



wwPDB EM Validation Summary Report ⓘ

Mar 19, 2024 – 02:39 PM JST

PDB ID : 5X0Y
EMDB ID : EMD-6700
Title : Complex of Snf2-Nucleosome complex with Snf2 bound to SHL2 of the nucleosome
Authors : Li, M.; Liu, X.; Xia, X.; Chen, Z.; Li, X.
Deposited on : 2017-01-23
Resolution : 4.69 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.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

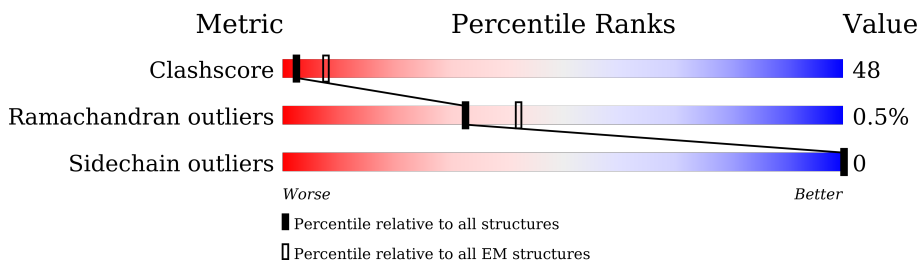
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.69 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.



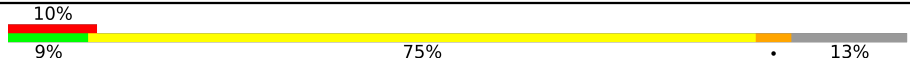
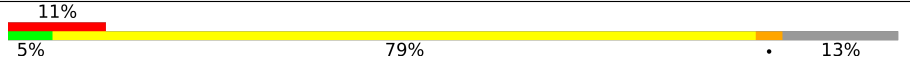
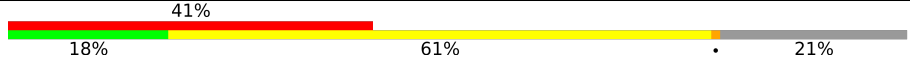
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	135	
1	E	135	
2	B	102	
2	F	102	
3	C	129	
3	G	129	
4	D	122	
4	H	122	

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Mol	Chain	Length	Quality of chain
5	I	167	
6	J	167	
7	O	735	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 16798 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 Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	98	800	505	153	139	3	0	0
1	E	95	778	491	148	136	3	0	0

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	87	703	443	142	117	1	0	0
2	F	86	672	424	130	117	1	0	0

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	C	107	811	510	158	143	0	0
3	G	107	815	513	159	143	0	0

- Molecule 4 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	93	718	451	128	137	2	0	0
4	H	93	726	457	130	137	2	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	29	THR	SER	see sequence details	UNP P02281

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Chain	Residue	Modelled	Actual	Comment	Reference
H	29	THR	SER	see sequence details	UNP P02281

- Molecule 5 is a DNA chain called DNA (167-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	I	146	2975	1413	540	876	146	0	0

- Molecule 6 is a DNA chain called DNA (167-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	J	146	3011	1425	564	876	146	0	0

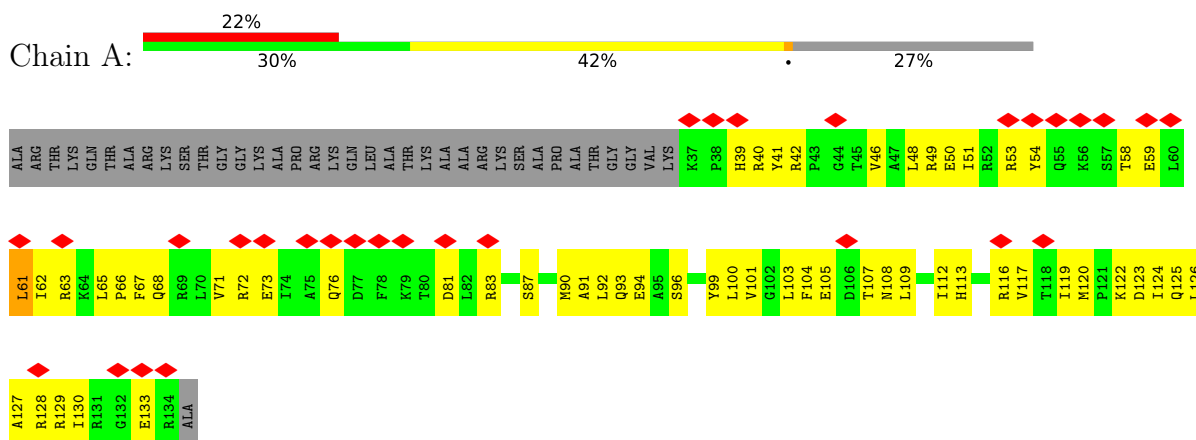
- Molecule 7 is a protein called Transcription regulatory protein SNF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	O	583	4789	3045	846	881	17	0	0

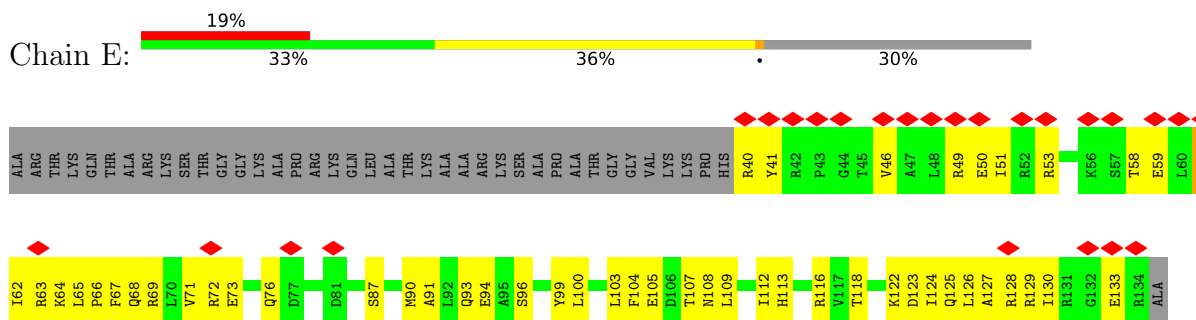
3 Residue-property plots [i](#)

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.

