B	845	THR
1	B	858	VAL
1	B	918	VAL
1	B	928	ILE
1	B	940	LEU
1	B	975	VAL
1	B	1004	PHE
1	B	1056	VAL
1	B	1069	VAL
1	B	1078	HIS
1	B	1109	LEU
1	B	1159	THR
1	B	1190	THR
1	B	1204	ASP
1	B	1272	VAL
1	B	1282	CYS
1	B	1320	THR
1	B	1371	LEU
1	B	1375	VAL
1	B	1410	LEU
1	B	1412	CYS
1	B	1465	TRP
1	B	1488	ASP
1	B	1513	VAL
1	B	1514	THR
2	C	48	GLN
2	C	63	VAL
2	C	78	ILE
2	C	86	MET
2	C	88	PHE
2	C	107	LEU
2	C	139	CYS
2	C	159	MET
2	C	165	LEU
2	C	167	LEU
2	C	181	CYS
2	C	197	CYS
2	C	201	TRP

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Mol	Chain	Res	Type
2	C	204	LEU
2	C	205	CYS
2	G	52	GLU
2	G	63	VAL
2	G	88	PHE
2	G	139	CYS
2	G	152	ASN
2	G	167	LEU
2	G	176	ASN
2	G	179	LEU
2	G	197	CYS
2	G	201	TRP
2	G	204	LEU
2	G	205	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1239	GLN
1	A	1491	ASN
2	C	176	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

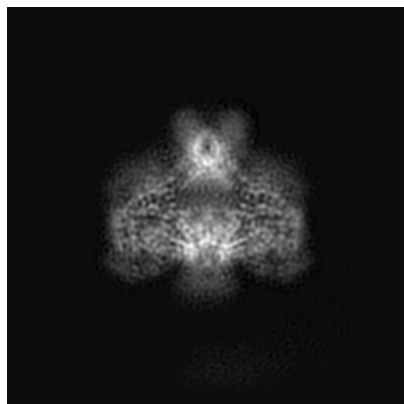
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34739. These allow visual inspection of the internal detail of the map and identification of artifacts.

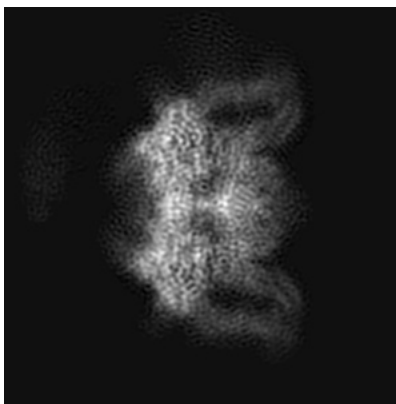
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

