



Full wwPDB EM Validation Report ⓘ

Mar 12, 2025 – 02:13 PM JST

PDB ID : 9JUK
EMDB ID : EMD-61828
Title : Structure of Arabidopsis thaliana ABCB1 with AMP-PNP bound in the inward-facing conformation
Authors : Chen, Q.; Su, N.; Guo, J.
Deposited on : 2024-10-08
Resolution : 3.30 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.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

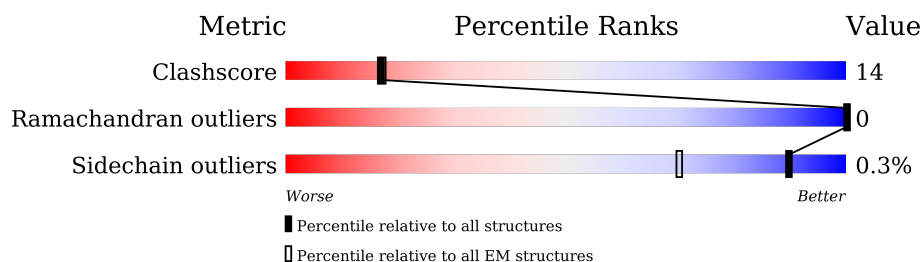
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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 ≥ 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>14%</div> <div>61%</div> <div>27%</div> <div>12%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9035 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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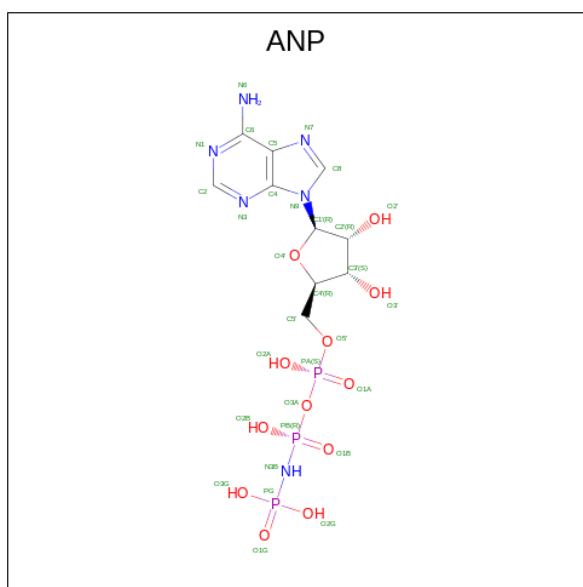
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Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	HIS	-	expression tag	UNP Q9ZR72
A	-11	PRO	-	expression tag	UNP Q9ZR72
A	-10	GLN	-	expression tag	UNP Q9ZR72
A	-9	PHE	-	expression tag	UNP Q9ZR72
A	-8	GLU	-	expression tag	UNP Q9ZR72
A	-7	LYS	-	expression 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: 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	

LYS	L1221	K1153	Q1073	L1000	V857	A754
GLU	S1222	T1154	R1074	K1003	L862	L755
ASP	T1223	Y1155	P1078	I1006	D873	N758
ASP	I1224	V1156	S1079	E1007	L874	T759
ALA	R1225	G1157	S1080	P1008	E875	L760
	N1226	E1158	G1081	D1009	A876	Q761
	A1227	R1159	R1082	D1010	T882	W765
	H1228	G1160	V1083	P1011	I889	V768
	V1229	V1161	M1084	D1012	V882	L772
	I1230	G1162	I1085	T1013	T773	
	A1231	L1163	D1086	T1014	K903	
		S1164	G1087	P1015	I904	
	D1234	Q1167	K1088	D1018	V905	
	D1235	K1168	D1089	R1019	R906	
	G1236	Q1169	I1090	L1020	L907	
	K1237	R1170	K1091	R1021	Y908	
	V1238	I1173	Y1093	G1022	T909	
	A1239	A1174	N1094	E1023	A910	
	E1240	R1175	L1095	V1024	N911	
	Q1241	A1176	K1096	E1025	N787	
	Q1242	L1177	A1097	I1026	E788	
	G1243	V1178	I1098	L1027	F792	
	S1243	R1179	R1099	H1028	E798	
	H1244	K1180	K1100	D1030	S799	
	S1245	I1183	H1101	F1031	A800	
	H1246	M1184	I1102	S1032	R801	
	L1247	L1185	A1103	R1036	L806	
	L1248	L1186	I1104	P1037	N812	
	K1249	D1187	E1106	D1038	V813	
	N1250	E1188	P1109	I1039	R814	
	H1251	A1189	C1110	Q1040	D819	
	P1252	T1190	L1111	I1041	R820	
	D1253	S1191	G1113	F1042	I824	
	G1254	A1192	T1114	R1043	G838	
	T1255	L1193	Y1117	D1044	L841	
	Y1256	D1194	E1118	L1045	G842	
	A1257	A1195	N1119	S1046	W843	
	R1258	E1196	Y1122	L1047	R844	
	M1259	S1197	A1127	R1048	L847	
	I1260	E1198	E1131	A1049	V850	
	Q1261	R1199	I1132	R1050	A851	
	Q1262	S1200	I1133	A1051	V852	
	L1263	Q1202	Q1134	G1052	P853	
	R1264	L1205	L1138	T1054	P854	
	PHE	D1206	E1150	L1055	V855	
	THR		G1151	A1056	L999	
	HIS		Y1152	L1057		
	THR			V1058		
	GLN			G1059		
	VAL					
	ILE					
	GLY					
	MET					
	THR					
	SER					
	GLY					
	SER					
	SER					
	ARG					
	VAL					

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	224069	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	0.136	Depositor
Minimum map value	-0.094	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	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

5.1 Standard geometry

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	0.26	0/9137	0.49	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

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	9115	247	0
2	A	2	0	0	0	0
3	A	62	0	26	3	0
All	All	9035	0	9141	247	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 14.