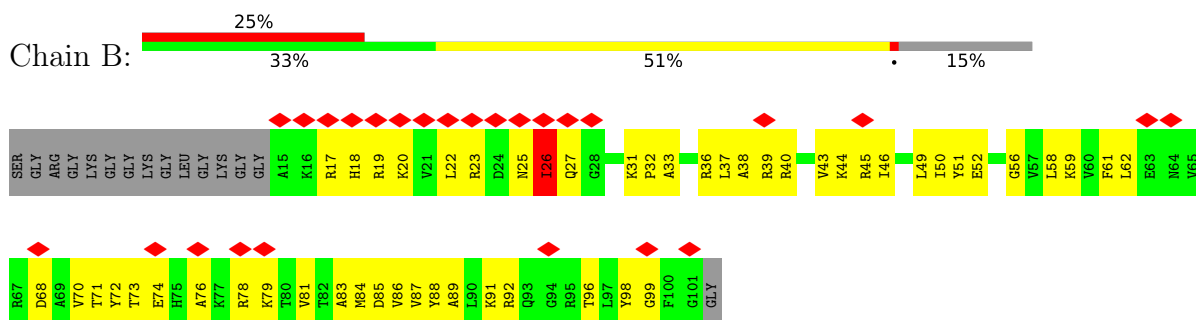
- Molecule 1: Histone H3.2



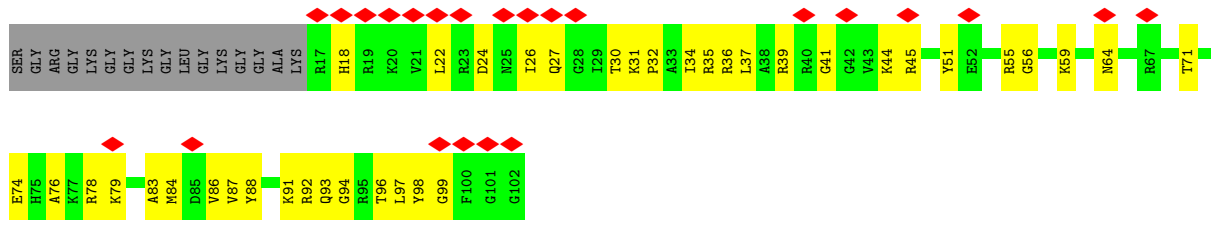
- Molecule 1: Histone H3.2



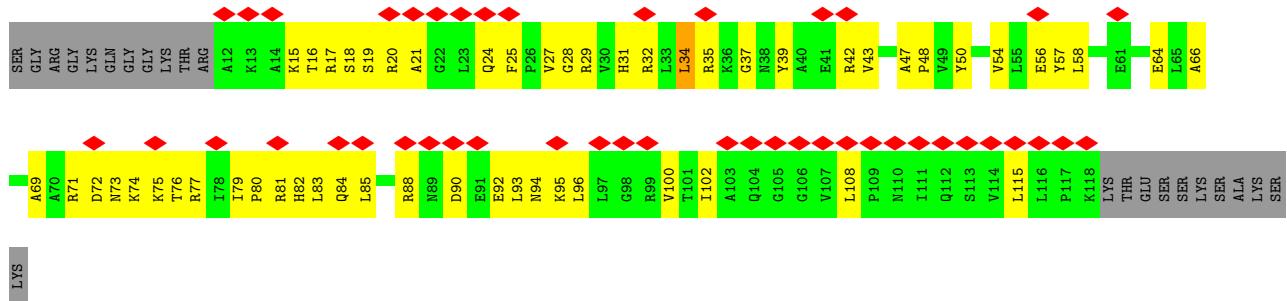
- Molecule 2: Histone H4



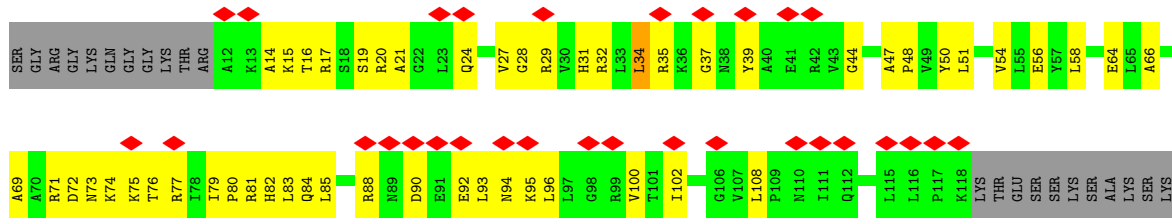
- Molecule 2: Histone H4



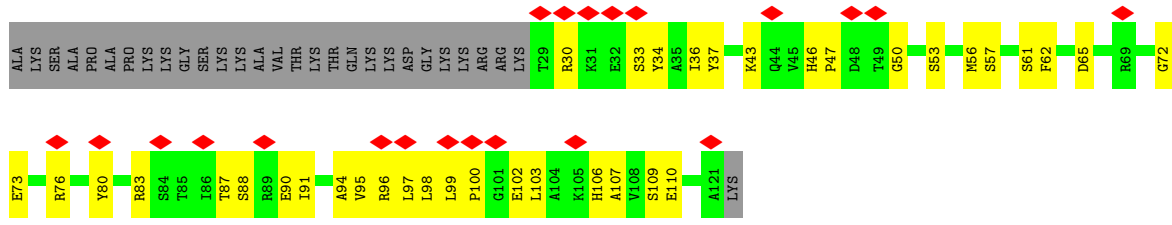
• Molecule 3: Histone H2A



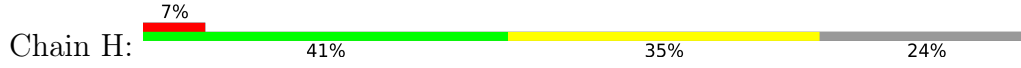
• Molecule 3: Histone H2A

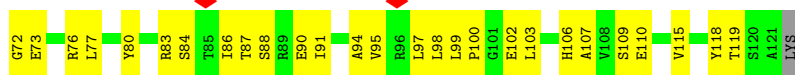
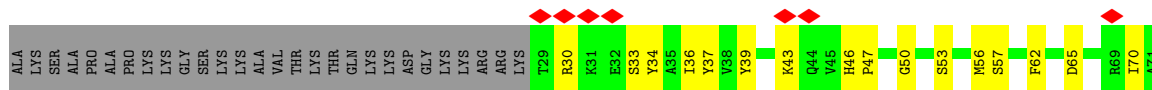


• Molecule 4: Histone H2B 1.1

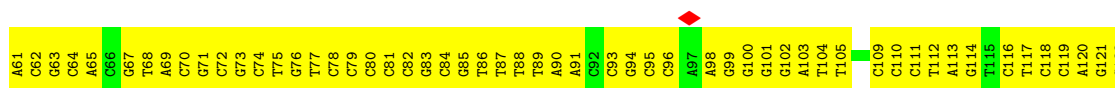
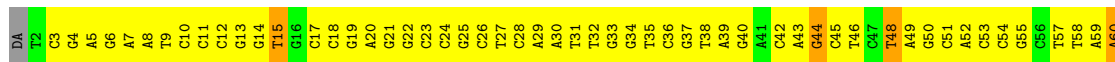
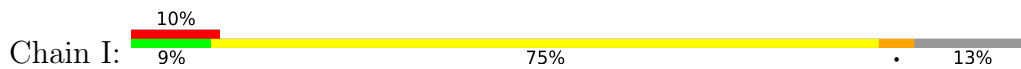


