



## Full wwPDB EM Validation Report ⓘ

Mar 12, 2025 – 02:12 PM JST

PDB ID : 9JUO  
EMDB ID : EMD-61832  
Title : Structure of Arabidopsis thaliana ABCB1 with AMP-PNP bound in the inward-facing conformation under IAA condition  
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

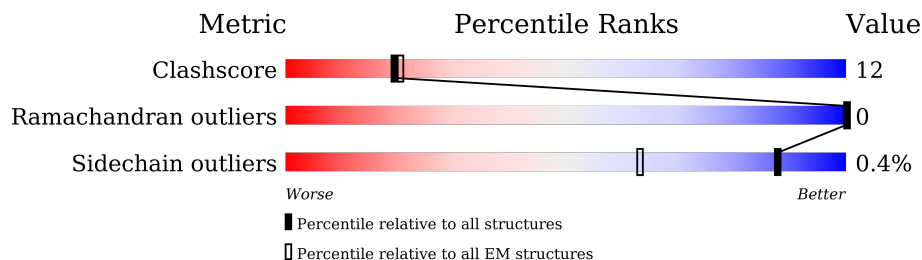
# 1 Overall quality at a glance

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>23%</div> <div>63%</div> <div>23%</div> <div>14%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8858 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	1144	Total	C	N	O	S	0	0
			8794	5625	1506	1623	40		

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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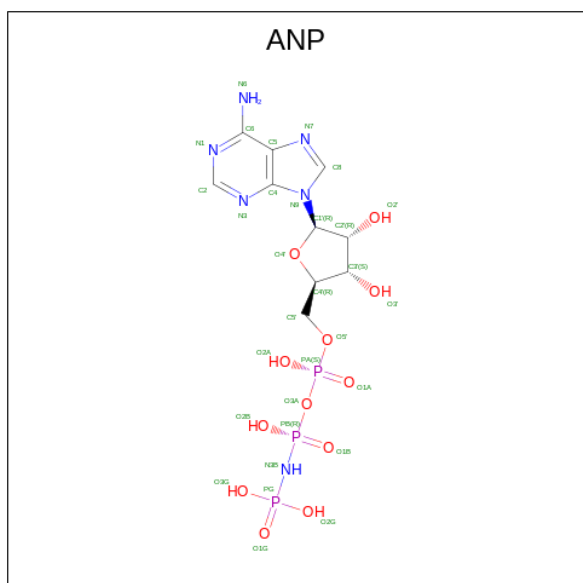
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Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	HIS	-	expression tag	UNP Q9ZR72
A	-11	PRO	-	expression tag	UNP Q9ZR72
A	-10	GLN	-	expression tag	UNP Q9ZR72
A	-9	PHE	-	expression tag	UNP Q9ZR72
A	-8	GLU	-	expression tag	UNP Q9ZR72
A	-7	LYS	-	expression 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).

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

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula:  $C_{10}H_{17}N_6O_{12}P_3$ ) (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	

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



PRO	R844	R994	V1058	C1126	T1190	ASP
GLY	L845	S995	G1059	A1127	S1191	GLY
ILE	A846	E998	P1060	T1128	A1192	ILE
TYR	V848	L999	S1061	E1129	L1193	TYR
ALA	L849	L1000	G1062	A1130	D1194	ALA
ARG	V850	D1001	C1063	E1131	A1195	ARG
MET		R1002	G1064	I1132	E1196	MET
ILE	T860	K1003	K1065	I1133	S1197	ILE
GLN	V861	T1004	I1069	Q1134	E1198	GLN
LEU	L862	E1005	I1072	A1135	R1199	LEU
GLN	Q863	I1006	Q1073	A1136	S1200	GLN
ARG	K864	E1007	R1074	T1137	V1201	ARG
ARG	Q883	P1008	F1075	L1138	Q1202	ARG
THR	I889	D1009	E1076	A1139	E1203	THR
THR		P1010	E1077	S1140	A1204	THR
GLN	V905	D1011	P1078	H1141	L1205	GLN
VAL	T909	D1012	S1079	H1142	D1206	VAL
ILE		T1013	S1080	K1143	Q1207	ILE
GLY	Y930	V1016	S1081	F1144	Q1208	GLY
NET	G931	P1017	G1082	I1145	A1209	NET
THR		D1018	R1083	S1146	C1210	THR
SER	L945	R1019	M1084	A1147	S1211	SER
GLY	S949	L1020	I1085	L1148	G1212	GLY
SER	W950	R1021	D1086	E1150	R1216	SER
SER	L951	G1022	G1087	G1151	V1217	SER
ARG	V952	E1023	K1088	K1153	A1218	ARG
VAL	K953	E1025	I1090	T1154	H1219	VAL
LYS		L1026	R1091	V1155	R1220	LYS
GLU	T962	K1027	K1092	G1157	L1221	GLU
ASP	I963	H1028	Y1093	E1158	S1222	ASP
ASP	R964	I1029	N1094	R1159	T1223	ASP
ALA	V965	D1030	K1096	G1160	I1224	ALA
	F966	F1031	A1097	V1161	R1225	
	M967	S1035	I1098	Q1162	N1226	
	V968	R1036	R1099	L1163	A1227	
	M970	P1037	K1100	S1164	H1228	
	V971	D1038	H1101	G1165	V1229	
	S972	I1039	T1104	G1166	I1230	
	A976	Q1040	V1105	Q1167	A1231	
	T979	I1041	P1106	K1168	V1232	
	L980	F1042	Q1107	R1170	I1233	
	T981	R1043	E1108	I1171	D1234	
	L982	D1044	P1109	A1174	D1235	
	A983	L1045	T1114	G1175	G1236	
	P984	S1046	I1115	V1176	K1237	
	D985	L1047	Y1116	R1179	V1238	
	F986	R1048	E1118	K1180	A1239	
	I987	A1049	N1119	A1181	E1240	
	K988	R1050	T1120	M1184	Q1241	
	A992	A1051	G1123	L1185	G1242	
	M993	G1052	H1124	L1186	S1243	
		K1053	E1125	D1187	HIS	SER
		T1054		E1188	SER	SER
		L1055		A1189	HIS	HIS
		A1056			LEU	LEU
					LEU	LEU
					LYS	LYS
					ASN	ASN
					HIS	HIS

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	157897	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 ( $e^-/\text{\AA}^2$ )	52	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	0.082	Depositor
Minimum map value	-0.040	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.014	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

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	0.31	0/8955	0.48	0/12121

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	8794	0	8936	221	0
2	A	2	0	0	0	0
3	A	62	0	26	0	0
All	All	8858	0	8962	221	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 12.

