



Full wwPDB EM Validation Report ⓘ

May 8, 2025 – 02:21 PM JST

PDB ID : 9JUK / pdb_00009juk
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.dev118
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.43.1

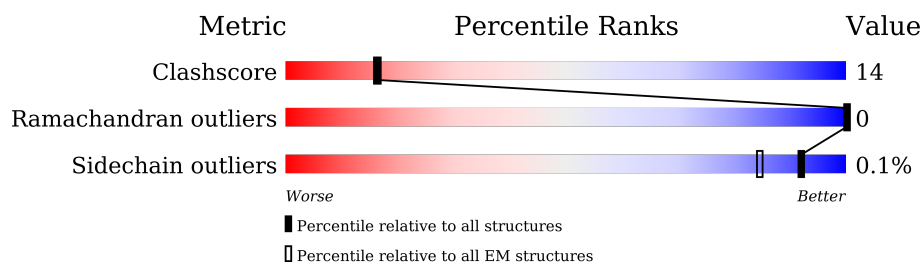
1 Overall quality at a glance

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>60%</div> <div>28%</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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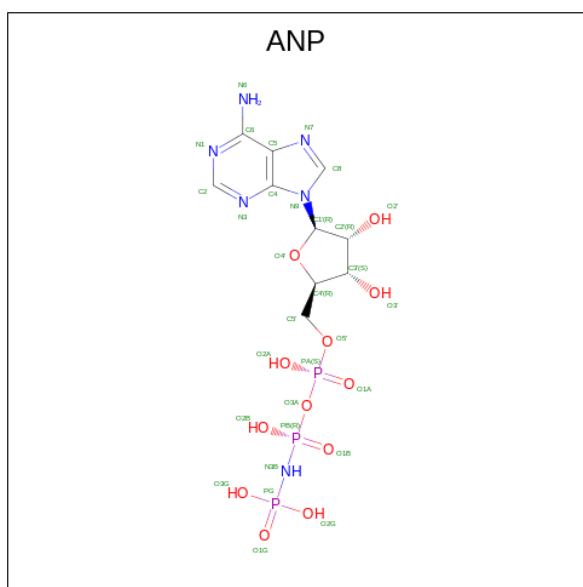
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Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	HIS	-	expression tag	UNP Q9ZR72
A	-11	PRO	-	expression tag	UNP Q9ZR72
A	-10	GLN	-	expression tag	UNP Q9ZR72
A	-9	PHE	-	expression tag	UNP Q9ZR72
A	-8	GLU	-	expression tag	UNP Q9ZR72
A	-7	LYS	-	expression 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 (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