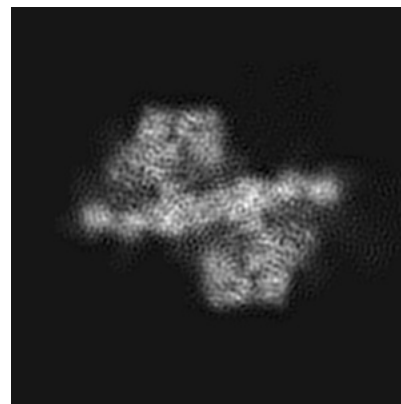
6.1.1 Primary map



X

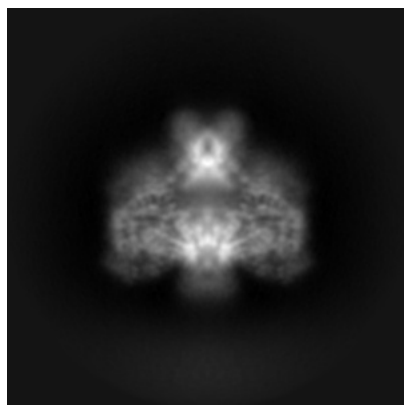


Y

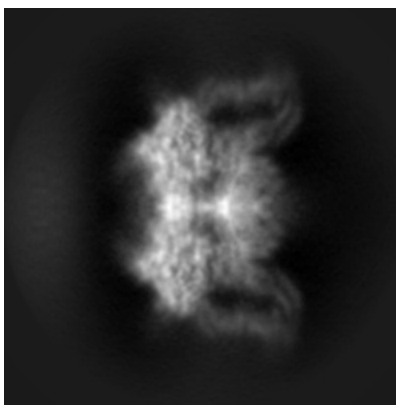


Z

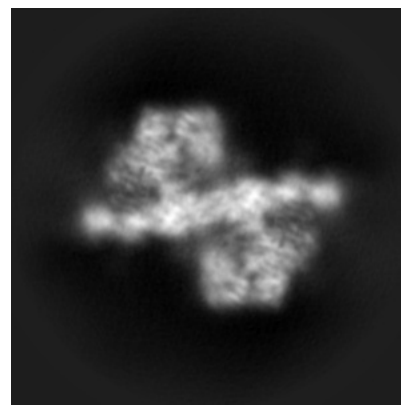
6.1.2 Raw map



X



Y

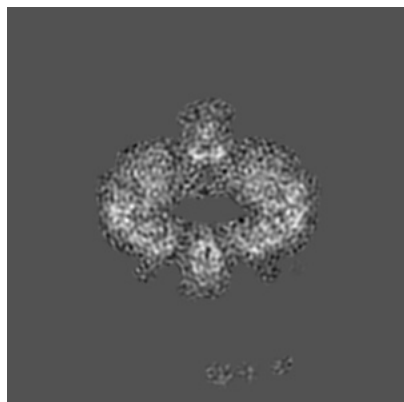


Z

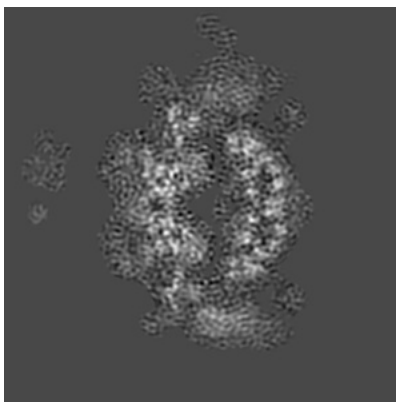
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

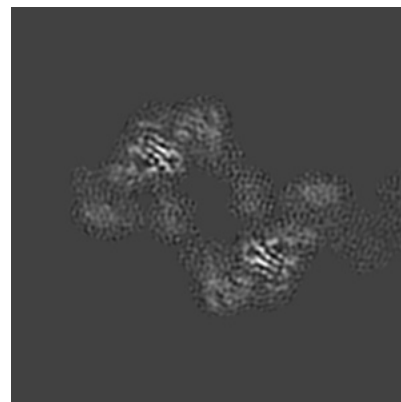
6.2.1 Primary map



X Index: 128

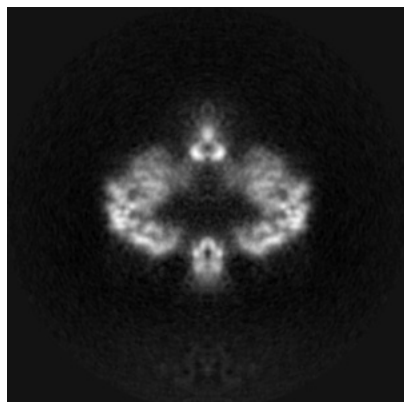


Y Index: 128

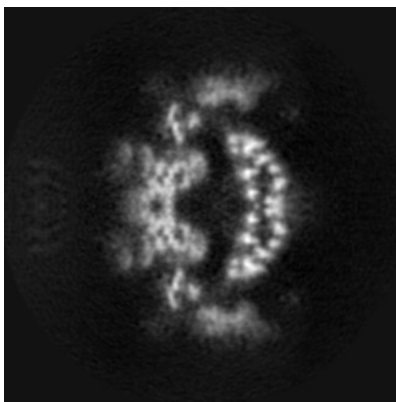


Z Index: 128

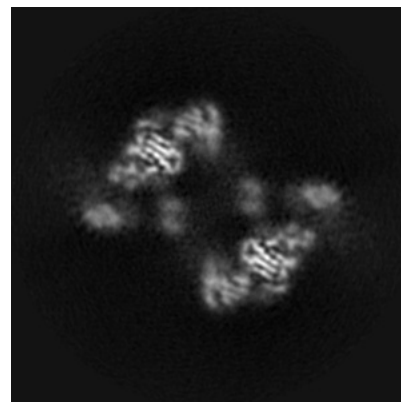
6.2.2 Raw map



X Index: 128



Y Index: 128

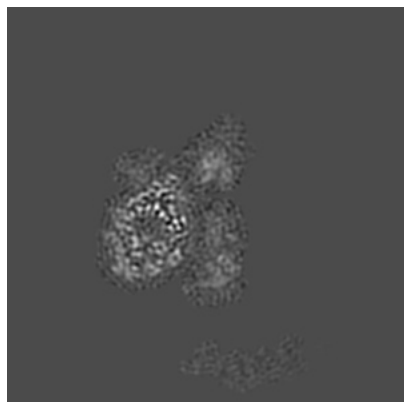


Z Index: 128

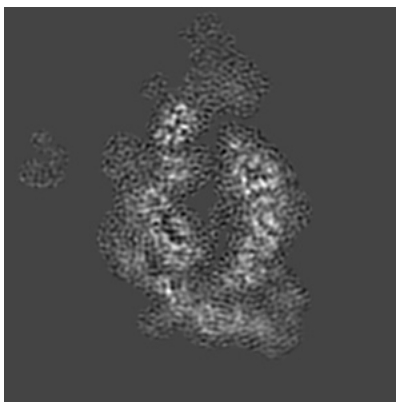
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