All (221) 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:770:GLU:HG2	1:A:814:ARG:HH21	1.35	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:727:VAL:HG12	1:A:736:MET:HG3	1.62	0.80
1:A:1095:LEU:HD21	1:A:1099:ARG:HH11	1.46	0.79
1:A:549:LEU:HB3	1:A:552:PHE:HB3	1.65	0.77
1:A:157:MET:HG2	1:A:334:ALA:HA	1.67	0.77
1:A:375:PHE:H	1:A:386:LEU:HB3	1.50	0.77
1:A:389:PHE:HB2	1:A:582:VAL:HG22	1.67	0.76
1:A:844:ARG:HD2	1:A:951:LEU:HD21	1.65	0.75
1:A:1093:TYR:CE2	1:A:1098:ILE:HG13	2.23	0.73
1:A:809:ASP:O	1:A:813:VAL:HG12	1.88	0.72
1:A:789:MET:HG3	1:A:1075:PHE:CD2	2.25	0.72
1:A:821:ILE:O	1:A:824:ILE:HG22	1.92	0.69
1:A:812:ASN:HD22	1:A:813:VAL:N	1.91	0.68
1:A:795:GLU:O	1:A:798:GLU:HG3	1.95	0.67
1:A:839:PHE:HD2	1:A:843:TRP:HD1	1.41	0.66
1:A:776:VAL:O	1:A:780:MET:HG3	1.97	0.65
1:A:413:VAL:HG13	1:A:529:LEU:HD23	1.80	0.64
1:A:809:ASP:HA	1:A:812:ASN:HD21	1.62	0.63
1:A:75:ASN:HB2	1:A:82:MET:HB3	1.79	0.63
1:A:773:THR:HB	1:A:814:ARG:HB2	1.81	0.63
1:A:838:GLY:HA2	1:A:965:VAL:HG22	1.80	0.63
1:A:1136:ALA:HB1	1:A:1141:ALA:HB3	1.80	0.63
1:A:584:GLU:OE2	1:A:588:HIS:NE2	2.32	0.63
1:A:1013:THR:HG21	1:A:1094:ASN:HB2	1.81	0.63
1:A:511:GLN:O	1:A:514:ARG:HB2	1.99	0.63
1:A:1008:PRO:HB2	1:A:1096:LYS:HE3	1.79	0.63
1:A:1136:ALA:HA	1:A:1139:ALA:HB3	1.80	0.61
1:A:409:LYS:HB3	1:A:559:LEU:HD11	1.82	0.61
1:A:1104:ILE:HG22	1:A:1106:PRO:HD3	1.81	0.61
1:A:966:PHE:O	1:A:970:MET:HG2	2.00	0.61
1:A:1120:ILE:HG22	1:A:1178:VAL:HG21	1.82	0.61
1:A:441:TRP:O	1:A:445:GLN:NE2	2.34	0.61
1:A:546:GLN:HA	1:A:551:ARG:HH12	1.66	0.61
1:A:1137:THR:HA	1:A:1142:HIS:HB2	1.82	0.61
1:A:569:ARG:NH2	1:A:588:HIS:O	2.34	0.61
1:A:349:PRO:HG2	1:A:352:GLU:HB2	1.82	0.60
1:A:1029:ILE:HD11	1:A:1045:LEU:HD23	1.83	0.60
1:A:820:ARG:HB3	1:A:986:PHE:CE1	2.36	0.60
1:A:1181:ALA:O	1:A:1212:ARG:NH1	2.35	0.58
1:A:241:MET:HB3	1:A:1099:ARG:HH22	1.67	0.58
1:A:66:ALA:HB2	1:A:309:ALA:HB2	1.85	0.57
1:A:1186:LEU:HD11	1:A:1205:LEU:HD22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:THR:OG1	1:A:141:GLU:OE2	2.16	0.57
1:A:545:VAL:O	1:A:551:ARG:NH1	2.38	0.57
1:A:68:LEU:HD22	1:A:945:LEU:HD13	1.86	0.56
1:A:812:ASN:HD22	1:A:813:VAL:H	1.52	0.56
1:A:484:ASN:OD1	1:A:514:ARG:NH1	2.38	0.56
1:A:823:VAL:O	1:A:826:GLN:HG2	2.04	0.56
1:A:773:THR:CB	1:A:814:ARG:HB2	2.36	0.56
1:A:780:MET:HG2	1:A:1000:LEU:HD11	1.88	0.56
1:A:845:LEU:HD22	1:A:962:THR:HG22	1.89	0.55
1:A:1114:THR:HG23	1:A:1115:THR:HG23	1.88	0.55
1:A:688:ARG:NH2	1:A:1001:ASP:OD2	2.35	0.55
1:A:396:GLY:HA2	1:A:554:ILE:HA	1.87	0.55
1:A:1187:ASP:HA	1:A:1217:VAL:HG22	1.88	0.55
1:A:427:VAL:HG13	1:A:434:LEU:HD12	1.89	0.55
1:A:798:GLU:HB2	1:A:801:ARG:HB3	1.87	0.55
1:A:355:SER:OG	1:A:440:ARG:NH2	2.40	0.55
1:A:995:SER:O	1:A:998:GLU:HG3	2.07	0.54
1:A:116:GLU:HA	1:A:159:GLN:HE22	1.73	0.54
1:A:144:THR:HG23	1:A:889:ILE:HG22	1.89	0.54
1:A:773:THR:HB	1:A:814:ARG:HG3	1.89	0.54
1:A:485:ALA:HB3	1:A:514:ARG:HH12	1.72	0.54
1:A:439:LEU:HD11	1:A:443:ARG:HH21	1.72	0.54
1:A:797:ASN:HB3	1:A:802:ILE:HD11	1.88	0.54
1:A:1088:LYS:HZ1	1:A:1098:ILE:HD11	1.72	0.53
1:A:111:TRP:HB3	1:A:163:SER:O	2.07	0.53
1:A:843:TRP:CG	1:A:844:ARG:N	2.76	0.53
1:A:83:MET:HG3	1:A:953:LYS:HD3	1.91	0.52
1:A:704:SER:O	1:A:707:SER:HB3	2.09	0.52
1:A:290:LEU:HD13	1:A:724:VAL:HG21	1.90	0.52
1:A:237:ILE:HA	1:A:240:VAL:HB	1.91	0.52
1:A:1116:ILE:O	1:A:1120:ILE:HG12	2.10	0.52
1:A:1186:LEU:HB2	1:A:1216:VAL:HA	1.92	0.52
1:A:1069:ILE:HA	1:A:1072:ILE:HG22	1.91	0.51
1:A:157:MET:HG3	1:A:337:ALA:HB3	1.92	0.51
1:A:354:ASN:HB3	1:A:418:ARG:HH21	1.74	0.51
1:A:35:PHE:HE1	1:A:125:LYS:HD2	1.75	0.51
1:A:370:LEU:HD22	1:A:391:LEU:HD23	1.92	0.51
1:A:1028:HIS:ND1	1:A:1044:ASP:OD1	2.44	0.51
1:A:1074:ARG:NH1	1:A:1090:ILE:O	2.43	0.51
1:A:843:TRP:O	1:A:844:ARG:HB3	2.11	0.51
1:A:382:ASP:OD1	1:A:383:VAL:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1117:TYR:HB2	1:A:1152:TYR:HB3	1.93	0.51
1:A:234:VAL:HG11	1:A:799:SER:HA	1.92	0.50
1:A:371:LYS:HG2	1:A:372:ASN:H	1.76	0.50
1:A:1093:TYR:HD2	1:A:1095:LEU:H	1.57	0.50
1:A:402:VAL:HG13	1:A:561:ILE:HD12	1.93	0.50
1:A:370:LEU:HA	1:A:427:VAL:HG23	1.94	0.50
1:A:705:VAL:O	1:A:708:VAL:HG22	2.12	0.50
1:A:773:THR:HG21	1:A:814:ARG:HD2	1.95	0.49
1:A:1062:GLY:H	1:A:1065:LYS:HZ1	1.60	0.49
1:A:35:PHE:CE1	1:A:125:LYS:HD2	2.47	0.49
1:A:1166:GLY:O	1:A:1170:ARG:HG2	2.12	0.49
1:A:1168:LYS:HA	1:A:1171:ILE:HD12	1.93	0.49
1:A:417:GLU:OE2	1:A:448:LEU:HB2	2.12	0.49
1:A:849:LEU:HD23	1:A:969:LEU:HB2	1.95	0.49
1:A:79:VAL:HA	1:A:82:MET:HG2	1.95	0.48
1:A:532:GLU:HA	1:A:560:ILE:HG12	1.95	0.48
1:A:831:MET:HE1	1:A:976:ALA:HB2	1.95	0.48
1:A:1058:VAL:HG13	1:A:1059:GLY:N	2.28	0.48
1:A:120:THR:O	1:A:124:ILE:HG12	2.14	0.48
1:A:302:THR:OG1	1:A:303:ASN:N	2.47	0.48
1:A:795:GLU:CD	1:A:801:ARG:HH22	2.17	0.48
1:A:500:VAL:HA	1:A:505:LEU:HB2	1.95	0.47
1:A:862:LEU:HD23	1:A:930:TYR:HA	1.96	0.47
1:A:847:LEU:HA	1:A:850:VAL:HG22	1.95	0.47
1:A:475:GLU:O	1:A:478:GLU:HG2	2.14	0.47
1:A:150:ALA:HA	1:A:153:THR:HG22	1.96	0.47
1:A:842:GLN:HB3	1:A:965:VAL:HG21	1.97	0.47
1:A:1031:PHE:HB3	1:A:1078:PRO:HA	1.96	0.47
1:A:780:MET:HB3	1:A:780:MET:HE2	1.67	0.47
1:A:1025:GLU:HB2	1:A:1084:MET:HB3	1.95	0.47
1:A:1055:LEU:HD23	1:A:1057:LEU:H	1.79	0.47
1:A:761:GLN:HG3	1:A:762:HIS:N	2.30	0.47
1:A:839:PHE:HD2	1:A:843:TRP:CD1	2.29	0.47
1:A:844:ARG:HB3	1:A:844:ARG:CZ	2.43	0.47
1:A:761:GLN:HE22	1:A:826:GLN:HE22	1.62	0.47
1:A:831:MET:CE	1:A:976:ALA:HB2	2.45	0.47
1:A:845:LEU:O	1:A:849:LEU:HD13	2.15	0.47
1:A:1095:LEU:HD21	1:A:1099:ARG:NH1	2.25	0.47
1:A:246:GLU:HB2	1:A:785:LEU:HD13	1.97	0.46
1:A:397:LYS:HE3	1:A:572:ASP:HB3	1.97	0.46
1:A:401:LEU:HD12	1:A:577:LEU:HD22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:VAL:CG1	1:A:799:SER:HA	2.45	0.46
1:A:461:LYS:HE2	1:A:496:PHE:O	2.15	0.46
1:A:1018:ASP:N	1:A:1018:ASP:OD1	2.48	0.46
1:A:829:ALA:O	1:A:833:VAL:HG22	2.16	0.46
1:A:1136:ALA:HB2	1:A:1174:ALA:HB2	1.97	0.46
1:A:794:GLN:HB3	1:A:796:GLU:CD	2.36	0.46
1:A:808:LEU:HA	1:A:811:ASN:HD21	1.81	0.46
1:A:530:LEU:HD21	1:A:544:LEU:HD21	1.96	0.46
1:A:796:GLU:HA	1:A:801:ARG:CZ	2.46	0.46
1:A:905:VAL:O	1:A:909:THR:HG23	2.16	0.46
1:A:1234:ASP:N	1:A:1234:ASP:OD1	2.46	0.46
1:A:1123:GLY:O	1:A:1179:ARG:NE	2.41	0.46
1:A:375:PHE:N	1:A:386:LEU:HB3	2.26	0.45
1:A:1058:VAL:HG13	1:A:1059:GLY:H	1.81	0.45
1:A:401:LEU:H	1:A:401:LEU:HD23	1.81	0.45
1:A:409:LYS:HE2	1:A:559:LEU:HD21	1.99	0.45
1:A:988:LYS:HB3	1:A:988:LYS:HE2	1.69	0.45
1:A:359:VAL:HG12	1:A:359:VAL:O	2.16	0.45
1:A:521:MET:SD	1:A:548:ALA:HA	2.57	0.45
1:A:981:THR:O	1:A:984:PRO:HD2	2.17	0.45
1:A:1006:ILE:HG23	1:A:1074:ARG:HH21	1.81	0.45
1:A:1098:ILE:O	1:A:1101:HIS:N	2.38	0.45
1:A:1170:ARG:HH12	1:A:1197:SER:HB2	1.80	0.45
1:A:82:MET:HG3	1:A:83:MET:N	2.32	0.45
1:A:307:ALA:O	1:A:311:MET:HG3	2.16	0.45
1:A:812:ASN:HD21	1:A:992:ALA:HB1	1.82	0.45
1:A:963:ILE:O	1:A:967:MET:HG2	2.16	0.45
1:A:1135:ALA:O	1:A:1138:LEU:N	2.37	0.45
1:A:368:VAL:O	1:A:393:VAL:N	2.50	0.44
1:A:1167:GLN:O	1:A:1171:ILE:HG13	2.17	0.44
1:A:508:SER:HB3	1:A:511:GLN:HB2	1.99	0.44
1:A:758:ASN:HA	1:A:761:GLN:HG2	1.99	0.44
1:A:723:ALA:O	1:A:727:VAL:HG23	2.17	0.44
1:A:791:TRP:O	1:A:797:ASN:ND2	2.50	0.44
1:A:231:GLU:O	1:A:235:VAL:HG23	2.17	0.44
1:A:367:LEU:HB2	1:A:395:ALA:HB2	1.99	0.44
1:A:1025:GLU:OE2	1:A:1050:ARG:NH2	2.50	0.44
1:A:513:GLN:O	1:A:517:ILE:HG12	2.17	0.44
1:A:67:ASP:HB3	1:A:89:TYR:CZ	2.53	0.44
1:A:241:MET:HB3	1:A:1099:ARG:NH2	2.31	0.44
1:A:860:THR:O	1:A:864:LYS:HG2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1041:ILE:O	1:A:1042:PHE:HB2	2.18	0.43
1:A:374:ASP:OD2	1:A:384:LYS:NZ	2.41	0.43
1:A:1029:ILE:HG12	1:A:1045:LEU:HB3	1.99	0.43
1:A:494:ASP:HB2	1:A:498:THR:HG23	1.99	0.43
1:A:686:PHE:HA	1:A:993:MET:HE1	2.00	0.43
1:A:824:ILE:HG13	1:A:979:THR:HG23	1.99	0.43
1:A:1065:LYS:H	1:A:1233:ILE:HD11	1.83	0.43
1:A:1116:ILE:HD13	1:A:1154:THR:HB	2.01	0.43
1:A:374:ASP:HA	1:A:386:LEU:HD23	2.01	0.43
1:A:507:LEU:HD12	1:A:512:LYS:HD3	2.01	0.43
1:A:554:ILE:O	1:A:554:ILE:HG13	2.19	0.43
1:A:773:THR:HB	1:A:814:ARG:CG	2.48	0.43
1:A:86:VAL:HG11	1:A:949:SER:HB3	2.01	0.43
1:A:176:PHE:HA	1:A:317:GLY:HA2	2.01	0.43
1:A:457:ALA:HB1	1:A:883:GLN:HE22	1.83	0.43
1:A:820:ARG:HB3	1:A:986:PHE:HE1	1.80	0.43
1:A:1028:HIS:N	1:A:1045:LEU:O	2.51	0.43
1:A:464:ILE:HD11	1:A:515:ILE:HG23	2.01	0.42
1:A:773:THR:HB	1:A:814:ARG:CB	2.46	0.42
1:A:1148:LEU:HD13	1:A:1154:THR:HG21	2.00	0.42
1:A:812:ASN:ND2	1:A:992:ALA:CB	2.82	0.42
1:A:361:LEU:HD21	1:A:432:GLN:HG3	2.02	0.42
1:A:409:LYS:HG2	1:A:577:LEU:HD23	2.01	0.42
1:A:820:ARG:CB	1:A:986:PHE:CE1	3.03	0.42
1:A:316:ILE:HD13	1:A:316:ILE:HA	1.92	0.42
1:A:194:THR:O	1:A:198:VAL:HG23	2.20	0.42
1:A:830:LEU:HD22	1:A:972:SER:HA	2.01	0.42
1:A:980:LEU:HD23	1:A:980:LEU:HA	1.83	0.42
1:A:794:GLN:HB3	1:A:796:GLU:OE2	2.20	0.42
1:A:79:VAL:HB	1:A:953:LYS:HG3	2.02	0.42
1:A:484:ASN:HD21	1:A:514:ARG:HG2	1.84	0.42
1:A:1056:ALA:HB1	1:A:1224:ILE:HB	2.02	0.42
1:A:1199:ARG:O	1:A:1203:GLU:OE1	2.38	0.42
1:A:1221:LEU:HA	1:A:1224:ILE:HG12	2.01	0.42
1:A:682:GLN:HG2	1:A:686:PHE:HE2	1.83	0.42
1:A:1088:LYS:HE2	1:A:1088:LYS:HB3	1.62	0.42
1:A:275:LEU:HD23	1:A:758:ASN:HD21	1.85	0.41
1:A:555:GLY:O	1:A:556:ARG:HG3	2.19	0.41
1:A:101:TRP:CD1	1:A:931:GLY:HA3	2.55	0.41
1:A:1088:LYS:NZ	1:A:1098:ILE:HD11	2.35	0.41
1:A:1028:HIS:O	1:A:1081:GLY:HA2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1142:HIS:O	1:A:1142:HIS:ND1	2.53	0.41
1:A:1060:PRO:HG2	1:A:1063:CYS:SG	2.60	0.41
1:A:847:LEU:O	1:A:850:VAL:HG22	2.20	0.41
1:A:56:CYS:O	1:A:60:LEU:HD23	2.21	0.41
1:A:821:ILE:HG23	1:A:822:SER:N	2.36	0.41
1:A:369:GLU:HA	1:A:392:SER:HA	2.03	0.40
1:A:371:LYS:HG2	1:A:372:ASN:N	2.37	0.40
1:A:559:LEU:O	1:A:559:LEU:HD23	2.21	0.40
1:A:370:LEU:HB3	1:A:390:CYS:HA	2.03	0.40
1:A:371:LYS:N	1:A:390:CYS:SG	2.89	0.40
1:A:441:TRP:O	1:A:444:GLN:HB2	2.21	0.40
1:A:539:SER:O	1:A:543:LYS:HE2	2.22	0.40
1:A:764:PHE:O	1:A:768:VAL:HG12	2.21	0.40
1:A:457:ALA:HA	1:A:501:GLY:HA2	2.04	0.40
1:A:813:VAL:CG2	1:A:993:MET:HB3	2.52	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	1140/1327 (86%)	1080 (95%)	60 (5%)	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	930/1087 (86%)	926 (100%)	4 (0%)	89	94