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

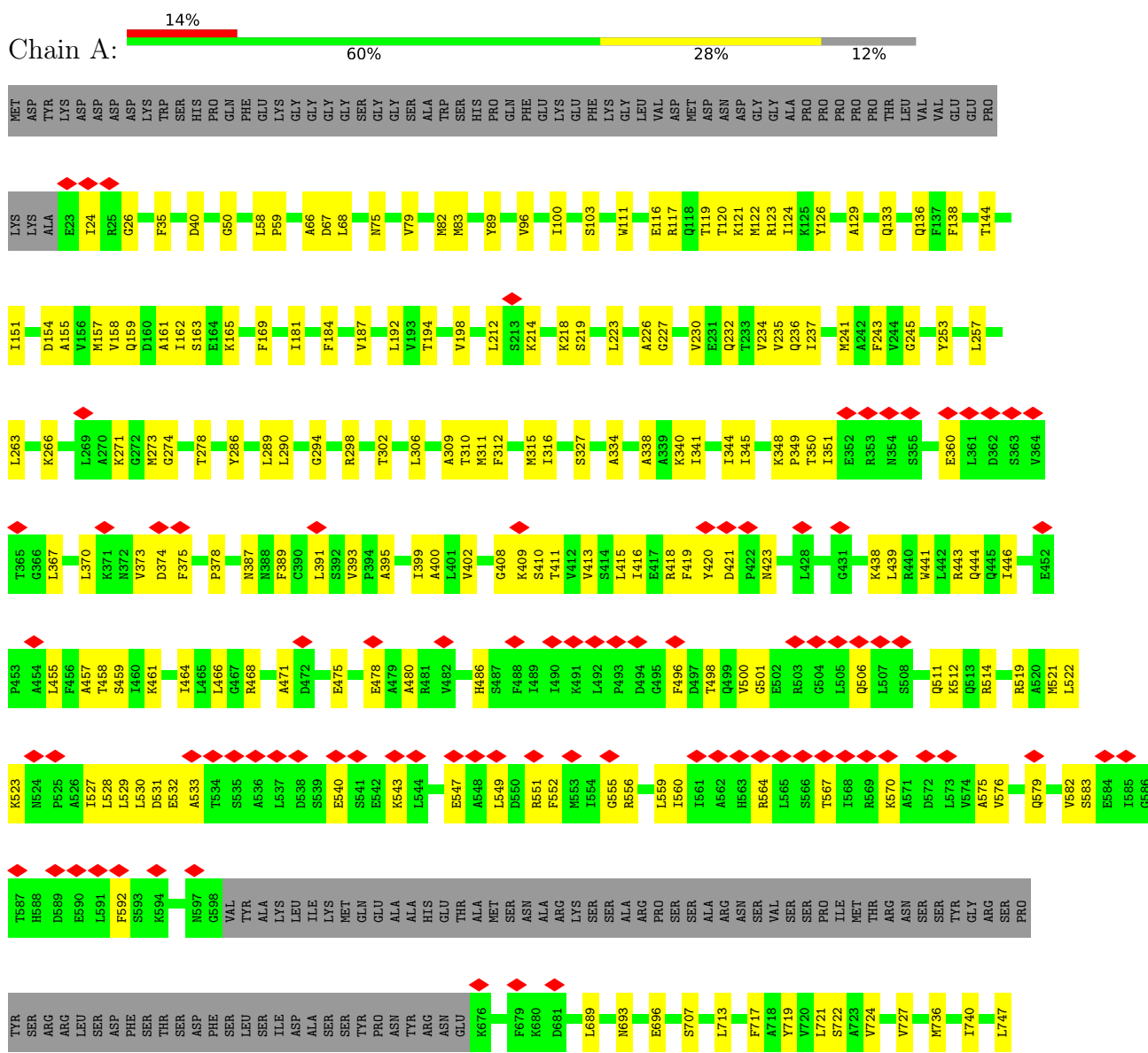


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	6	12	3	
3	A	1	Total	C	N	O	P	0
			31	10	6	12	3	

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: ABC transporter B family member 1