• Molecule 4: Histone H2B 1.1

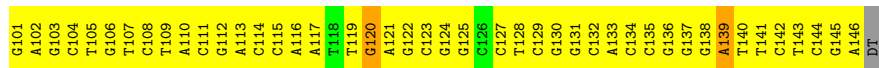
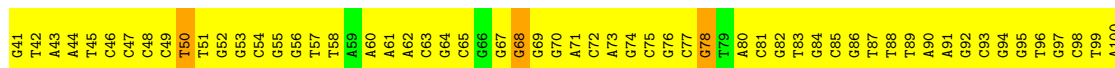
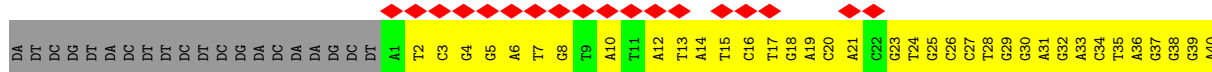
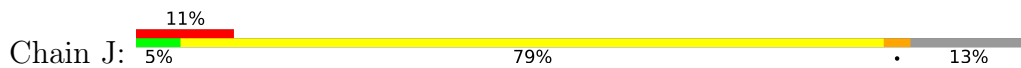




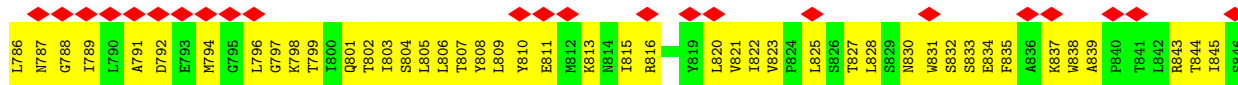
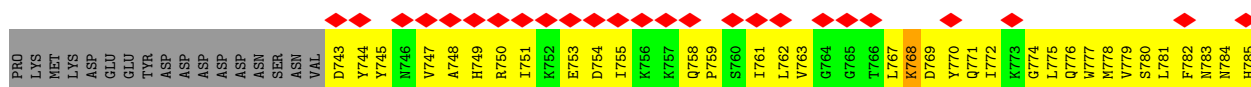
• Molecule 5: DNA (167-MER)



• Molecule 6: DNA (167-MER)



• Molecule 7: Transcription regulatory protein SNF2



THR	LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLY	SER	E1269	L1209	F1149	K1088	L1027	D967	S907	F847
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	L1210	L1211	A1150	F1089	K1028	K968	L908	K848
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	L1212	L1213	F1152	E1090	Y1029	T969	T909	G849
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	T1214	T1215	D1153	D1093	R1030	E970	N911	S850
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	L1216	L1217	S1154	R1094	L1032	L971	T912	P851
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	N1218	N1219	E1155	I1095	PHE	S972	H913	N852
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	V1220	V1221	L1160	L1096	GLY	E973	Y914	R854
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	L1222	L1223	L1161	P1097	ASP	E974	H915	K855
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	E1218	E1219	F1159	K1098	GLN	E975	A916	A856
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	V1220	V1221	L1160	L1099	ASN	T976	D917	K857
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	L1222	L1223	L1162	T1102	ASN	L977	Y918	Q858
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	E1223	E1224	S1162	G1103	LYS	L978	R919	A859
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	R1224	R1225	T1163	H1104	LYS	L979	L920	K860
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	A1225	A1226	R1164	R1105	MET	V979	I921	I861
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	Y1226	Y1227	A1165	V1106	VAL	R980	T923	A863
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	K1227	K1228	G1166	L1107	GLY	R981	G924	G864
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	L1228	L1229	G1167	I1108	LEU	H984	P926	E865
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	D1230	D1231	L1168	F1109	G1047	K985	L927	F866
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	I1231	I1232	G1169	F1110	F1048	V986	Q928	D867
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	D1232	D1233	L1170	M1112	N1049	V987	Q928	V868
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	G1233	G1234	L1171	T1113	N1050	R988	N929	V869
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	K1234	K1235	N1171	Q1114	Q1051	P989	L931	L870
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	V1235	V1236	L1172	I1115	I1052	F990	R932	T871
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	I1236	I1237	Q1173	M1116	M1053	L991	E933	F873
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	Q1237	Q1238	T1174	D1117	Q1054	L992	E833	E874
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	A1238	A1239	A1175	I1118	K1056	R993	W835	Y875
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	G1239	G1240	L1176	M1119	K1057	R994	I876	I876
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	K1240	K1241	L1177	D1120	K1058	K996	I877	I877
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	F1241	F1242	V1178	E1121	C1059	K997	L838	K878
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	D1242	D1243	I1179	F1122	C1080	F940	F940	E879
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	N1243	N1244	I1180	R1124	N1060	V999	V941	R880
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	K1244	K1245	F1181	Y1125	H1061	E1000	L942	L882
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	S1245	S1246	D1182	I1126	P1062	E1001	P943	L883
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	T1246	T1247	L1183	N1127	F1063	K1001	K944	L884
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	E1246	E1247	D1184	K1129	F1065	L1003	I945	S884
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	E1249	E1250	L1185	Y1130	E1066	P1004	F946	K885
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	Q1250	Q1251	H1186	L1131	V1068	D1005	N947	V886
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	E1251	E1252	P1187	H1136	V1069	K1006	S948	W888
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	L1253	L1254	D1190	D1134	E1070	V1007	V949	V889
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	A1252	A1253	L1191	G1135	Q1071	E1008	K950	H890
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	L1254	L1255	Q1192	H1137	I1072	K1009	S951	M891
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	R1255	R1256	Q1193	T1137	M1073	V1010	F952	I892
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	Q1194	Q1195	Q1194	K1138	P1074	V1011	F952	I893
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	D1196	D1197	D1195	S1139	T1075	K1012	D953	I894
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	R1196	R1197	R1196	D1140	R1076	C1013	E954	E895
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	A1197	A1198	H1198	E1141	E1077	K1014	G896	V896
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	H1198	H1199	H1198	R1142	E1080	M1015	G896	V896
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	R1199	R1200	R1199	S1143	D1080	M1015	G896	V896
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	I1200	I1201	I1200	E1144	I1082	S1016	G896	V896
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	G1201	G1202	G1201	L1145	W1083	L1018	M899	K900
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	Q1202	Q1203	Q1202	L1146	R1084	Q1019	K900	K900
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	K1203	K1204	K1203	R1147	V1085	Q1020	K901	A902
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	N1204	N1205	N1204	L1148	A1086	I1021	N901	A902
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	E1205	E1206	E1205	L1208	G1087	I1022	Q903	Q903
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	V1206	V1207	V1206	L1208	G1087	Y1023	S904	S904
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	R1207	R1208	R1207	L1208	G1087	Q1024	S904	S904
LYS	GLU	ASP	ALA	ILE	GLU	GLY	VAL	GLU	GLY	SER	I1208	I1209	I1208	L1208	G1087	Q1025	L906	L906

