



## Full wwPDB EM Validation Report ⓘ

Mar 12, 2025 – 02:21 PM JST

PDB ID : 9JUM  
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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev117  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41.2

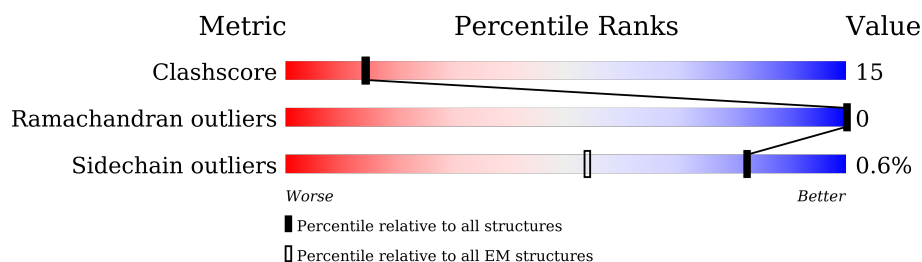
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.10 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>25%</div> <div>60%</div> <div>28%</div> <div>12%</div> </div>

## 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

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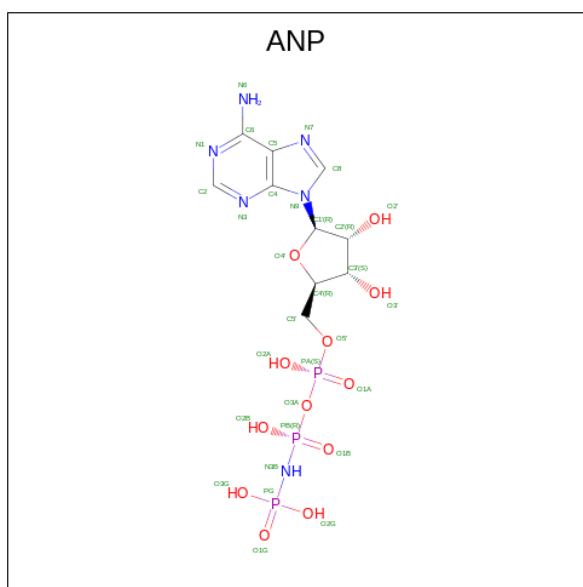
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Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	HIS	-	expression tag	UNP Q9ZR72
A	-11	PRO	-	expression tag	UNP Q9ZR72
A	-10	GLN	-	expression tag	UNP Q9ZR72
A	-9	PHE	-	expression tag	UNP Q9ZR72
A	-8	GLU	-	expression tag	UNP Q9ZR72
A	-7	LYS	-	expression 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 (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

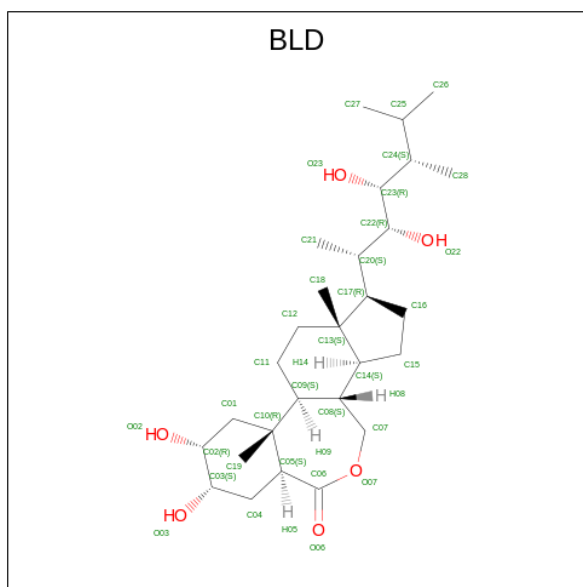
Mol	Chain	Residues	Atoms	AltConf
2	A	2	Total Mg 2 2	0

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>) (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 (three-letter code: BLD) (formula:  $C_{28}H_{48}O_6$ ) (labeled as "Ligand of Interest" by depositor).