SER	V1216	P1149	K1085	S995	P854	L750
SER	H1219	E1150	I1069	E998	V855	L754
ARG	L1221	G1151	Q1073	L1000	V856	A754
VAL	L1222	Y1152	R1074	K1003	V857	L755
LYS	S1222	T1154	P1078	I1006	L862	N758
GLU	T1223	Y1155	S1079	E1007	N759	T759
ASP	I1224	V1156	S1080	P1008	L874	L760
ALA	R1225	E1157	G1081	D1009	E875	Q761
	N1226	E1158	R1082	D1010	A876	
	A1227	E1159	V1083	P1011	T882	W765
	H1228	G1160	M1084	D1012	V768	
	V1229	V1161	I1085	T1013	L772	
	I1230	Q1162	D1086	D1014	T773	
	A1231	L1163	G1087	P1015	V776	
	D1234	S1164	K1088	D1018	R777	
	D1235	Q1167	D1089	R1018	M780	
	G1236	K1168	I1090	R1019	L781	
	K1237	Q1169	R1091	L1020	K786	
	V1238	R1170	K1092	R1021	N787	
	A1239	I1173	Y1093	G1022	E788	
	E1240	A1174	N1094	E1023	F792	
	Q1241	R1175	K1095	V1024	E798	
	G1242	A1176	K1096	E1025	S799	
	S1243	L1177	I1097	L1026	A800	
	H1244	V1178	I1098	L916	R801	
	S1245	R1179	R1099	Y930	L806	
	H1246	K1180	K1100	H1027	N812	
	L1247	I1183	H1101	H1028	V813	
	L1248	M1184	I1102	I1029	R814	
	K1249	L1185	A1103	D1030	D819	
	N1250	L1186	I1104	F1031	R820	
	H1251	D1187	E1106	S1032	I824	
	P1252	E1188	P1109	R1036	G838	
	D1253	A1189	C1110	D1037	L841	
	G1254	E1190	L1111	D1038	Q842	
	I1255	T1190	F1112	I1039	W843	
	Y1256	S1191	G1113	Q1040	R844	
	A1257	A1192	T1114	I1041	L845	
	R1258	L1193	Y1117	F1042	A846	
	M1259	D1194	E1118	R1043	L847	
	I1260	A1195	N1119	D1044	V850	
	Q1261	E1196	Y1122	L1045	A851	
	L1262	S1197	A1127	S1046	V852	
	Q1263	E1198	E1131	L1047	F853	
	R1264	I1199	I1132	R1048		
	PHE	S1200	I1133	A1049		
THR	THR	V1201	Q1134	R1050		
HIS	HIS	Q1202	L1138	A1051		
THR	THR	L1205	A1147	G1052		
GLN	GLN	D1206	L1148	K1053		
VAL	VAL	C1209		T1054		
ILE	ILE	G1210		L1055		
GLY	GLY	G1211		A1056		
MET	MET	R1212		L1057		
THR	THR			V1058		
SER	SER			G1059		
GLY	GLY					
SER	SER					

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 [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	0.16	0/9137	0.34	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	9115	255	0
2	A	2	0	0	0	0
3	A	62	0	26	3	0
All	All	9035	0	9141	255	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 (255) 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:286:TYR:HE1	1:A:315:MET:HE3	1.49	0.75
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:298:ARG:HB2	1:A:736:MET:HE1	1.75	0.67
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: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: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:780:MET:HE3	1:A:806:LEU:HG	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1199:ARG:NH1	1:A:1202:GLN:OE1	2.34	0.60
1:A:521:MET:HE1	1:A:549:LEU:HD21	1.83	0.60
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:689:LEU:HD22	1:A:993:MET:HE2	1.88	0.55
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:122:MET:SD	1:A:157:MET:HE1	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:912:LEU:C	1:A:915:PRO:HD2	2.38	0.49
1:A:389:PHE:HB2	1:A:582:VAL:HG12	1.95	0.48
1:A:689:LEU:HD21	1:A:772:LEU:HD21	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:286:TYR:CE1	1:A:315:MET:HE3	2.39	0.47
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:241:MET:HE2	1:A:241:MET:HB3	1.89	0.46
1:A:1058:VAL:HG23	1:A:1059:GLY:N	2.30	0.46
1:A:475:GLU:HA	1:A:478:GLU:CD	2.41	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:970:MET:HE2	1:A:970:MET:HA	2.01	0.42
1:A:400:ALA:O	1:A:575:ALA:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:843:TRP:C	1:A:845:LEU:H	2.28	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
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:531:ASP:C	1:A:532:GLU:HG3	2.45	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: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:521:MET:HE2	1:A:521:MET:HA	2.02	0.41
1:A:1019:ARG:HH22	1:A:1180:LYS:HG2	1.85	0.41
1:A:1192:ALA:C	1:A:1193:LEU:HD12	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:696:GLU:HB2	1:A:768:VAL:HG23	2.03	0.40
1:A:843:TRP:O	1:A:844:ARG:HB3	2.20	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%)	948 (100%)	1 (0%)	92	96