All (247) 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:418:ARG:HD2	1:A:439:LEU:HD13	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:MET:HG2	1:A:334:ALA:HA	1.66	0.78
1:A:812:ASN:HD21	1:A:988:LYS:HG2	1.50	0.76
1:A:693:ASN:HB2	1:A:772:LEU:HD13	1.69	0.73
1:A:124:ILE:HD12	1:A:909:THR:HG22	1.73	0.71
1:A:576:VAL:HG13	1:A:583:SER:HB2	1.73	0.71
1:A:758:ASN:OD1	1:A:761:GLN:NE2	2.24	0.71
1:A:461:LYS:NZ	1:A:496:PHE:O	2.24	0.70
1:A:528:LEU:HD21	1:A:530:LEU:HG	1.74	0.70
1:A:532:GLU:HB3	1:A:560:ILE:HA	1.75	0.68
1:A:235:VAL:HG23	1:A:236:GLN:HG2	1.75	0.68
1:A:798:GLU:HB3	1:A:801:ARG:HG3	1.75	0.68
1:A:1109:PRO:HG3	1:A:1169:GLN:HG3	1.75	0.67
1:A:1186:LEU:HB2	1:A:1216:VAL:HA	1.76	0.67
1:A:151:ILE:HG22	1:A:882:THR:HG23	1.74	0.67
1:A:75:ASN:HB2	1:A:82:MET:HB3	1.76	0.66
1:A:820:ARG:O	1:A:824:ILE:HG12	1.95	0.66
1:A:116:GLU:HG3	1:A:916:LEU:HD12	1.77	0.66
1:A:1078:PRO:O	1:A:1091:ARG:NH2	2.29	0.66
1:A:1024:VAL:HG12	1:A:1049:ALA:HB3	1.76	0.66
1:A:719:TYR:HE1	1:A:841:LEU:HD11	1.61	0.65
1:A:1220:ARG:NH2	1:A:1223:THR:O	2.29	0.65
1:A:444:GLN:HA	1:A:523:LYS:HE3	1.79	0.65
1:A:273:MET:HA	1:A:759:THR:HG22	1.79	0.65
1:A:1224:ILE:HD13	1:A:1230:ILE:HD11	1.78	0.64
1:A:360:GLU:HB3	1:A:438:LYS:HD2	1.80	0.63
1:A:409:LYS:HB3	1:A:559:LEU:HD22	1.80	0.63
1:A:286:TYR:HE1	1:A:315:MET:HE3	1.63	0.63
1:A:1049:ALA:HB2	1:A:1055:LEU:HD11	1.81	0.63
1:A:1026:LEU:O	1:A:1046:SER:HA	1.98	0.63
1:A:521:MET:HE1	1:A:549:LEU:HD21	1.79	0.63
1:A:466:LEU:HD21	1:A:519:ARG:HE	1.64	0.62
1:A:527:ILE:HA	1:A:556:ARG:HG3	1.80	0.62
1:A:471:ALA:HB1	1:A:475:GLU:HB2	1.82	0.62
1:A:506:GLN:HB2	1:A:511:GLN:HB3	1.82	0.61
1:A:498:THR:HG22	1:A:501:GLY:H	1.65	0.61
1:A:1042:PHE:H	1:A:1236:GLY:HA3	1.65	0.61
1:A:351:ILE:HG13	1:A:439:LEU:HD21	1.83	0.60
1:A:555:GLY:O	1:A:556:ARG:NH1	2.30	0.60
1:A:374:ASP:HB3	1:A:423:ASN:H	1.67	0.60
1:A:1190:THR:OG1	1:A:1219:HIS:NE2	2.29	0.60
1:A:1199:ARG:NH1	1:A:1202:GLN:OE1	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:ARG:NH2	1:A:151:ILE:O	2.34	0.60
1:A:1117:TYR:HB2	1:A:1152:TYR:HB3	1.84	0.60
1:A:24:ILE:HG22	1:A:26:GLY:H	1.67	0.59
1:A:1053:LYS:HE2	1:A:1228:HIS:HB3	1.84	0.59
1:A:119:THR:O	1:A:123:ARG:HG3	2.03	0.58
1:A:68:LEU:HD22	1:A:945:LEU:HD13	1.84	0.58
1:A:1057:LEU:HA	1:A:1230:ILE:HG23	1.86	0.57
1:A:773:THR:HB	1:A:814:ARG:HG2	1.86	0.57
1:A:136:GLN:HG2	1:A:378:PRO:HG2	1.86	0.57
1:A:155:ALA:HA	1:A:159:GLN:HB3	1.87	0.56
1:A:511:GLN:HA	1:A:514:ARG:HG2	1.85	0.56
1:A:693:ASN:HD21	1:A:768:VAL:HG22	1.71	0.56
1:A:480:ALA:HB1	1:A:486:HIS:HB2	1.85	0.56
1:A:119:THR:HG21	1:A:159:GLN:HB2	1.88	0.56
1:A:187:VAL:HG22	1:A:302:THR:HG21	1.86	0.56
1:A:370:LEU:HD13	1:A:391:LEU:HD23	1.87	0.56
1:A:1020:LEU:H	1:A:1101:HIS:HE1	1.53	0.56
1:A:1036:ARG:NH2	3:A:1304:ANP:HI'	2.20	0.55
1:A:387:ASN:ND2	1:A:579:GLN:O	2.39	0.55
1:A:1023:GLU:HA	1:A:1049:ALA:O	2.06	0.55
1:A:907:LEU:O	1:A:911:ASN:ND2	2.39	0.55
1:A:458:THR:HG22	1:A:459:SER:H	1.71	0.55
1:A:994:ARG:HD2	1:A:995:SER:N	2.21	0.55
1:A:83:MET:SD	1:A:949:SER:OG	2.58	0.54
1:A:1099:ARG:O	1:A:1179:ARG:NH1	2.41	0.54
1:A:788:GLU:HG3	1:A:1006:ILE:HG12	1.90	0.54
1:A:1198:GLU:O	1:A:1202:GLN:HG3	2.07	0.54
1:A:226:ALA:HB1	1:A:253:TYR:HE1	1.73	0.54
1:A:340:LYS:O	1:A:344:ILE:HD12	2.07	0.53
1:A:413:VAL:HG23	1:A:559:LEU:HD21	1.90	0.53
1:A:1013:THR:OG1	1:A:1094:ASN:OD1	2.23	0.53
1:A:124:ILE:HD13	1:A:908:TYR:CD2	2.44	0.53
1:A:966:PHE:O	1:A:970:MET:HG2	2.08	0.53
1:A:1040:GLN:NE2	1:A:1041:ILE:O	2.42	0.53
1:A:455:LEU:HD12	1:A:512:LYS:HE3	1.91	0.53
1:A:1112:PHE:O	1:A:1119:ASN:ND2	2.32	0.53
1:A:446:ILE:HA	1:A:527:ILE:HB	1.91	0.53
1:A:468:ARG:HD3	1:A:471:ALA:HB2	1.91	0.53
1:A:713:LEU:HD23	1:A:750:LEU:HD22	1.91	0.52
1:A:905:VAL:O	1:A:909:THR:HG23	2.09	0.52
1:A:854:PRO:HA	1:A:857:VAL:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:776:VAL:O	1:A:780:MET:HG3	2.08	0.52
1:A:1058:VAL:HG23	1:A:1059:GLY:H	1.75	0.52
1:A:286:TYR:CE1	1:A:315:MET:HE3	2.44	0.52
1:A:1009:ASP:OD1	1:A:1096:LYS:NZ	2.39	0.52
1:A:212:LEU:HD13	1:A:271:LYS:HB2	1.92	0.52
1:A:1220:ARG:HH21	1:A:1224:ILE:HA	1.75	0.52
1:A:66:ALA:HB2	1:A:309:ALA:HB2	1.91	0.52
1:A:120:THR:O	1:A:124:ILE:HG12	2.09	0.52
1:A:35:PHE:HB3	1:A:121:LYS:HD2	1.92	0.51
1:A:850:VAL:HA	1:A:853:PHE:HB2	1.91	0.51
1:A:458:THR:HG22	1:A:459:SER:N	2.25	0.51
1:A:464:ILE:HG22	1:A:522:LEU:HD12	1.93	0.51
1:A:1167:GLN:HA	1:A:1170:ARG:HE	1.74	0.51
1:A:1163:LEU:HD13	1:A:1167:GLN:HB2	1.91	0.51
1:A:312:PHE:O	1:A:316:ILE:HG12	2.10	0.51
1:A:367:LEU:HD21	1:A:395:ALA:HB2	1.93	0.51
1:A:1088:LYS:HE2	1:A:1092:LYS:HD2	1.93	0.50
1:A:564:ARG:NH2	1:A:592:PHE:O	2.44	0.50
1:A:40:ASP:OD1	1:A:117:ARG:NE	2.27	0.50
1:A:144:THR:HG23	1:A:889:ILE:HG22	1.94	0.50
1:A:234:VAL:HG12	1:A:792:PHE:HE2	1.76	0.50
1:A:311:MET:O	1:A:315:MET:HG2	2.12	0.50
1:A:257:LEU:HD21	1:A:777:ARG:HD2	1.93	0.50
1:A:159:GLN:HG3	1:A:874:LEU:HD22	1.93	0.50
1:A:290:LEU:HD13	1:A:724:VAL:HG21	1.94	0.50
1:A:1015:PRO:HA	1:A:1094:ASN:HD21	1.76	0.50
1:A:133:GLN:HA	1:A:349:PRO:HB3	1.93	0.49
1:A:253:TYR:CD2	1:A:781:LEU:HD22	2.47	0.49
1:A:1093:TYR:HB2	1:A:1098:ILE:HD11	1.94	0.49
1:A:1220:ARG:HB3	1:A:1224:ILE:HG22	1.94	0.49
1:A:243:PHE:HE2	1:A:1175:ARG:HD2	1.76	0.49
1:A:350:THR:HG22	1:A:420:TYR:HE2	1.76	0.49
1:A:1038:ASP:OD1	1:A:1039:ILE:N	2.45	0.49
1:A:1049:ALA:HA	1:A:1055:LEU:HD21	1.93	0.49
1:A:1163:LEU:O	1:A:1168:LYS:NZ	2.45	0.49
1:A:1211:GLY:O	1:A:1212:ARG:NE	2.36	0.49
1:A:532:GLU:OE1	1:A:533:ALA:N	2.44	0.49
1:A:798:GLU:HG2	1:A:799:SER:N	2.28	0.49
1:A:226:ALA:HB1	1:A:253:TYR:CE1	2.47	0.49
1:A:862:LEU:HD23	1:A:930:TYR:HA	1.95	0.49
1:A:389:PHE:HB2	1:A:582:VAL:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:689:LEU:HD21	1:A:772:LEU:HD21	1.95	0.48
1:A:780:MET:HE1	1:A:806:LEU:HA	1.95	0.48
1:A:1102:ILE:HG12	1:A:1183:ILE:HB	1.95	0.48
1:A:79:VAL:HB	1:A:953:LYS:HG2	1.94	0.48
1:A:35:PHE:HE2	1:A:122:MET:HG3	1.78	0.48
1:A:237:ILE:HG13	1:A:241:MET:HG3	1.96	0.48
1:A:194:THR:O	1:A:198:VAL:HG23	2.14	0.48
1:A:214:LYS:HG2	1:A:218:LYS:HE2	1.95	0.48
1:A:1069:ILE:O	1:A:1073:GLN:HG3	2.14	0.48
1:A:1167:GLN:O	1:A:1170:ARG:HG2	2.14	0.48
1:A:375:PHE:HE2	1:A:419:PHE:HB2	1.78	0.47
1:A:138:PHE:HD2	1:A:892:VAL:HG11	1.79	0.47
1:A:1074:ARG:HD3	1:A:1095:LEU:HD13	1.97	0.47
1:A:402:VAL:HG13	1:A:576:VAL:HG23	1.96	0.47
1:A:547:GLU:HA	1:A:551:ARG:HH12	1.79	0.47
1:A:707:SER:HA	1:A:761:GLN:OE1	2.15	0.47
1:A:717:PHE:HD1	1:A:747:LEU:HD11	1.80	0.47
1:A:129:ALA:O	1:A:133:GLN:HG2	2.14	0.47
1:A:416:ILE:HG22	1:A:446:ILE:HD13	1.97	0.47
1:A:66:ALA:HB2	1:A:309:ALA:CB	2.45	0.47
1:A:1222:SER:HA	1:A:1244:HIS:HE1	1.80	0.47
1:A:441:TRP:HA	1:A:444:GLN:NE2	2.29	0.47
1:A:66:ALA:HB1	1:A:306:LEU:HD23	1.97	0.47
1:A:375:PHE:HA	1:A:421:ASP:HB2	1.97	0.46
1:A:157:MET:HG2	1:A:334:ALA:CA	2.43	0.46
1:A:1175:ARG:HA	1:A:1178:VAL:HG12	1.97	0.46
1:A:232:GLN:HA	1:A:235:VAL:HG22	1.98	0.46
1:A:289:LEU:HB3	1:A:311:MET:SD	2.56	0.46
1:A:263:LEU:HD23	1:A:263:LEU:HA	1.78	0.46
1:A:373:VAL:HG11	1:A:389:PHE:CE1	2.51	0.46
1:A:123:ARG:NH1	1:A:154:ASP:HB3	2.30	0.46
1:A:1058:VAL:HG23	1:A:1059:GLY:N	2.30	0.46
1:A:560:ILE:HD12	1:A:567:THR:HG21	1.98	0.45
1:A:227:GLY:HA2	1:A:230:VAL:HG12	1.97	0.45
1:A:439:LEU:HD11	1:A:443:ARG:HH21	1.81	0.45
1:A:1103:ALA:HB2	1:A:1179:ARG:HG2	1.98	0.45
1:A:1029:ILE:HG13	1:A:1042:PHE:HB3	1.98	0.45
1:A:780:MET:HG2	1:A:1000:LEU:HD11	1.99	0.45
1:A:1031:PHE:CD1	1:A:1040:GLN:HG2	2.52	0.45
1:A:958:ASP:OD1	1:A:959:PHE:N	2.47	0.45
1:A:1022:GLY:HA2	1:A:1183:ILE:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1084:MET:HA	1:A:1089:ASP:HA	1.97	0.45
1:A:410:SER:H	3:A:1303:ANP:HNB1	1.64	0.45
1:A:111:TRP:HB3	1:A:163:SER:O	2.17	0.45
1:A:294:GLY:HA3	1:A:740:ILE:HD13	1.98	0.45
1:A:393:VAL:HG12	1:A:399:ILE:HG21	1.98	0.45
1:A:838:GLY:HA2	1:A:965:VAL:HG22	1.97	0.45
1:A:126:TYR:HA	1:A:345:ILE:HG12	1.99	0.44
1:A:457:ALA:HA	1:A:500:VAL:HG11	1.98	0.44
1:A:758:ASN:HA	1:A:761:GLN:HG2	2.00	0.44
1:A:819:ASP:N	1:A:819:ASP:OD1	2.50	0.44
1:A:824:ILE:HD12	1:A:979:THR:HG23	1.99	0.44
1:A:713:LEU:HD13	1:A:754:ALA:HA	1.99	0.44
1:A:157:MET:SD	1:A:338:ALA:HB2	2.57	0.44
1:A:912:LEU:C	1:A:915:PRO:HD2	2.38	0.44
1:A:1027:LYS:HE2	1:A:1027:LYS:HB3	1.87	0.44
1:A:161:ALA:HA	1:A:165:LYS:HB2	2.00	0.44
1:A:349:PRO:HB2	1:A:351:ILE:HG22	2.00	0.44
1:A:67:ASP:HB3	1:A:89:TYR:CZ	2.53	0.43
1:A:1234:ASP:O	1:A:1237:LYS:NZ	2.41	0.43
1:A:812:ASN:ND2	1:A:988:LYS:HG2	2.24	0.43
1:A:991:GLN:HG3	1:A:994:ARG:NH2	2.32	0.43
1:A:995:SER:O	1:A:998:GLU:HG2	2.17	0.43
1:A:408:GLY:H	3:A:1303:ANP:H5'2	1.83	0.43
1:A:1104:ILE:HG22	1:A:1185:LEU:HD12	1.99	0.43
1:A:411:THR:O	1:A:415:LEU:HD23	2.19	0.43
1:A:786:LYS:HA	1:A:1008:PRO:HG3	2.00	0.43
1:A:266:LYS:HD3	1:A:266:LYS:HA	1.88	0.43
1:A:438:LYS:O	1:A:439:LEU:HB3	2.17	0.42
1:A:348:LYS:HD2	1:A:348:LYS:N	2.34	0.42
1:A:754:ALA:O	1:A:758:ASN:HB2	2.18	0.42
1:A:58:LEU:HB2	1:A:59:PRO:HD3	2.00	0.42
1:A:1058:VAL:O	1:A:1065:LYS:HE2	2.19	0.42
1:A:138:PHE:HE2	1:A:892:VAL:HG21	1.83	0.42
1:A:416:ILE:HG21	1:A:529:LEU:HD11	2.01	0.42
1:A:400:ALA:O	1:A:575:ALA:HB3	2.19	0.42
1:A:1026:LEU:HB3	1:A:1029:ILE:HG21	2.01	0.42
1:A:1074:ARG:HH11	1:A:1091:ARG:HA	1.85	0.42
1:A:852:VAL:O	1:A:856:VAL:HG23	2.20	0.42
1:A:187:VAL:HB	1:A:310:THR:HG21	2.01	0.42
1:A:50:GLY:O	1:A:103:SER:HB3	2.19	0.42
1:A:458:THR:HG21	1:A:907:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1138:LEU:HD22	1:A:1177:LEU:HG	2.01	0.42
1:A:219:SER:O	1:A:223:LEU:HG	2.20	0.42
1:A:1104:ILE:HG22	1:A:1185:LEU:HB2	2.00	0.42
1:A:184:PHE:HE1	1:A:192:LEU:HG	1.85	0.42
1:A:722:SER:OG	1:A:964:ARG:HA	2.20	0.41
1:A:312:PHE:HZ	1:A:721:LEU:HD21	1.85	0.41
1:A:765:TRP:HA	1:A:768:VAL:HG12	2.03	0.41
1:A:1003:LYS:HA	1:A:1003:LYS:HD2	1.84	0.41
1:A:274:GLY:O	1:A:278:THR:HG23	2.20	0.41
1:A:948:ALA:HB1	1:A:962:THR:HB	2.02	0.41
1:A:1155:TYR:CE2	1:A:1160:GLY:HA2	2.56	0.41
1:A:169:PHE:HB2	1:A:327:SER:HB3	2.02	0.41
1:A:570:LYS:HD2	1:A:570:LYS:H	1.86	0.41
1:A:126:TYR:CD1	1:A:341:ILE:HG23	2.56	0.41
1:A:375:PHE:CG	1:A:421:ASP:HB2	2.56	0.41
1:A:540:GLU:HA	1:A:543:LYS:HG2	2.01	0.41
1:A:727:VAL:O	1:A:736:MET:HG3	2.21	0.41
1:A:755:LEU:O	1:A:759:THR:HG23	2.20	0.41
1:A:1096:LYS:HG3	1:A:1097:ALA:N	2.35	0.41
1:A:1131:GLU:HA	1:A:1134:GLN:HG3	2.03	0.41
1:A:843:TRP:O	1:A:844:ARG:HB3	2.20	0.41
1:A:847:LEU:HD23	1:A:847:LEU:HA	1.89	0.41
1:A:903:LYS:NZ	1:A:906:ARG:HE	2.19	0.41
1:A:230:VAL:O	1:A:234:VAL:HG22	2.21	0.41
1:A:475:GLU:HA	1:A:478:GLU:CD	2.41	0.41
1:A:1019:ARG:HH22	1:A:1180:LYS:HG2	1.85	0.41
1:A:1222:SER:HA	1:A:1244:HIS:CE1	2.54	0.41
1:A:245:GLY:HA3	1:A:1122:TYR:OH	2.20	0.41
1:A:873:ASP:HB3	1:A:876:ALA:HB3	2.03	0.41
1:A:1151:GLY:O	1:A:1154:THR:OG1	2.29	0.41
1:A:123:ARG:CZ	1:A:154:ASP:HB3	2.51	0.40
1:A:181:ILE:HD13	1:A:181:ILE:HA	1.95	0.40
1:A:1013:THR:HB	1:A:1092:LYS:O	2.21	0.40
1:A:96:VAL:O	1:A:100:ILE:HG13	2.21	0.40
1:A:727:VAL:HG12	1:A:736:MET:HG3	2.02	0.40
1:A:158:VAL:HG23	1:A:162:ILE:HD11	2.02	0.40
1:A:528:LEU:HD22	1:A:552:PHE:CZ	2.56	0.40
1:A:461:LYS:N	1:A:461:LYS:HD2	2.36	0.40
1:A:521:MET:HA	1:A:521:MET:HE2	2.03	0.40
1:A:696:GLU:HB2	1:A:768:VAL:HG23	2.03	0.40
1:A:1093:TYR:CB	1:A:1098:ILE:HD11	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	1161/1327 (88%)	1104 (95%)	57 (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	949/1087 (87%)	946 (100%)	3 (0%)	91	94

