



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 12:13 PM UTC

PDB ID : 9JUM / pdb_00009jum
EMDB ID : EMD-61830
Title : Structure of Arabidopsis thaliana ABCB1 with brassinolide and AMP-PNP bound in the inward-facing conformation
Authors : Chen, Q.; Su, N.; Guo, J.
Deposited on : 2024-10-08
Resolution : 3.10 Å(reported)

This is a Full wwPDB EM Validation 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.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

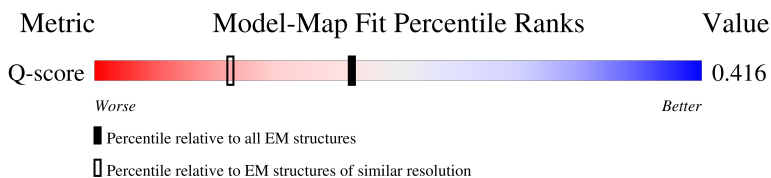
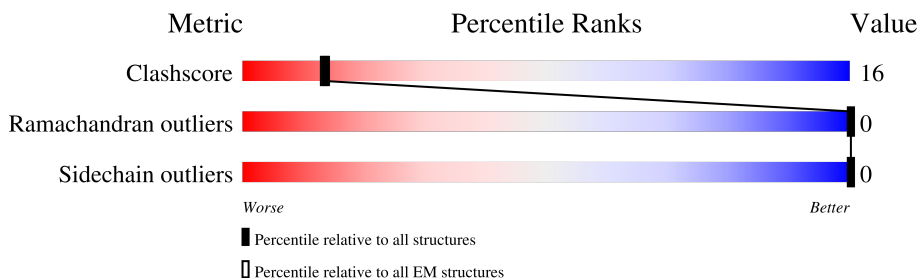
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	14724 (2.60 - 3.60)

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	1327	25% 59% 29% 12%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9069 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 ABC transporter B family member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1165	Total	C	N	O	S	0	0
			8971	5736	1543	1651	41		

There are 41 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-40	MET	-	initiating methionine	UNP Q9ZR72
A	-39	ASP	-	expression tag	UNP Q9ZR72
A	-38	TYR	-	expression tag	UNP Q9ZR72
A	-37	LYS	-	expression tag	UNP Q9ZR72
A	-36	ASP	-	expression tag	UNP Q9ZR72
A	-35	ASP	-	expression tag	UNP Q9ZR72
A	-34	ASP	-	expression tag	UNP Q9ZR72
A	-33	ASP	-	expression tag	UNP Q9ZR72
A	-32	LYS	-	expression tag	UNP Q9ZR72
A	-31	TRP	-	expression tag	UNP Q9ZR72
A	-30	SER	-	expression tag	UNP Q9ZR72
A	-29	HIS	-	expression tag	UNP Q9ZR72
A	-28	PRO	-	expression tag	UNP Q9ZR72
A	-27	GLN	-	expression tag	UNP Q9ZR72
A	-26	PHE	-	expression tag	UNP Q9ZR72
A	-25	GLU	-	expression tag	UNP Q9ZR72
A	-24	LYS	-	expression tag	UNP Q9ZR72
A	-23	GLY	-	expression tag	UNP Q9ZR72
A	-22	GLY	-	expression tag	UNP Q9ZR72
A	-21	GLY	-	expression tag	UNP Q9ZR72
A	-20	GLY	-	expression tag	UNP Q9ZR72
A	-19	SER	-	expression tag	UNP Q9ZR72
A	-18	GLY	-	expression tag	UNP Q9ZR72
A	-17	GLY	-	expression tag	UNP Q9ZR72
A	-16	SER	-	expression tag	UNP Q9ZR72
A	-15	ALA	-	expression tag	UNP Q9ZR72
A	-14	TRP	-	expression tag	UNP Q9ZR72
A	-13	SER	-	expression tag	UNP Q9ZR72

Continued on next page...

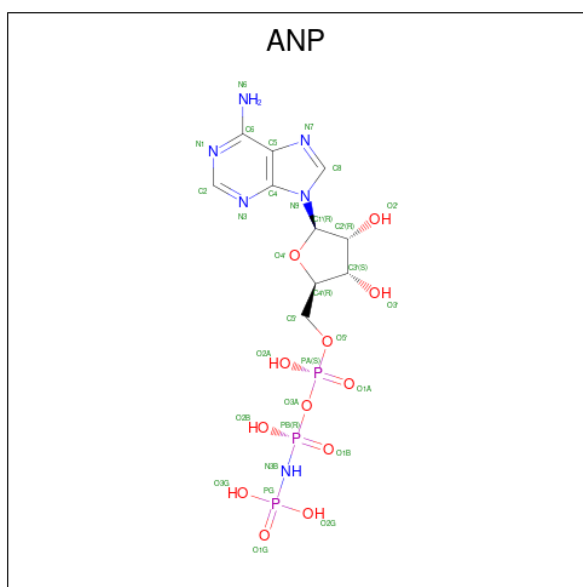
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	HIS	-	expression tag	UNP Q9ZR72
A	-11	PRO	-	expression tag	UNP Q9ZR72
A	-10	GLN	-	expression tag	UNP Q9ZR72
A	-9	PHE	-	expression tag	UNP Q9ZR72
A	-8	GLU	-	expression tag	UNP Q9ZR72
A	-7	LYS	-	expression tag	UNP Q9ZR72
A	-6	GLU	-	expression tag	UNP Q9ZR72
A	-5	PHE	-	expression tag	UNP Q9ZR72
A	-4	LYS	-	expression tag	UNP Q9ZR72
A	-3	GLY	-	expression tag	UNP Q9ZR72
A	-2	LEU	-	expression tag	UNP Q9ZR72
A	-1	VAL	-	expression tag	UNP Q9ZR72
A	0	ASP	-	expression tag	UNP Q9ZR72

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

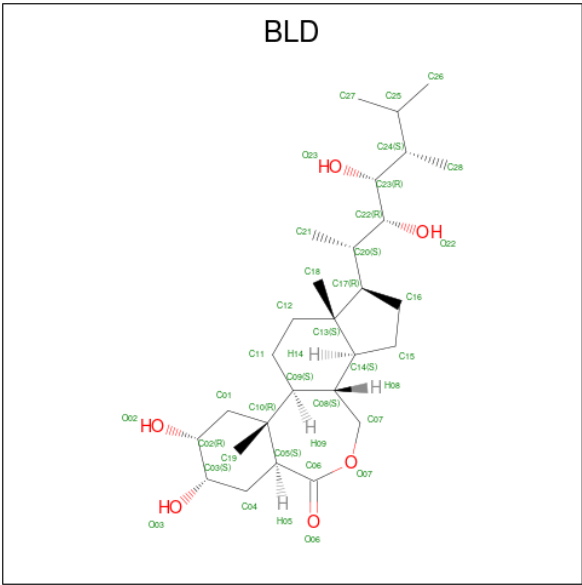
Mol	Chain	Residues	Atoms	AltConf
2	A	2	Total Mg 2 2	0

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	6	12	3	
3	A	1	Total	C	N	O	P	0
			31	10	6	12	3	

- Molecule 4 is Brassinolide (CCD ID: BLD) (formula: C₂₈H₄₈O₆) (labeled as "Ligand of Interest" by depositor).

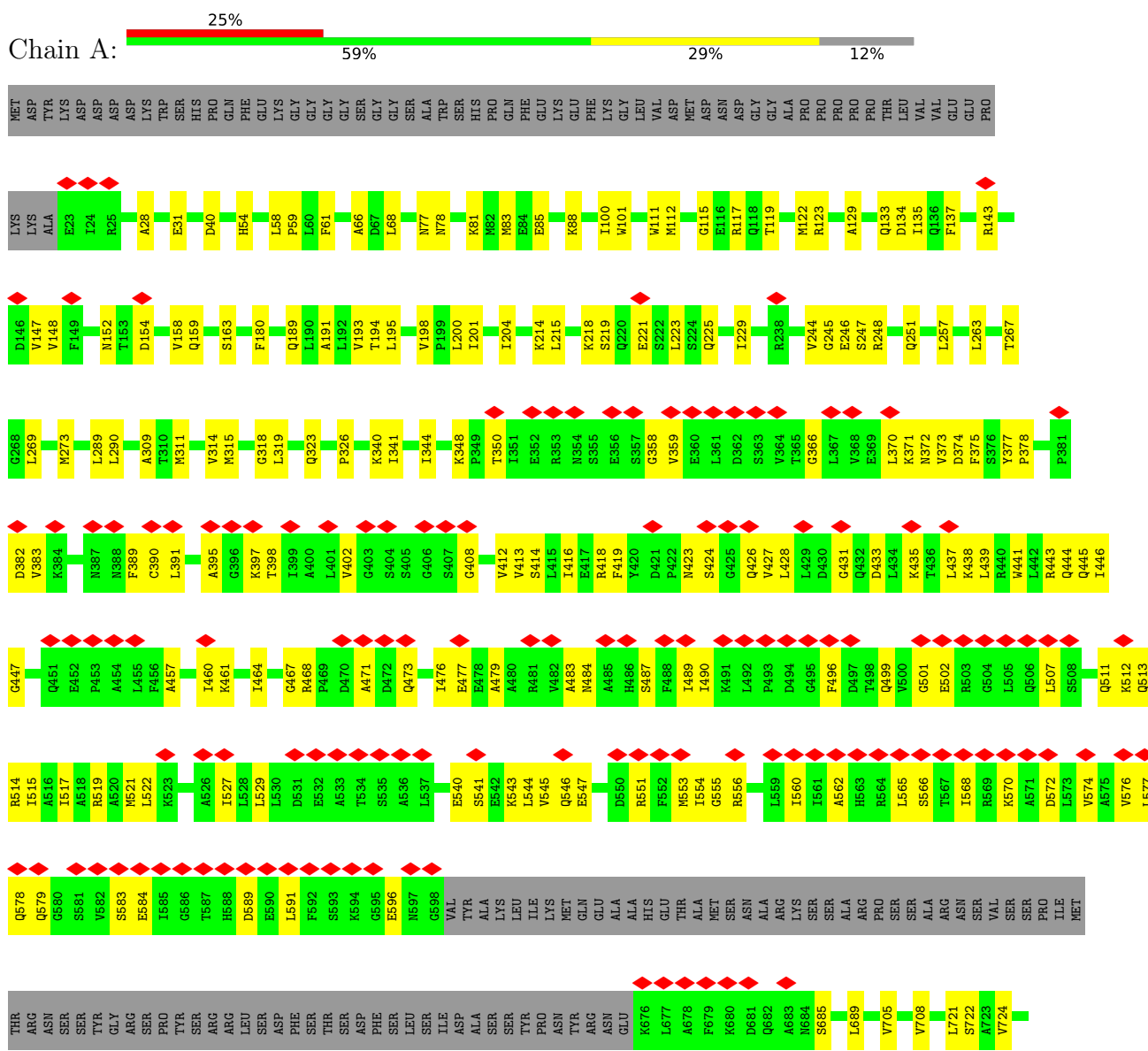


Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			34	28	6	

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: ABC transporter B family member 1