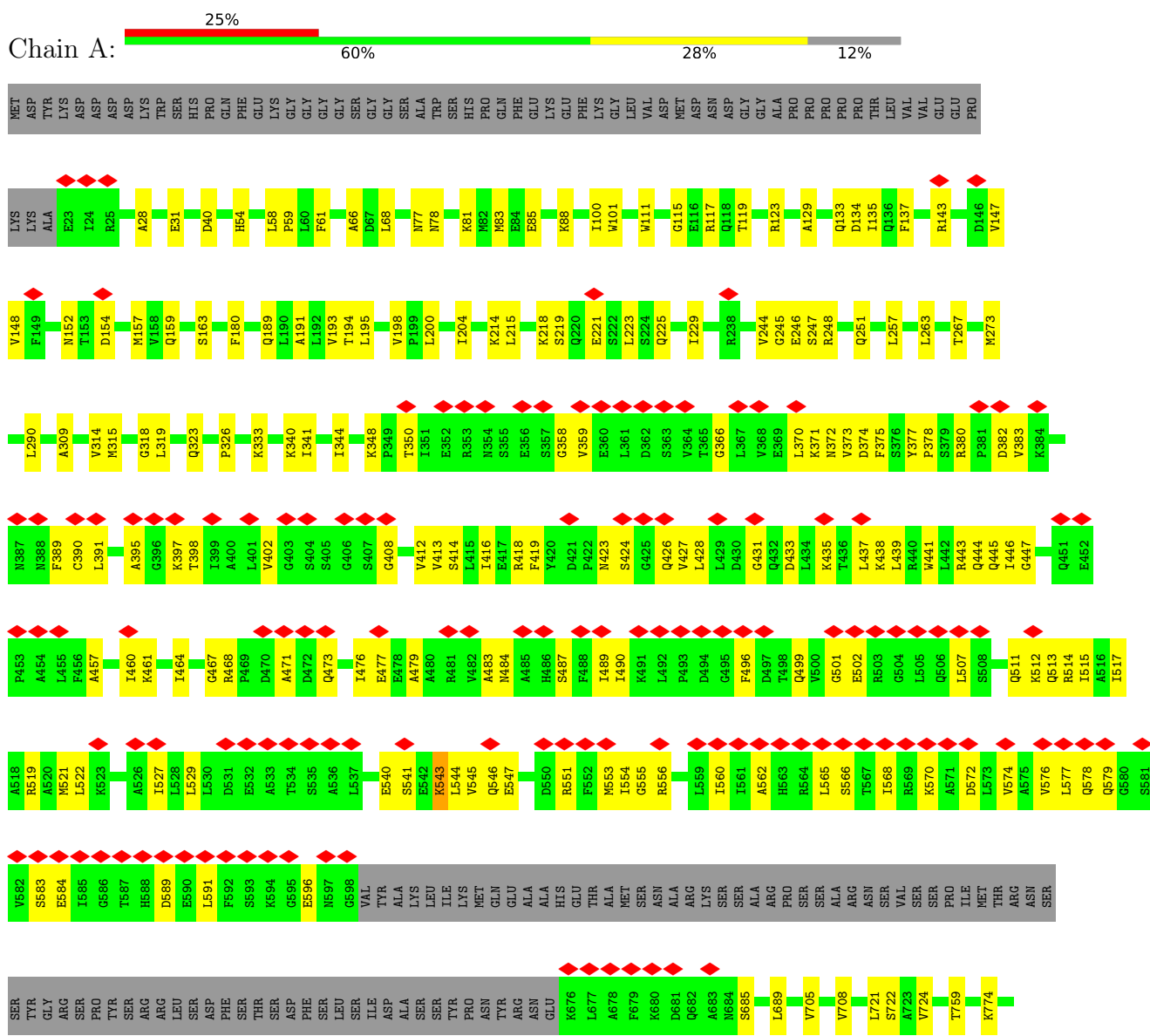


Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			34	28	6	

### 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



SER	H1219	G1157	Y1093	Y1033	K953	R777
ARG	R1220	E1158	M1094	P1094	S957	E778
VAL	L1221	R1159	L1095	S1035	D958	K786
LYS	S1222	G1160	K1096	R1036	R964	N787
GLU	T1223	Q1161	A1097	P1037	V965	E788
ASP	I1224	V1162	I1098	D1038	A976	M789
ASP	R1225	L1163	K1100	I1039	A977	A790
ALA	N1226	G1166	H1101	Q1040	E978	F792
	A1227	Q1167	I1102	I1041	T979	D793
	H1228	K1168	A1103	F1042	L980	Q794
	V1229	Q1169	I1104	R1043	T981	E795
	I1230	R1170	V1105	D1044	L982	E796
	A1231	I1171	E1108	L1045	P984	N797
	V1232	A1172	L1111	L1046	D985	R801
	I1233	I1173	F1112	L1047	F986	A807
	D1234	A1174	G1113	R1048	T987	L808
	D1235	L1177	T1114	A1049	K988	N811
	G1236	V1178	T1115	R1050	Q991	D819
	K1237	R1179	I1116	A1051	A992	R820
	V1238	K1180	Y1117	G1052	N993	V823
	A1239	A1181	E1118	L1055	R994	I824
	E1240	E1182	M1119	T1054	S995	N827
	Q1241	I1183	I1120	L1056	E998	G838
	G1242	M1184	A1121	L1057	D1001	Q842
	S1243	L1185	Y1122	V1058	E1005	L849
	H1244	L1186	G1123	G1059	I1006	V852
	S1245	D1187	H1124	P1060	E1007	V861
	H1246	E1188	E1125	S1061	P1008	T868
	L1247	A1189	G1126	G1062	D1009	D873
	L1248	T1190	A1127	C1063	D1010	L874
	K1249	S1191	T1128	G1064	P1011	E875
	N1250	A1192	E1129	K1065	D1012	R893
	H1251	L1193	A1130	S1066	T1013	D873
	P1252	D1194	E1131	S1067	T1014	L874
	D1253	A1195	I1132	V1068	P1015	E875
	G1254	E1196	Q1134	I1069	V1016	R893
	I1255	S1197	A1135	S1070	P1017	R893
	Y1256	E1198	A1136	L1071	Q1073	E913
	A1257	R1199	T1137	I1072	F1075	P914
	R1258	S1200	L1138	Q1074	D1018	E913
	M1259	V1201	A1141	R1074	L1020	P914
	I1260	Q1202	H1142	Y1076	R1021	R918
	Q1261	E1203	K1143	E1077	G1022	G931
	L1262	A1204	F1144	P1078	E1023	Y938
	Q1263	L1205	I1145	S1079	V1024	L945
	D1206	D1206	S1146	S1080	E1025	
	Q1207	Q1207	A1147	G1081	L1026	
PHE	R1264	A1208	L1148	R1082	K1027	
THR	THR	C1209	P1149	V1083	H1028	
HTS	THR	S1210	E1150	M1084	I1029	
THR	THR	G1211	G1151	T1086	D1030	
GLN	VAL	R1212	Y1152	G1087	F1031	
ILE	GLY	T1213	Y1155	D1088	I1032	
GLY	GLY	S1214	V1156	K1089		
MET	MET	I1215		I1090		
THR	THR	T1216		D1091		
SER	SER	V1217		K1092		
GLY	GLY	A1218				
SER	SER					

## 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: MG, ANP, 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	0.30	0/9137	0.51	0/12366

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	8971	0	9114	278	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	279	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 15.

All (279) 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	1.52	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: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:1086:ASP:HB3	1:A:1088:LYS:HZ1	1.59	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
1:A:473:GLN:HA	1:A:476:ILE:HD12	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:218:LYS:O	1:A:221:GLU:HG3	2.04	0.57
1:A:555:GLY:C	1:A:556:ARG:HD2	2.24	0.57
1:A:115:GLY:HA3	1:A:163:SER:HB3	1.87	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1177:LEU:O	1:A:1180:LYS:NZ	2.29	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: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
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: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:1220:ARG:NE	1:A:1221:LEU:O	2.47	0.46
1:A:246:GLU:OE2	1:A:1096:LYS:NZ	2.29	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:157:MET:HE1	1:A:333:LYS:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:789:MET:HE2	1:A:1075:PHE:CE1	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1150:GLU:OE2	1:A:1150:GLU:N	2.50	0.43
1:A:83:MET:HE1	1:A:953:LYS:CB	2.37	0.43
1:A:774:LYS:HG2	1:A:778:GLU:OE2	2.17	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: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:1019:ARG:HH21	1:A:1182:GLU:CD	2.23	0.42
1:A:1102:ILE:HG12	1:A:1183:ILE:HB	2.00	0.42
1:A:572:ASP:OD1	1:A:572:ASP:N	2.53	0.42
1:A:977:ALA:C	1:A:979:THR:H	2.23	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
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:1061:SER:HA	1:A:1065:LYS:HZ1	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:83:MET:HE1	1:A:953:LYS:HD2	2.02	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: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: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: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: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
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 ⓘ

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%)	943 (99%)	6 (1%)	84	91

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	380	ARG
1	A	543	LYS
1	A	1033	TYR
1	A	1143	LYS
1	A	1159	ARG
1	A	1258	ARG

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	152	ASN
1	A	444	GLN
1	A	445	GLN
1	A	484	ASN
1	A	758	ASN
1	A	1169	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

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	1303	2	29,33,33	1.19	5 (17%)	31,52,52	1.14	3 (9%)
4	BLD	A	1305	-	36,37,37	0.37	0	46,59,59	1.19	3 (6%)
3	ANP	A	1304	2	29,33,33	1.21	5 (17%)	31,52,52	1.17	3 (9%)

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	1303	2	-	4/14/38/38	0/3/3/3
4	BLD	A	1305	-	-	8/20/85/85	0/4/4/4
3	ANP	A	1304	2	-	3/14/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1304	ANP	PG-O1G	3.27	1.51	1.46
3	A	1303	ANP	PG-O1G	3.12	1.51	1.46
3	A	1303	ANP	PB-O1B	2.95	1.50	1.46
3	A	1304	ANP	PB-O1B	2.86	1.50	1.46
3	A	1304	ANP	PB-O2B	-2.21	1.50	1.56
3	A	1303	ANP	PB-O2B	-2.17	1.50	1.56
3	A	1304	ANP	PG-O2G	-2.09	1.51	1.56
3	A	1303	ANP	PG-O2G	-2.08	1.51	1.56
3	A	1304	ANP	PG-O3G	-2.04	1.51	1.56
3	A	1303	ANP	PG-O3G	-2.04	1.51	1.56

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1305	BLD	O07-C06-O06	4.64	123.96	116.72
3	A	1304	ANP	O2B-PB-O1B	4.09	118.50	109.92
3	A	1303	ANP	O2B-PB-O1B	4.03	118.38	109.92
4	A	1305	BLD	C01-C10-C05	2.97	111.80	107.06
4	A	1305	BLD	C07-O07-C06	-2.68	117.22	121.01
3	A	1304	ANP	C5-C6-N6	2.32	123.87	120.35
3	A	1303	ANP	C5-C6-N6	2.30	123.84	120.35
3	A	1303	ANP	O3G-PG-O1G	-2.14	108.07	113.45
3	A	1304	ANP	O2G-PG-O1G	-2.10	108.17	113.45

There are no chirality outliers.

All (15) torsion outliers are listed below:

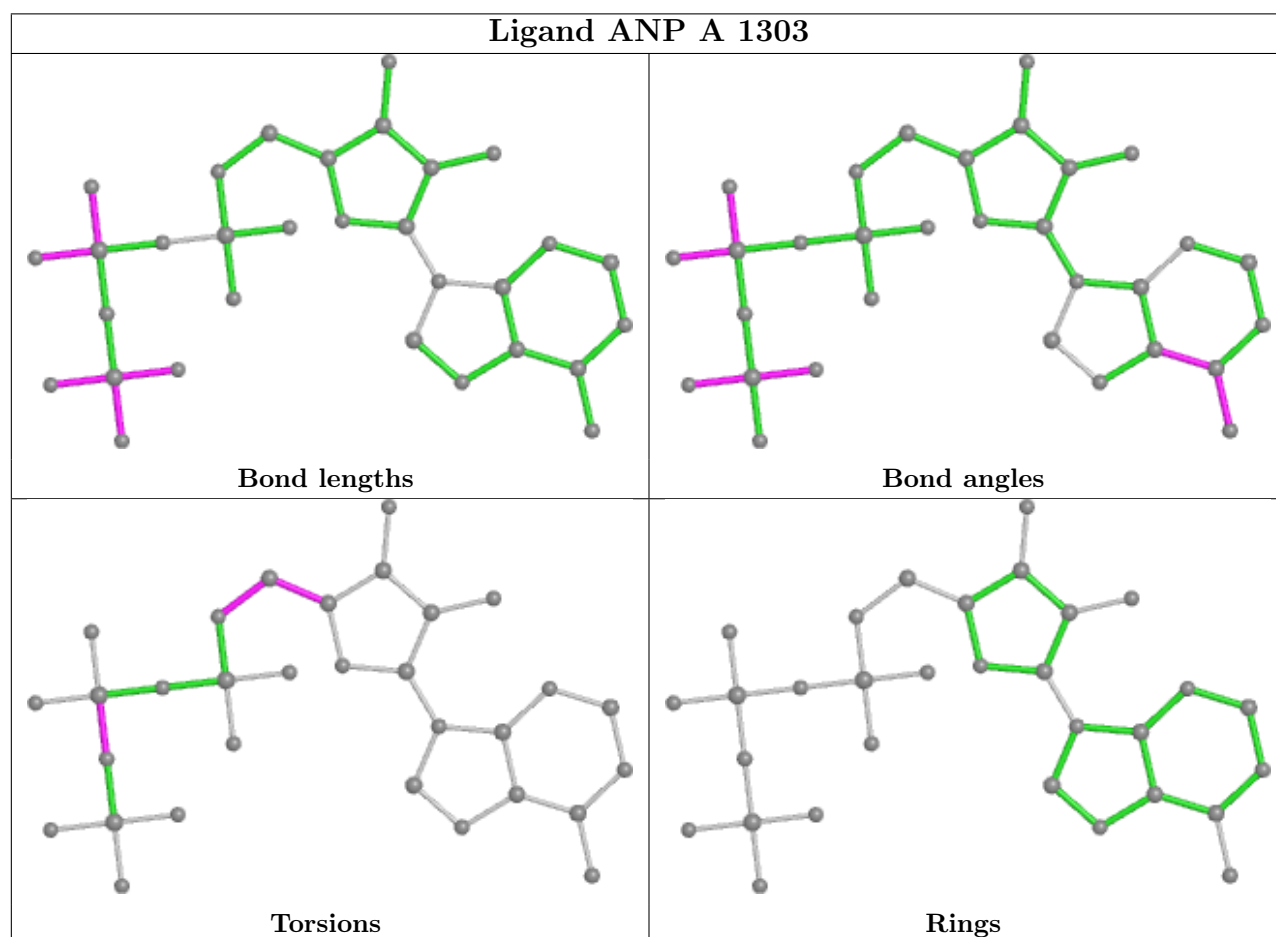
Mol	Chain	Res	Type	Atoms
3	A	1303	ANP	PG-N3B-PB-O1B
4	A	1305	BLD	C22-C23-C24-C28
4	A	1305	BLD	O22-C22-C23-O23
4	A	1305	BLD	O23-C23-C24-C28
3	A	1304	ANP	C3'-C4'-C5'-O5'
3	A	1303	ANP	O4'-C4'-C5'-O5'
4	A	1305	BLD	O23-C23-C24-C25
3	A	1304	ANP	PG-N3B-PB-O3A
4	A	1305	BLD	C20-C22-C23-C24
4	A	1305	BLD	C22-C23-C24-C25
3	A	1304	ANP	O4'-C4'-C5'-O5'
4	A	1305	BLD	C20-C22-C23-O23
4	A	1305	BLD	O22-C22-C23-C24
3	A	1303	ANP	C3'-C4'-C5'-O5'
3	A	1303	ANP	C4'-C5'-O5'-PA

There are no ring outliers.

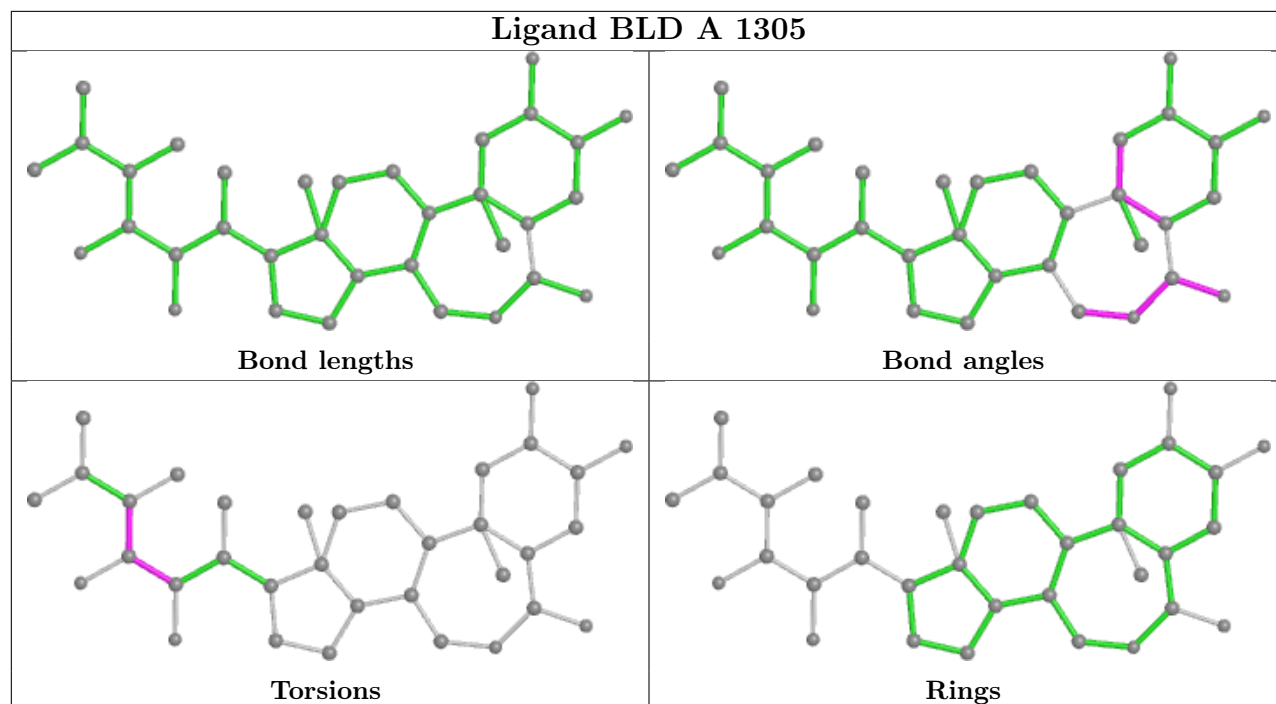
3 monomers are involved in 3 short contacts:

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

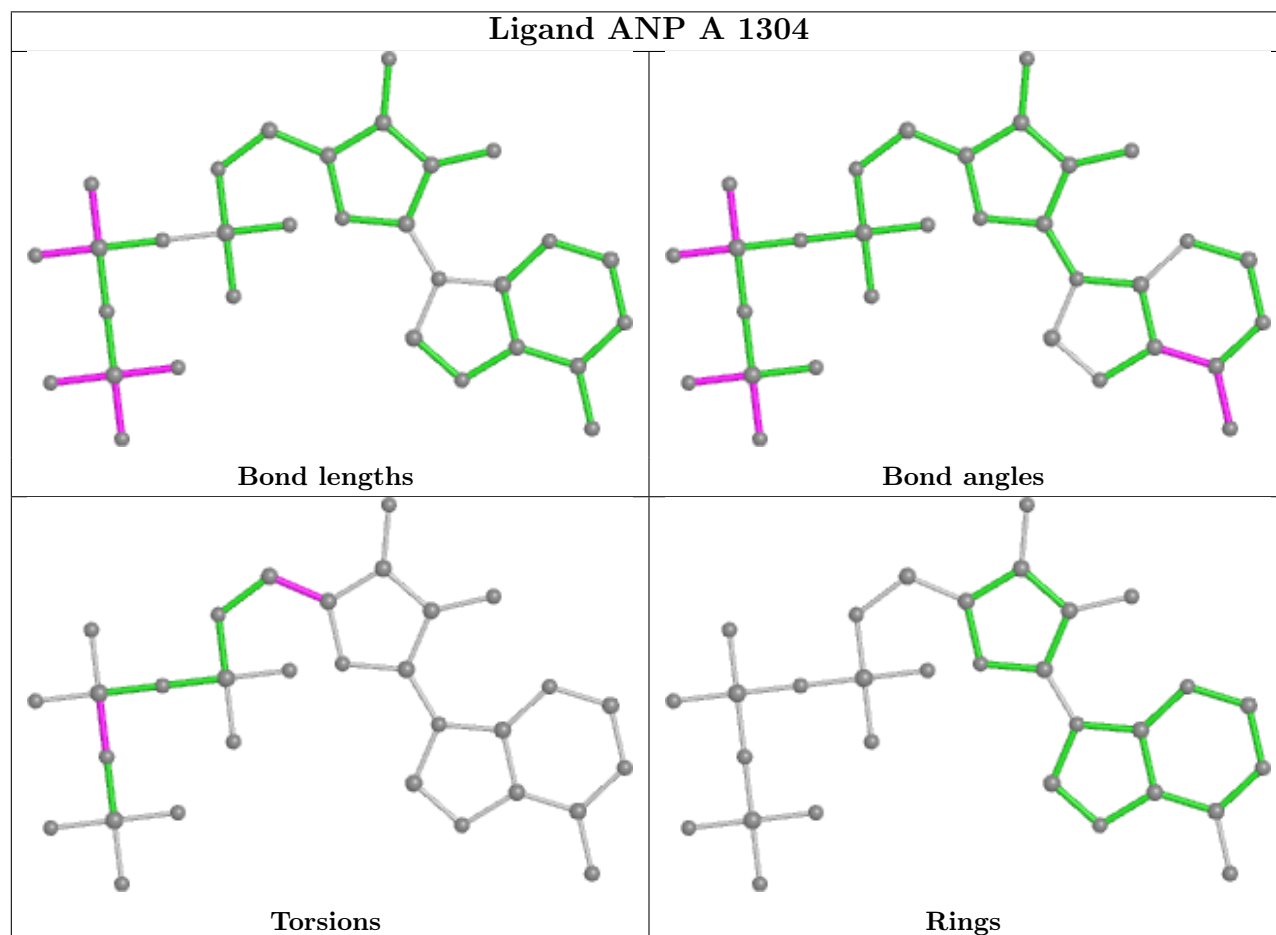
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 BLD A 1305