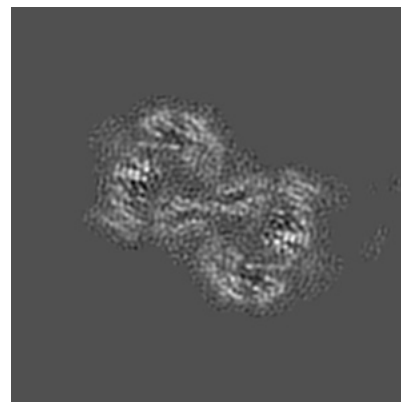
6.3.1 Primary map



X Index: 164

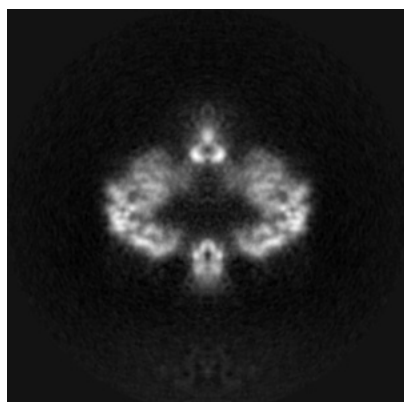


Y Index: 123

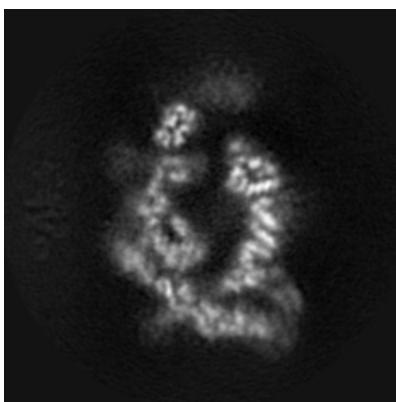


Z Index: 106

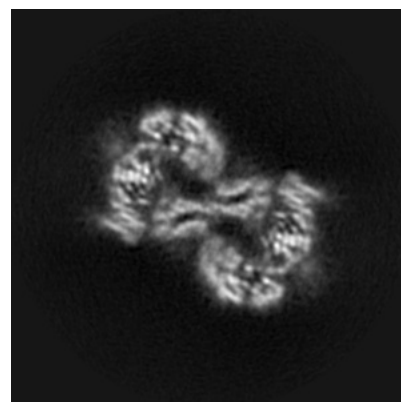
6.3.2 Raw map



X Index: 128



Y Index: 122



Z Index: 106

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0217. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

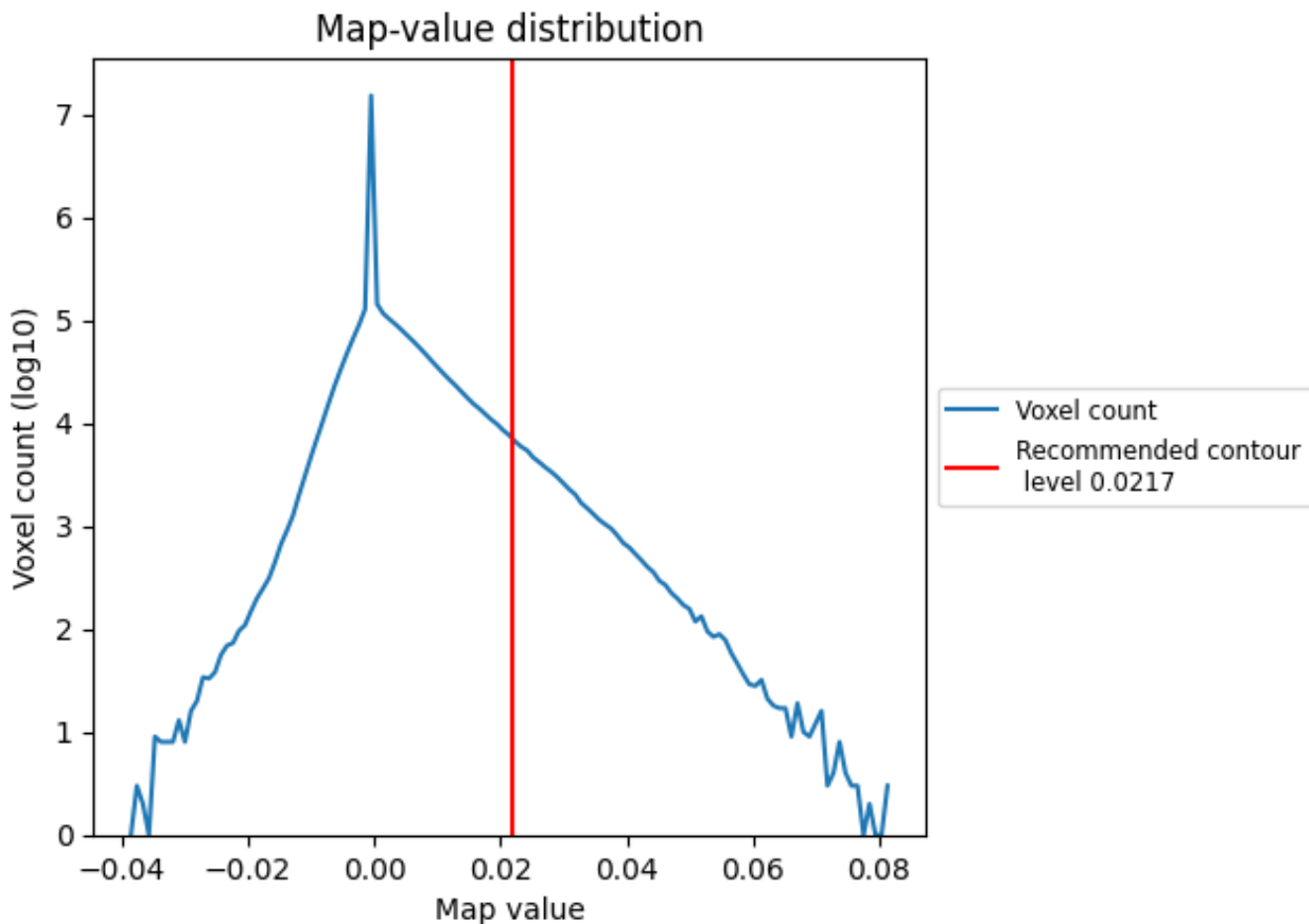
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