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	814	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	75	ASN
1	A	236	GLN
1	A	261	GLN
1	A	323	GLN
1	A	347	HIS
1	A	812	ASN
1	A	863	GLN
1	A	1119	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	4 (12%)
3	ANP	A	1304	-	29,33,33	1.20	5 (17%)	31,52,52	1.18	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	-	3/14/38/38	0/3/3/3
3	ANP	A	1304	-	-	4/14/38/38	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:

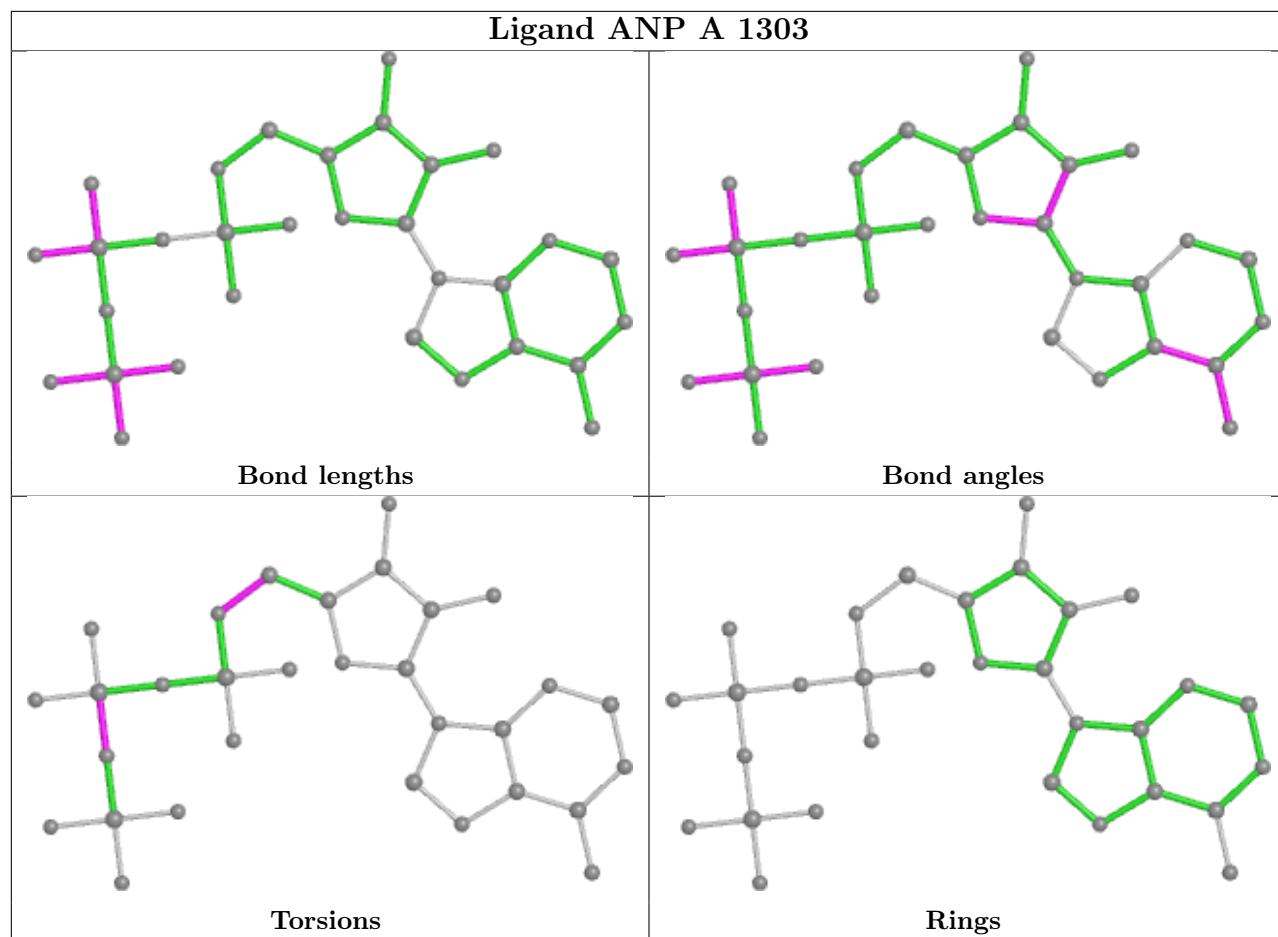
Mol	Chain	Res	Type	Atoms
3	A	1303	ANP	PG-N3B-PB-O1B
3	A	1303	ANP	PG-N3B-PB-O3A
3	A	1304	ANP	PB-N3B-PG-O1G
3	A	1304	ANP	PG-N3B-PB-O1B
3	A	1304	ANP	PG-N3B-PB-O3A
3	A	1304	ANP	O4'-C4'-C5'-O5'
3	A	1303	ANP	C4'-C5'-O5'-PA