## Ligand ANP A 1304



## 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.

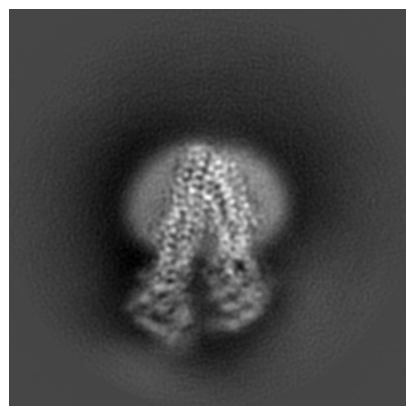
## 6 Map visualisation [i](#)

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.

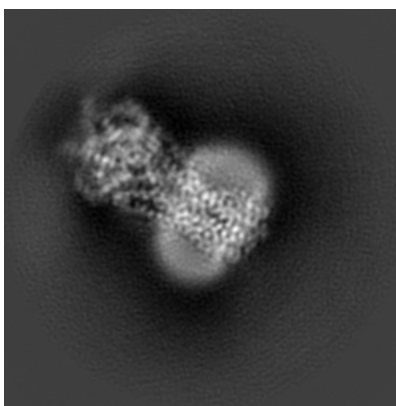
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

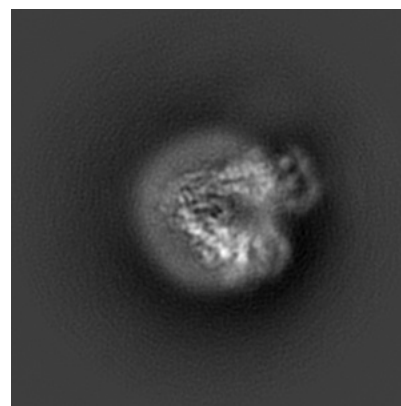
#### 6.1.1 Primary map



X

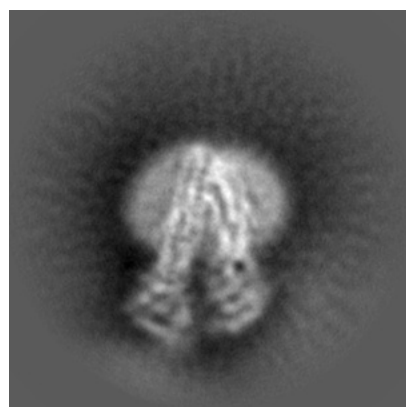


Y

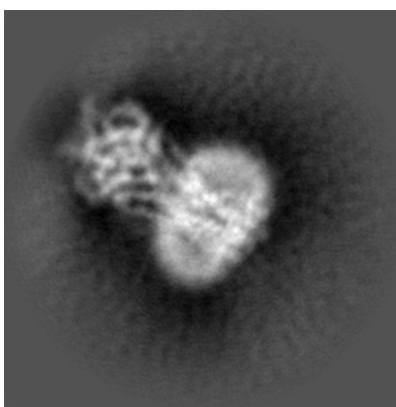


Z

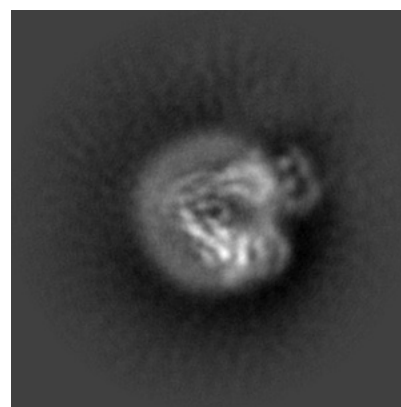
#### 6.1.2 Raw map



X



Y

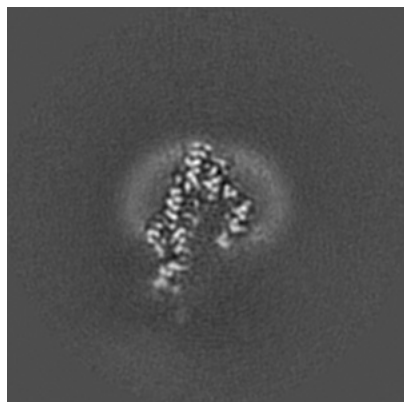


Z

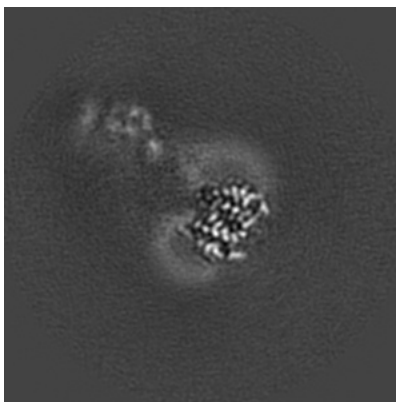
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