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	90725	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)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.093	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0341	Depositor
Map size (Å)	337.92, 337.92, 337.92	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.57	0/812	0.67	1/1091 (0.1%)
1	E	0.57	0/788	0.67	1/1057 (0.1%)
2	B	0.62	0/711	0.68	0/950
2	F	0.62	0/680	0.66	0/912
3	C	0.49	0/821	0.63	1/1112 (0.1%)
3	G	0.48	0/825	0.64	1/1116 (0.1%)
4	D	0.59	0/729	0.61	0/985
4	H	0.59	0/737	0.62	0/993
5	I	1.34	0/3333	1.11	6/5137 (0.1%)
6	J	1.36	1/3381 (0.0%)	1.04	4/5221 (0.1%)
7	O	0.45	0/4864	0.65	2/6536 (0.0%)
All	All	0.93	1/17681 (0.0%)	0.85	16/25110 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	E	0	1
2	B	0	1
7	O	0	5
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	68	DG	C3'-O3'	-5.87	1.36	1.44

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	120	DG	O4'-C4'-C3'	-7.85	101.29	106.00
5	I	15	DT	O4'-C4'-C3'	-7.37	101.55	104.50
5	I	48	DT	O4'-C4'-C3'	-7.21	101.61	104.50
5	I	60	DA	O4'-C1'-N9	6.42	112.50	108.00
5	I	44	DG	O4'-C4'-C3'	-6.09	102.06	104.50

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	58	THR	Peptide
2	B	26	ILE	Peptide
1	E	58	THR	Peptide
7	O	768	LYS	Peptide
7	O	839	ALA	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	800	0	829	60	0
1	E	778	0	813	45	0
2	B	703	0	757	74	0
2	F	672	0	698	44	0
3	C	811	0	849	62	0
3	G	815	0	860	51	0
4	D	718	0	725	53	0
4	H	726	0	747	45	0
5	I	2975	0	1639	262	0
6	J	3011	0	1639	309	0
7	O	4789	0	4882	638	0
All	All	16798	0	14438	1477	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 48.

The worst 5 of 1477 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)
7:O:1233:GLY:O	7:O:1237:GLN:HB2	1.22	1.32
7:O:876:ILE:O	7:O:880:ARG:HB2	1.41	1.17
7:O:1232:ASP:O	7:O:1236:ILE:HB	1.42	1.16
7:O:1301:ASP:O	7:O:1305:SER:HB2	1.60	1.02
5:I:111:DC:O2	6:J:37:DG:N2	1.93	1.01

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	96/135 (71%)	88 (92%)	8 (8%)	0	100	100
1	E	93/135 (69%)	85 (91%)	8 (9%)	0	100	100
2	B	85/102 (83%)	69 (81%)	15 (18%)	1 (1%)	13	50
2	F	84/102 (82%)	81 (96%)	3 (4%)	0	100	100
3	C	105/129 (81%)	99 (94%)	6 (6%)	0	100	100
3	G	105/129 (81%)	99 (94%)	6 (6%)	0	100	100
4	D	91/122 (75%)	83 (91%)	8 (9%)	0	100	100
4	H	91/122 (75%)	83 (91%)	8 (9%)	0	100	100
7	O	569/735 (77%)	483 (85%)	81 (14%)	5 (1%)	17	56
All	All	1319/1711 (77%)	1170 (89%)	143 (11%)	6 (0%)	32	68

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	26	ILE
7	O	1163	THR
7	O	958	THR
7	O	979	VAL
7	O	679	ILE

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	84/110 (76%)	84 (100%)	0	100	100
1	E	82/110 (74%)	82 (100%)	0	100	100
2	B	72/78 (92%)	72 (100%)	0	100	100
2	F	67/78 (86%)	67 (100%)	0	100	100
3	C	81/101 (80%)	81 (100%)	0	100	100
3	G	82/101 (81%)	82 (100%)	0	100	100
4	D	77/102 (76%)	77 (100%)	0	100	100
4	H	79/102 (78%)	79 (100%)	0	100	100
7	O	525/667 (79%)	525 (100%)	0	100	100
All	All	1149/1449 (79%)	1149 (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 23 such sidechains are listed below:

Mol	Chain	Res	Type
7	O	929	ASN
7	O	1051	GLN
7	O	1025	GLN
7	O	1054	GLN
2	F	93	GLN

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

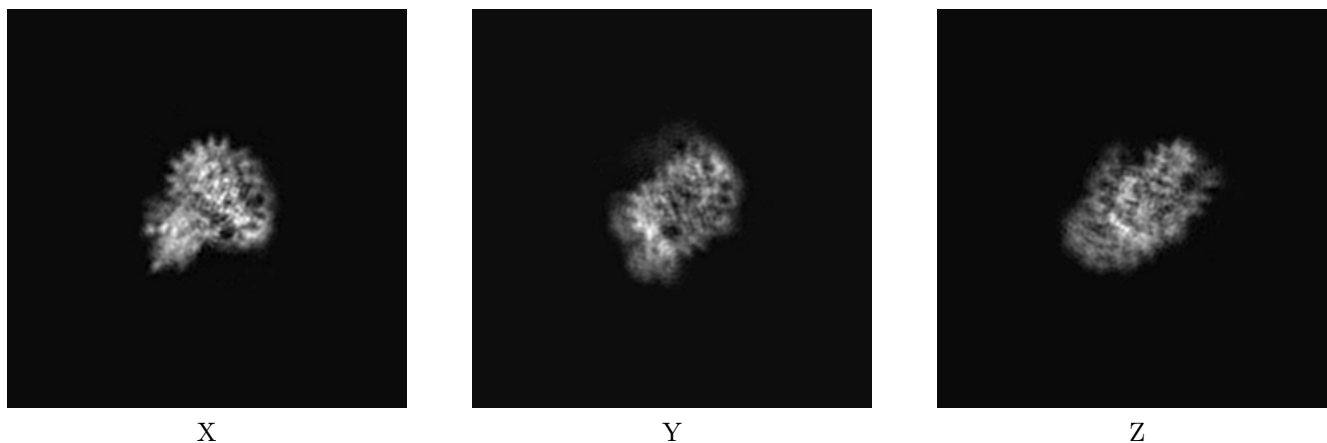
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6700. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