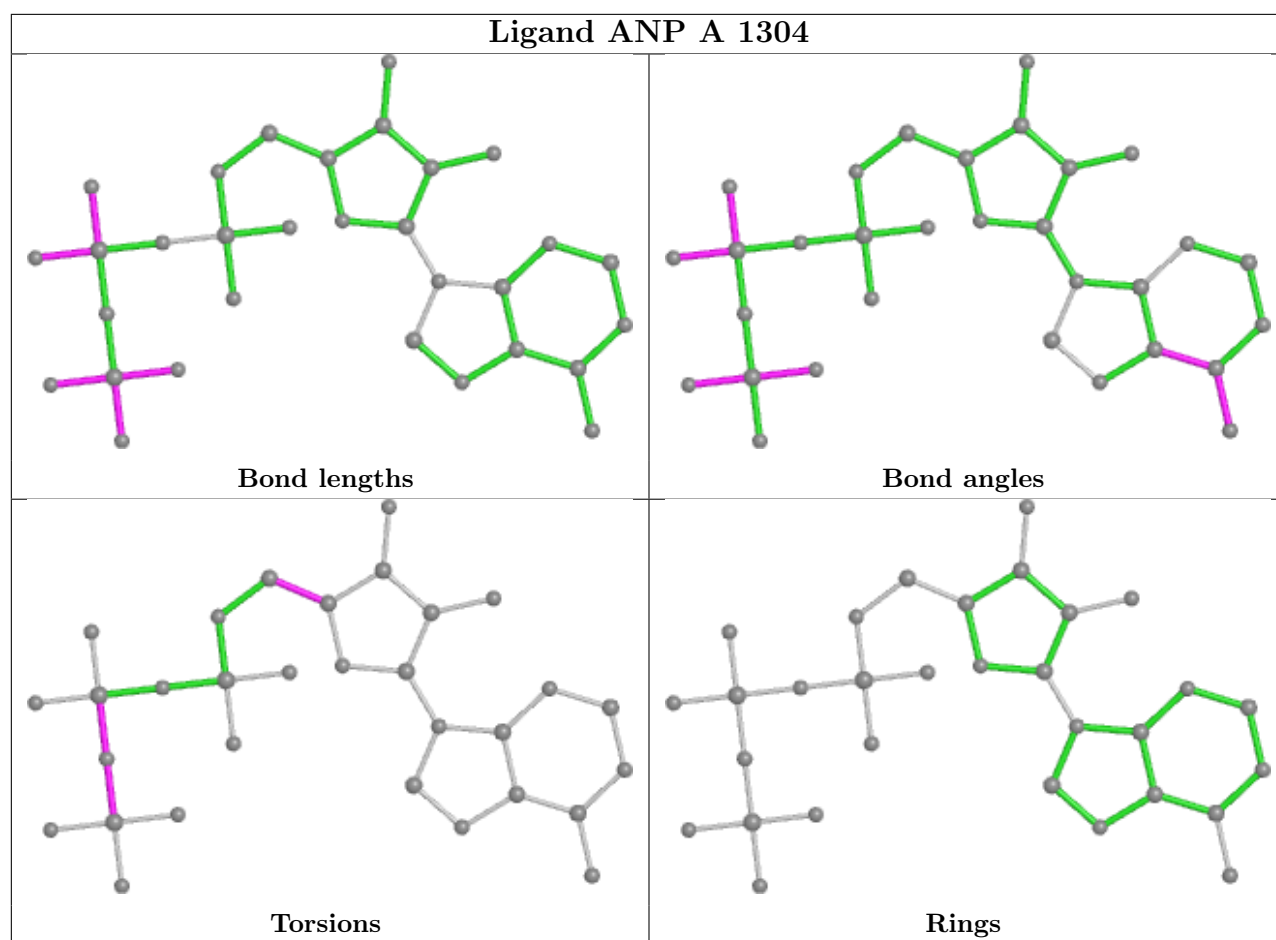
There are no ring outliers.