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	418	ARG
1	A	676	LYS
1	A	814	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	70	ASN
1	A	261	GLN

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Mol	Chain	Res	Type
1	A	812	ASN
1	A	1040	GLN
1	A	1101	HIS

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 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	1304	-	29,33,33	1.20	5 (17%)	31,52,52	1.18	3 (9%)
3	ANP	A	1303	2	29,33,33	1.20	5 (17%)	31,52,52	1.17	4 (12%)

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	-	-	4/14/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ANP	A	1303	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	3.18	1.51	1.46
3	A	1303	ANP	PG-O1G	3.13	1.51	1.46
3	A	1303	ANP	PB-O1B	2.96	1.50	1.46
3	A	1304	ANP	PB-O1B	2.93	1.50	1.46
3	A	1304	ANP	PB-O2B	-2.21	1.50	1.56
3	A	1303	ANP	PB-O2B	-2.20	1.50	1.56
3	A	1304	ANP	PG-O2G	-2.06	1.51	1.56
3	A	1303	ANP	PG-O2G	-2.06	1.51	1.56
3	A	1303	ANP	PG-O3G	-2.05	1.51	1.56
3	A	1304	ANP	PG-O3G	-2.04	1.51	1.56

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1304	ANP	O2B-PB-O1B	4.18	118.69	109.92
3	A	1303	ANP	O2B-PB-O1B	4.02	118.36	109.92
3	A	1304	ANP	C5-C6-N6	2.27	123.80	120.35
3	A	1303	ANP	O4'-C1'-C2'	-2.25	103.64	106.93
3	A	1303	ANP	C5-C6-N6	2.25	123.77	120.35
3	A	1303	ANP	O3G-PG-O1G	-2.05	108.30	113.45
3	A	1304	ANP	O3G-PG-O1G	-2.01	108.39	113.45

There are no chirality outliers.