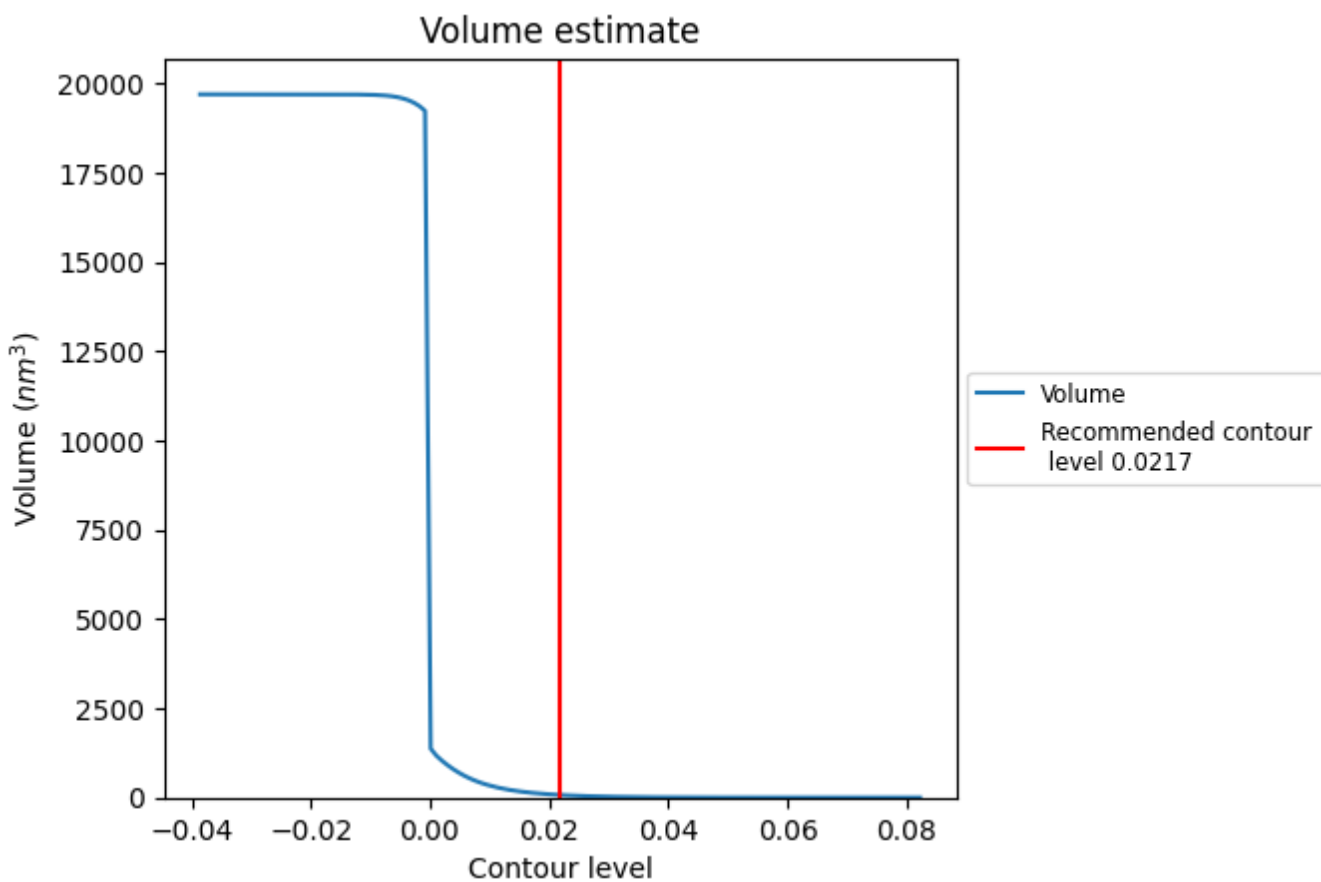
This section contains the results of statistical analysis of the map.