HIS	Q1207	F1144	G1081	R1019	T759
THR	A1208	I1145	R1082	L1020	K774
GLN	C1209	S1146	V1083	R1021	K777
VAL	S1210	A1147	I1085	G1022	E778
ILE	G1211	L1148	D1086	V1023	K779
GLY	P1149	E1150	G1087	E1024	M780
MET	E1151	G1151	K1088	E1025	K786
THR	S1214	Y1152	D1089	L1026	N787
GLY	I1215	Y1155	I1090	K1027	E788
SER	V1216	V1156	I1091	H1028	M789
SER	V1217	G1157	R1092	I1029	A790
SER	A1218	E1158	L1095	D1030	M791
ARG	H1219	R1159	K1096	F1031	F792
VAL	R1220	G1160	A1097	S1035	D793
LYS	L1221	V1161	I1098	R1036	Q794
GLU	L1221	Q1162	R1099	P1037	E795
ASP	S1222	L1163	K1100	D1040	E796
ASP	T1223	G1166	H1101	I1041	N797
ALA	I1224	Q1167	I1102	F1042	R801
	R1225	K1168	A1103	R1043	A807
	N1226	Q1169	V1105	D1044	L808
	A1227	R1170	E1108	L1045	N811
	H1228	I1171	L1111	S1046	D819
	V1229	A1172	F1112	L1047	R820
	I1230	A1174	G1113	R1048	V823
	A1231	L1177	T1114	A1049	I824
	V1232	V1178	T1115	A1050	N827
	I1233	K1180	I1116	A1051	G838
	D1234	A1181	Y1117	G1052	Q842
	D1235	E1182	E1118	K1053	L849
	G1236	I1183	N1119	T1054	V852
	K1237	M1184	I1120	L1055	V861
	V1238	L1185	A1121	A1056	T868
	A1239	L1186	Y1122	L1057	D873
	E1240	D1187	G1123	G1059	L874
	Q1241	E1188	H1124	P1060	E875
	G1242	A1189	E1125	S1061	R893
	S1243	T1190	C1126	G1062	E913
	H1244	S1191	T1128	S1061	P914
	S1245	A1192	E1129	C1063	R818
	H1246	L1193	A1130	G1064	C919
	L1247	D1194	E1131	K1065	
	L1248	A1195	I1132	S1066	
	K1249	E1196	I1133	S1067	
	N1250	S1197	Q1134	V1068	
	H1251	E1198	A1135	I1069	
	P1252	R1199	T1137	S1070	
	D1253	S1200	L1138	I1071	
	G1254	V1201	A1141	I1072	
	I1255	Q1202	H1142	Q1073	
	I1256	E1203	K1143	R1074	
	Y1257	A1204		F1075	
	A1257	L1205		Y1076	
	R1258	D1206		E1077	
	M1259			P1078	
	I1260			S1079	
	Q1261			S1080	
	L1262				
	Q1263				
	R1264				
	PHE				
	THR				

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	105302	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1400	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.053	Depositor
Minimum map value	-0.021	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.013	Depositor
Map size (Å)	223.2, 223.2, 223.2	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93, 0.93, 0.93	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: ANP, MG, BLD

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	0.25	0/9137	0.44	1/12366 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	1254	GLY	CA-C-O	-6.12	118.25	122.22

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	8971	0	9114	290	0
2	A	2	0	0	0	0
3	A	62	0	26	2	0
4	A	34	0	48	1	0
All	All	9069	0	9188	291	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 16.