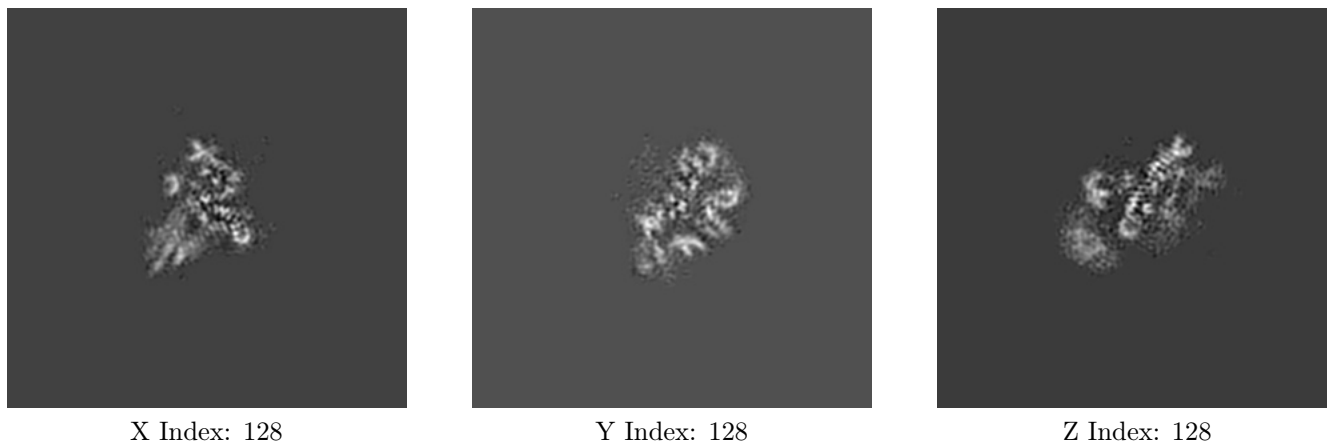
6.1.1 Primary map



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

6.2 Central slices [i](#)

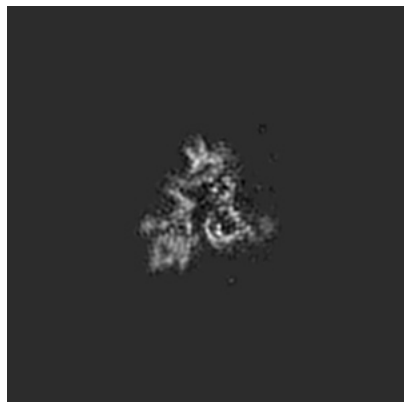
6.2.1 Primary map



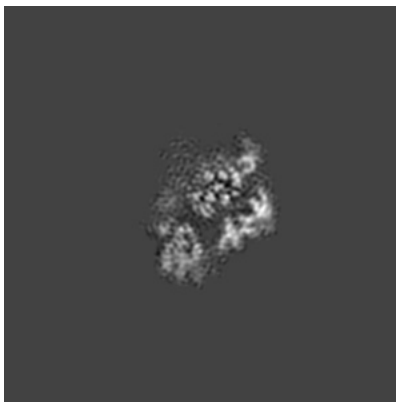
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

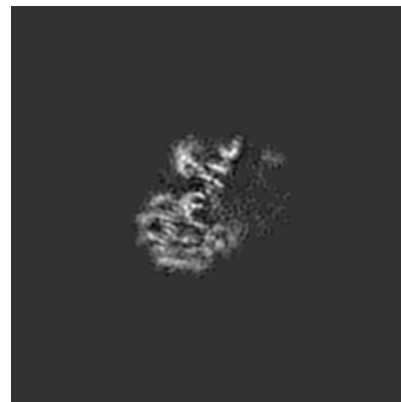
6.3.1 Primary map



X Index: 118



Y Index: 122

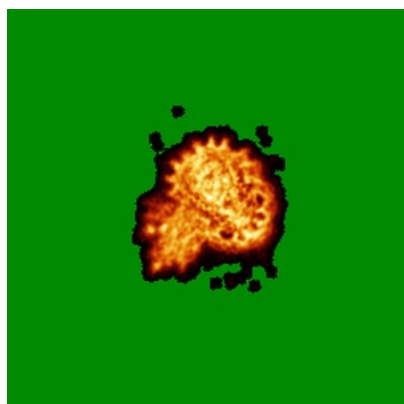


Z Index: 113

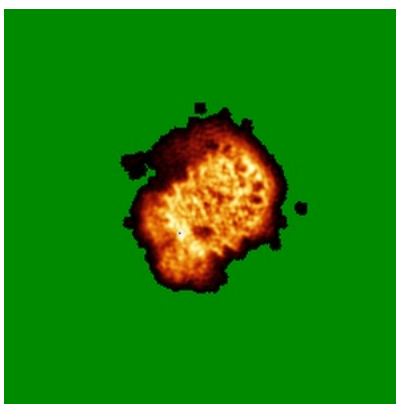
The images above show the largest variance slices of the map in three orthogonal directions.

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

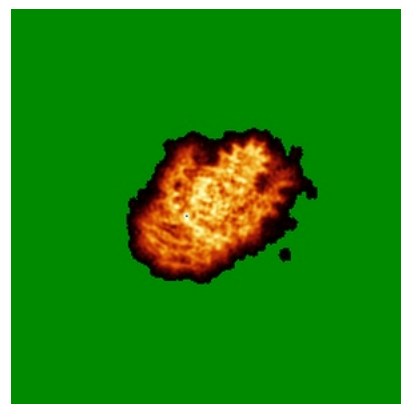
6.4.1 Primary map



X



Y

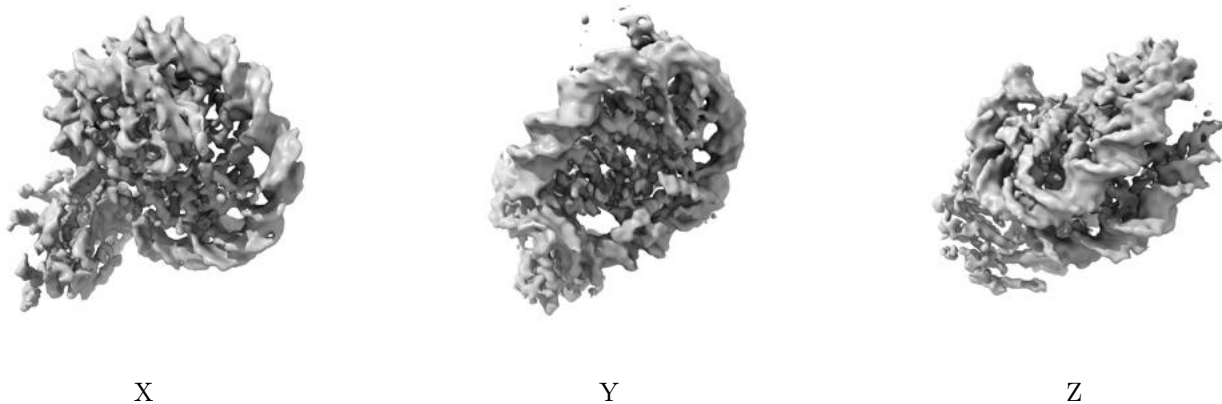


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0341. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