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.

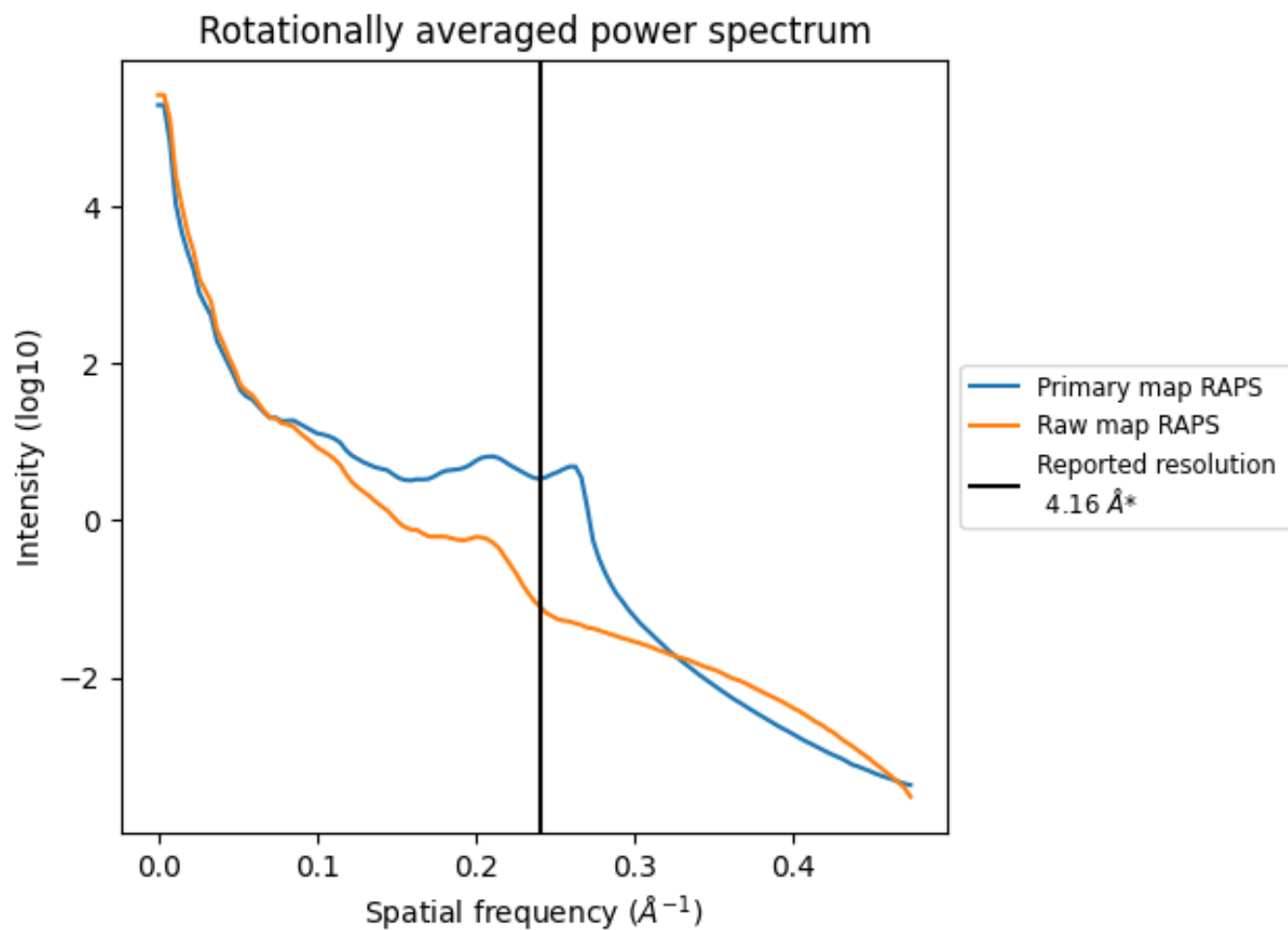
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 73 nm³; this corresponds to an approximate mass of 66 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum i