All (291) 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:83:MET:HE1	1:A:953:LYS:HB2	1.51	0.91
1:A:215:LEU:HB3	1:A:267:THR:HG22	1.58	0.86
1:A:1026:LEU:HB2	1:A:1047:LEU:HB2	1.62	0.82
1:A:1195:ALA:HB1	1:A:1199:ARG:HH12	1.44	0.82
1:A:1050:ARG:HB3	1:A:1053:LYS:HB3	1.59	0.81
1:A:257:LEU:HB3	1:A:774:LYS:HG3	1.64	0.79
1:A:578:GLN:HE22	1:A:583:SER:HB3	1.48	0.77
1:A:1021:ARG:HE	1:A:1086:ASP:HA	1.50	0.77
1:A:370:LEU:HD12	1:A:373:VAL:HG21	1.65	0.76
1:A:373:VAL:HG22	1:A:427:VAL:HG22	1.68	0.76
1:A:789:MET:SD	1:A:789:MET:N	2.57	0.74
1:A:1186:LEU:HB2	1:A:1216:VAL:HG22	1.70	0.74
1:A:257:LEU:HD11	1:A:777:ARG:HD2	1.69	0.73
1:A:370:LEU:HD22	1:A:416:ILE:HD11	1.71	0.72
1:A:248:ARG:HH22	1:A:1125:GLU:HA	1.54	0.72
1:A:1025:GLU:HB2	1:A:1084:MET:HB2	1.72	0.71
1:A:489:ILE:HG13	1:A:490:ILE:HD12	1.73	0.70
1:A:791:TRP:O	1:A:797:ASN:ND2	2.23	0.70
1:A:483:ALA:HB1	1:A:521:MET:HG3	1.74	0.69
1:A:1086:ASP:HB3	1:A:1088:LYS:HZ1	1.57	0.69
1:A:395:ALA:HA	1:A:556:ARG:HH22	1.57	0.69
1:A:371:LYS:HA	1:A:390:CYS:HA	1.75	0.69
1:A:408:GLY:HA2	3:A:1303:ANP:H5'1	1.75	0.68
1:A:1221:LEU:HD22	1:A:1260:ILE:HG23	1.75	0.68
1:A:1246:HIS:HA	1:A:1249:LYS:HG2	1.76	0.67
1:A:1042:PHE:HZ	1:A:1068:VAL:HG22	1.59	0.67
1:A:40:ASP:OD1	1:A:117:ARG:NH1	2.29	0.66
1:A:1221:LEU:HD12	1:A:1222:SER:HB3	1.78	0.65
1:A:789:MET:HA	1:A:792:PHE:HB2	1.77	0.65
1:A:1203:GLU:OE2	1:A:1207:GLN:NE2	2.30	0.65
1:A:1114:THR:HG23	1:A:1115:THR:HG23	1.77	0.64
1:A:290:LEU:HD13	1:A:724:VAL:HG21	1.79	0.64
1:A:389:PHE:HE1	1:A:391:LEU:HB2	1.62	0.64
1:A:1026:LEU:HD12	1:A:1029:ILE:HG13	1.79	0.64
1:A:1021:ARG:NH2	1:A:1087:GLY:H	1.96	0.64
1:A:468:ARG:HE	1:A:471:ALA:HB2	1.62	0.64
1:A:1059:GLY:HA2	1:A:1256:TYR:CE1	2.33	0.63
1:A:1059:GLY:HA2	1:A:1256:TYR:HE1	1.62	0.63
1:A:1120:ILE:HD11	1:A:1171:ILE:HB	1.80	0.63
1:A:198:VAL:HG11	1:A:318:GLY:HA3	1.80	0.63
1:A:398:THR:HA	1:A:556:ARG:HG3	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:GLN:HA	1:A:476:ILE:HD12	1.79	0.63
1:A:555:GLY:C	1:A:556:ARG:HD2	2.24	0.62
1:A:371:LYS:NZ	1:A:372:ASN:OD1	2.28	0.62
1:A:225:GLN:O	1:A:229:ILE:HD12	2.01	0.61
1:A:722:SER:HB3	1:A:964:ARG:HA	1.82	0.61
1:A:1061:SER:HA	1:A:1065:LYS:HZ1	1.66	0.61
1:A:842:GLN:HE21	1:A:957:SER:HB2	1.66	0.61
1:A:66:ALA:HB2	1:A:309:ALA:HB2	1.81	0.61
1:A:1187:ASP:HA	1:A:1217:VAL:HG12	1.83	0.60
1:A:290:LEU:HD23	1:A:311:MET:HE1	1.83	0.60
1:A:373:VAL:HB	1:A:389:PHE:HB3	1.84	0.59
1:A:1040:GLN:HB2	1:A:1043:ARG:HH22	1.68	0.59
1:A:112:MET:HE1	1:A:922:LYS:HE3	1.84	0.59
1:A:457:ALA:HA	1:A:501:GLY:HA3	1.84	0.59
1:A:1053:LYS:HD3	1:A:1228:HIS:HB3	1.84	0.59
1:A:1074:ARG:HB2	1:A:1090:ILE:HD12	1.84	0.59
1:A:1169:GLN:HE22	1:A:1173:ILE:HD11	1.68	0.58
1:A:861:VAL:HG13	1:A:980:LEU:HD21	1.85	0.58
1:A:246:GLU:OE2	1:A:1096:LYS:NZ	2.29	0.57
1:A:218:LYS:O	1:A:221:GLU:HG3	2.04	0.57
1:A:115:GLY:HA3	1:A:163:SER:HB3	1.87	0.57
1:A:1177:LEU:O	1:A:1180:LYS:NZ	2.29	0.57
1:A:1068:VAL:O	1:A:1072:ILE:HG12	2.04	0.57
1:A:560:ILE:HD13	1:A:568:ILE:HB	1.87	0.57
1:A:1143:LYS:HD2	1:A:1144:PHE:N	2.20	0.57
1:A:1040:GLN:HB2	1:A:1043:ARG:HH12	1.70	0.56
1:A:689:LEU:HD11	1:A:993:MET:HG3	1.87	0.56
1:A:1021:ARG:HH21	1:A:1087:GLY:H	1.54	0.56
1:A:1158:GLU:HB2	1:A:1159:ARG:HH11	1.70	0.56
1:A:1243:SER:O	1:A:1247:LEU:N	2.32	0.56
1:A:838:GLY:HA2	1:A:965:VAL:HG22	1.89	0.55
1:A:540:GLU:O	1:A:543:LYS:HG3	2.07	0.54
1:A:1220:ARG:HA	1:A:1263:GLN:HE22	1.71	0.54
1:A:1089:ASP:HB3	1:A:1091:ARG:HG3	1.89	0.54
1:A:389:PHE:HE2	1:A:577:LEU:HD13	1.71	0.54
1:A:568:ILE:HD11	1:A:574:VAL:HG11	1.90	0.54
1:A:976:ALA:O	1:A:979:THR:OG1	2.25	0.54
1:A:1005:GLU:HG2	1:A:1006:ILE:HG13	1.90	0.54
1:A:1038:ASP:OD1	1:A:1039:ILE:N	2.41	0.54
1:A:366:GLY:H	1:A:554:ILE:HD11	1.73	0.54
1:A:1174:ALA:O	1:A:1178:VAL:HG23	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:ILE:HG22	1:A:522:LEU:HD11	1.90	0.53
1:A:788:GLU:HG2	1:A:790:ALA:H	1.74	0.53
1:A:269:LEU:HG	1:A:273:MET:HE2	1.90	0.53
1:A:513:GLN:O	1:A:517:ILE:HG12	2.09	0.53
1:A:913:GLU:HB3	1:A:914:PRO:HD3	1.91	0.53
1:A:808:LEU:HA	1:A:811:ASN:HD21	1.73	0.53
1:A:428:LEU:HA	1:A:433:ASP:HA	1.89	0.53
1:A:428:LEU:HD12	1:A:431:GLY:HA2	1.90	0.52
1:A:1182:GLU:HA	1:A:1212:ARG:HG2	1.91	0.52
1:A:58:LEU:HB2	1:A:59:PRO:HD3	1.90	0.52
1:A:289:LEU:HB3	1:A:311:MET:HE2	1.91	0.52
1:A:780:MET:HE3	1:A:999:LEU:HD23	1.91	0.52
1:A:1058:VAL:HG23	1:A:1219:HIS:HA	1.90	0.52
1:A:1168:LYS:HA	1:A:1171:ILE:HG12	1.92	0.52
1:A:122:MET:HE1	1:A:158:VAL:HG11	1.92	0.52
1:A:1111:LEU:HD21	1:A:1171:ILE:HD11	1.90	0.52
1:A:995:SER:O	1:A:998:GLU:HG3	2.09	0.52
1:A:382:ASP:OD1	1:A:383:VAL:N	2.43	0.52
1:A:1023:GLU:OE2	1:A:1051:ALA:N	2.43	0.52
1:A:820:ARG:HH21	1:A:986:PHE:HB2	1.73	0.52
1:A:1008:PRO:HA	1:A:1095:LEU:HD23	1.91	0.52
1:A:1097:ALA:HA	1:A:1100:LYS:HG2	1.91	0.52
1:A:566:SER:O	1:A:570:LYS:HG2	2.10	0.51
1:A:1029:ILE:HA	1:A:1081:GLY:HA3	1.92	0.51
1:A:1259:MET:O	1:A:1263:GLN:HG3	2.10	0.51
1:A:444:GLN:OE1	1:A:445:GLN:NE2	2.43	0.51
1:A:565:LEU:O	1:A:568:ILE:HG22	2.11	0.51
1:A:589:ASP:HB2	1:A:591:LEU:HD13	1.91	0.51
1:A:1043:ARG:H	1:A:1045:LEU:HD23	1.76	0.51
1:A:1129:GLU:O	1:A:1133:ILE:HG12	2.10	0.51
1:A:1123:GLY:O	1:A:1179:ARG:NH1	2.44	0.51
1:A:479:ALA:O	1:A:484:ASN:ND2	2.44	0.51
1:A:517:ILE:O	1:A:521:MET:HG2	2.11	0.51
1:A:1141:ALA:HA	1:A:1144:PHE:CE2	2.47	0.50
1:A:290:LEU:HD22	1:A:724:VAL:HG11	1.93	0.50
1:A:414:SER:HA	1:A:419:PHE:HD2	1.77	0.50
1:A:957:SER:OG	1:A:958:ASP:N	2.43	0.50
1:A:372:ASN:OD1	1:A:426:GLN:NE2	2.42	0.50
1:A:1095:LEU:O	1:A:1099:ARG:HG2	2.12	0.50
1:A:119:THR:HG22	1:A:123:ARG:HE	1.76	0.50
1:A:511:GLN:OE1	1:A:514:ARG:NH2	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:ILE:O	1:A:464:ILE:HG12	2.11	0.50
1:A:1021:ARG:HE	1:A:1086:ASP:CA	2.23	0.50
1:A:340:LYS:O	1:A:344:ILE:HD12	2.12	0.49
1:A:438:LYS:HG2	1:A:439:LEU:H	1.76	0.49
1:A:789:MET:HG3	1:A:1075:PHE:CE2	2.47	0.49
1:A:1028:HIS:HE1	1:A:1082:ARG:HB3	1.77	0.49
1:A:1082:ARG:HE	1:A:1083:VAL:H	1.58	0.49
1:A:487:SER:HB2	1:A:514:ARG:HH22	1.78	0.49
1:A:583:SER:OG	1:A:584:GLU:OE1	2.29	0.49
1:A:1073:GLN:O	1:A:1099:ARG:NH1	2.44	0.49
1:A:412:VAL:O	1:A:416:ILE:HG12	2.13	0.49
1:A:1021:ARG:HD2	1:A:1023:GLU:HB2	1.95	0.49
1:A:418:ARG:HH12	1:A:435:LYS:HA	1.77	0.49
1:A:562:ALA:HB1	1:A:596:GLU:HG3	1.94	0.49
1:A:439:LEU:HD11	1:A:443:ARG:HE	1.78	0.49
1:A:418:ARG:O	1:A:418:ARG:HG3	2.13	0.49
1:A:578:GLN:HG2	1:A:579:GLN:HG3	1.95	0.49
1:A:374:ASP:OD2	1:A:424:SER:OG	2.30	0.48
1:A:489:ILE:HG12	1:A:514:ARG:HH22	1.77	0.48
1:A:544:LEU:O	1:A:547:GLU:HG2	2.13	0.48
1:A:705:VAL:O	1:A:708:VAL:HG22	2.13	0.48
1:A:849:LEU:HA	1:A:852:VAL:HG22	1.95	0.48
1:A:823:VAL:HG23	1:A:982:LEU:HD12	1.95	0.48
1:A:991:GLN:O	1:A:994:ARG:HG3	2.14	0.48
1:A:358:GLY:HA2	1:A:437:LEU:HA	1.95	0.48
1:A:970:MET:HE2	1:A:970:MET:HA	1.96	0.48
1:A:1053:LYS:HG2	1:A:1054:THR:H	1.79	0.48
1:A:1064:GLY:O	1:A:1068:VAL:HG23	2.13	0.48
1:A:358:GLY:HA3	1:A:438:LYS:HE3	1.96	0.47
1:A:413:VAL:HG22	1:A:529:LEU:HD11	1.95	0.47
1:A:273:MET:HA	1:A:759:THR:HG22	1.96	0.47
1:A:1120:ILE:HB	1:A:1132:ILE:HD11	1.96	0.47
1:A:111:TRP:HB3	1:A:163:SER:O	2.15	0.47
1:A:68:LEU:HD22	1:A:945:LEU:HD21	1.96	0.47
1:A:119:THR:HG21	1:A:159:GLN:HB2	1.96	0.47
1:A:1066:SER:HA	1:A:1069:ILE:HG12	1.96	0.47
1:A:148:VAL:HG12	1:A:152:ASN:HD21	1.80	0.47
1:A:402:VAL:HB	1:A:576:VAL:HA	1.96	0.47
1:A:1036:ARG:HB2	3:A:1304:ANP:H2	1.97	0.47
1:A:370:LEU:HD23	1:A:391:LEU:HD23	1.96	0.47
1:A:1042:PHE:O	1:A:1043:ARG:HD3	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1069:ILE:HD12	1:A:1104:ILE:HD11	1.97	0.47
1:A:1114:THR:O	1:A:1155:TYR:HA	2.14	0.47
1:A:1019:ARG:HH21	1:A:1182:GLU:CD	2.23	0.46
1:A:247:SER:O	1:A:251:GLN:HG2	2.14	0.46
1:A:1020:LEU:HB3	1:A:1182:GLU:HG2	1.97	0.46
1:A:461:LYS:HB2	1:A:496:PHE:HB3	1.97	0.46
1:A:977:ALA:C	1:A:979:THR:H	2.23	0.46
1:A:1220:ARG:NE	1:A:1221:LEU:O	2.47	0.46
1:A:547:GLU:HB2	1:A:551:ARG:NH2	2.31	0.46
1:A:1086:ASP:HB3	1:A:1088:LYS:NZ	2.29	0.46
1:A:1205:LEU:HD11	1:A:1216:VAL:HG21	1.96	0.46
1:A:437:LEU:HD12	1:A:441:TRP:HZ3	1.81	0.46
1:A:464:ILE:HG21	1:A:476:ILE:HG23	1.97	0.46
1:A:54:HIS:CE1	1:A:100:ILE:HG23	2.50	0.46
1:A:245:GLY:HA3	1:A:1122:TYR:OH	2.16	0.46
1:A:512:LYS:HA	1:A:515:ILE:HD12	1.97	0.46
1:A:1105:VAL:HG12	1:A:1186:LEU:HA	1.97	0.46
1:A:402:VAL:HG22	1:A:560:ILE:HG21	1.98	0.45
1:A:468:ARG:HD2	1:A:471:ALA:H	1.81	0.45
1:A:1056:ALA:HB3	1:A:1230:ILE:HG13	1.97	0.45
1:A:1074:ARG:O	1:A:1074:ARG:HG2	2.16	0.45
1:A:1111:LEU:HD12	1:A:1119:ASN:HD22	1.82	0.45
1:A:1257:ALA:O	1:A:1261:GLN:HG2	2.15	0.45
1:A:1043:ARG:O	1:A:1237:LYS:NZ	2.35	0.45
1:A:1084:MET:HE1	1:A:1089:ASP:OD1	2.16	0.45
1:A:1145:ILE:HG21	1:A:1152:TYR:CE1	2.51	0.45
1:A:1195:ALA:HB1	1:A:1199:ARG:NH1	2.21	0.45
1:A:1143:LYS:HE3	1:A:1144:PHE:HD2	1.80	0.45
1:A:244:VAL:HG12	1:A:244:VAL:O	2.15	0.45
1:A:1051:ALA:O	1:A:1213:THR:HB	2.17	0.45
1:A:214:LYS:HE2	1:A:214:LYS:HB3	1.84	0.45
1:A:1130:ALA:O	1:A:1133:ILE:HB	2.17	0.45
1:A:129:ALA:O	1:A:133:GLN:HG2	2.17	0.45
1:A:685:SER:HB2	1:A:993:MET:SD	2.57	0.45
1:A:78:ASN:ND2	1:A:81:LYS:HE2	2.32	0.44
1:A:1065:LYS:H	1:A:1065:LYS:HG2	1.64	0.44
1:A:490:ILE:HG13	1:A:496:PHE:CE1	2.53	0.44
1:A:1019:ARG:HH21	1:A:1182:GLU:CG	2.30	0.44
1:A:101:TRP:CD1	1:A:931:GLY:HA3	2.52	0.44
1:A:154:ASP:HB2	1:A:341:ILE:HD11	2.00	0.44
1:A:194:THR:O	1:A:198:VAL:HG23	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:GLU:O	1:A:88:LYS:HG2	2.18	0.44
1:A:375:PHE:HA	1:A:423:ASN:OD1	2.17	0.44
1:A:397:LYS:H	1:A:556:ARG:NH2	2.15	0.44
1:A:467:GLY:HA3	1:A:519:ARG:HB2	1.99	0.44
1:A:1027:LYS:HA	1:A:1046:SER:HA	1.99	0.44
1:A:1058:VAL:O	1:A:1233:ILE:HG22	2.18	0.44
1:A:395:ALA:CA	1:A:556:ARG:HH22	2.27	0.43
1:A:135:ILE:H	1:A:135:ILE:HD12	1.83	0.43
1:A:1083:VAL:O	1:A:1084:MET:HE2	2.16	0.43
1:A:1112:PHE:HE2	1:A:1122:TYR:CD2	2.36	0.43
1:A:397:LYS:H	1:A:556:ARG:HH21	1.66	0.43
1:A:1150:GLU:OE2	1:A:1150:GLU:N	2.50	0.43
1:A:774:LYS:HG2	1:A:778:GLU:OE2	2.17	0.43
1:A:83:MET:HE3	1:A:953:LYS:HD2	2.00	0.43
1:A:290:LEU:HD11	1:A:721:LEU:HD23	2.00	0.43
1:A:359:VAL:H	1:A:437:LEU:HA	1.83	0.43
1:A:789:MET:H	1:A:789:MET:CE	2.31	0.43
1:A:323:GLN:O	1:A:326:PRO:HD2	2.18	0.43
1:A:1232:VAL:HG13	1:A:1256:TYR:CE2	2.54	0.43
1:A:1019:ARG:HH21	1:A:1182:GLU:HG3	1.83	0.43
1:A:1149:PRO:HB2	1:A:1150:GLU:OE2	2.18	0.42
4:A:1305:BLD:H121	4:A:1305:BLD:H23	1.71	0.42
1:A:134:ASP:O	1:A:137:PHE:HB3	2.20	0.42
1:A:219:SER:O	1:A:223:LEU:HG	2.20	0.42
1:A:446:ILE:HA	1:A:527:ILE:O	2.19	0.42
1:A:377:TYR:CG	1:A:378:PRO:HD2	2.54	0.42
1:A:823:VAL:HG13	1:A:827:ASN:OD1	2.19	0.42
1:A:1100:LYS:HA	1:A:1179:ARG:NH2	2.34	0.42
1:A:189:GLN:O	1:A:193:VAL:HG23	2.20	0.42
1:A:201:ILE:HD12	1:A:315:MET:HE1	2.01	0.42
1:A:218:LYS:CB	1:A:263:LEU:HD21	2.49	0.42
1:A:447:GLY:O	1:A:529:LEU:N	2.53	0.42
1:A:382:ASP:OD1	1:A:383:VAL:HG23	2.20	0.42
1:A:1014:THR:HG21	1:A:1094:ASN:N	2.35	0.42
1:A:414:SER:HB3	1:A:419:PHE:HB2	2.02	0.42
1:A:547:GLU:O	1:A:551:ARG:NE	2.53	0.42
1:A:83:MET:HB2	1:A:83:MET:HE2	1.49	0.42
1:A:1102:ILE:HG12	1:A:1183:ILE:HB	2.00	0.42
1:A:1134:GLN:HA	1:A:1137:THR:OG1	2.20	0.42
1:A:507:LEU:HD12	1:A:511:GLN:HB2	2.02	0.41
1:A:789:MET:HA	1:A:792:PHE:HD2	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1129:GLU:O	1:A:1132:ILE:HG22	2.20	0.41
1:A:460:ILE:HD11	1:A:496:PHE:HA	2.03	0.41
1:A:499:GLN:O	1:A:502:GLU:HG2	2.20	0.41
1:A:479:ALA:O	1:A:483:ALA:HB3	2.20	0.41
1:A:1163:LEU:HD23	1:A:1167:GLN:HB3	2.00	0.41
1:A:1232:VAL:HG21	1:A:1240:GLU:OE2	2.20	0.41
1:A:842:GLN:NE2	1:A:957:SER:HB2	2.32	0.41
1:A:1016:VAL:HA	1:A:1093:TYR:HE1	1.85	0.41
1:A:1185:LEU:HD23	1:A:1215:ILE:HB	2.02	0.41
1:A:61:PHE:CG	1:A:938:TYR:HE2	2.39	0.41
1:A:134:ASP:OD2	1:A:350:THR:OG1	2.34	0.41
1:A:348:LYS:HE3	1:A:348:LYS:HB3	1.93	0.41
1:A:541:SER:O	1:A:545:VAL:HG23	2.21	0.41
1:A:553:MET:SD	1:A:553:MET:N	2.94	0.41
1:A:578:GLN:C	1:A:579:GLN:HG3	2.45	0.41
1:A:807:ALA:O	1:A:811:ASN:ND2	2.53	0.41
1:A:28:ALA:HB3	1:A:31:GLU:OE1	2.21	0.41
1:A:112:MET:HE2	1:A:919:CYS:SG	2.60	0.41
1:A:143:ARG:O	1:A:147:VAL:HG23	2.21	0.41
1:A:191:ALA:HA	1:A:314:VAL:HG21	2.03	0.41
1:A:543:LYS:HA	1:A:546:GLN:OE1	2.21	0.41
1:A:786:LYS:HA	1:A:1008:PRO:HG3	2.03	0.41
1:A:820:ARG:O	1:A:824:ILE:HG12	2.20	0.41
1:A:967:MET:HB3	1:A:967:MET:HE3	1.88	0.41
1:A:1098:ILE:HG23	1:A:1102:ILE:HD12	2.02	0.41
1:A:1144:PHE:CE2	1:A:1170:ARG:HD2	2.56	0.41
1:A:1169:GLN:NE2	1:A:1173:ILE:HD11	2.33	0.41
1:A:1203:GLU:HG3	1:A:1207:GLN:HE22	1.86	0.41
1:A:200:LEU:O	1:A:204:ILE:HG12	2.20	0.40
1:A:246:GLU:CD	1:A:246:GLU:H	2.29	0.40
1:A:473:GLN:O	1:A:477:GLU:HG2	2.21	0.40
1:A:1240:GLU:HG3	1:A:1247:LEU:HD22	2.02	0.40
1:A:77:ASN:OD1	1:A:77:ASN:N	2.54	0.40
1:A:180:PHE:CZ	1:A:195:LEU:HD13	2.56	0.40
1:A:358:GLY:HA3	1:A:438:LYS:HB2	2.02	0.40
1:A:1144:PHE:O	1:A:1148:LEU:HG	2.21	0.40
1:A:423:ASN:OD1	1:A:423:ASN:N	2.54	0.40
1:A:572:ASP:OD1	1:A:572:ASP:N	2.53	0.40
1:A:1040:GLN:HB2	1:A:1043:ARG:NH1	2.36	0.40
1:A:1040:GLN:CB	1:A:1043:ARG:HH12	2.33	0.40
1:A:1074:ARG:NH1	1:A:1091:ARG:HB3	2.37	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:MET:O	1:A:319:LEU:HG	2.21	0.40
1:A:794:GLN:HG2	1:A:795:GLU:O	2.20	0.40
1:A:1117:TYR:HB2	1:A:1152:TYR:HB3	2.03	0.40
1:A:1131:GLU:HA	1:A:1134:GLN:OE1	2.22	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	1161/1327 (88%)	1113 (96%)	48 (4%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	949/1087 (87%)	949 (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. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	152	ASN
1	A	445	GLN
1	A	484	ASN
1	A	513	GLN
1	A	758	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](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