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	806	LEU
1	A	812	ASN
1	A	1038	ASP
1	A	1159	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	445	GLN
1	A	812	ASN
1	A	826	GLN
1	A	827	ASN
1	A	1142	HIS

### 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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	1.20	5 (17%)	31,52,52	1.17	3 (9%)
3	ANP	A	1304	2	29,33,33	1.22	5 (17%)	31,52,52	1.12	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	-	6/14/38/38	0/3/3/3
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	3.26	1.51	1.46
3	A	1303	ANP	PG-O1G	3.12	1.51	1.46
3	A	1303	ANP	PB-O1B	2.98	1.50	1.46
3	A	1304	ANP	PB-O1B	2.93	1.50	1.46
3	A	1304	ANP	PB-O2B	-2.22	1.50	1.56
3	A	1303	ANP	PB-O2B	-2.22	1.50	1.56
3	A	1303	ANP	PG-O3G	-2.07	1.51	1.56
3	A	1304	ANP	PG-O3G	-2.06	1.51	1.56
3	A	1303	ANP	PG-O2G	-2.06	1.51	1.56
3	A	1304	ANP	PG-O2G	-2.06	1.51	1.56

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1303	ANP	O2B-PB-O1B	4.19	118.71	109.92
3	A	1304	ANP	O2B-PB-O1B	4.06	118.44	109.92
3	A	1304	ANP	C5-C6-N6	2.29	123.83	120.35
3	A	1303	ANP	C5-C6-N6	2.24	123.76	120.35
3	A	1304	ANP	O3G-PG-O1G	-2.08	108.23	113.45
3	A	1303	ANP	O3G-PG-O1G	-2.03	108.36	113.45

There are no chirality outliers.