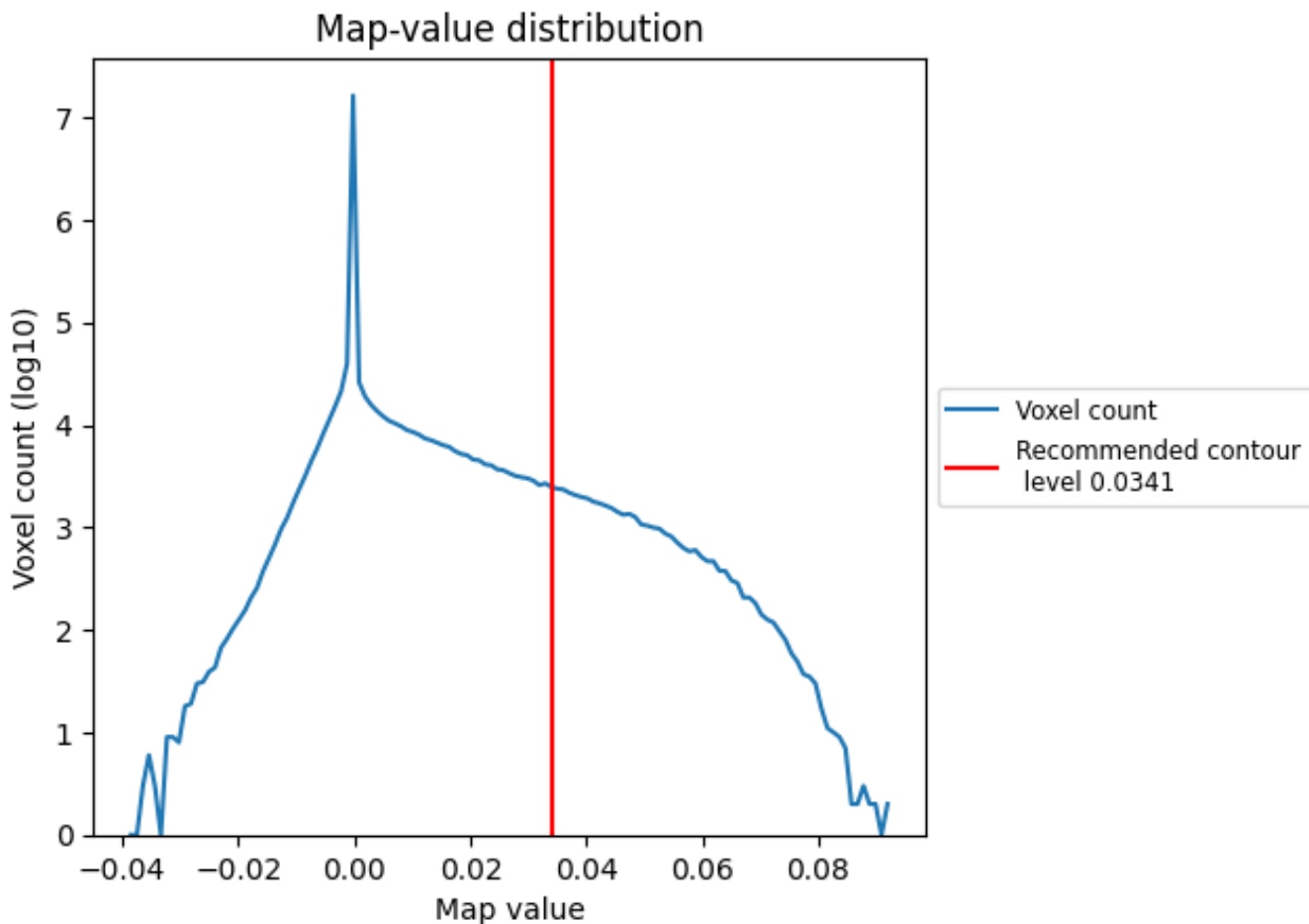
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

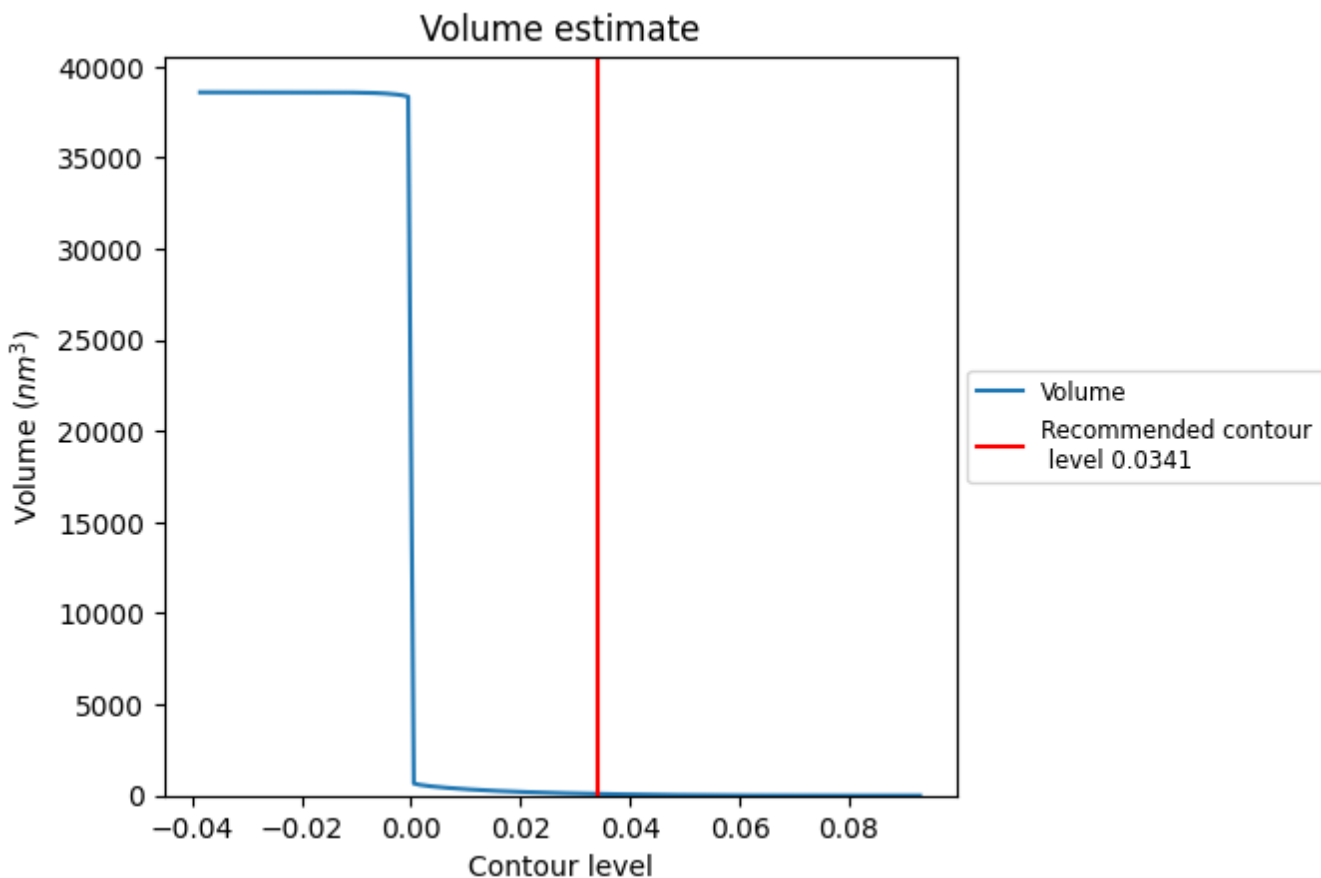
This section contains the results of statistical analysis of the map.