All (7) torsion outliers are listed below:

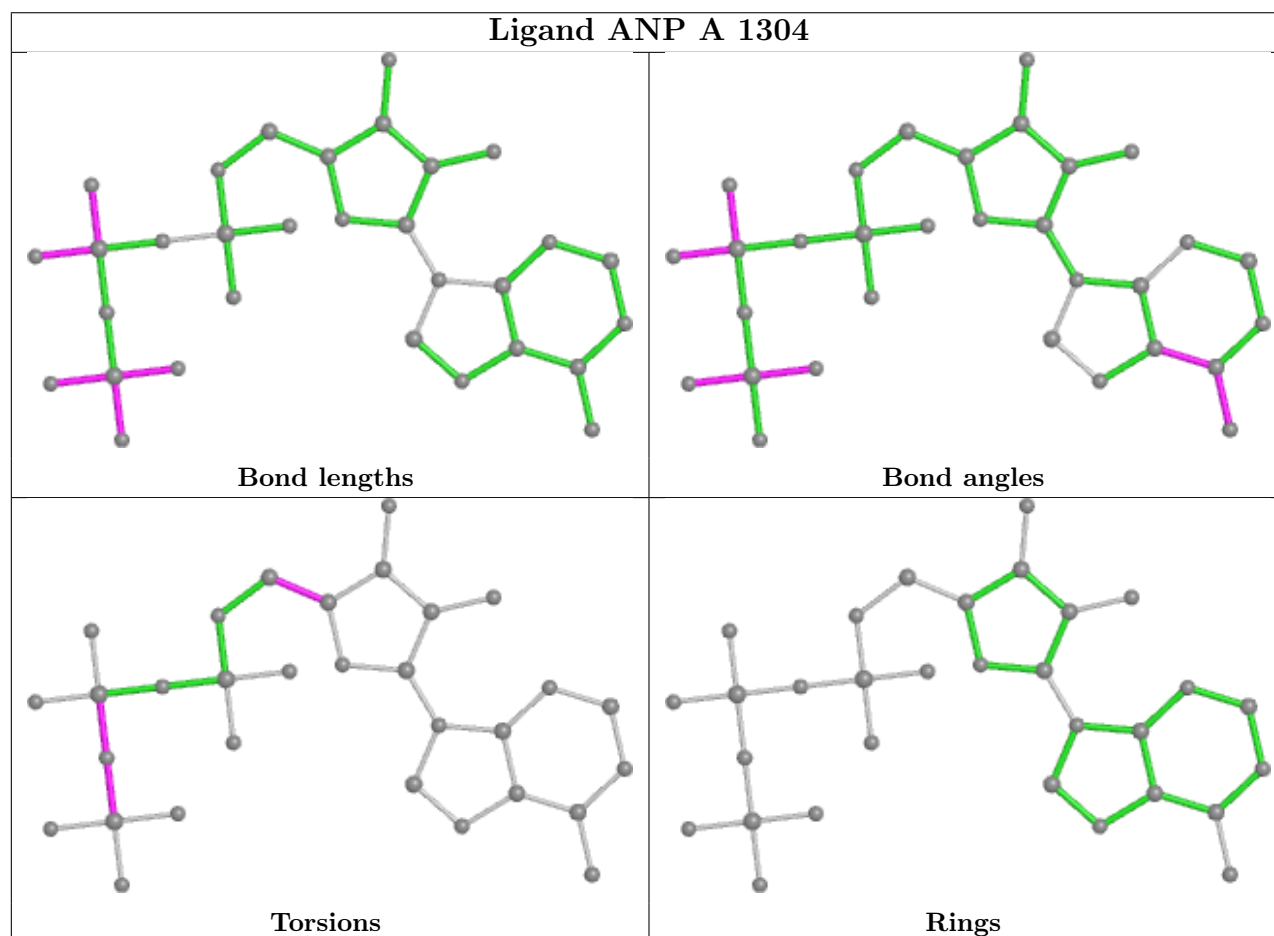
Mol	Chain	Res	Type	Atoms
3	A	1303	ANP	PG-N3B-PB-O1B
3	A	1303	ANP	PG-N3B-PB-O3A
3	A	1304	ANP	PB-N3B-PG-O1G
3	A	1304	ANP	PG-N3B-PB-O1B
3	A	1304	ANP	PG-N3B-PB-O3A
3	A	1304	ANP	O4'-C4'-C5'-O5'
3	A	1303	ANP	C4'-C5'-O5'-PA

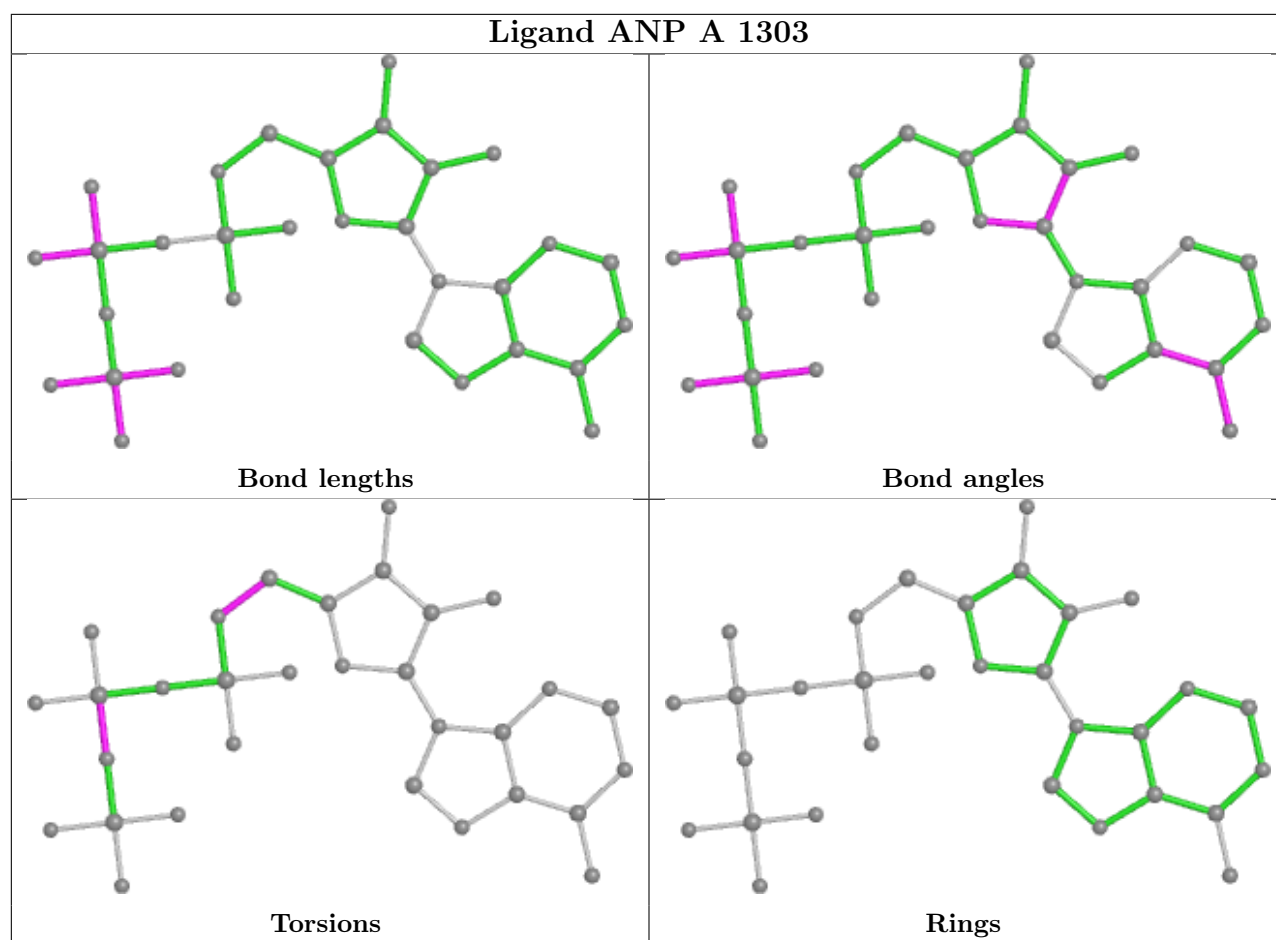
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1304	ANP	1	0
3	A	1303	ANP	2	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.





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.

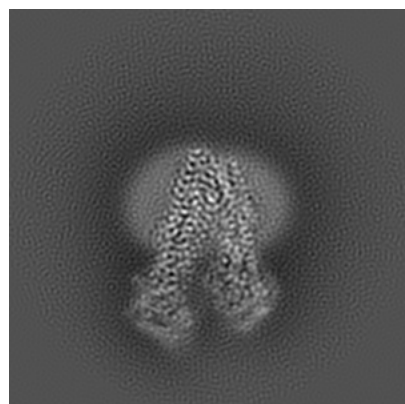
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61828. These allow visual inspection of the internal detail of the map and identification of artifacts.

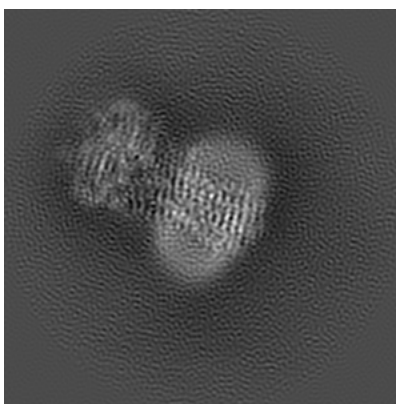
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