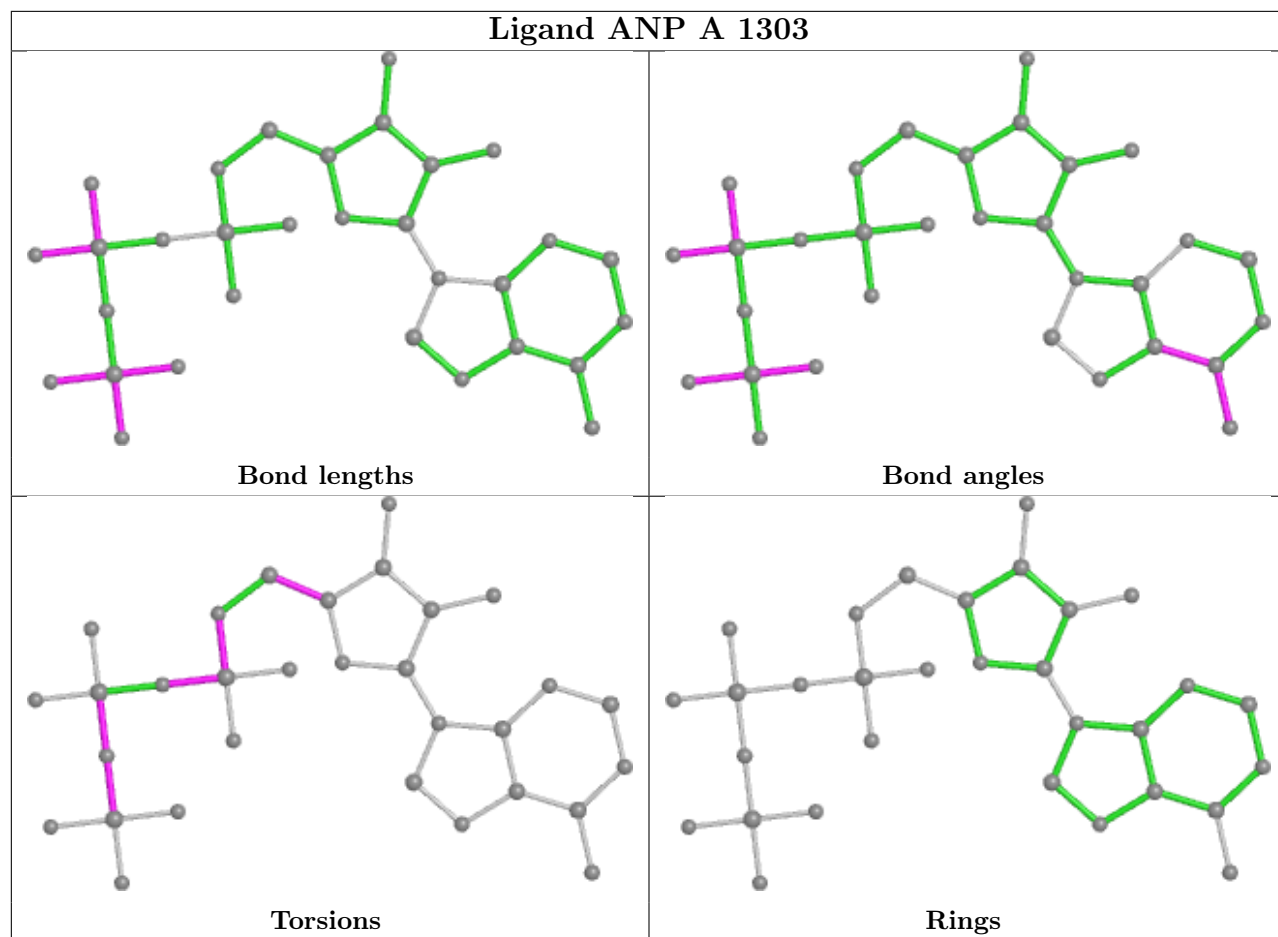
All (9) torsion outliers are listed below:

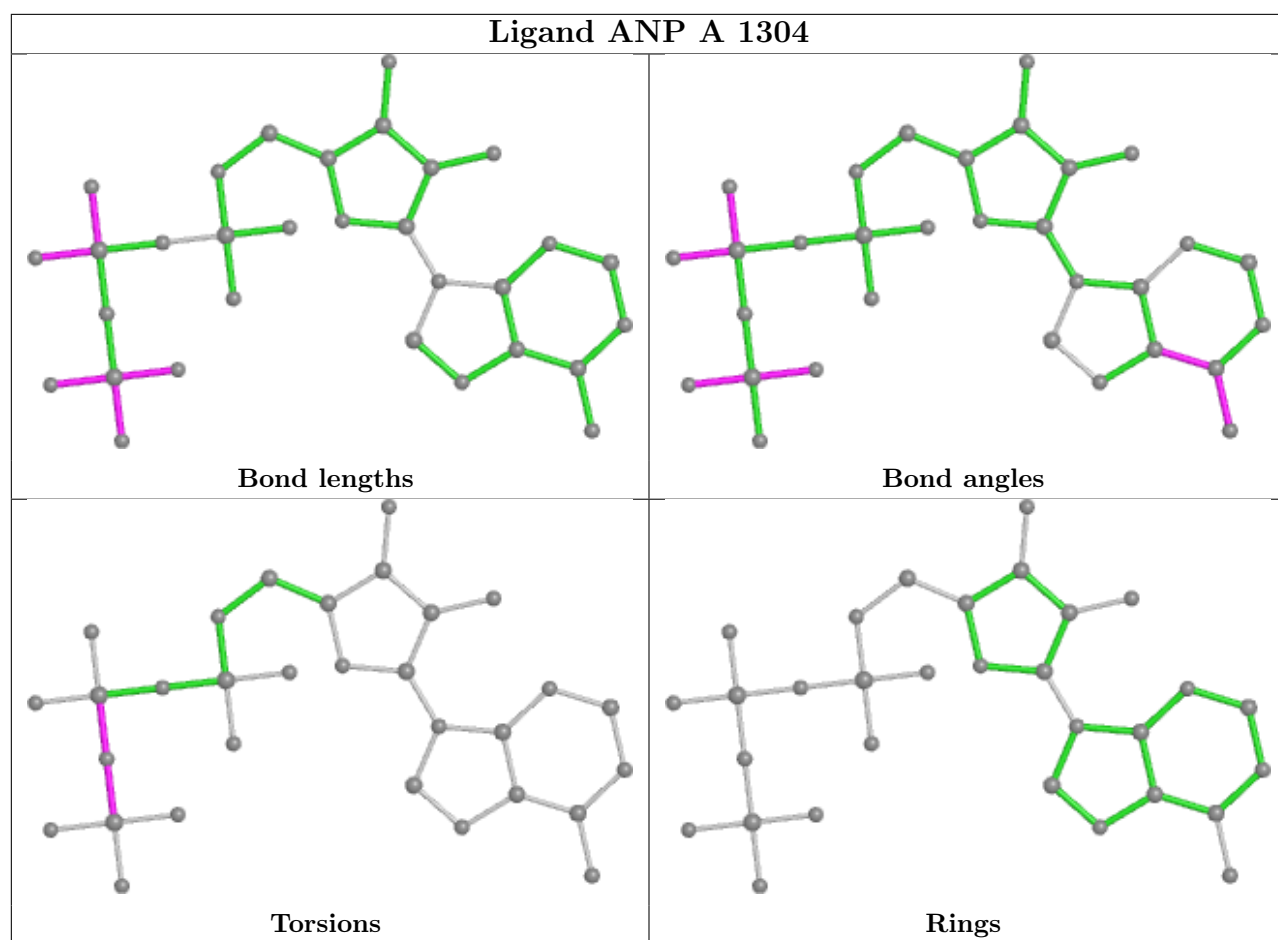
Mol	Chain	Res	Type	Atoms
3	A	1303	ANP	PB-N3B-PG-O1G
3	A	1303	ANP	PG-N3B-PB-O1B
3	A	1303	ANP	PB-O3A-PA-O5'
3	A	1304	ANP	PB-N3B-PG-O1G
3	A	1304	ANP	PG-N3B-PB-O1B
3	A	1304	ANP	PG-N3B-PB-O3A
3	A	1303	ANP	O4'-C4'-C5'-O5'
3	A	1303	ANP	C3'-C4'-C5'-O5'
3	A	1303	ANP	C5'-O5'-PA-O1A

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

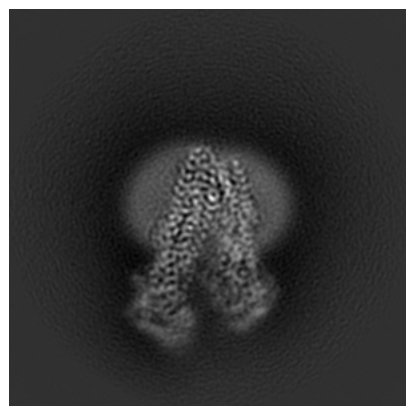
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61832. These allow visual inspection of the internal detail of the map and identification of artifacts.

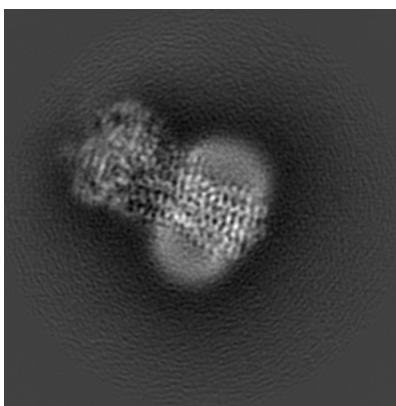
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

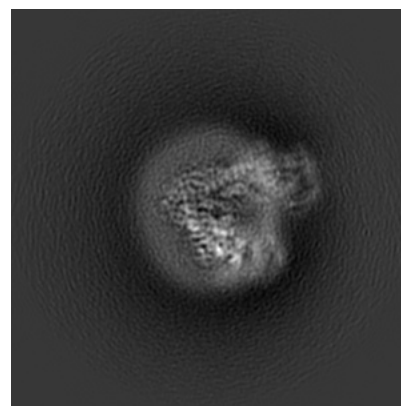
#### 6.1.1 Primary map



X

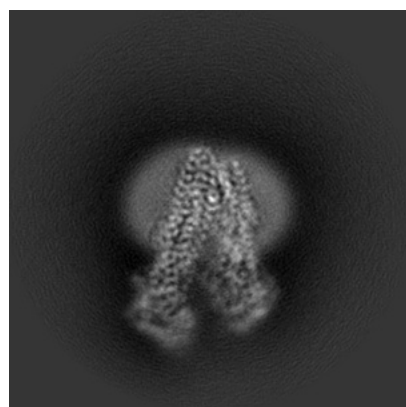


Y

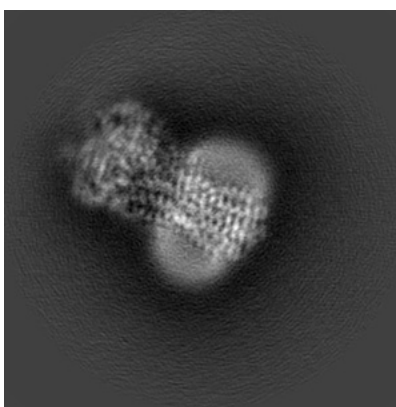


Z

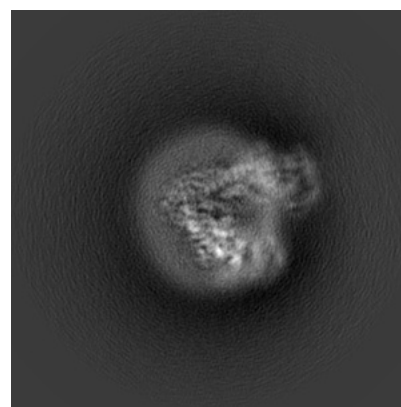
#### 6.1.2 Raw map



X



Y

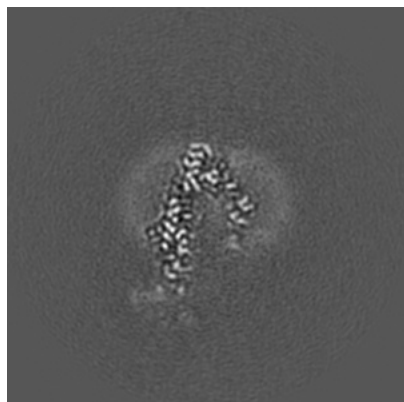


Z

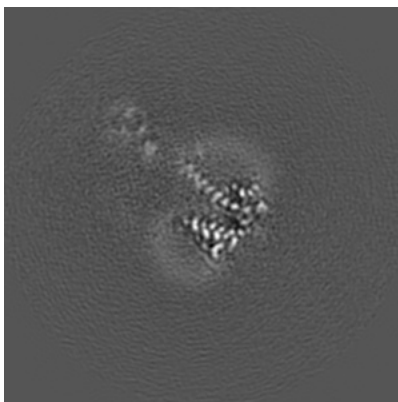
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