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.

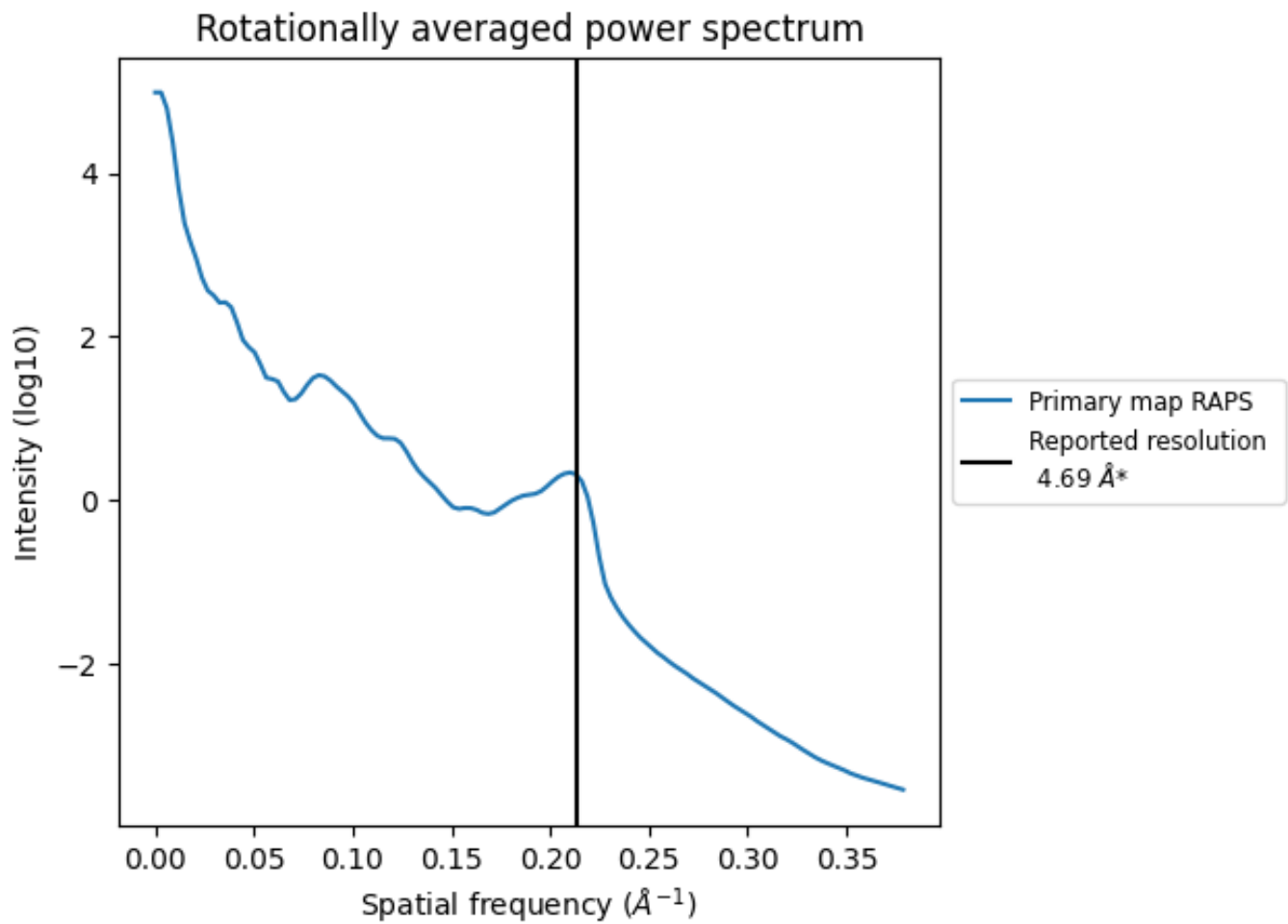
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 91 nm³; this corresponds to an approximate mass of 82 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 0.213\AA^{-1}

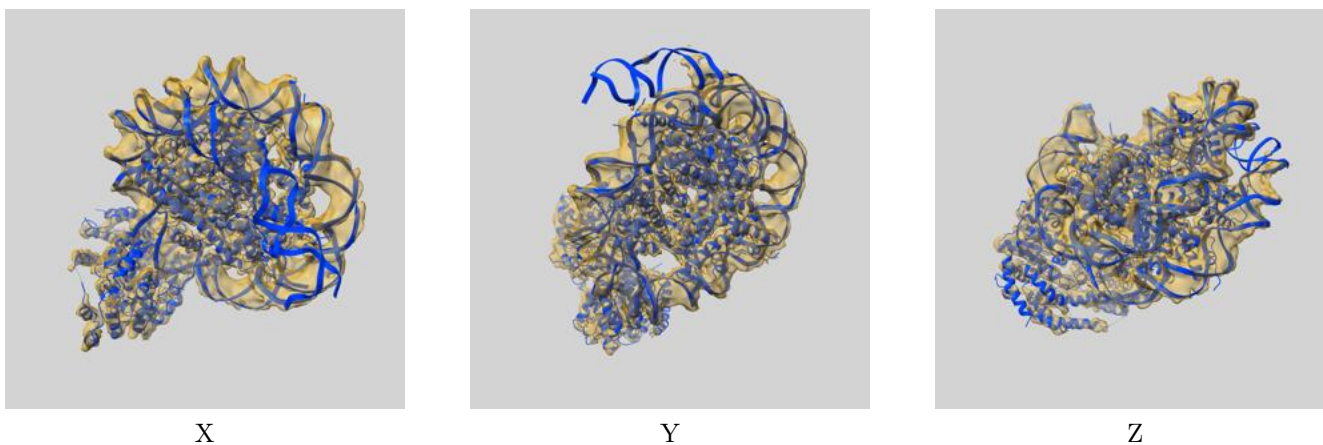
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

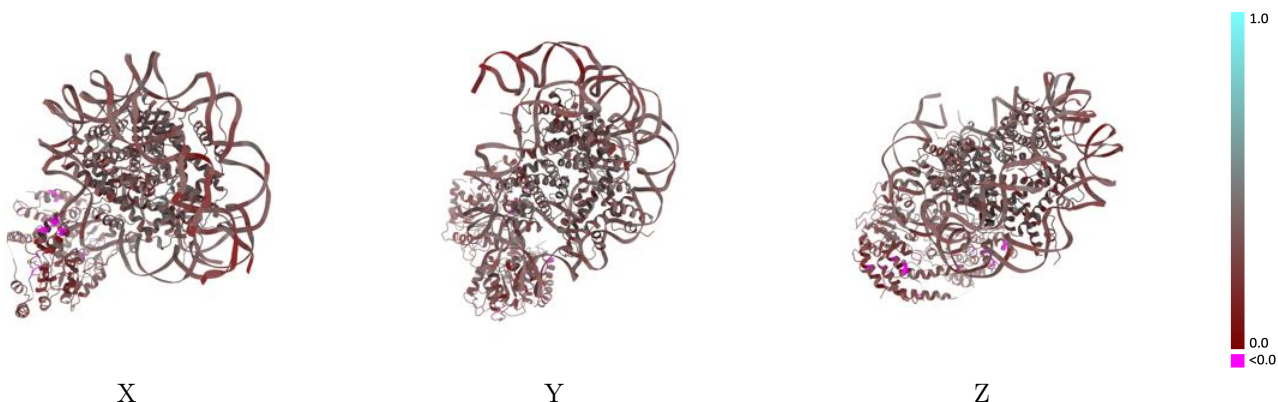
This section contains information regarding the fit between EMDB map EMD-6700 and PDB model 5X0Y. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