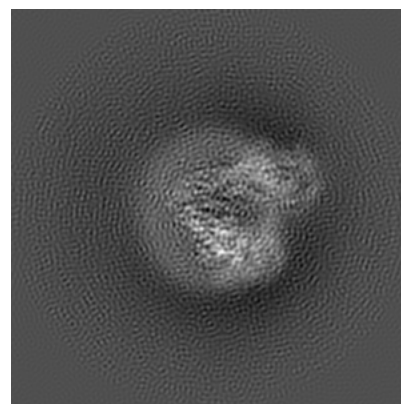
6.1.1 Primary map



X

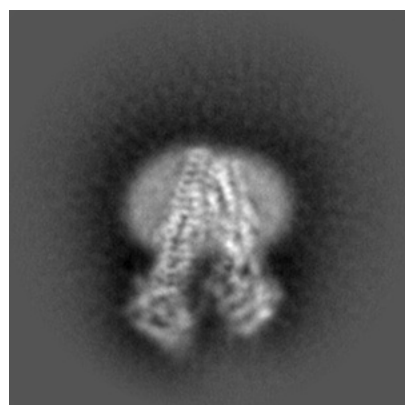


Y

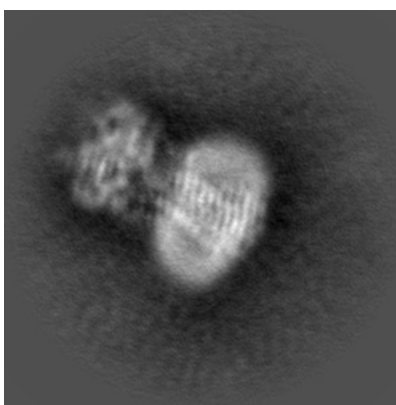


Z

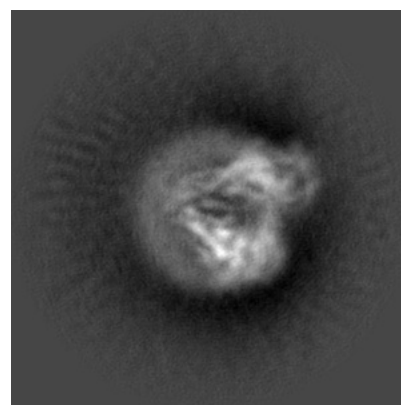
6.1.2 Raw map



X



Y

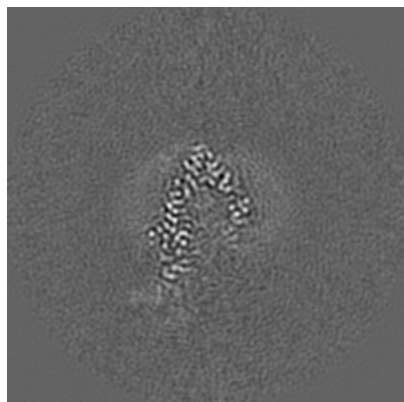


Z

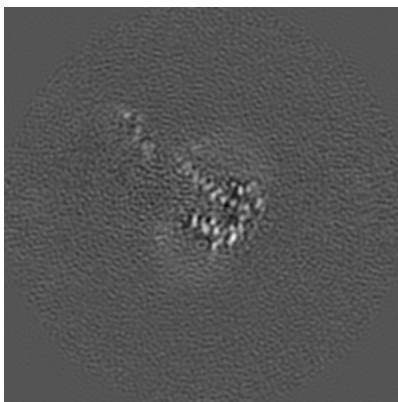
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

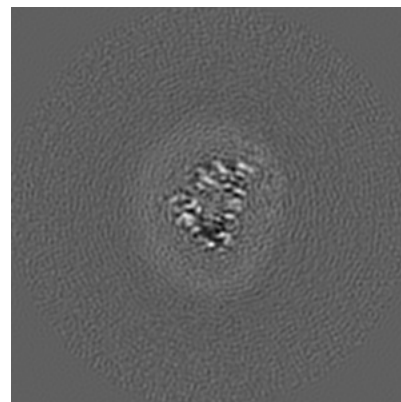
6.2.1 Primary map



X Index: 120

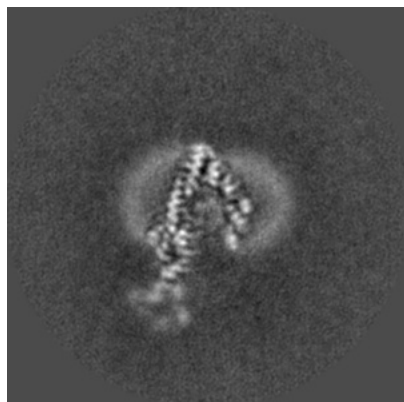


Y Index: 120

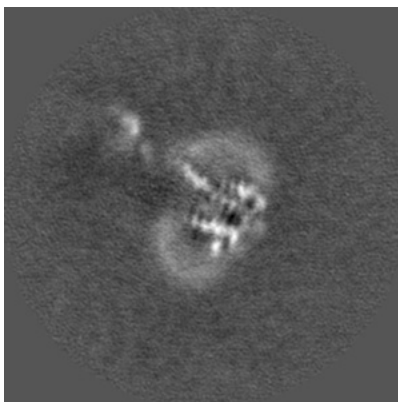


Z Index: 120

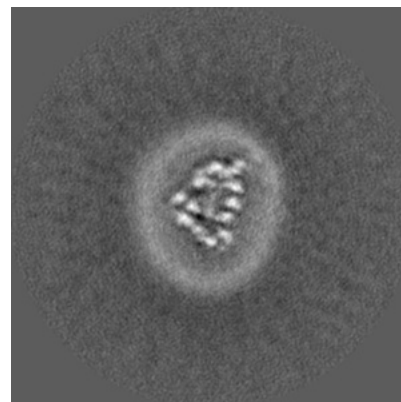
6.2.2 Raw map



X Index: 120



Y Index: 120

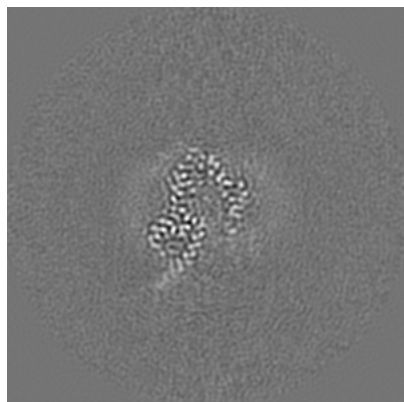


Z Index: 120

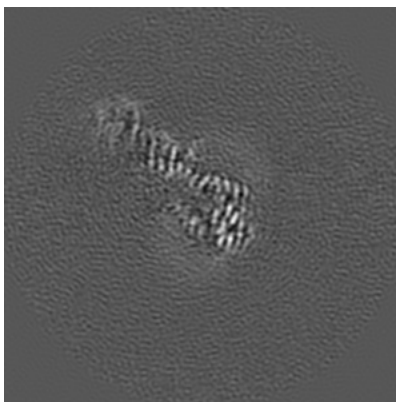
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

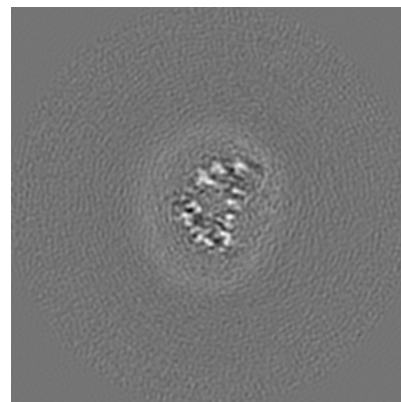
6.3.1 Primary map



X Index: 116

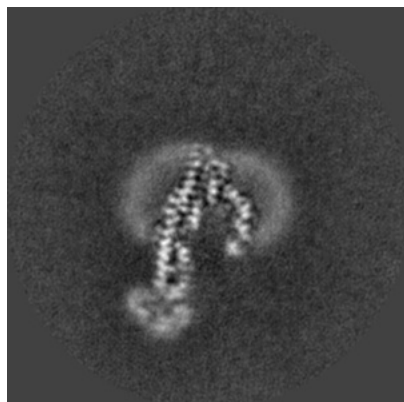


Y Index: 130

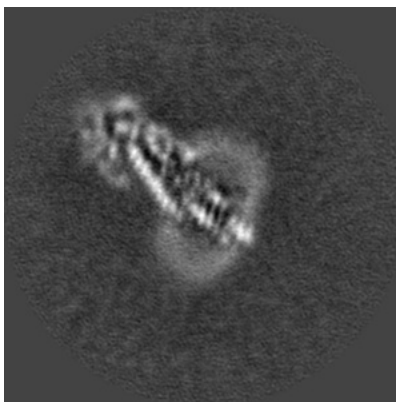


Z Index: 119

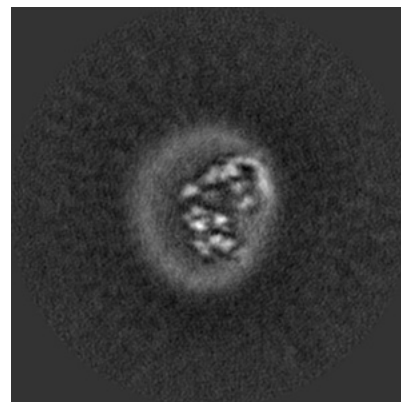
6.3.2 Raw map



X Index: 125



Y Index: 136

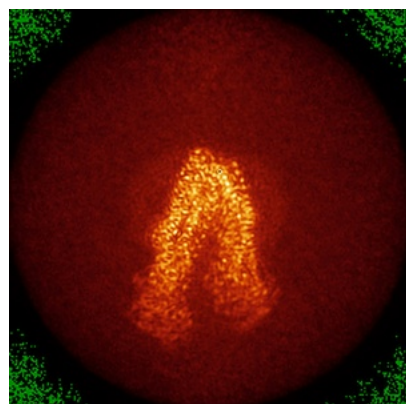


Z Index: 112

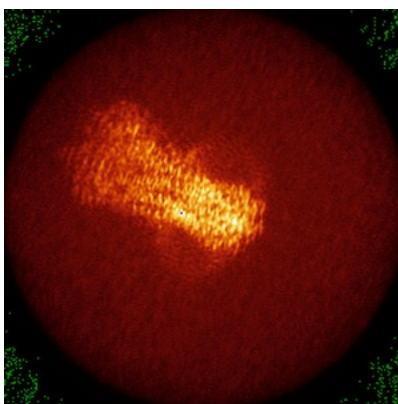
The images above show the largest variance slices of the map in three orthogonal directions.