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	$\# Z > 2$
3	ANP	A	1304	2	33,33,33	1.12	5 (15%)	45,52,52	0.90	2 (4%)
3	ANP	A	1303	2	33,33,33	1.10	5 (15%)	45,52,52	0.89	2 (4%)
4	BLD	A	1305	-	36,37,37	0.38	0	49,59,59	1.20	3 (6%)

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
3	ANP	A	1304	2	-	3/18/38/38	0/3/3/3
3	ANP	A	1303	2	-	4/18/38/38	0/3/3/3
4	BLD	A	1305	-	-	8/20/85/85	0/4/4/4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1304	ANP	PG-O1G	3.40	1.51	1.46
3	A	1303	ANP	PG-O1G	3.25	1.51	1.46
3	A	1303	ANP	PB-O1B	3.07	1.50	1.46
3	A	1304	ANP	PB-O1B	2.97	1.50	1.46
3	A	1304	ANP	PB-O2B	-2.25	1.50	1.56
3	A	1303	ANP	PB-O2B	-2.22	1.50	1.56
3	A	1304	ANP	PG-O2G	-2.14	1.51	1.56
3	A	1303	ANP	PG-O2G	-2.12	1.51	1.56
3	A	1304	ANP	PG-O3G	-2.09	1.51	1.56
3	A	1303	ANP	PG-O3G	-2.09	1.51	1.56

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1305	BLD	O07-C06-O06	4.60	123.96	116.97
3	A	1304	ANP	O2B-PB-O1B	4.03	118.50	109.87
3	A	1303	ANP	O2B-PB-O1B	3.97	118.38	109.87
4	A	1305	BLD	C01-C10-C05	3.00	111.80	107.11
4	A	1305	BLD	C07-O07-C06	-2.71	117.22	120.98
3	A	1303	ANP	O3G-PG-O1G	-2.15	108.07	113.45
3	A	1304	ANP	O2G-PG-O1G	-2.11	108.17	113.45

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1303	ANP	PG-N3B-PB-O1B
4	A	1305	BLD	C22-C23-C24-C28
4	A	1305	BLD	O22-C22-C23-O23
4	A	1305	BLD	O23-C23-C24-C28
3	A	1304	ANP	C3'-C4'-C5'-O5'
3	A	1303	ANP	O4'-C4'-C5'-O5'
4	A	1305	BLD	O23-C23-C24-C25
4	A	1305	BLD	C22-C23-C24-C25

Continued on next page...

Continued from previous page...

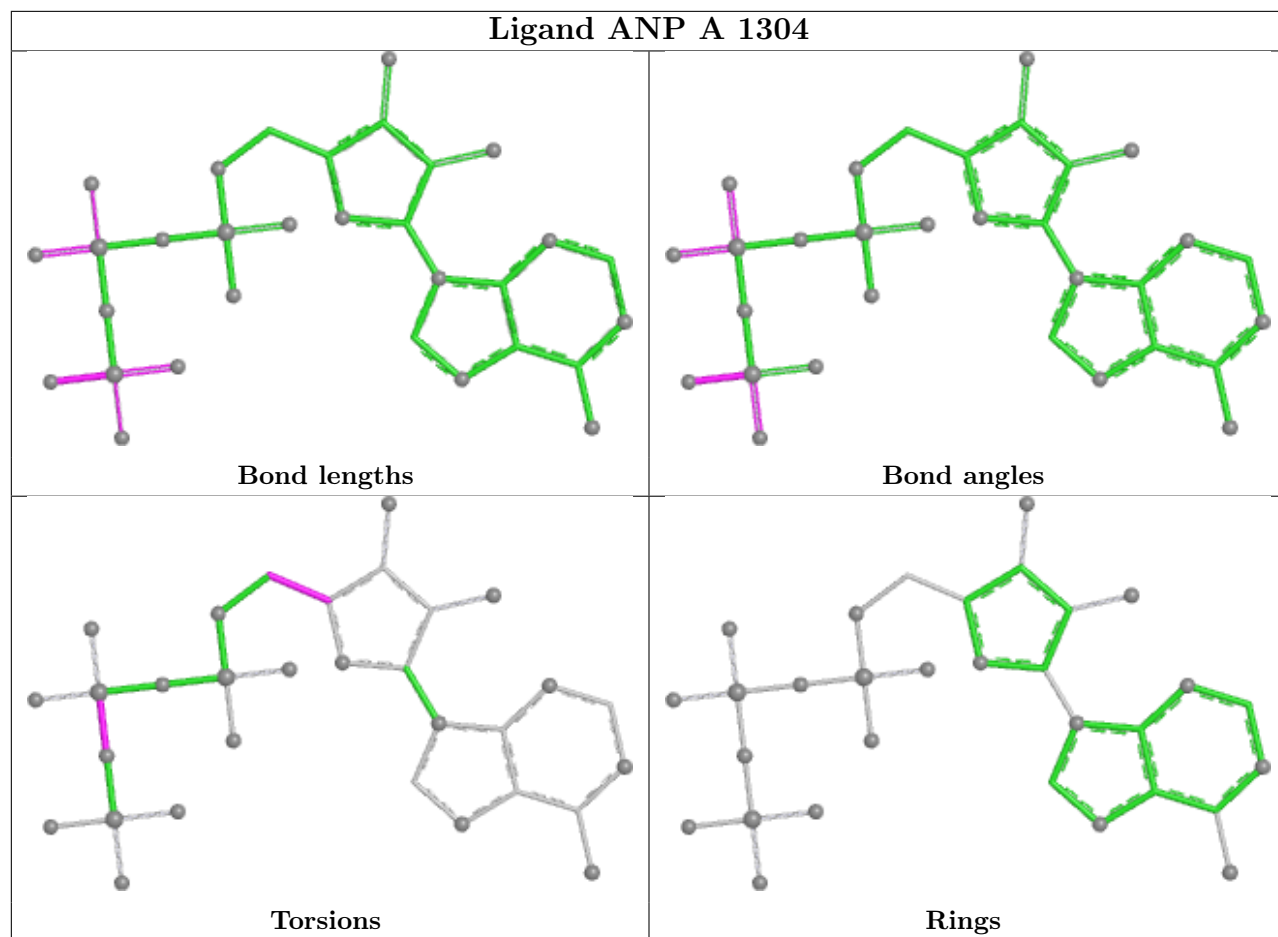
Mol	Chain	Res	Type	Atoms
3	A	1304	ANP	PG-N3B-PB-O3A
4	A	1305	BLD	C20-C22-C23-C24
4	A	1305	BLD	C20-C22-C23-O23
4	A	1305	BLD	O22-C22-C23-C24
3	A	1304	ANP	O4'-C4'-C5'-O5'
3	A	1303	ANP	C3'-C4'-C5'-O5'
3	A	1303	ANP	C4'-C5'-O5'-PA

There are no ring outliers.