2 monomers are involved in 3 short contacts:

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





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.

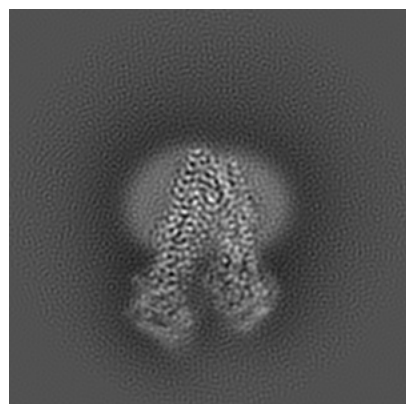
6 Map visualisation [i](#)

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.

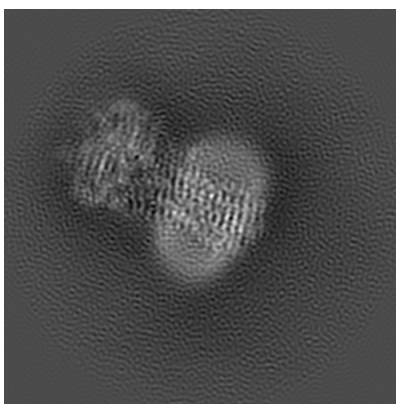
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

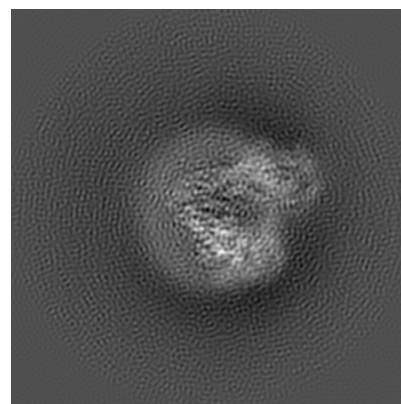
6.1.1 Primary map



X

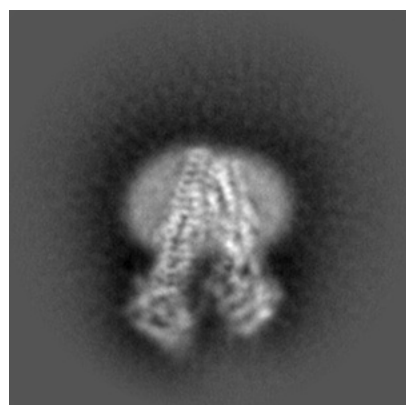


Y

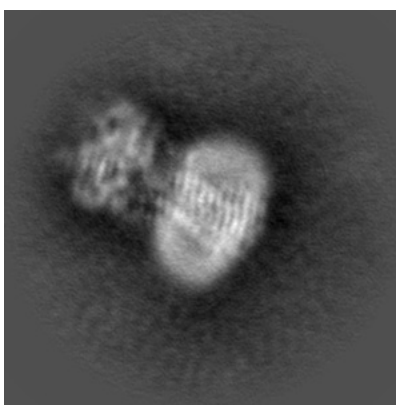


Z

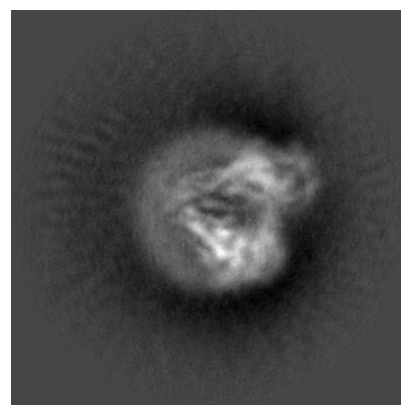
6.1.2 Raw map



X



Y

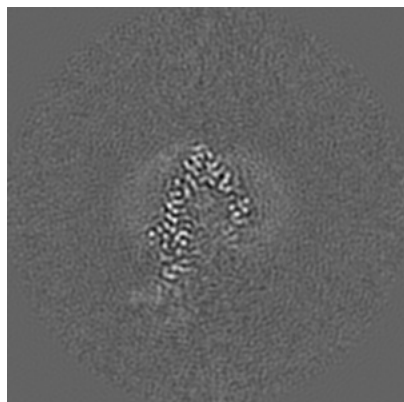


Z

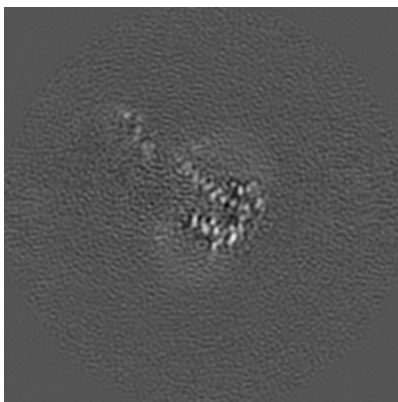
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