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

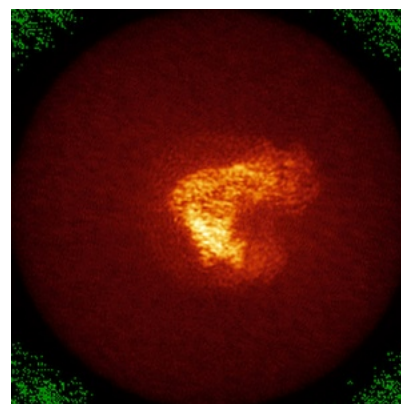
6.4.1 Primary map



X

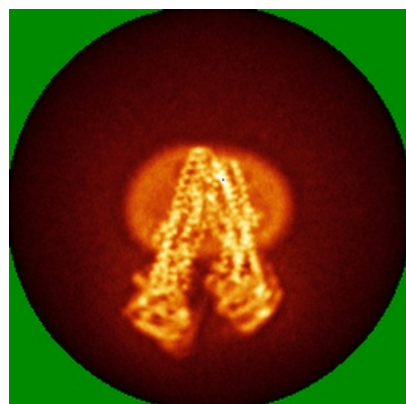


Y

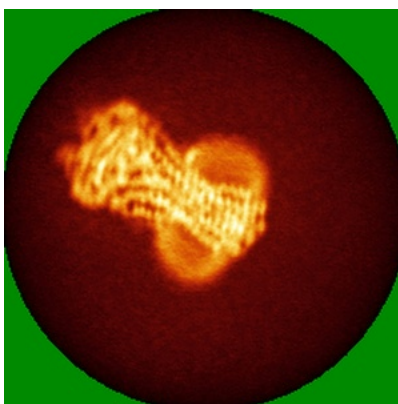


Z

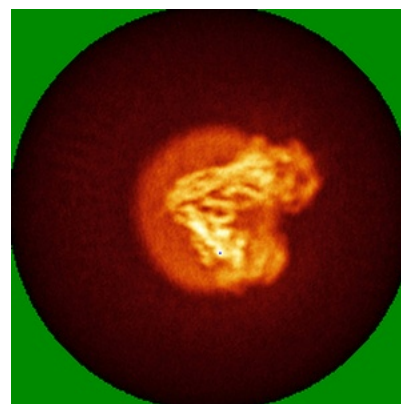
6.4.2 Raw map



X



Y

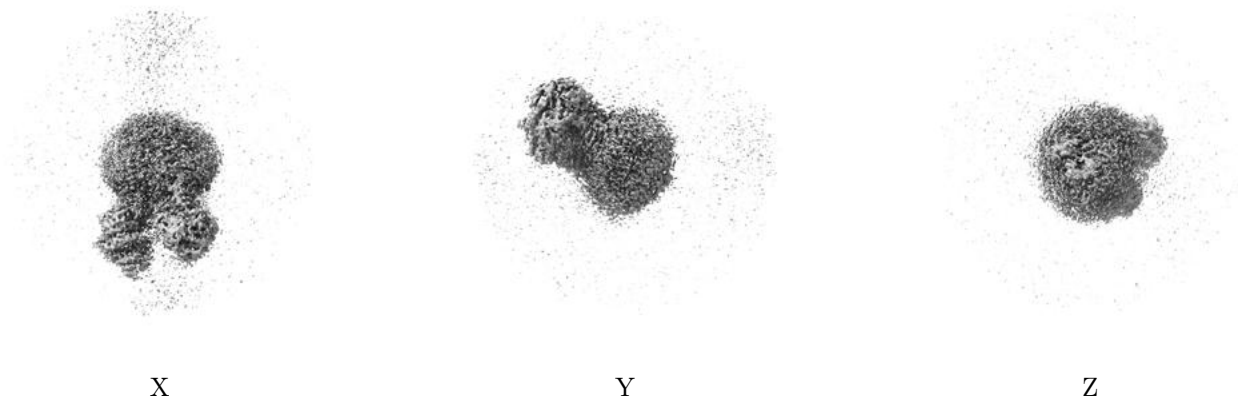


Z

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.

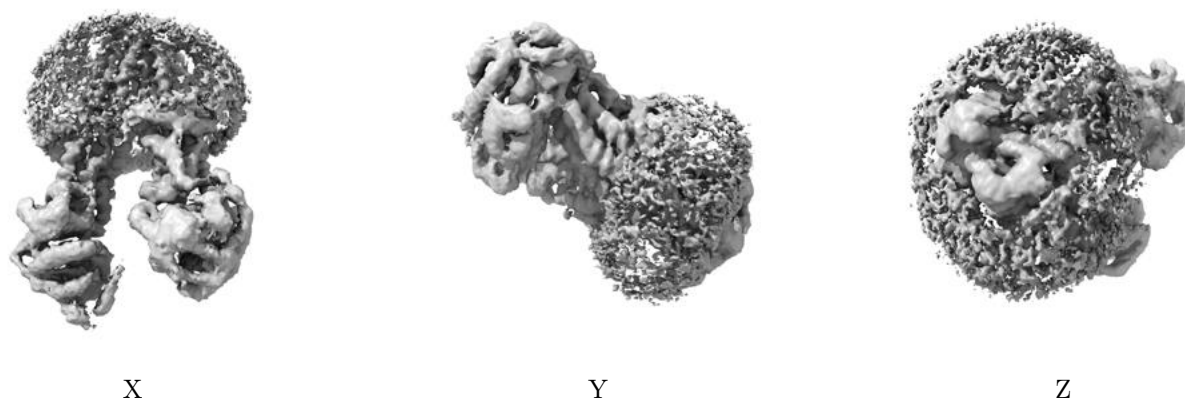
6.5 Orthogonal surface views [i](#)

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.

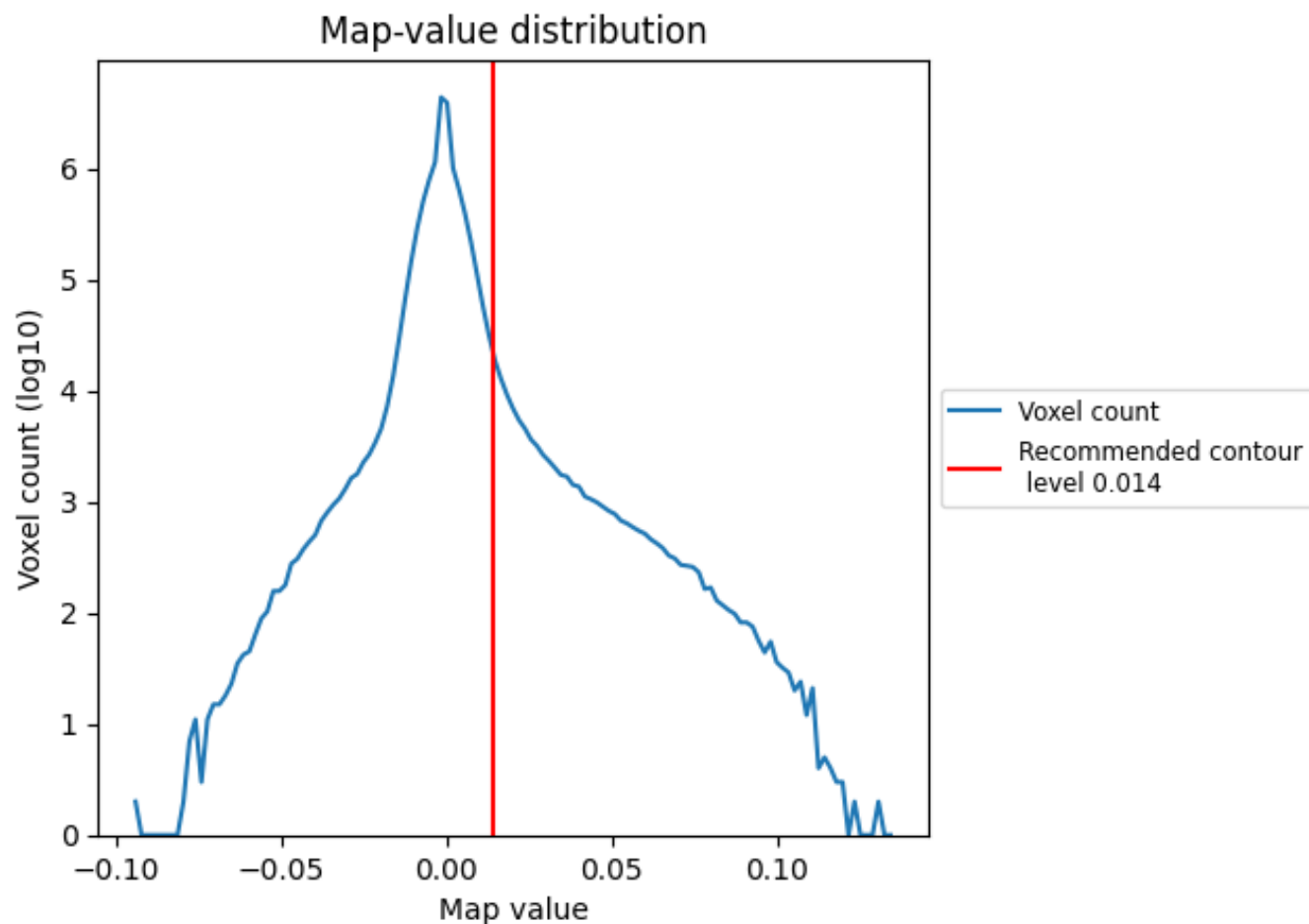
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