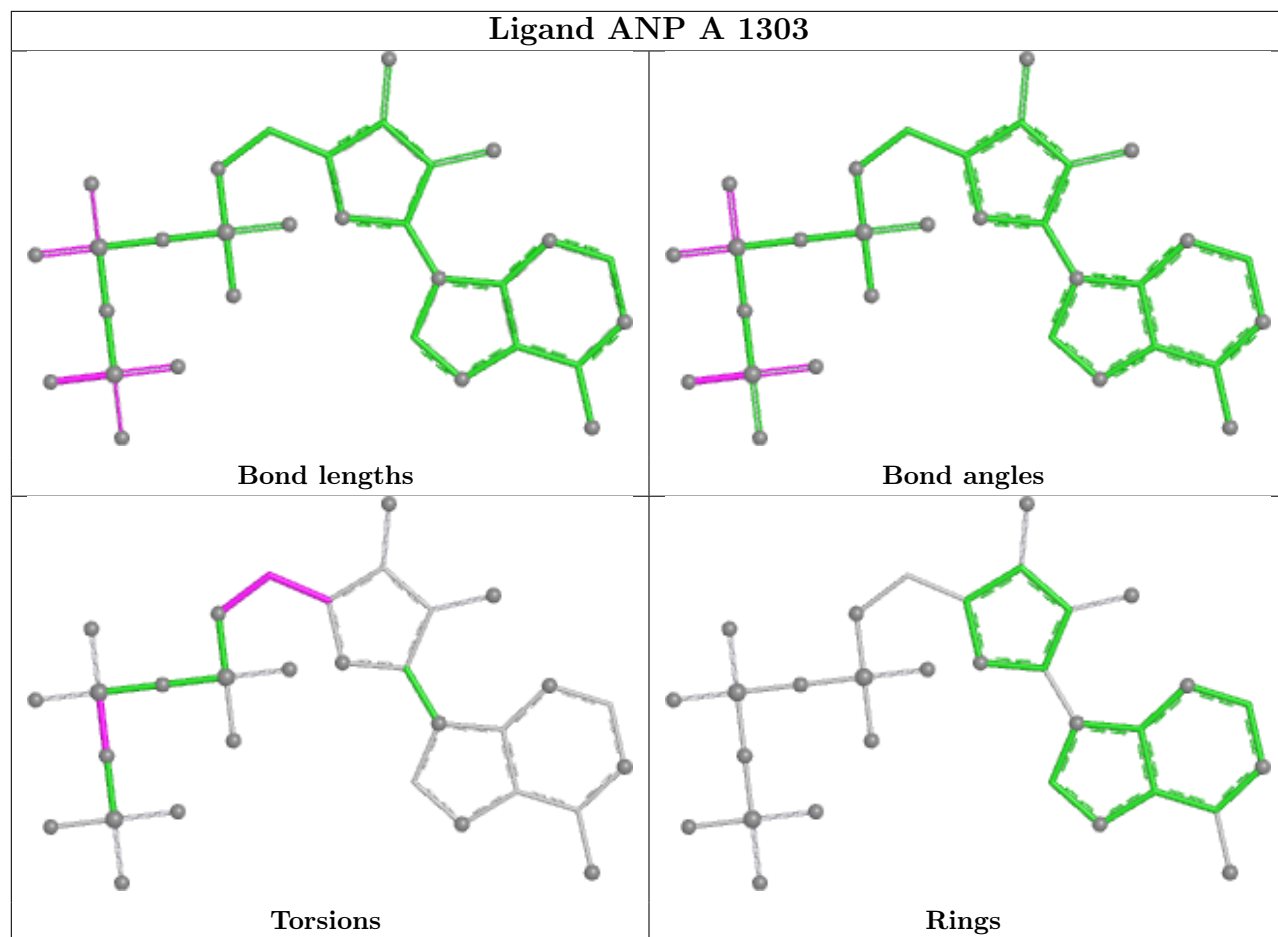
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1304	ANP	1	0
3	A	1303	ANP	1	0
4	A	1305	BLD	1	0

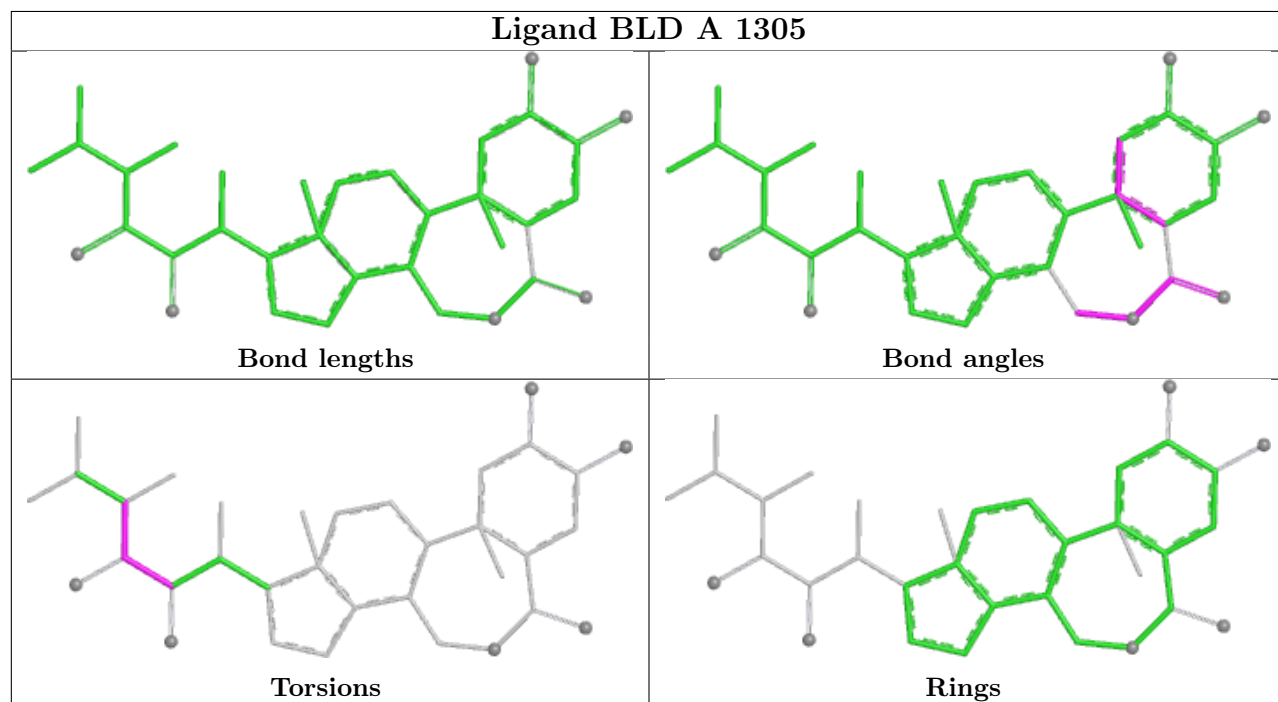
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



Ligand ANP A 1303



Ligand BLD A 1305



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.

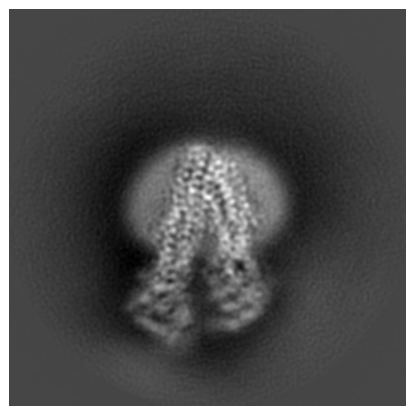
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61830. These allow visual inspection of the internal detail of the map and identification of artifacts.

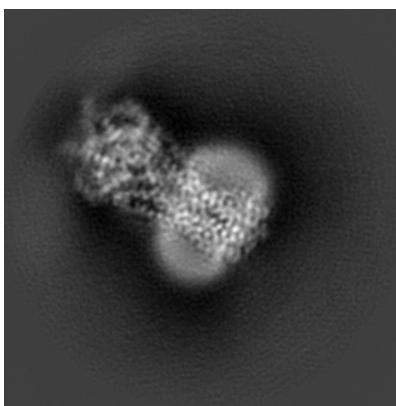
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

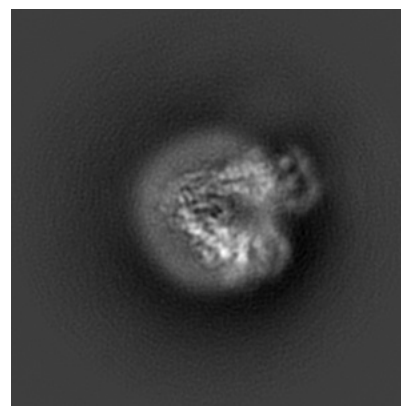
6.1.1 Primary map



X

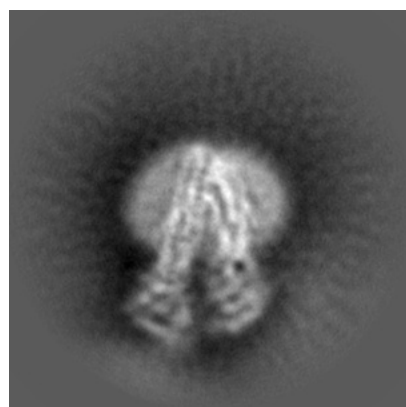


Y

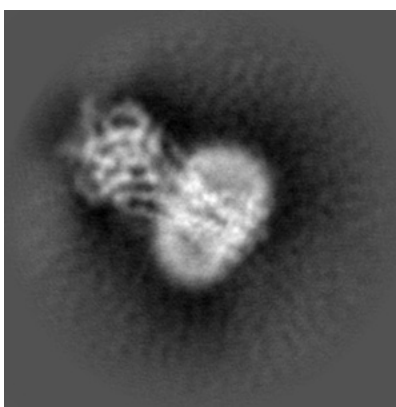


Z

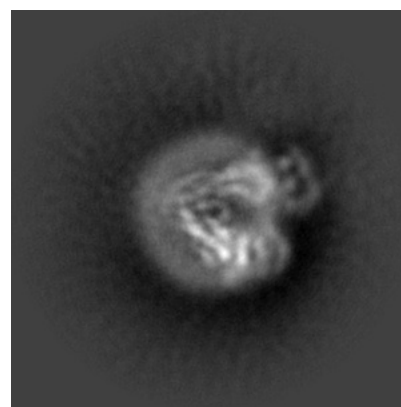
6.1.2 Raw map



X



Y

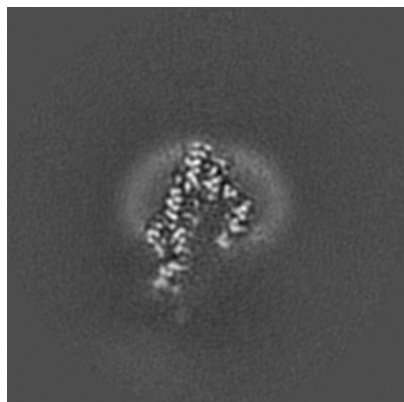


Z

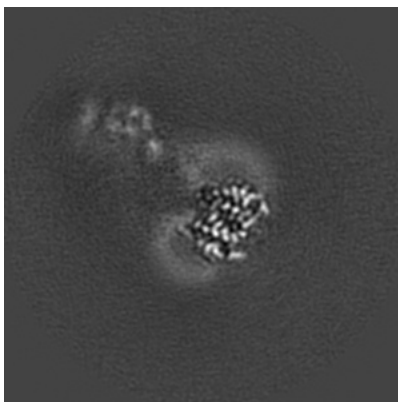
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