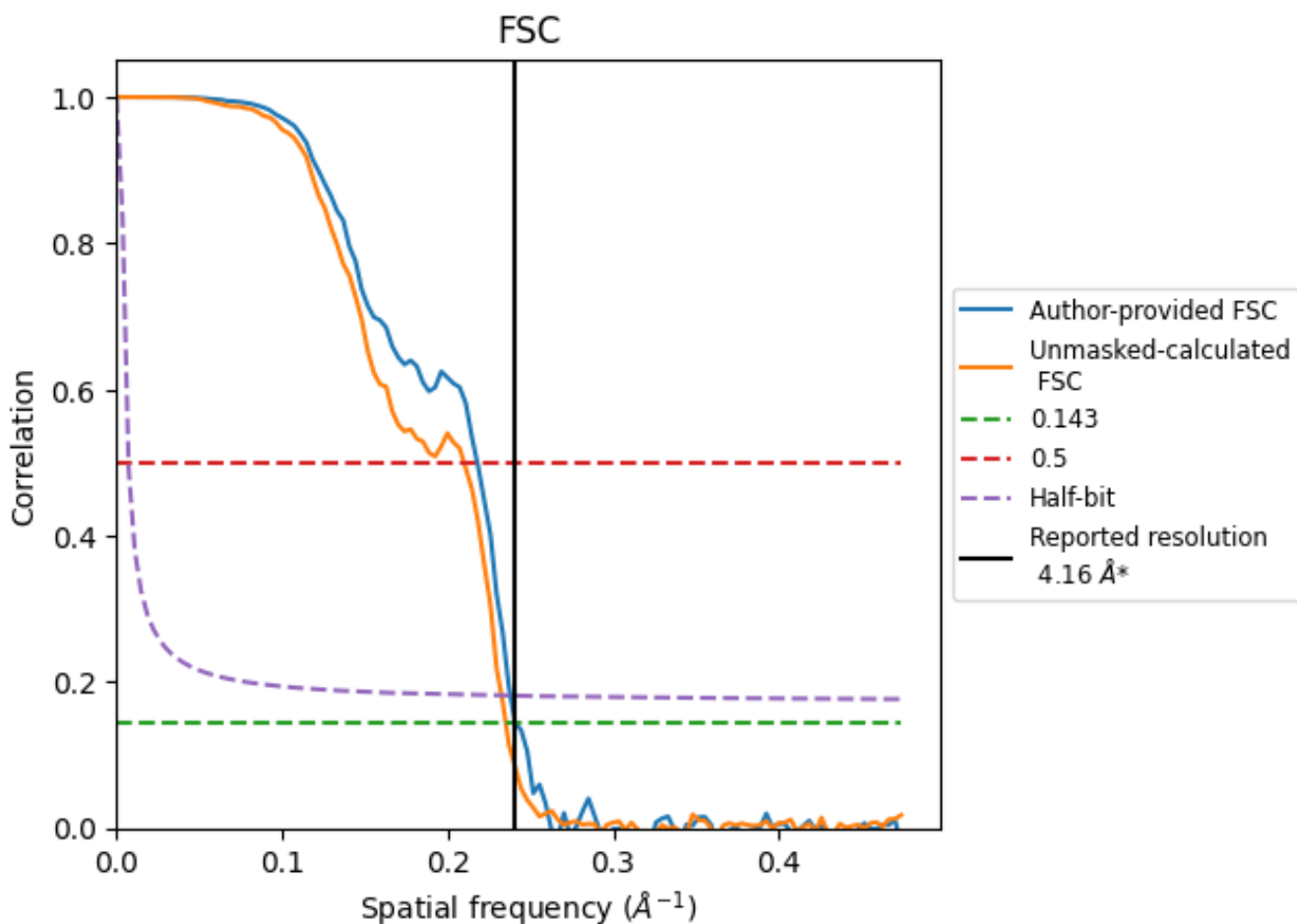


*Reported resolution corresponds to spatial frequency of 0.240 Å⁻¹

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 0.240 Å⁻¹

8.2 Resolution estimates [i](#)

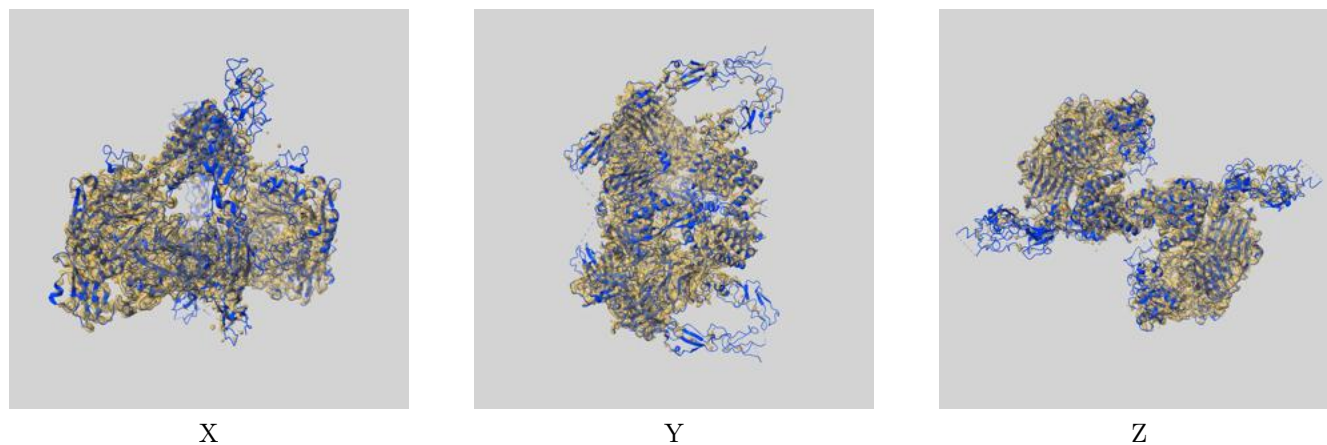
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.16	-	-
Author-provided FSC curve	4.15	4.59	4.20
Unmasked-calculated*	4.25	4.76	4.30