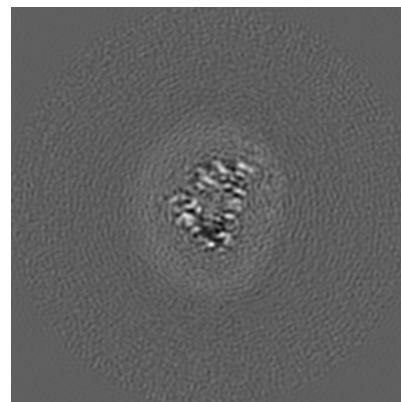
6.2.1 Primary map



X Index: 120

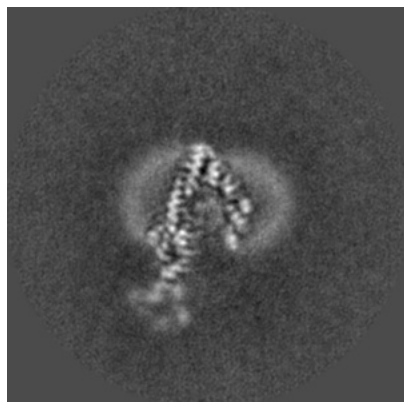


Y Index: 120

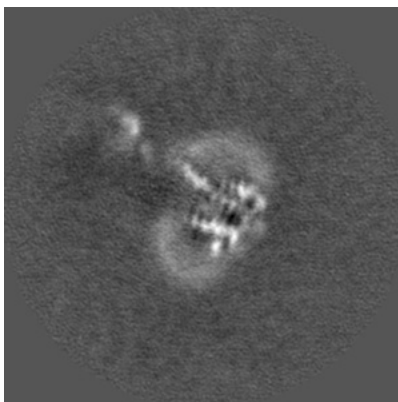


Z Index: 120

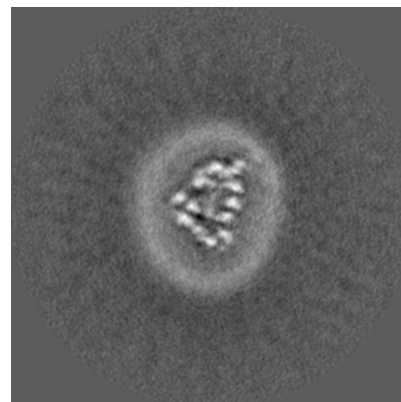
6.2.2 Raw map



X Index: 120



Y Index: 120

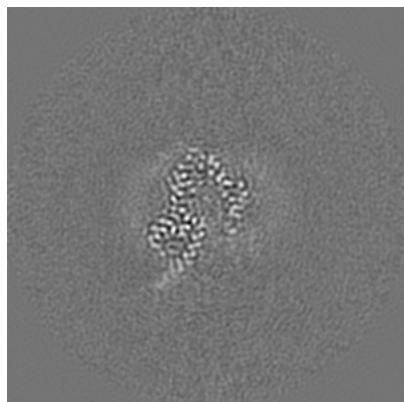


Z Index: 120