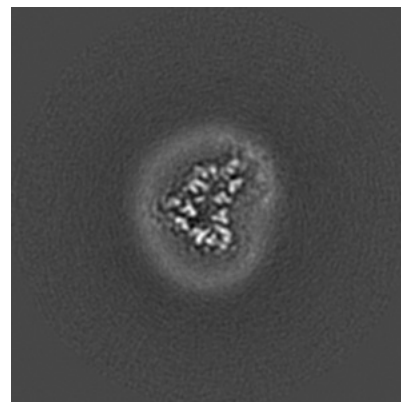
6.2.1 Primary map



X Index: 120

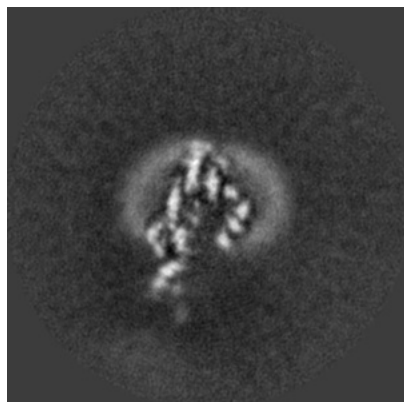


Y Index: 120

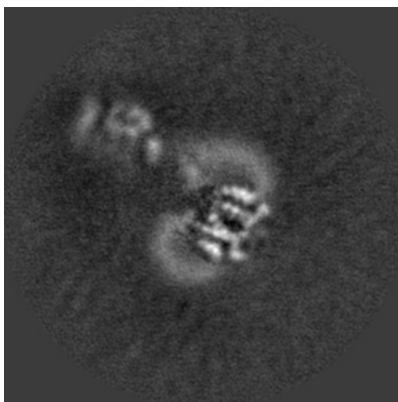


Z Index: 120

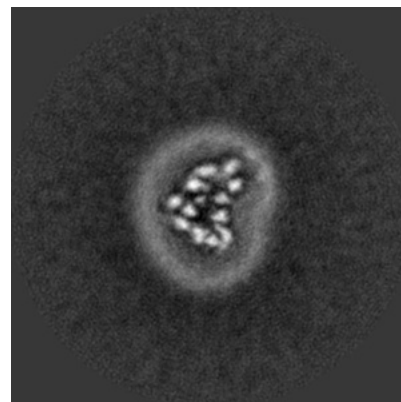
6.2.2 Raw map



X Index: 120



Y Index: 120

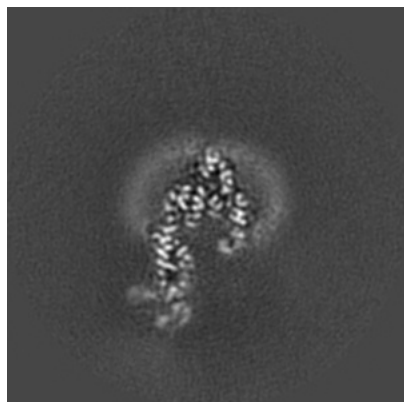


Z Index: 120

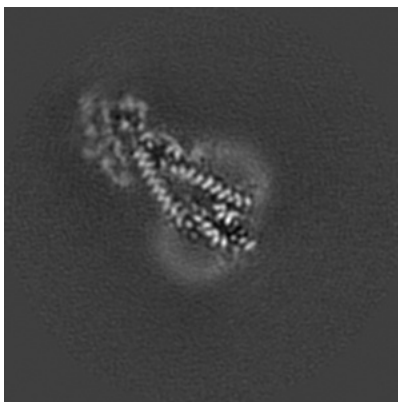
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

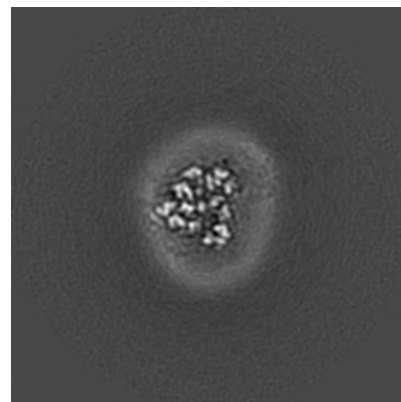
6.3.1 Primary map



X Index: 126

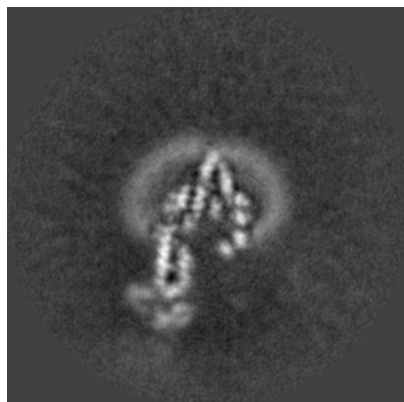


Y Index: 131

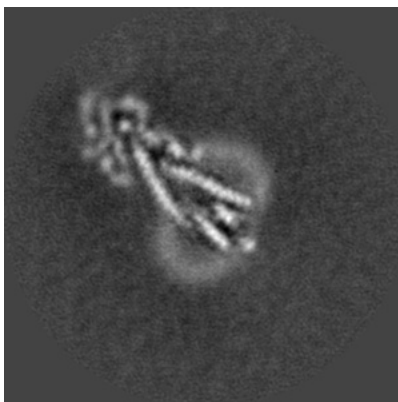


Z Index: 126

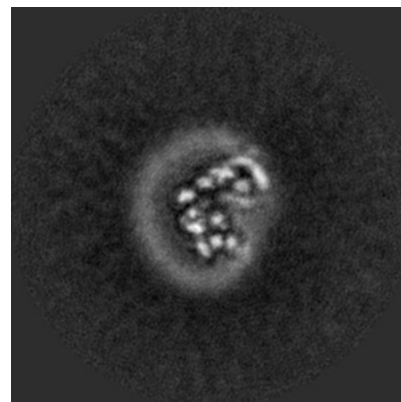
6.3.2 Raw map



X Index: 127



Y Index: 131

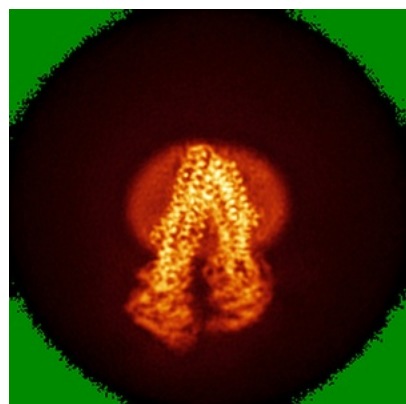


Z Index: 113

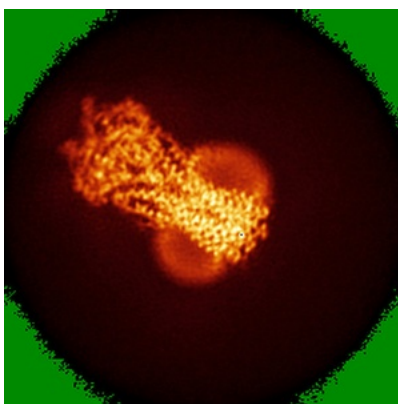
The images above show the largest variance slices of the map in three orthogonal directions.

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

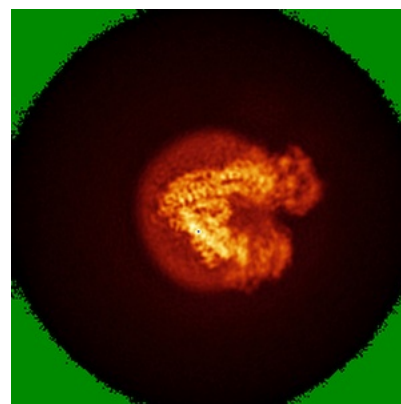
6.4.1 Primary map



X

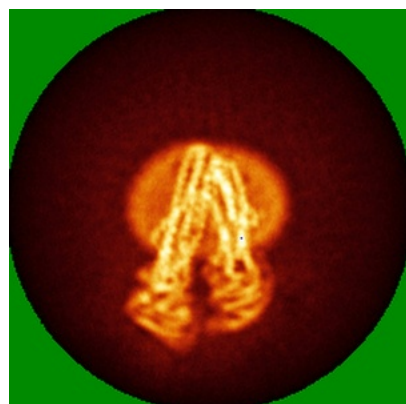


Y

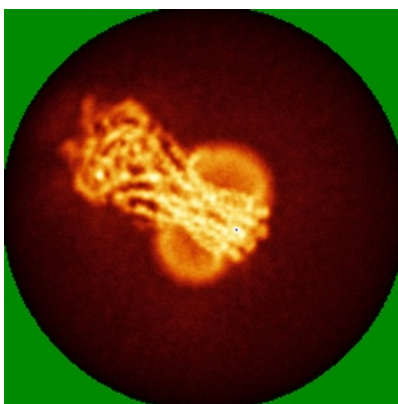


Z

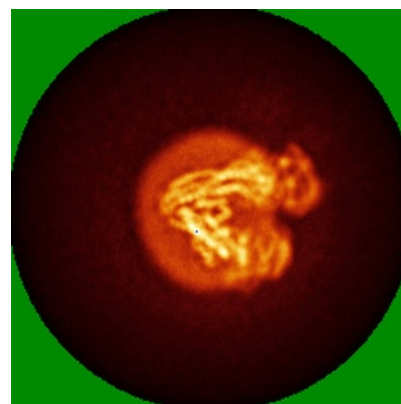
6.4.2 Raw map



X



Y

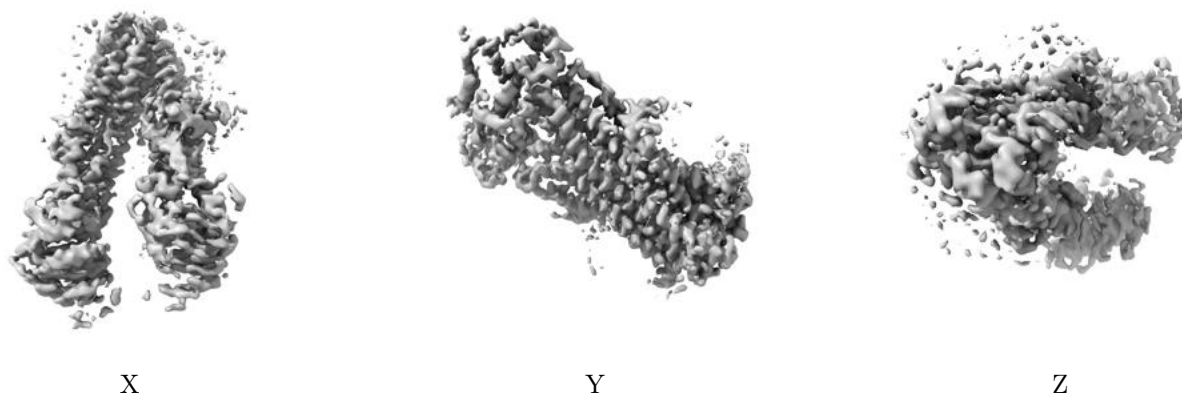


Z

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

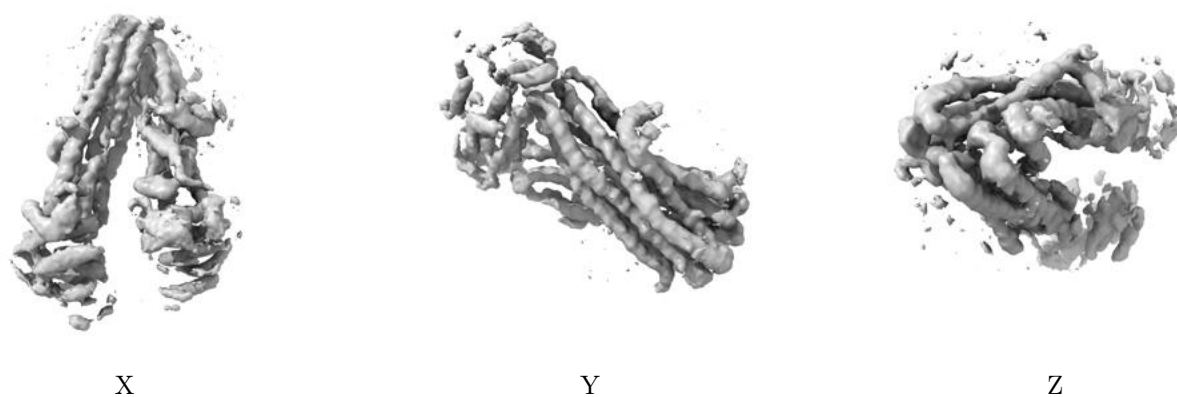
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.013. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