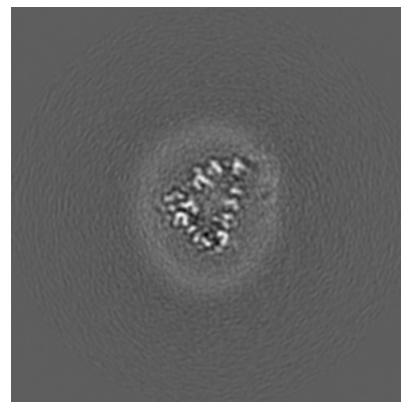
### 6.2.1 Primary map



X Index: 120

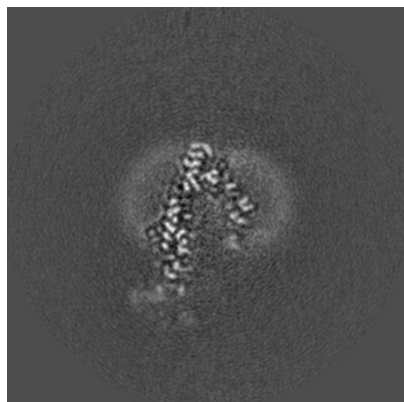


Y Index: 120

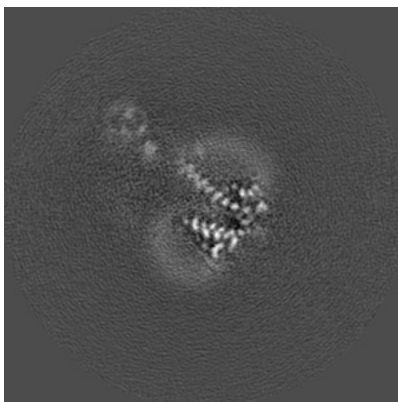


Z Index: 120

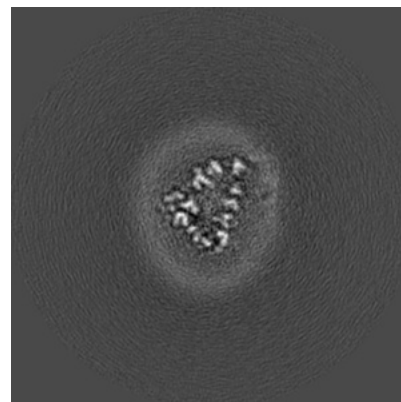
### 6.2.2 Raw map



X Index: 120



Y Index: 120

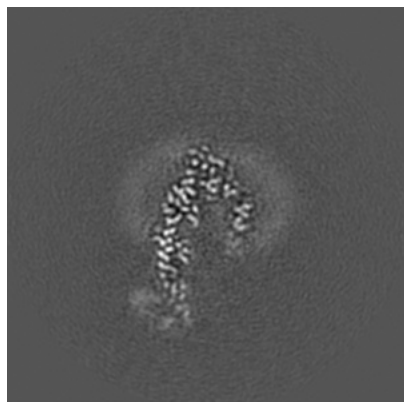


Z Index: 120

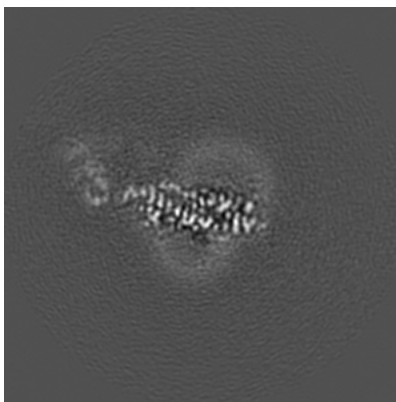
The images above show central slices of the map in three orthogonal directions.