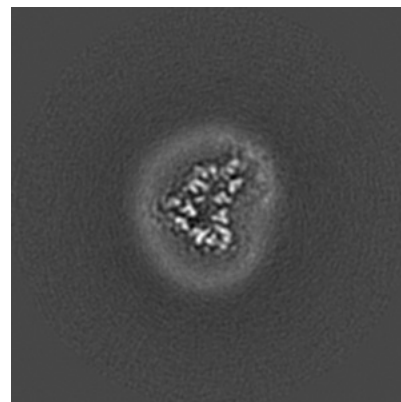
### 6.2.1 Primary map



X Index: 120

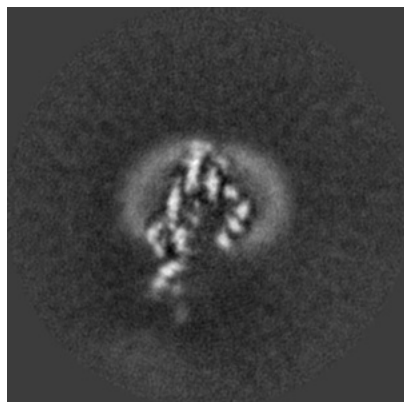


Y Index: 120

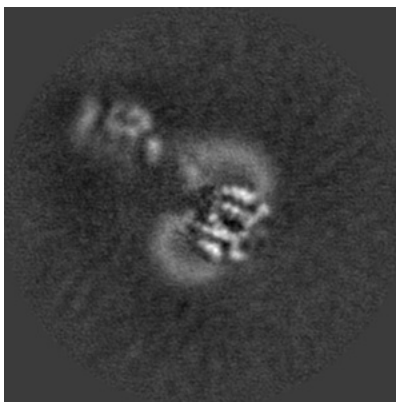


Z Index: 120

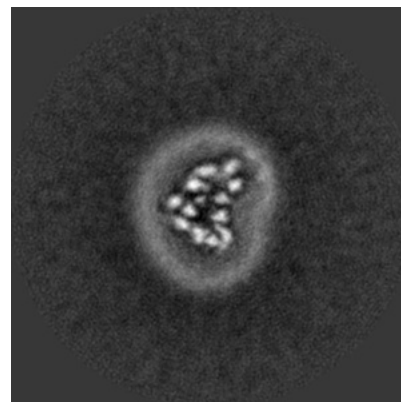
### 6.2.2 Raw map



X Index: 120



Y Index: 120



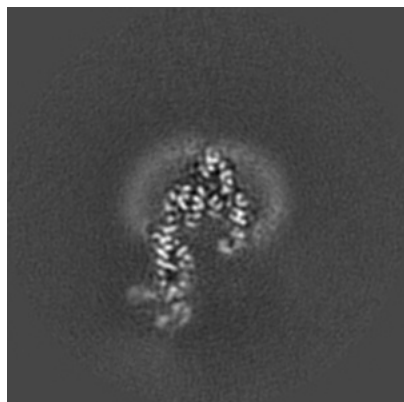
Z Index: 120

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

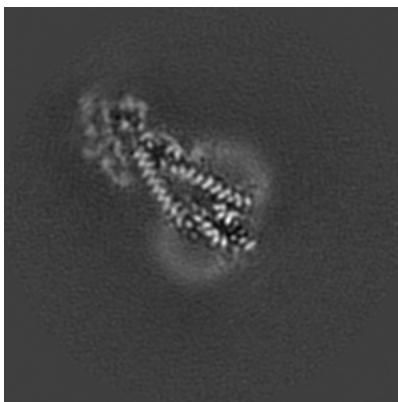


## 6.3 Largest variance slices [i](#)

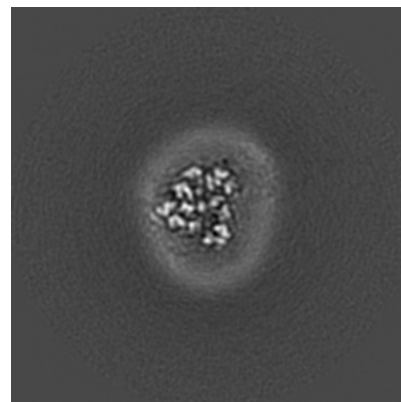
### 6.3.1 Primary map



X Index: 126

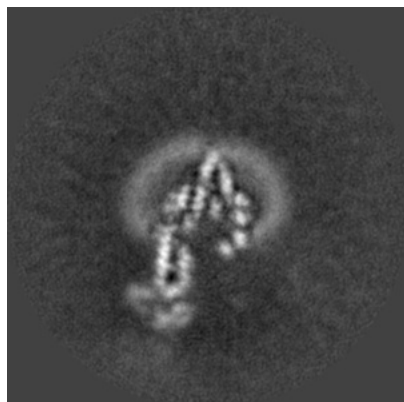


Y Index: 131

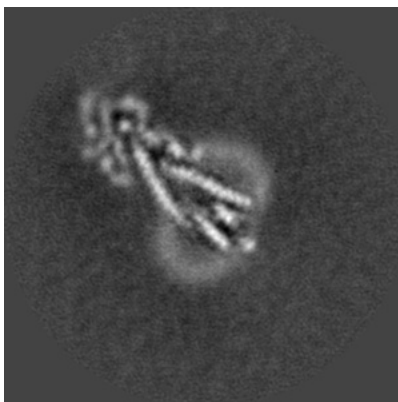


Z Index: 126

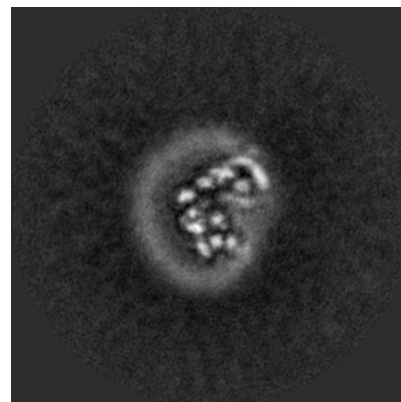
### 6.3.2 Raw map



X Index: 127



Y Index: 131

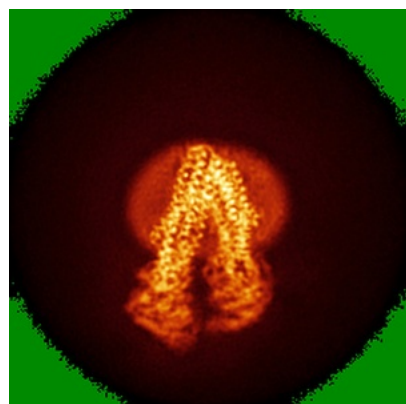


Z Index: 113

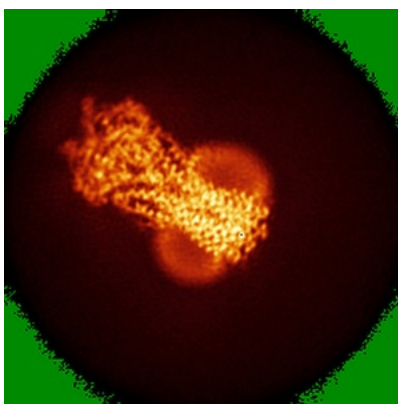
The images above show the largest variance slices of the map in three orthogonal directions.

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

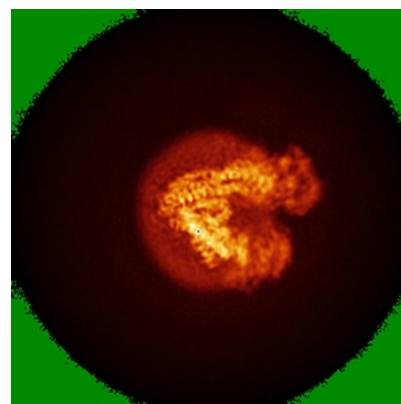
### 6.4.1 Primary map



X

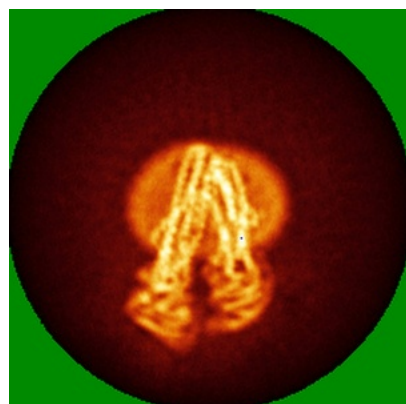


Y

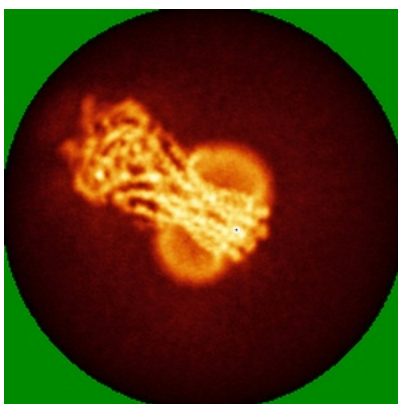


Z

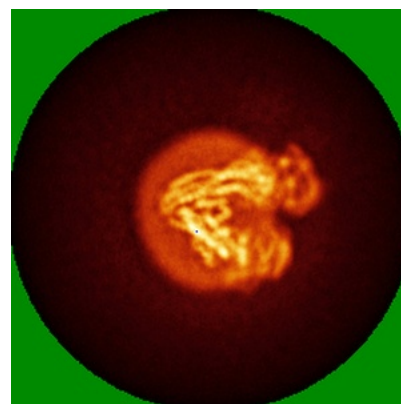
### 6.4.2 Raw map



X



Y

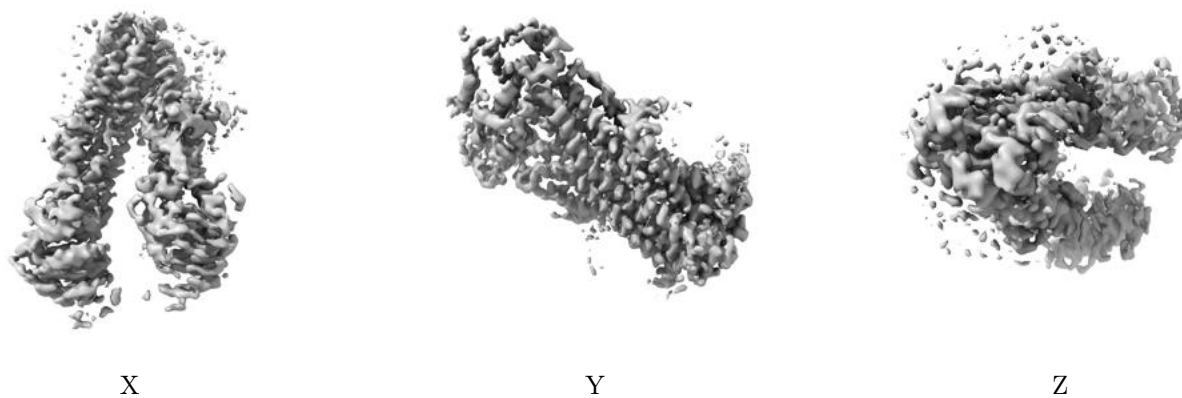


Z

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.