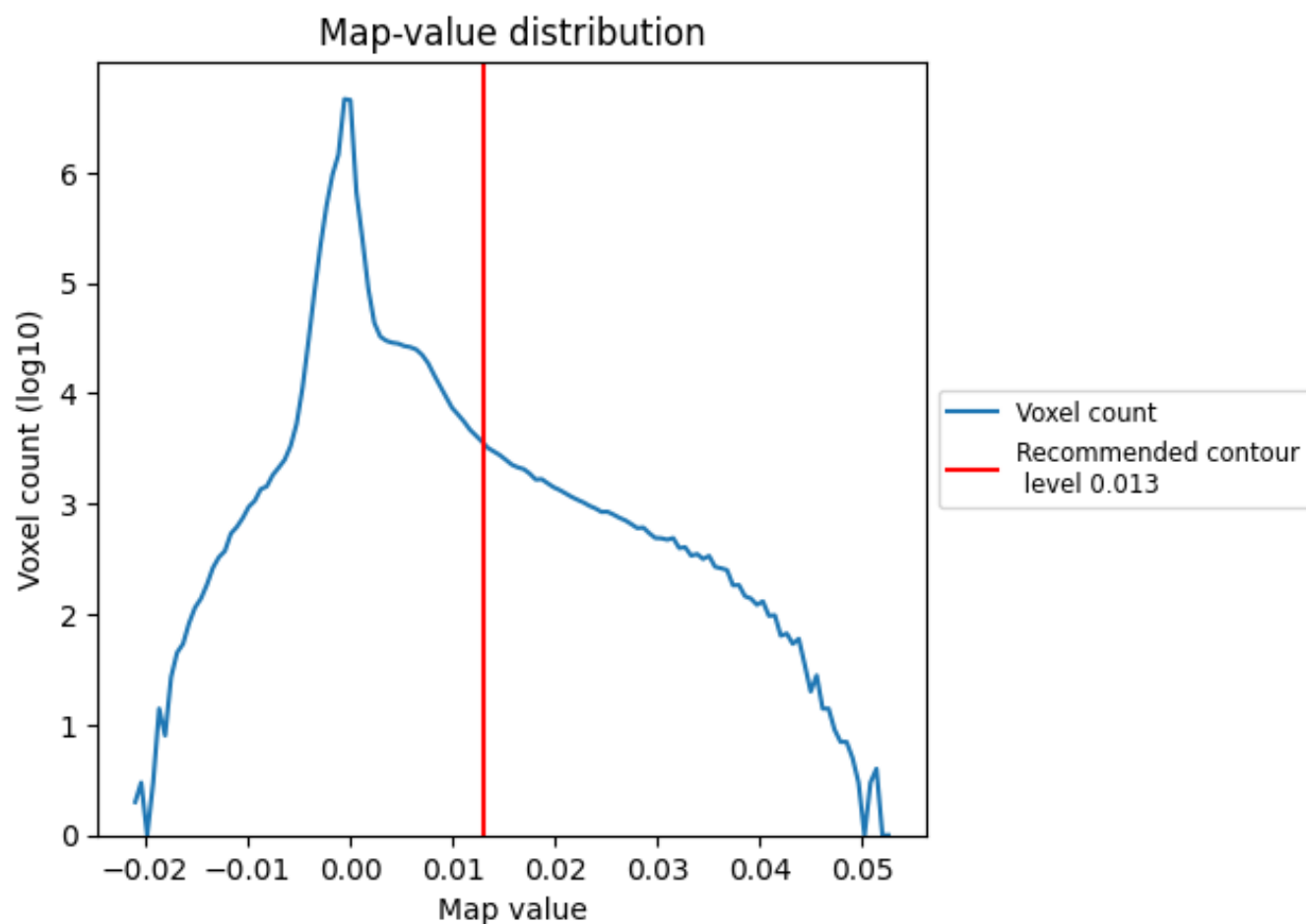
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

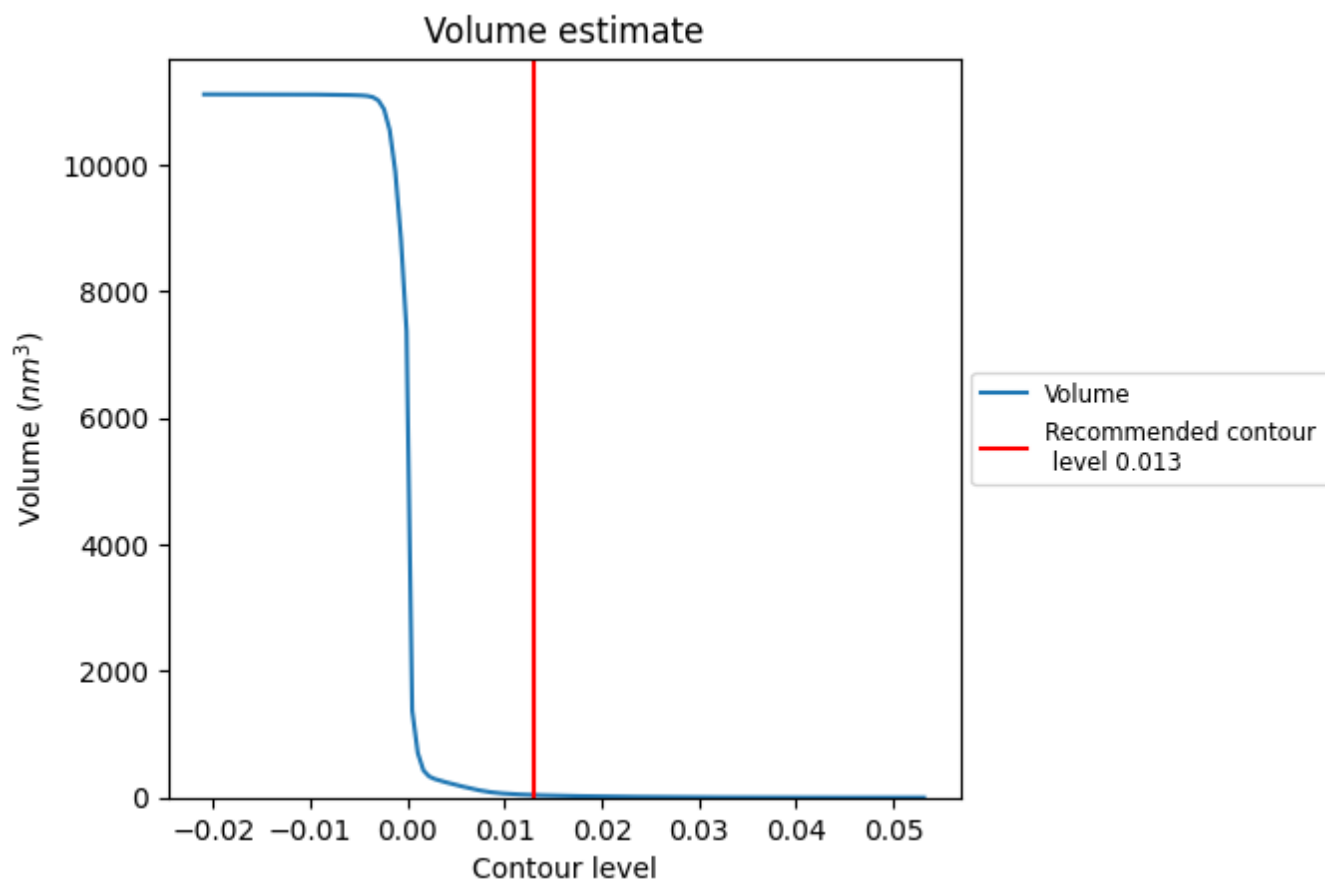
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

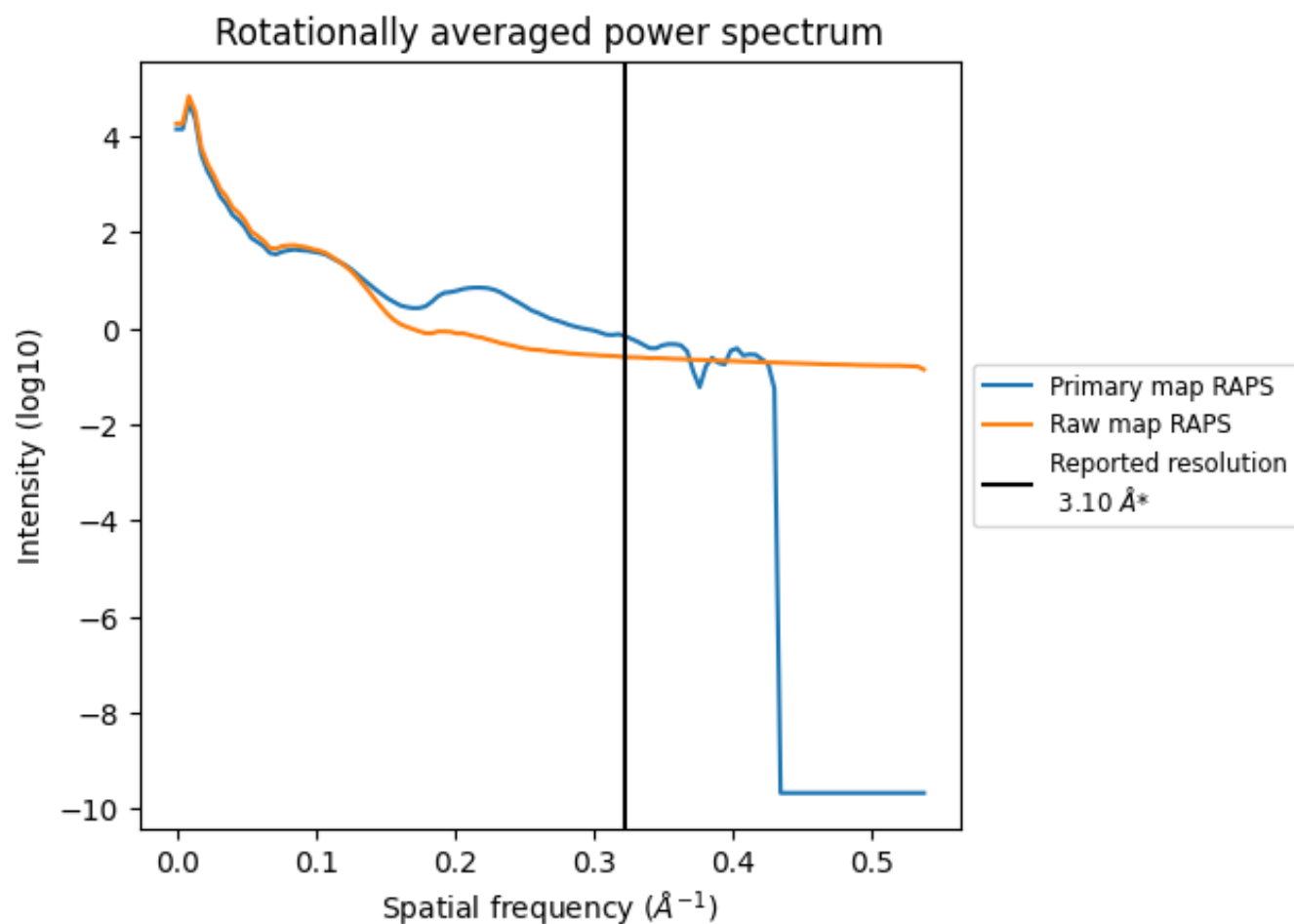
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 40 nm^3 ; this corresponds to an approximate mass of 36 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 ⓘ