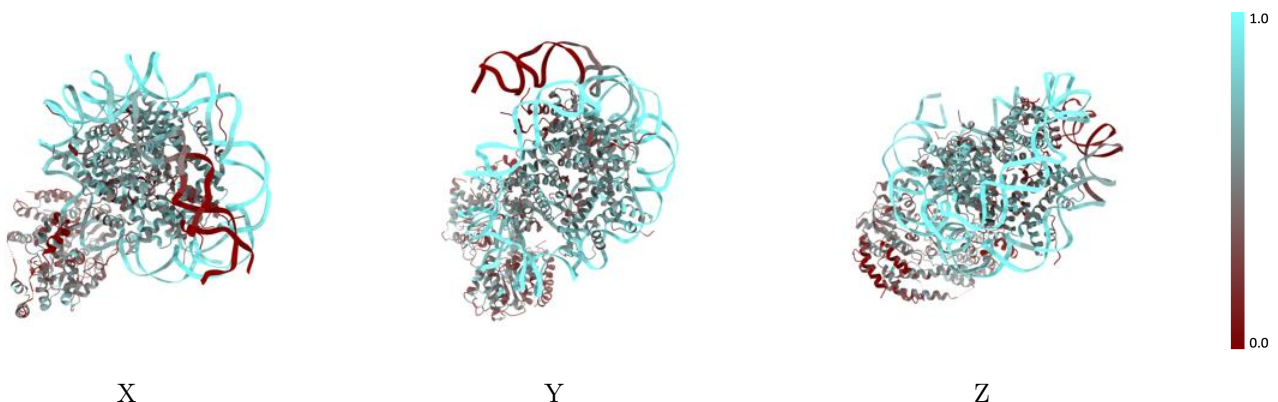
The images above show the 3D surface view of the map at the recommended contour level 0.0341 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



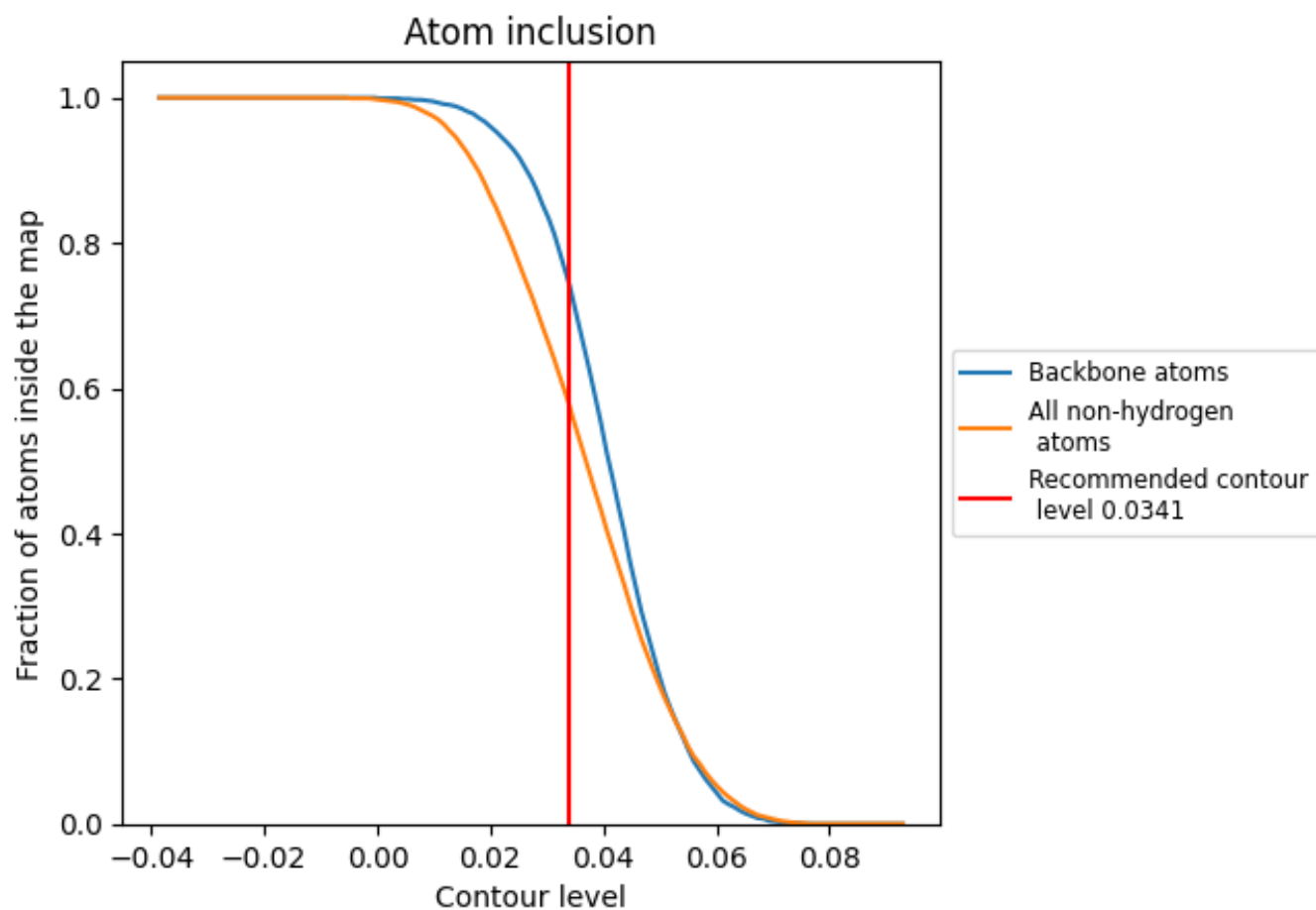
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0341).

























9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 57% 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 (0.0341) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5740	 0.3150
A	 0.5320	 0.3630
B	 0.5200	 0.3700
C	 0.4380	 0.3190
D	 0.5490	 0.3320
E	 0.5070	 0.3590
F	 0.5290	 0.3620
G	 0.5440	 0.3520
H	 0.6010	 0.3590
I	 0.7780	 0.3240
J	 0.7810	 0.3270
O	 0.3690	 0.2570