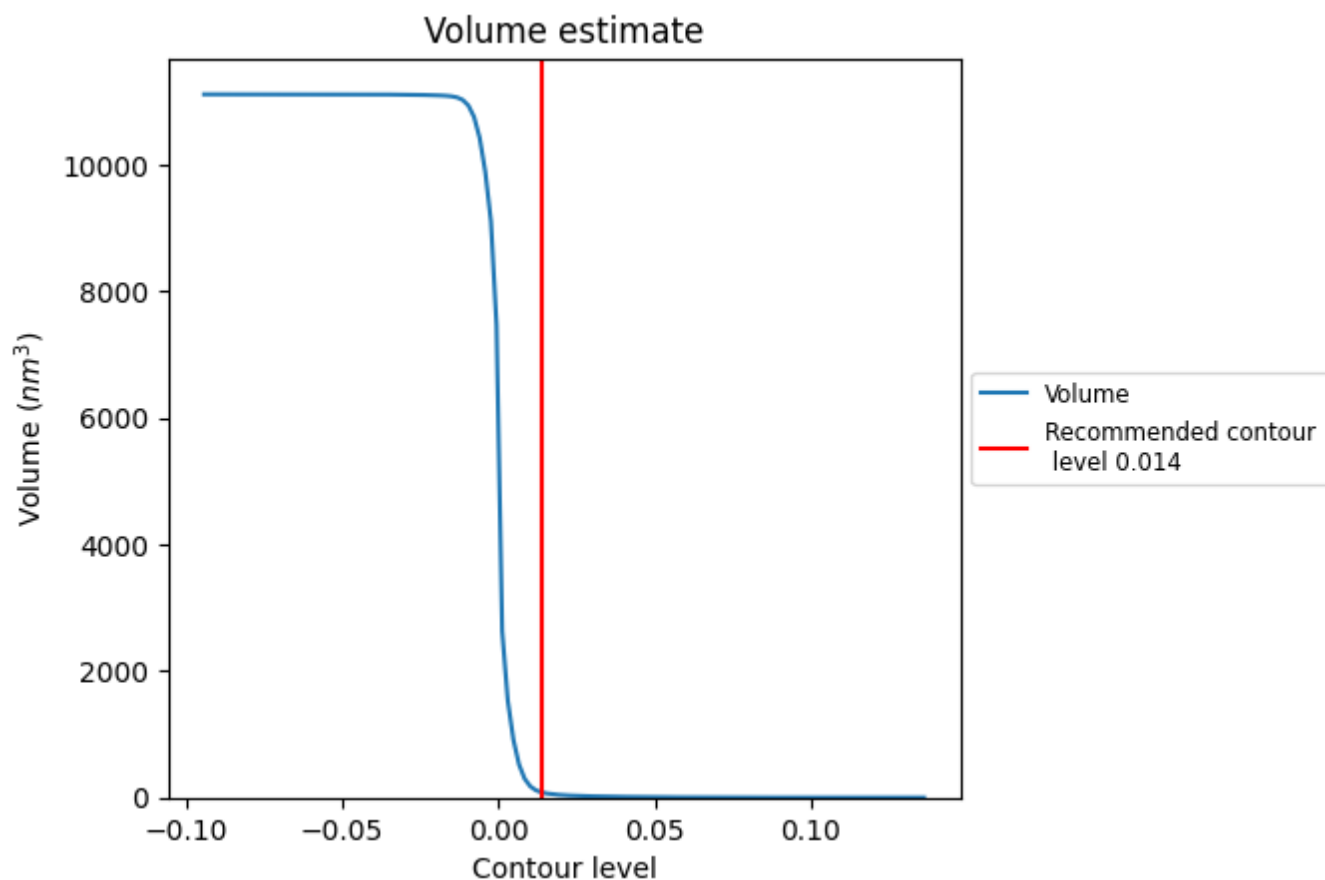
This section contains the results of statistical analysis of the map.

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.

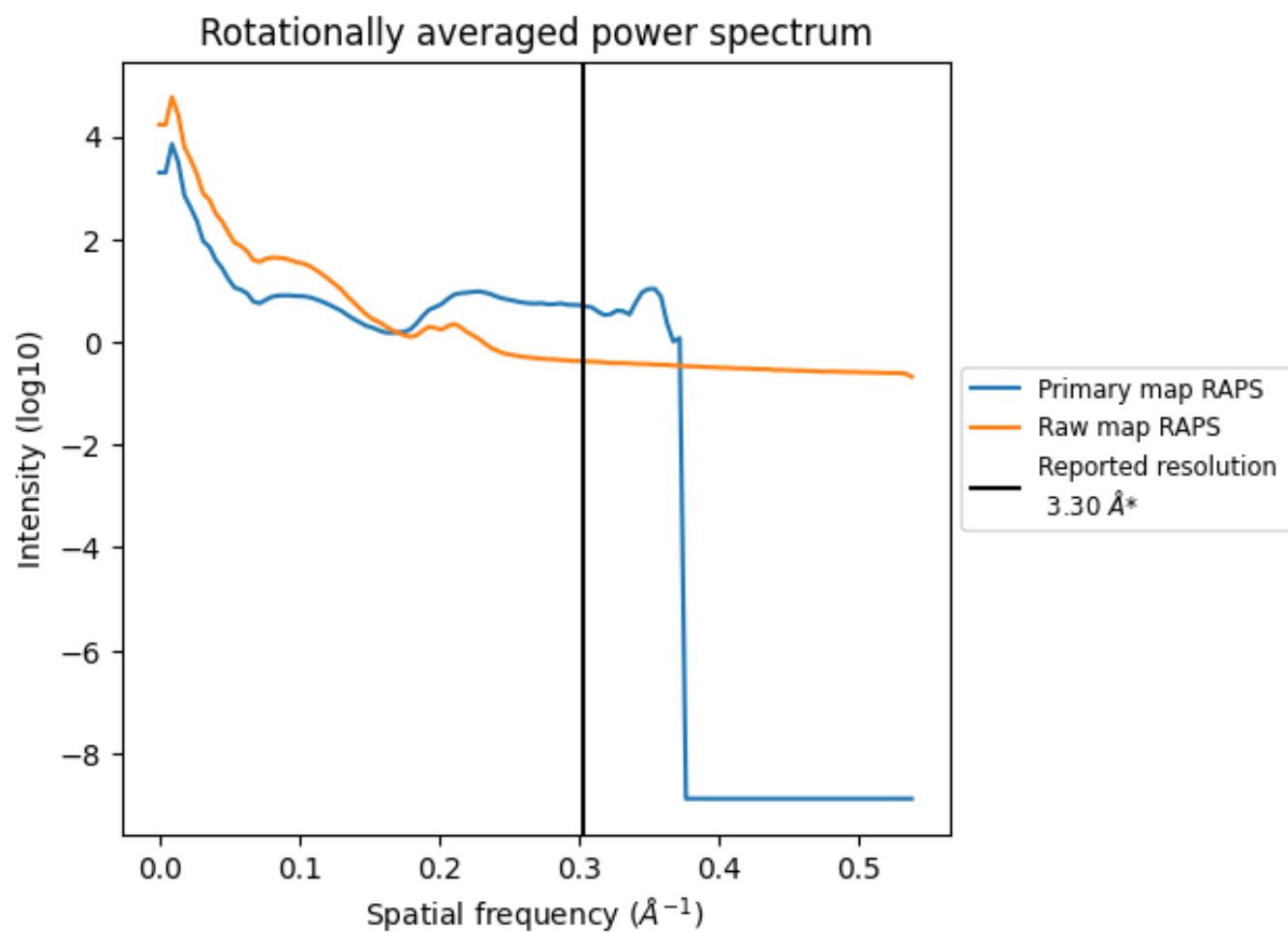
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 81 nm³; this corresponds to an approximate mass of 73 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 ⓘ