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

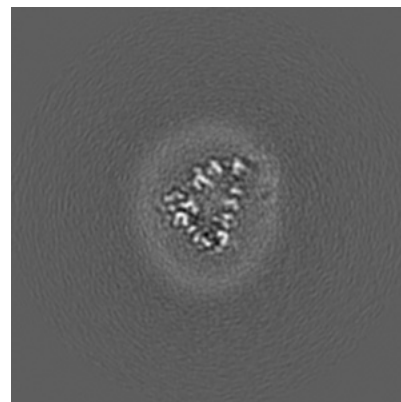
### 6.3.1 Primary map



X Index: 123

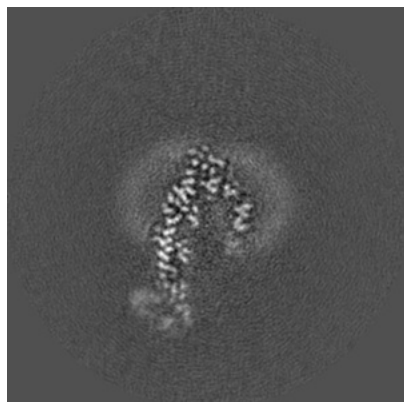


Y Index: 107

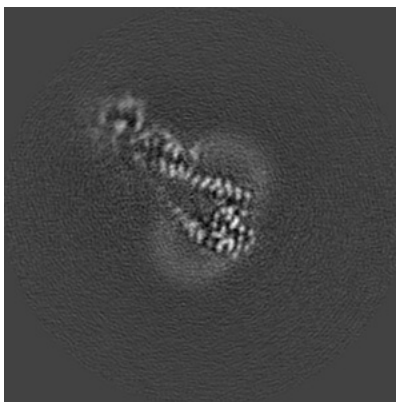


Z Index: 120

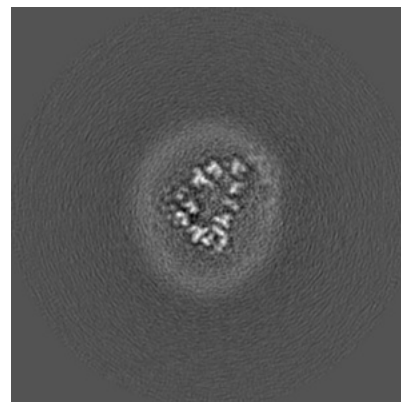
### 6.3.2 Raw map



X Index: 123



Y Index: 130



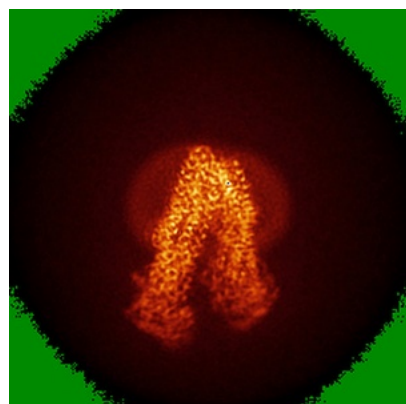
Z Index: 119

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

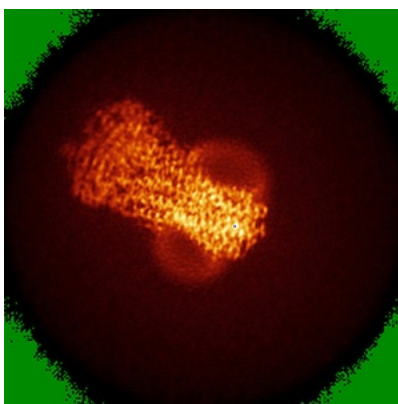


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

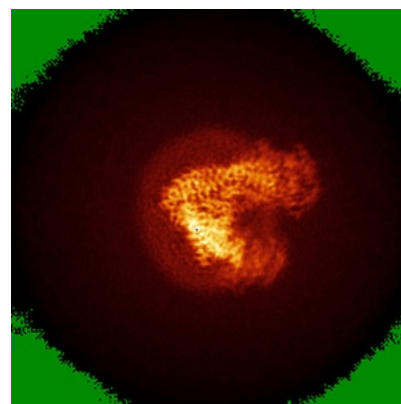
### 6.4.1 Primary map



X

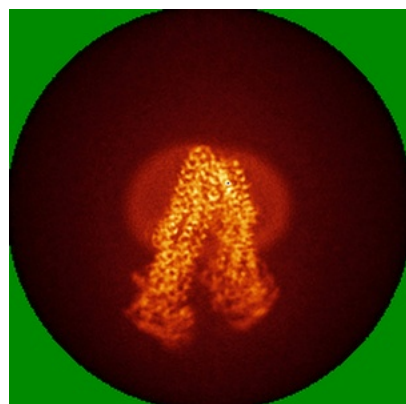


Y

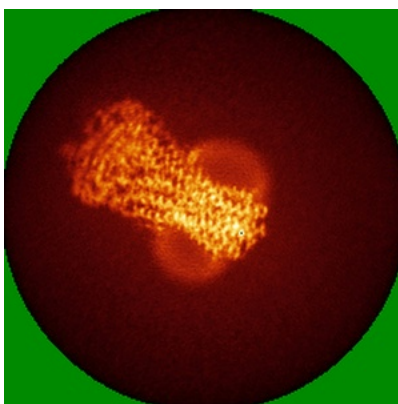


Z

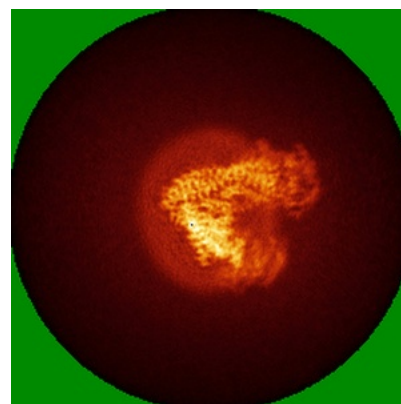
### 6.4.2 Raw map



X



Y



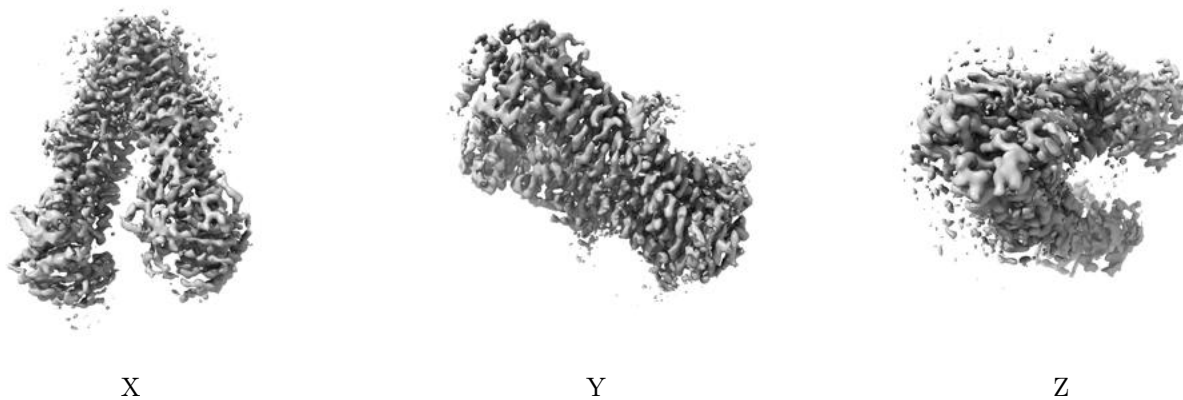
Z

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.



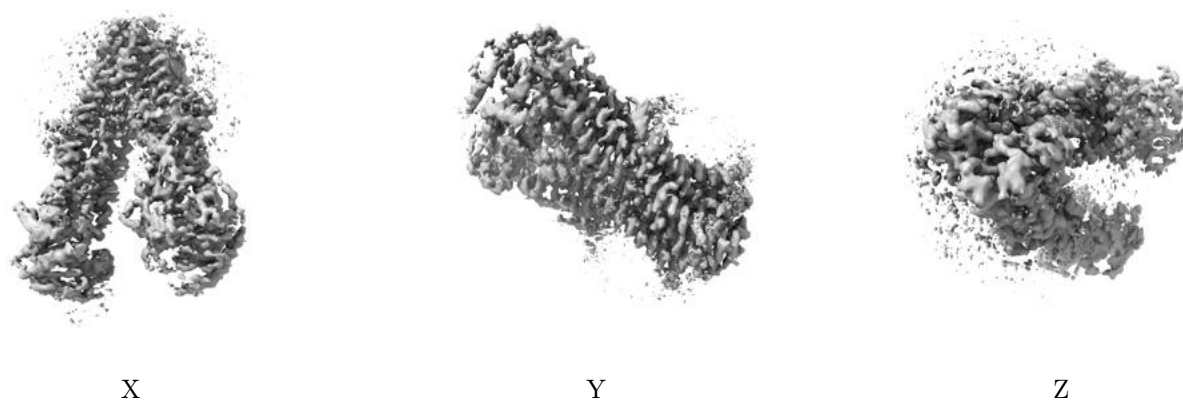
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.014. 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.

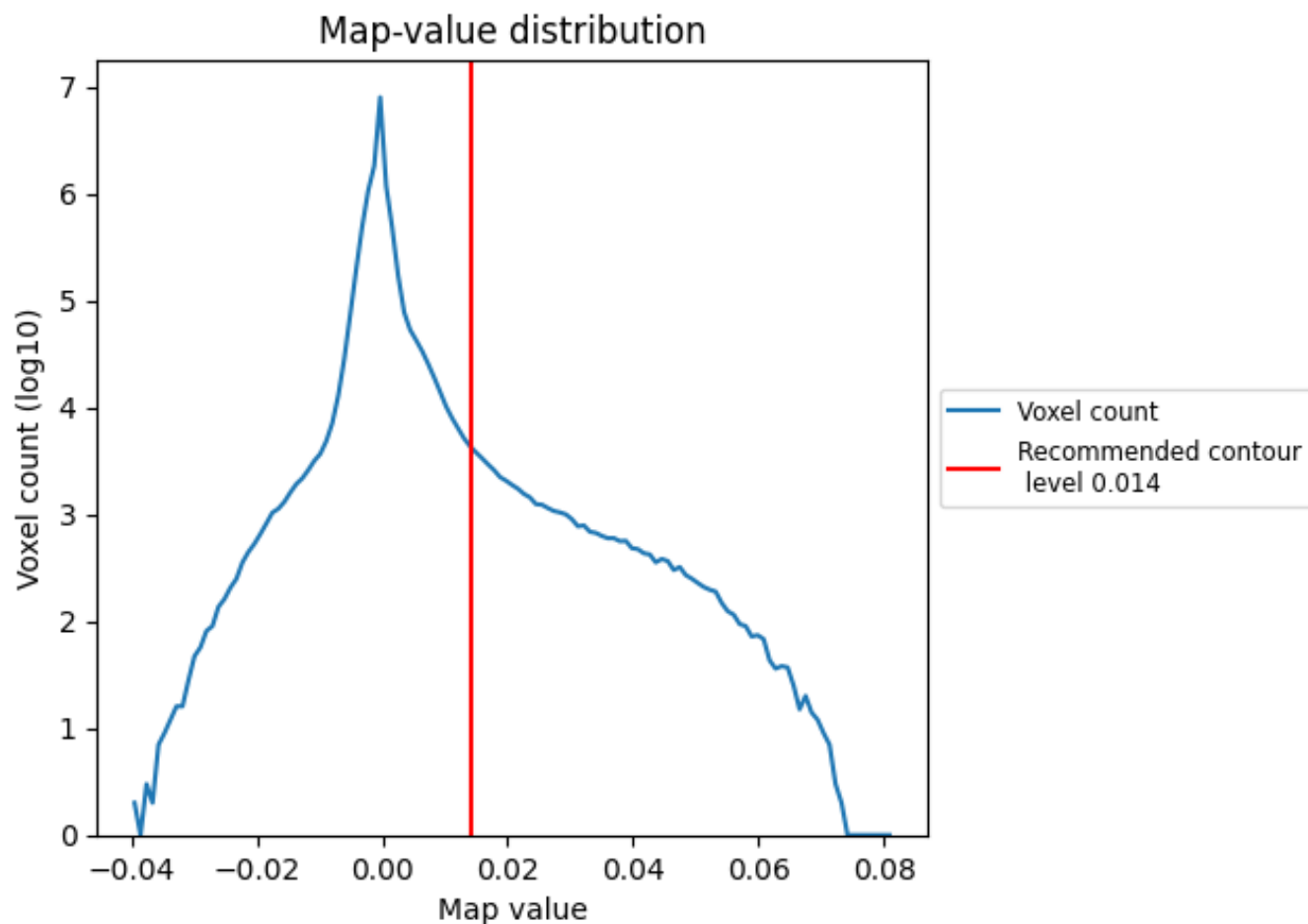
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