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

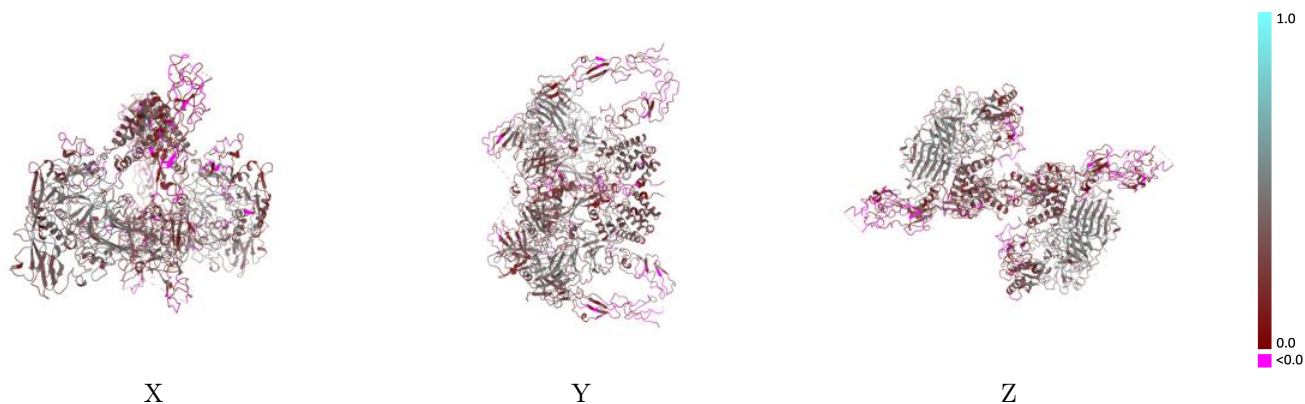
This section contains information regarding the fit between EMDB map EMD-34739 and PDB model 8HGH. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



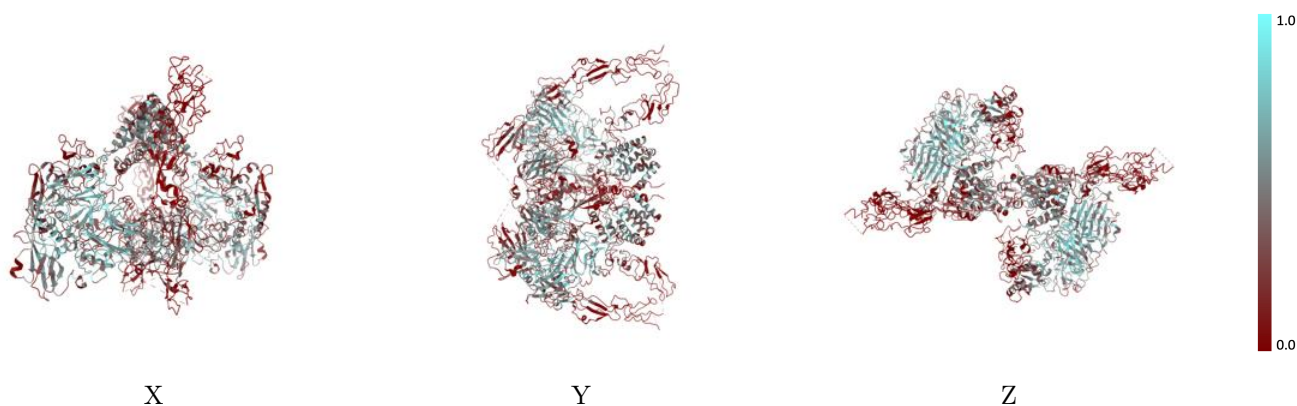
The images above show the 3D surface view of the map at the recommended contour level 0.0217 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