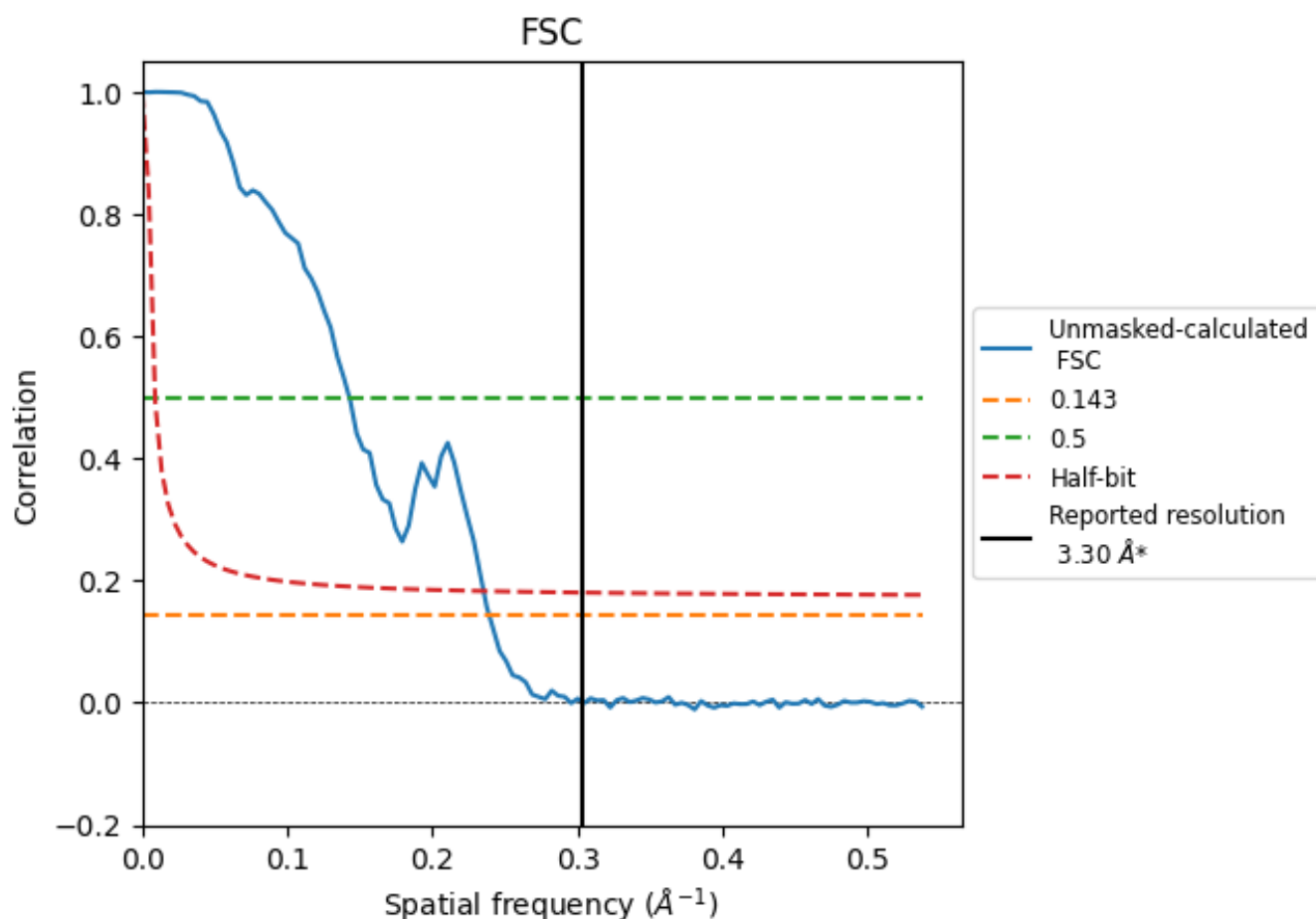


*Reported resolution corresponds to spatial frequency of 0.303 \AA^{-1}

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 0.303 \AA^{-1}

8.2 Resolution estimates [i](#)

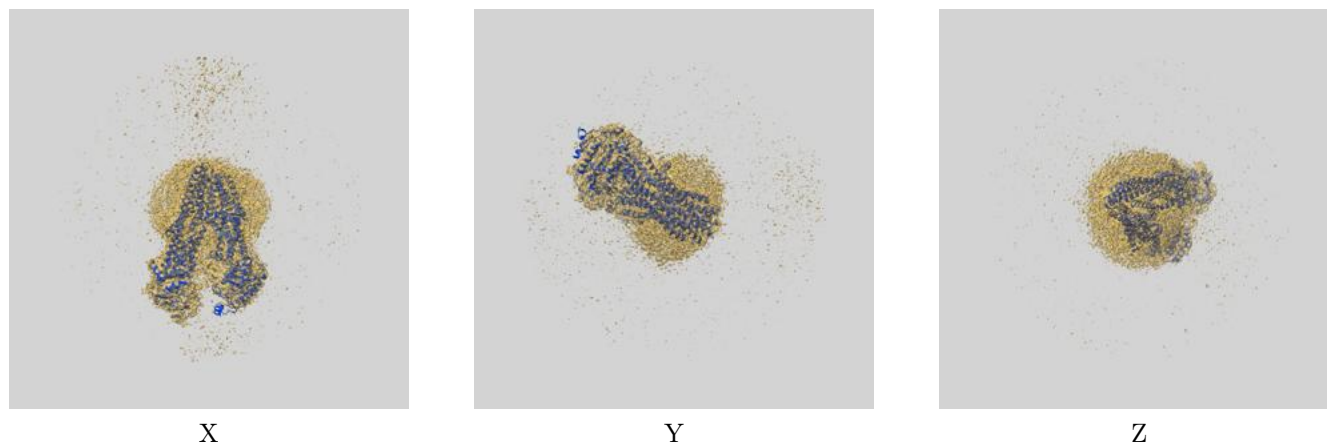
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.18	7.01	4.25

*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 4.18 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

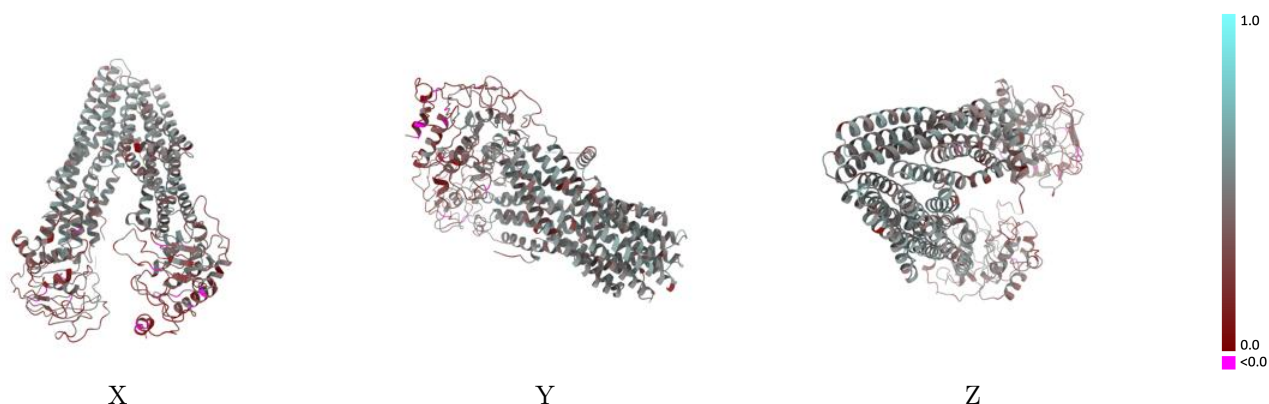
This section contains information regarding the fit between EMDB map EMD-61828 and PDB model 9JUK. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



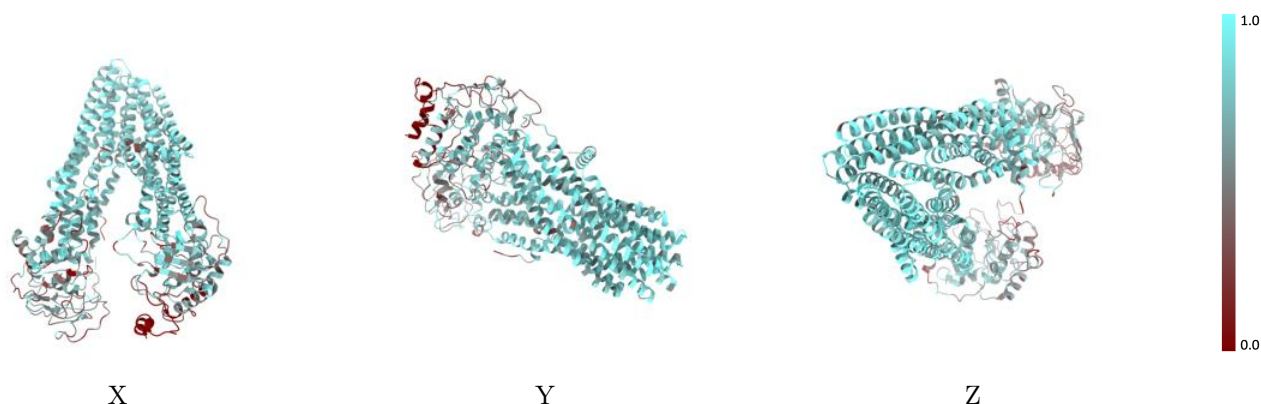
The images above show the 3D surface view of the map at the recommended contour level 0.014 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



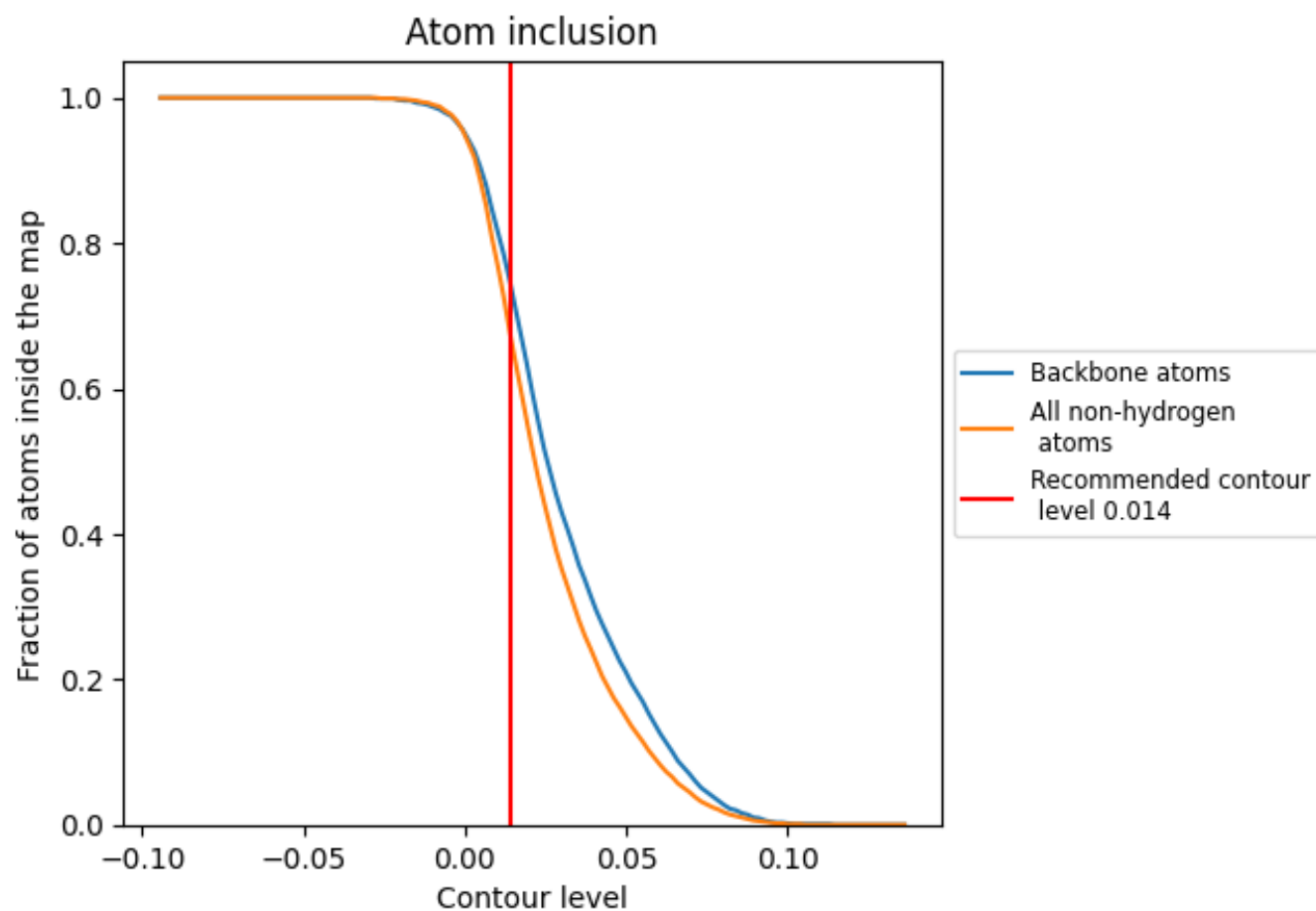
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 75% of all backbone atoms, 68% 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> 0.6760	<div></div> 0.4060
A	<div></div> 0.6760	<div></div> 0.4060