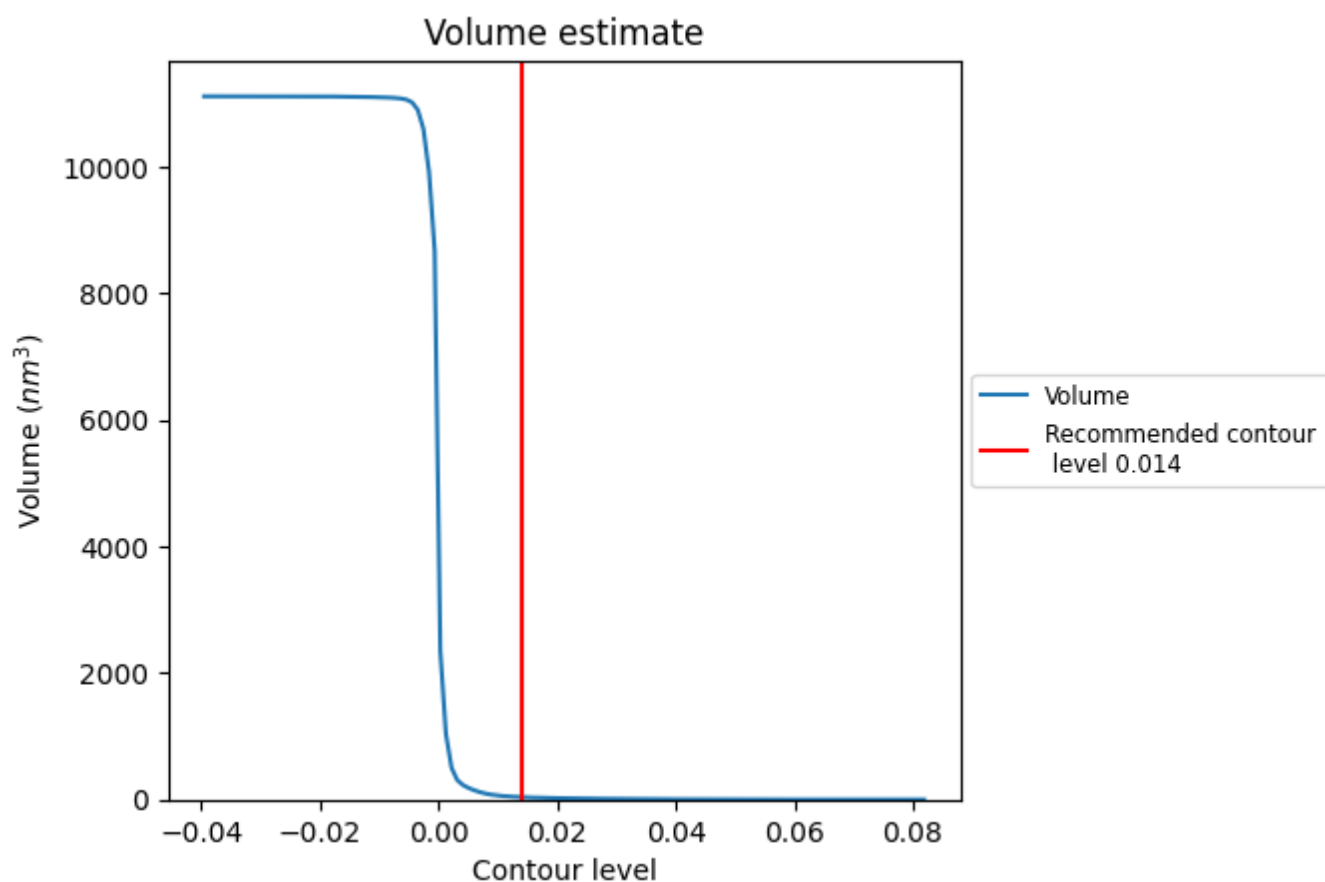
This section contains the results of statistical analysis of the map.

### 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.

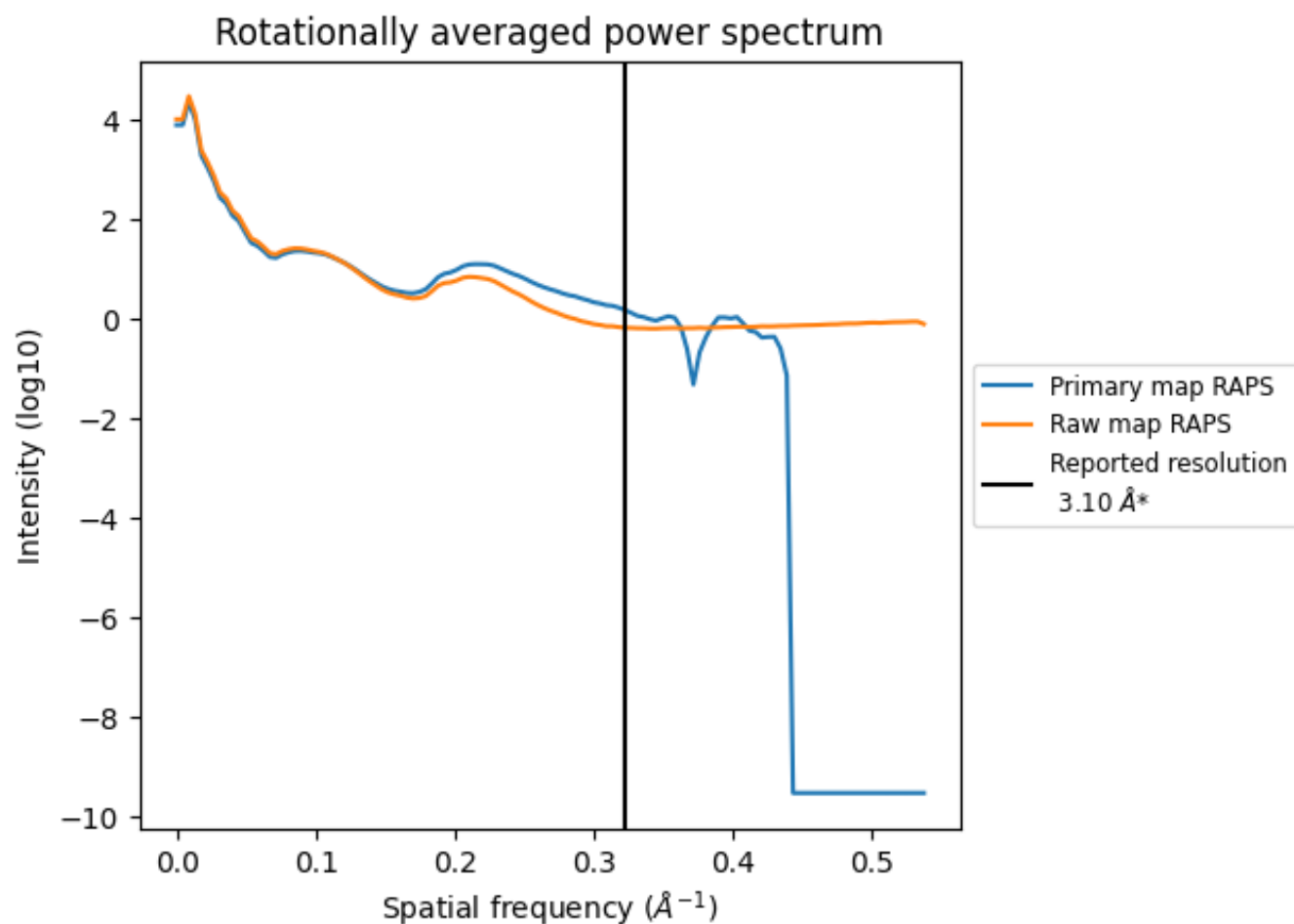
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 38  $\text{nm}^3$ ; this corresponds to an approximate mass of 34 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 ⓘ