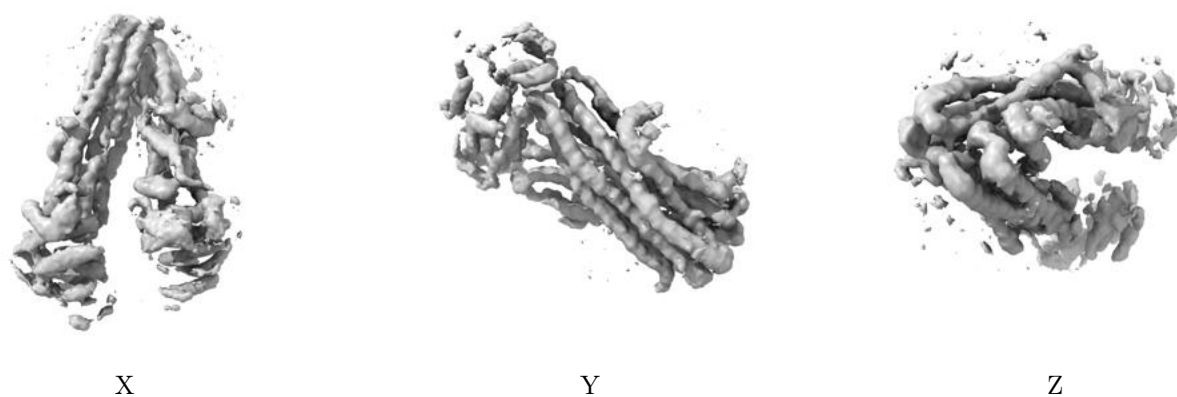
## 6.5 Orthogonal surface views [i](#)

### 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.

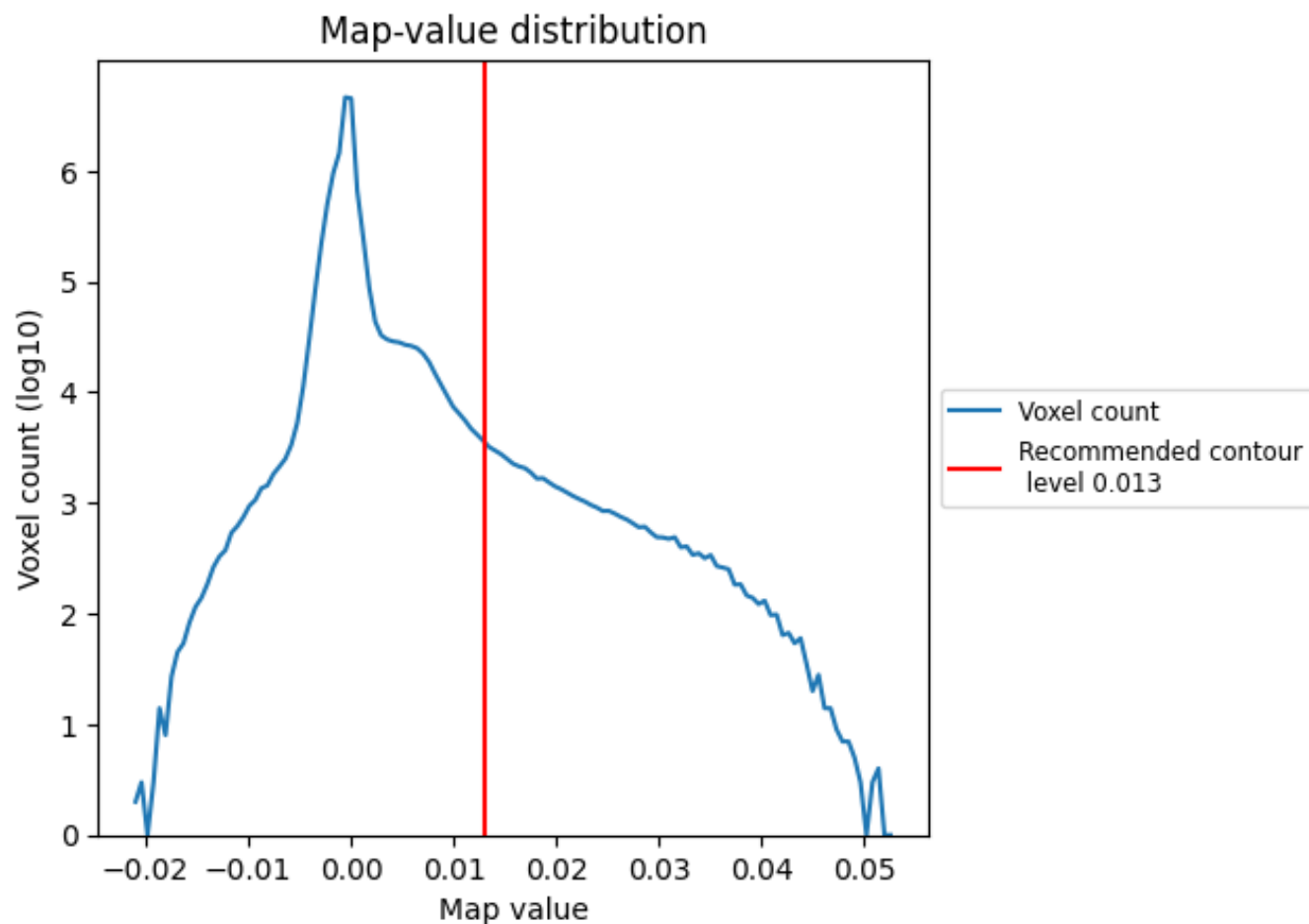
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

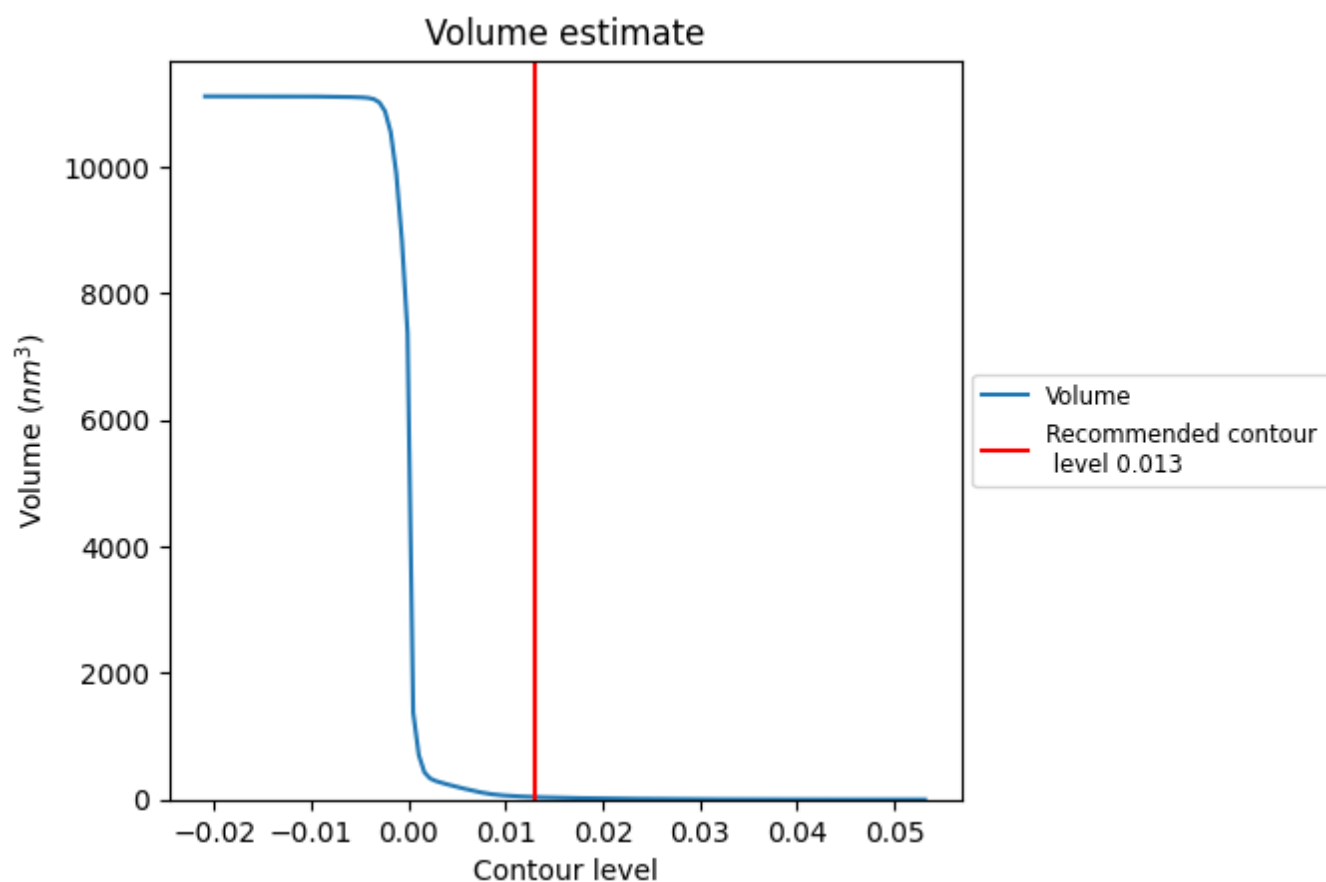
This section contains the results of statistical analysis of the map.