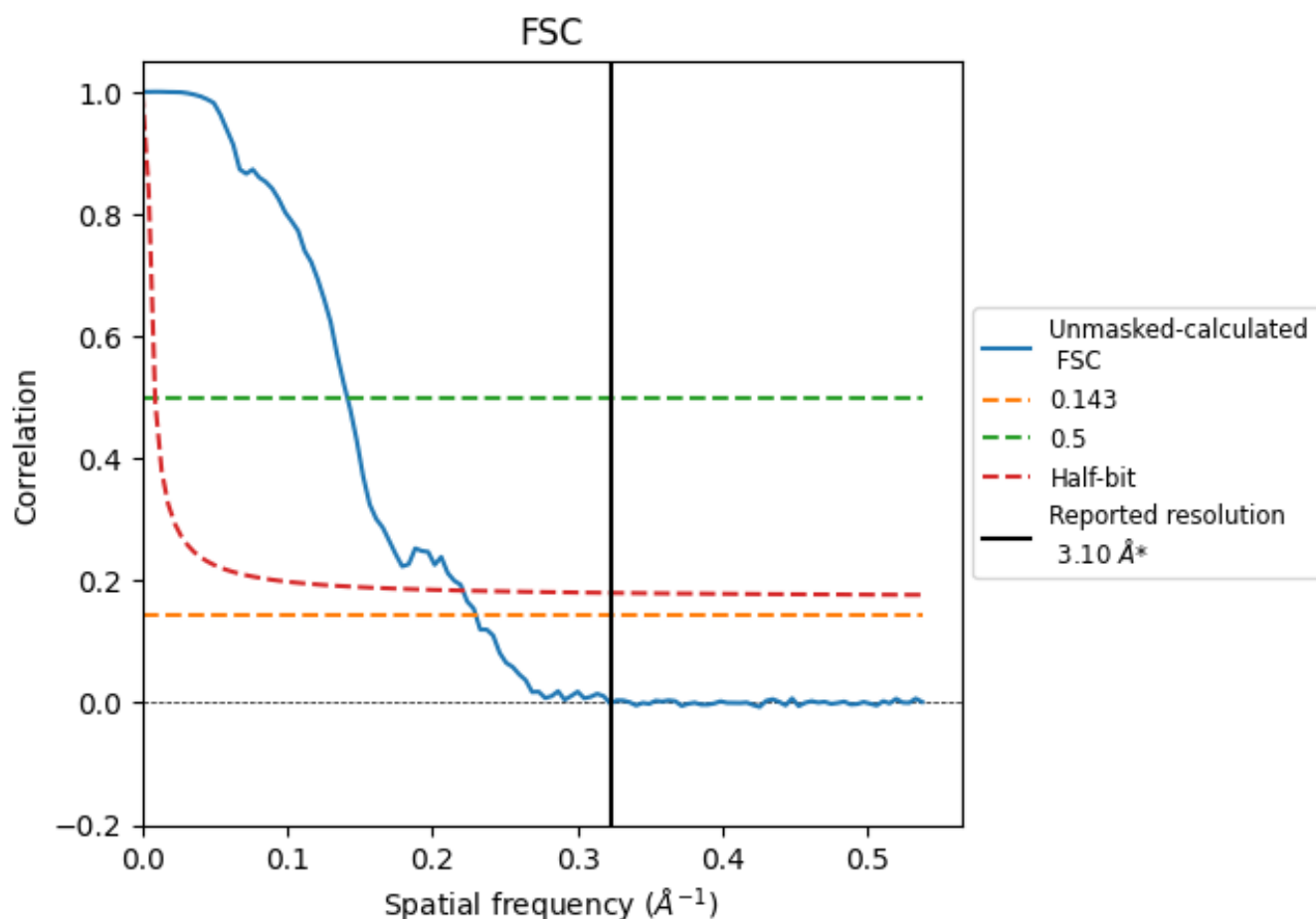


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

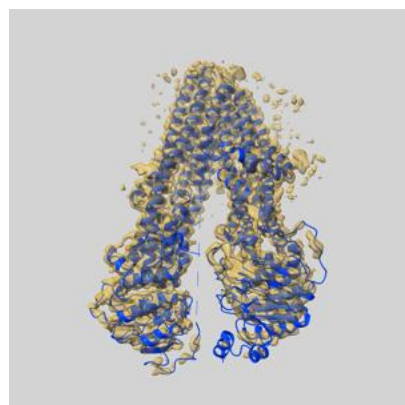
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.35	7.08	4.52

*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 4.35 differs from the reported value 3.1 by more than 10 %

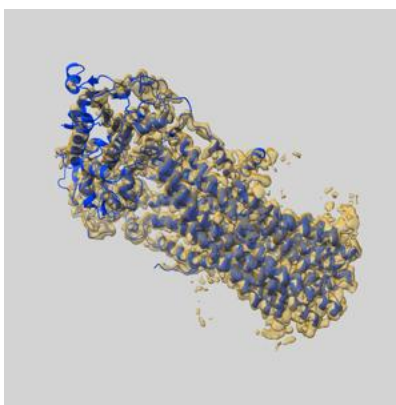
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-61830 and PDB model 9JUM. Per-residue inclusion information can be found in section [3](#) on page [6](#).

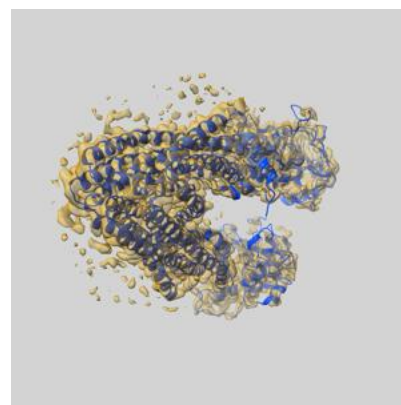
9.1 Map-model overlay [i](#)



X



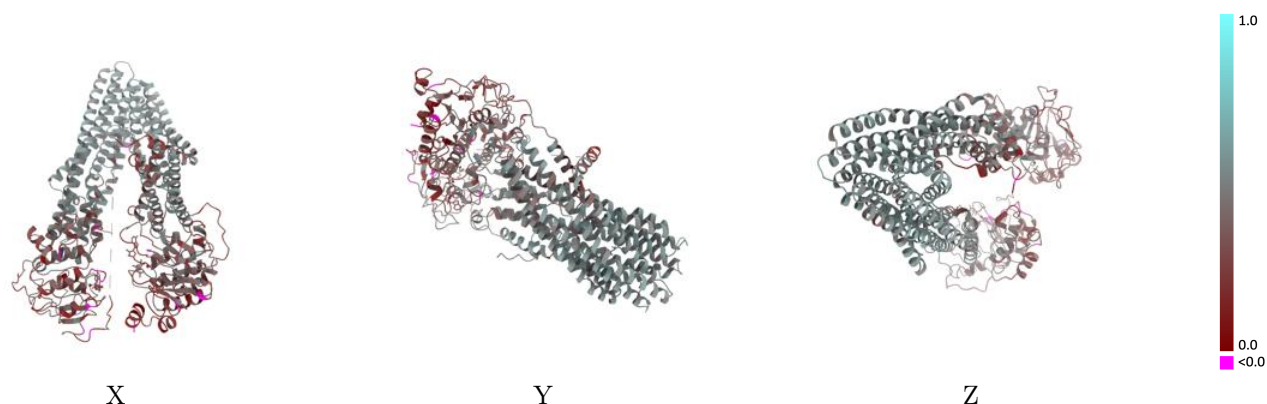
Y



Z

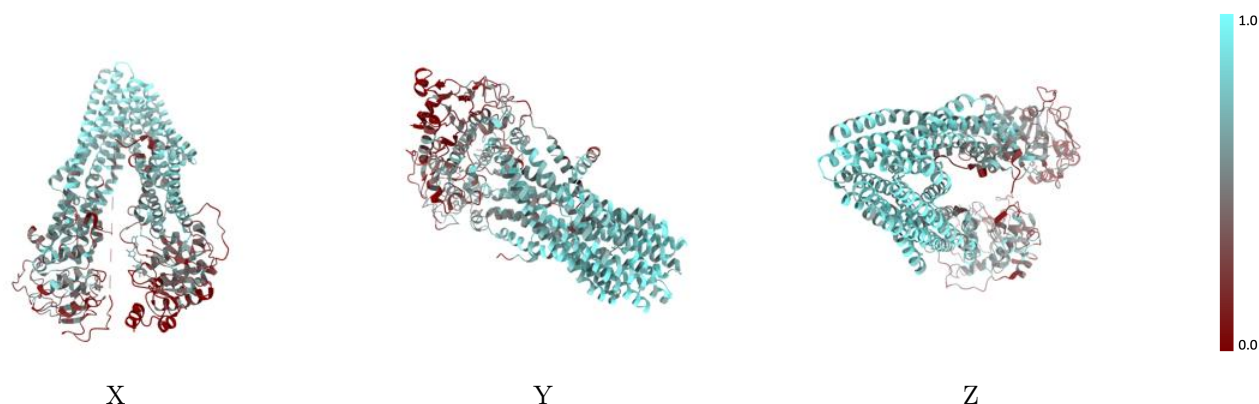
The images above show the 3D surface view of the map at the recommended contour level 0.013 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



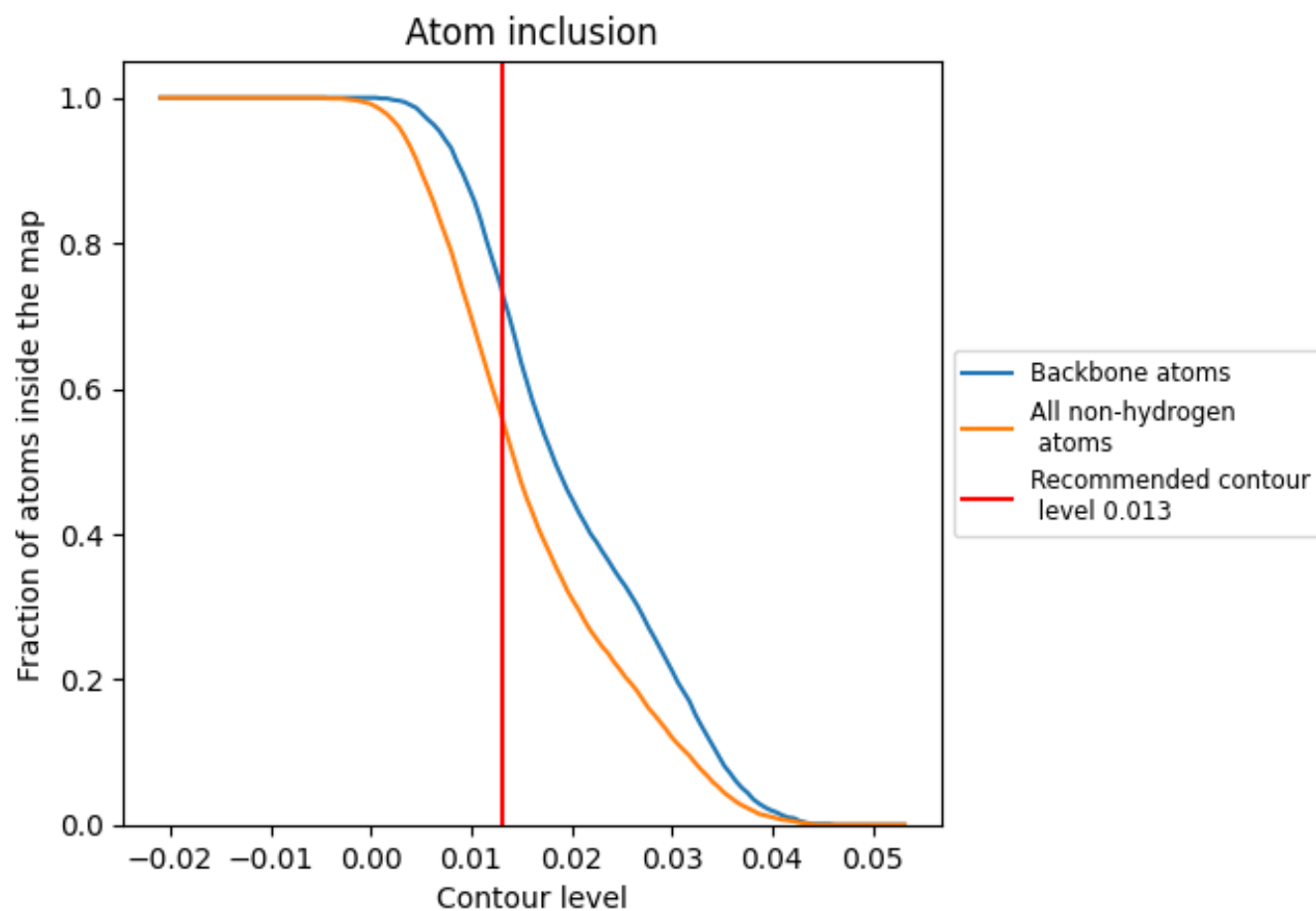
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.013).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 56% 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 (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5630	0.4160
A	0.5630	0.4160