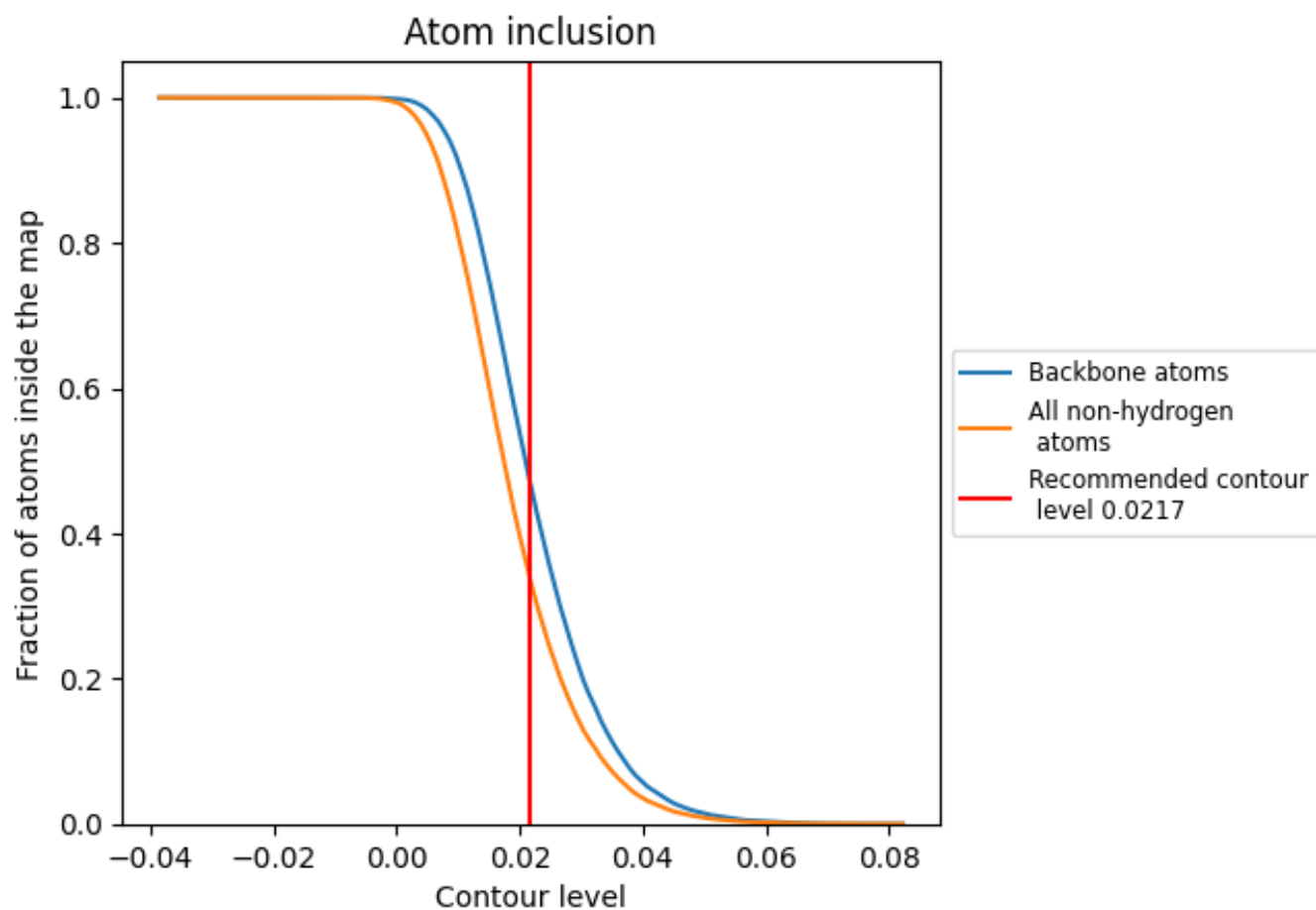
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0217).











9.4 Atom inclusion [i](#)



At the recommended contour level, 47% of all backbone atoms, 34% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.0217) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3361	 0.2950
A	 0.3265	 0.2920
B	 0.3324	 0.2970
C	 0.4088	 0.3080
G	 0.3761	 0.2910