### 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.

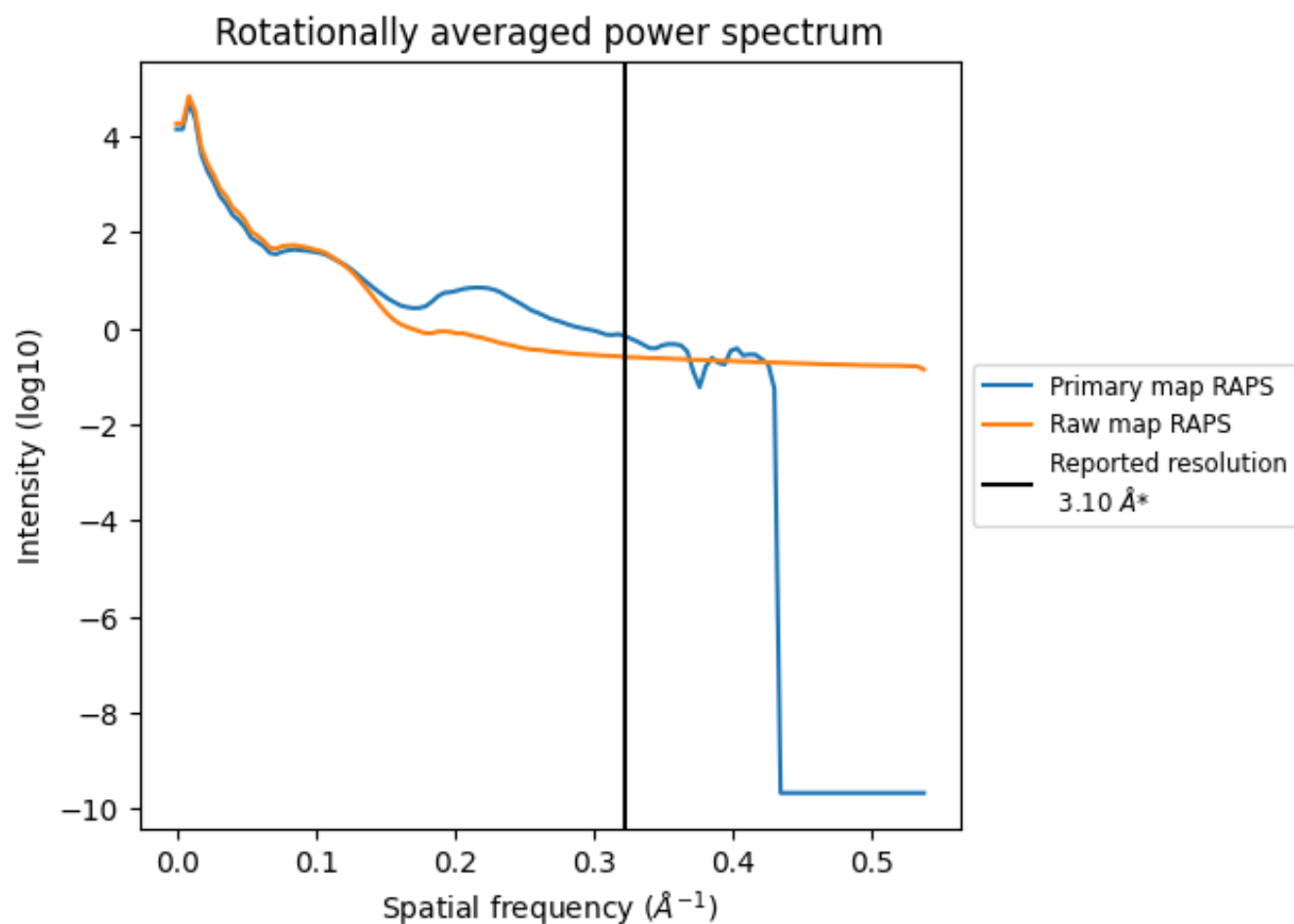
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 40 nm<sup>3</sup>; 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 ⓘ

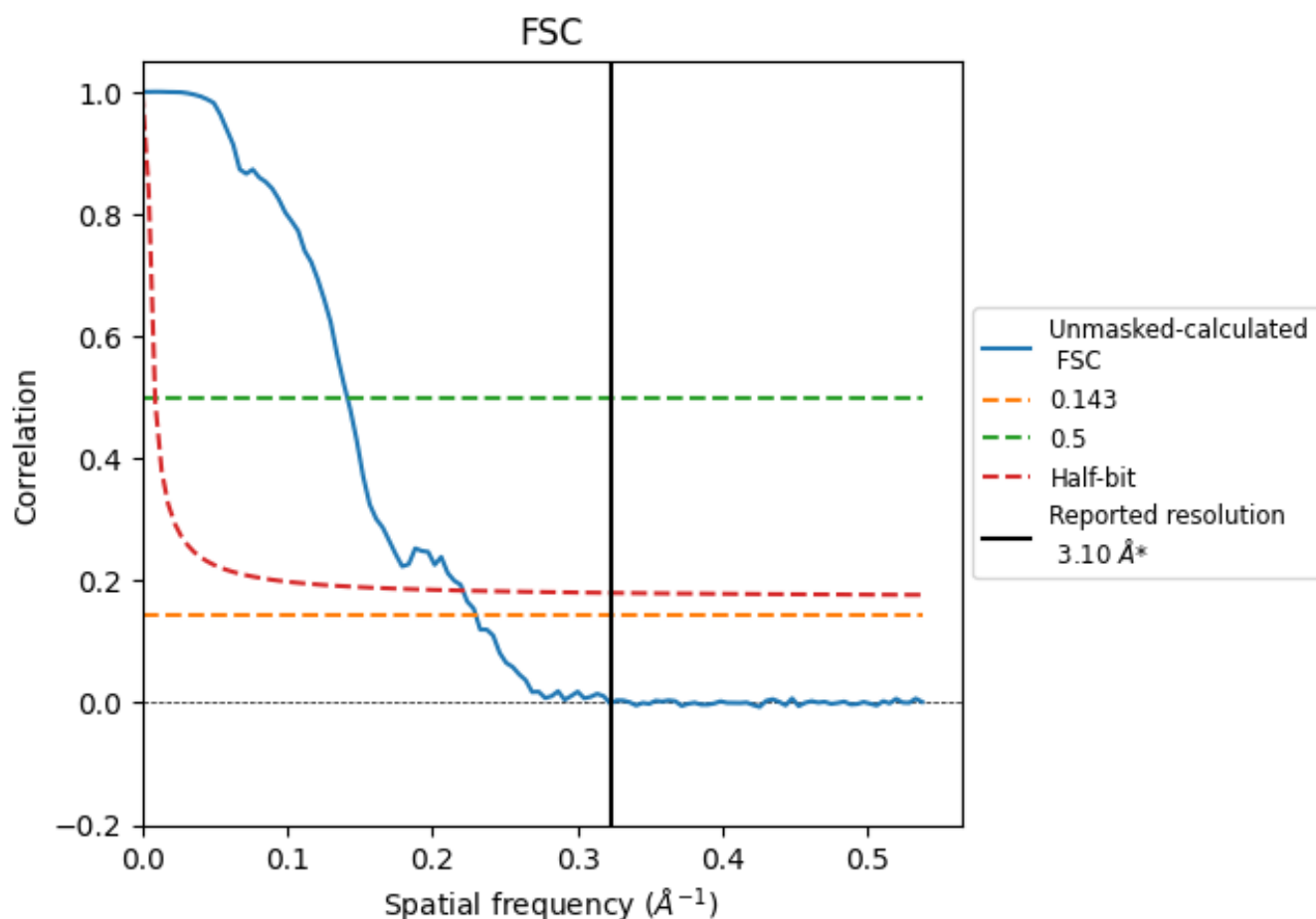


\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>

## 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 Å<sup>-1</sup>

## 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

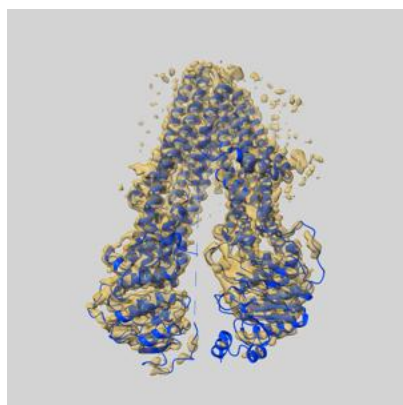
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.35 differs from the reported value 3.1 by more than 10 %



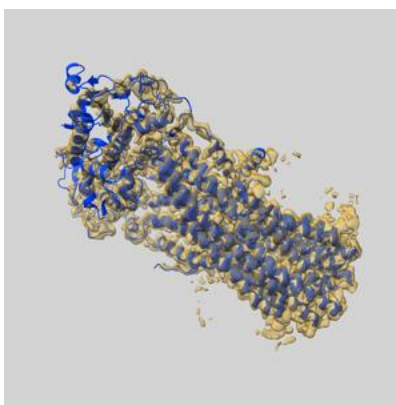
## 9 Map-model fit [i](#)

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](#).