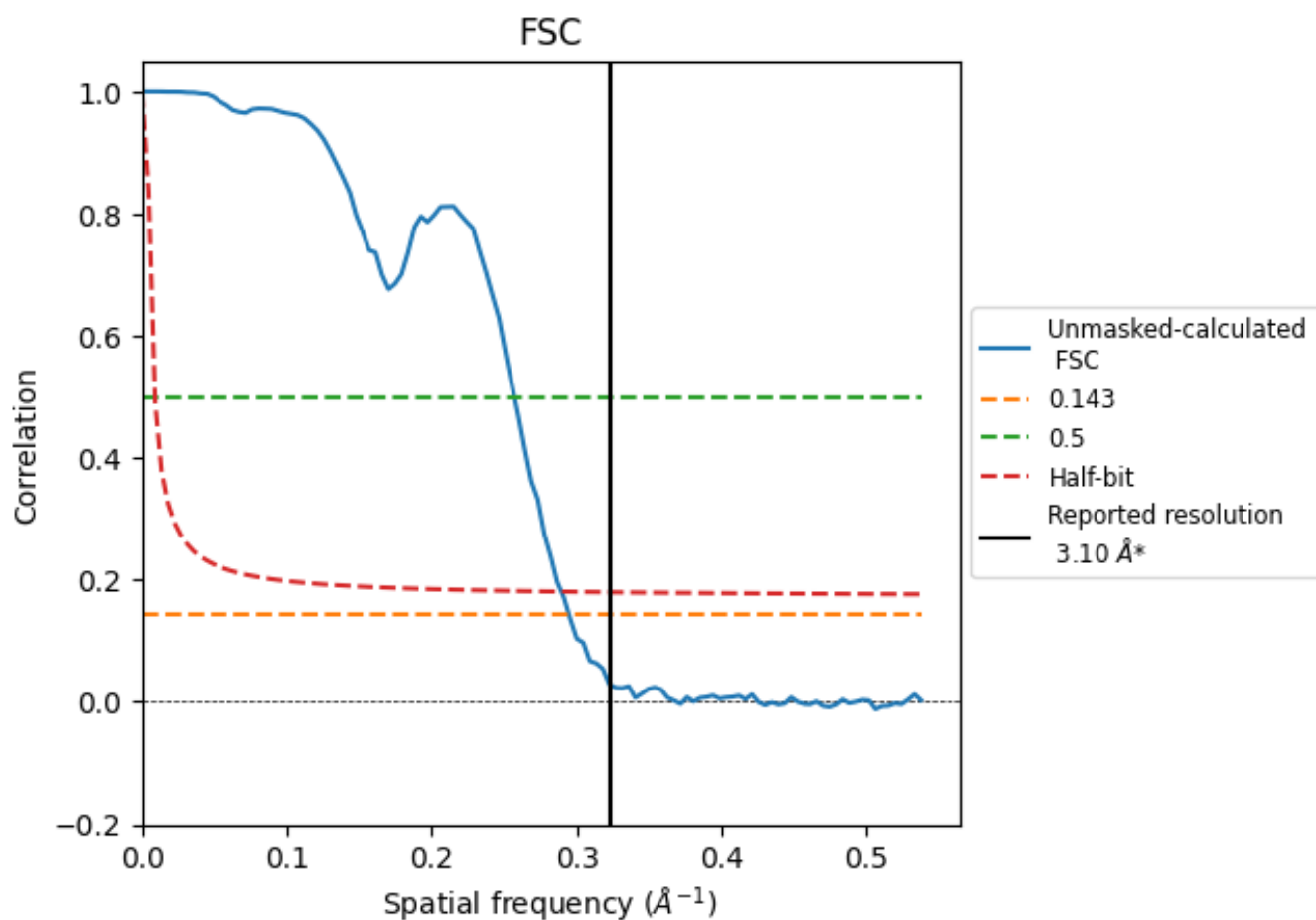


\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

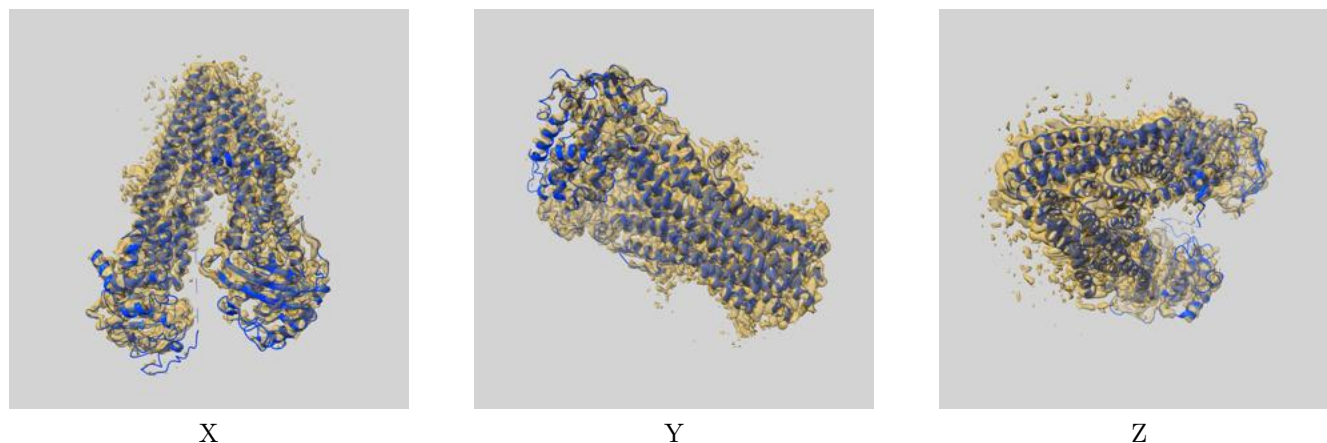
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.39	3.89	3.45

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

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

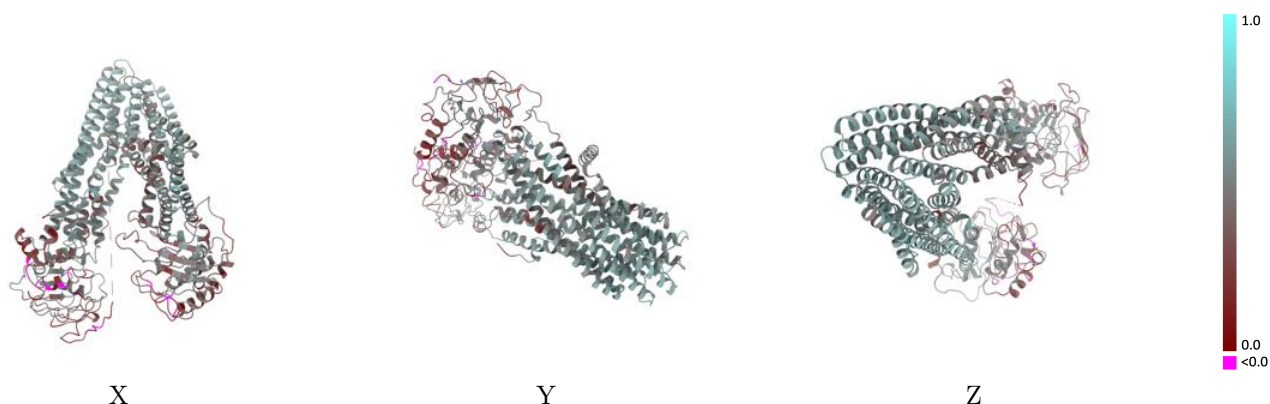
This section contains information regarding the fit between EMDB map EMD-61832 and PDB model 9JUO. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

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



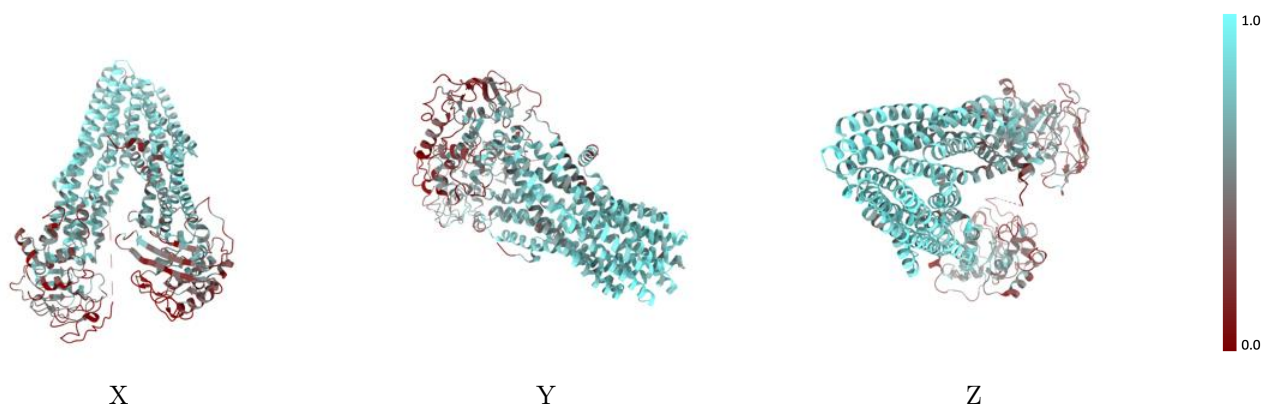
The images above show the 3D surface view of the map at the recommended contour level 0.014 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

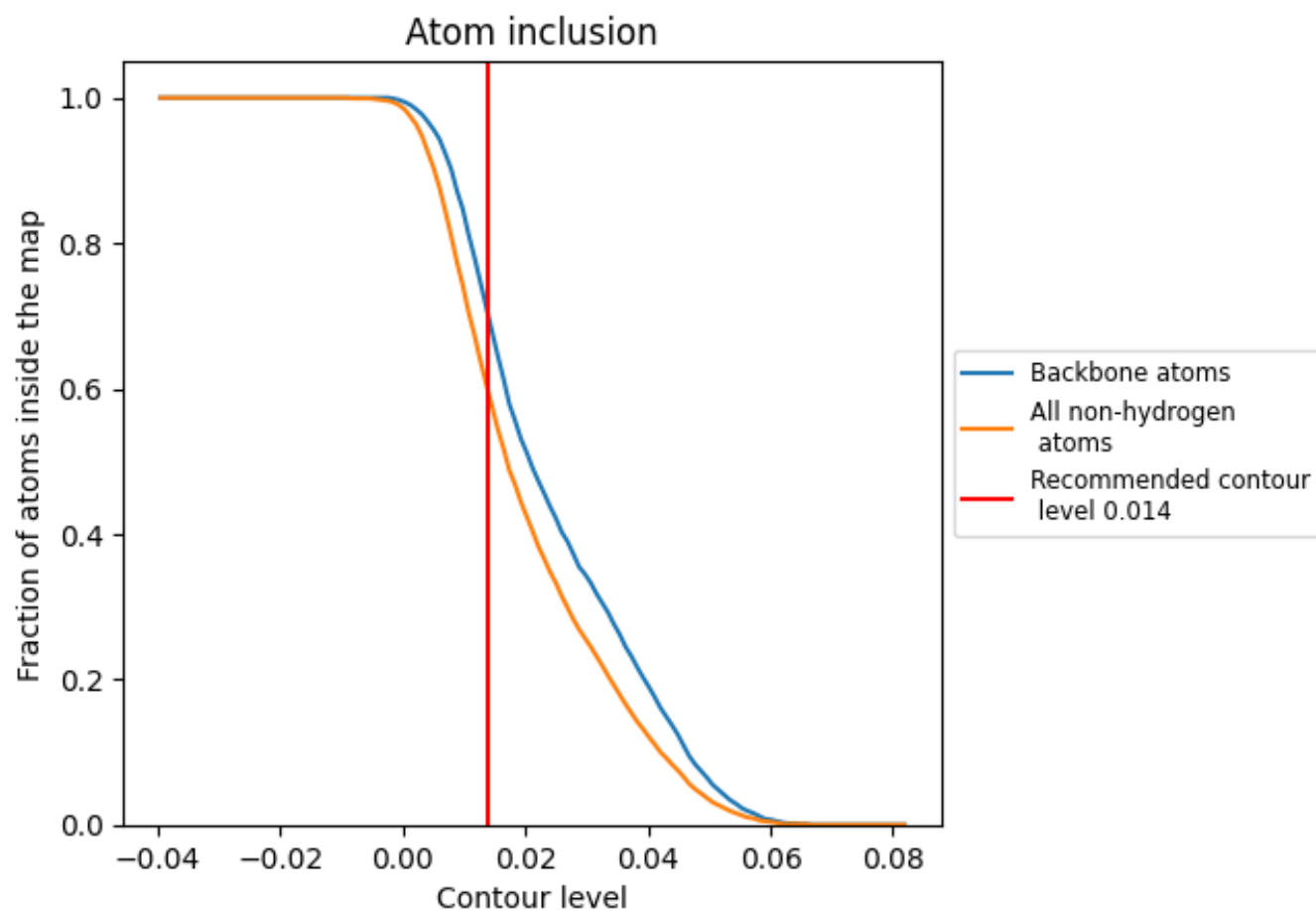
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.014).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 59% 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 (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5940	<div></div> 0.4610
A	<div></div> 0.5940	<div></div> 0.4610