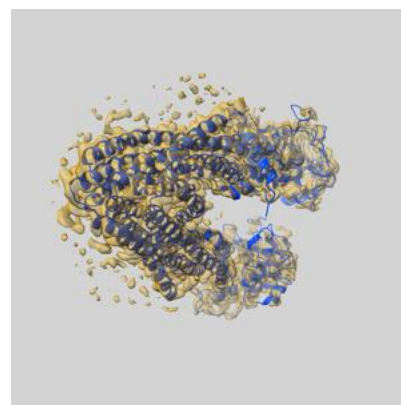
### 9.1 Map-model overlay [i](#)



X



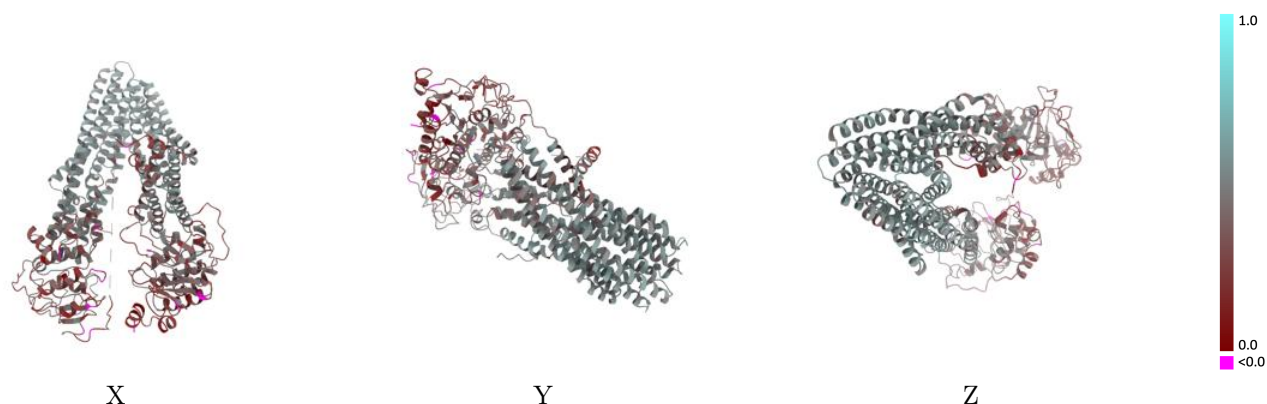
Y



Z

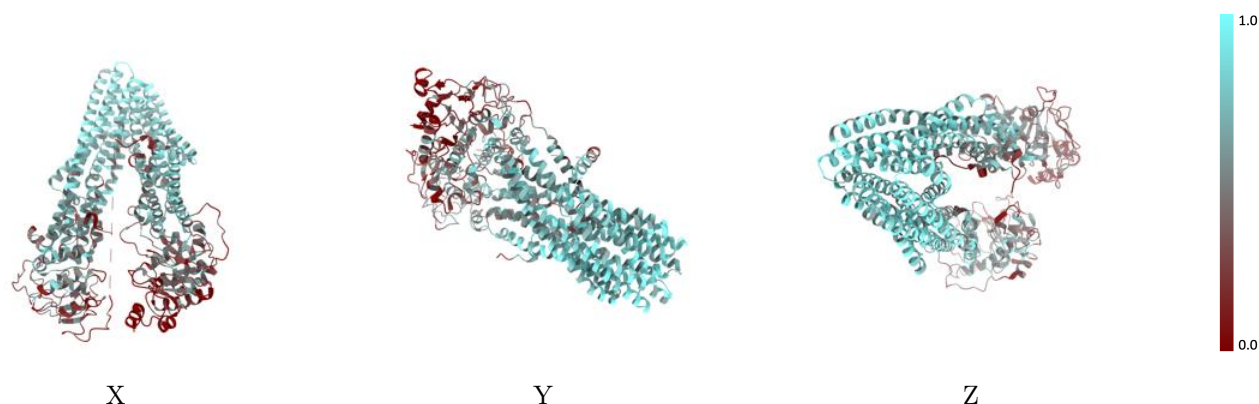
The images above show the 3D surface view of the map at the recommended contour level 0.013 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



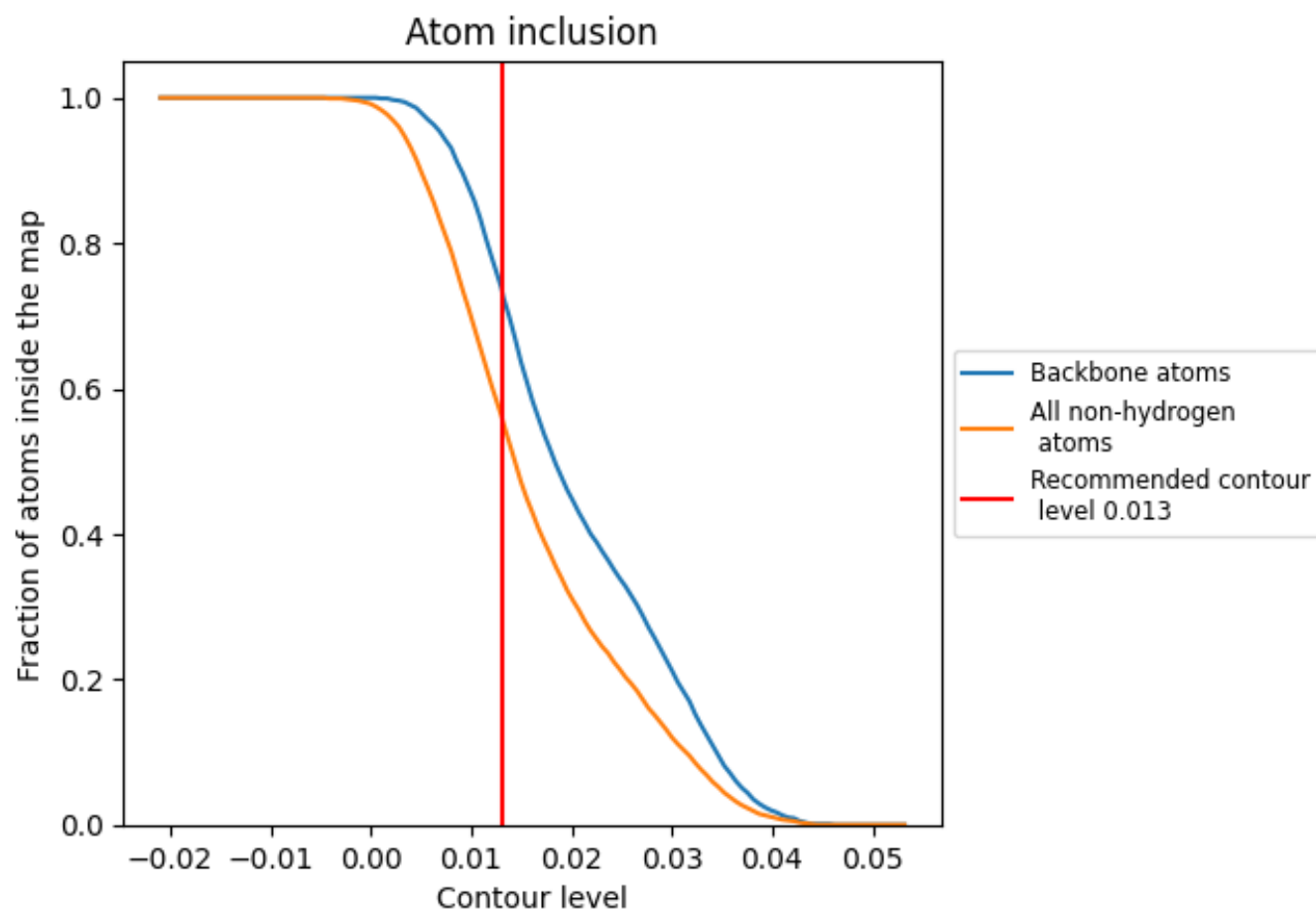
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	<div></div> 0.5630	<div></div> 0.4160
A	<div></div> 0.5630	<div></div> 0.4160