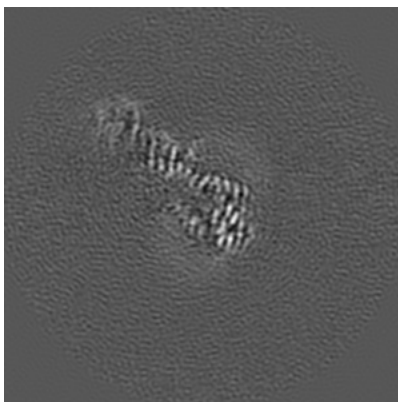
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

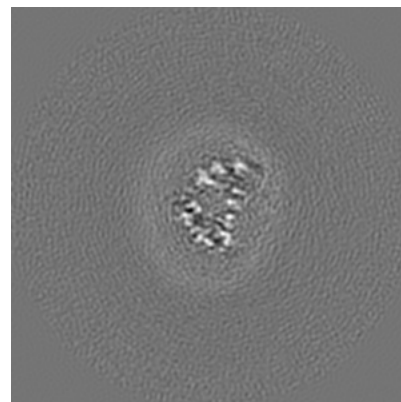
6.3.1 Primary map



X Index: 116

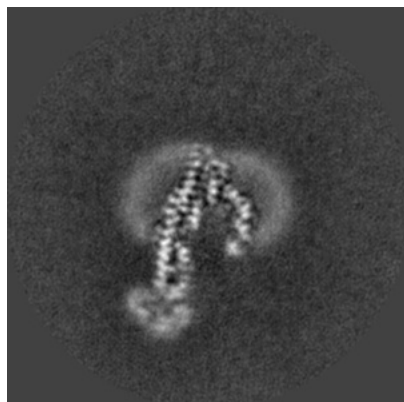


Y Index: 130

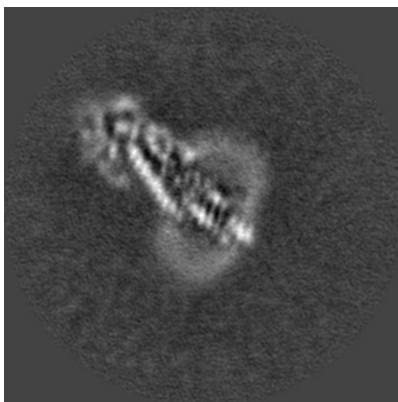


Z Index: 119

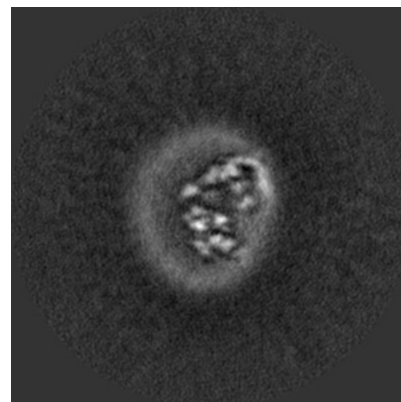
6.3.2 Raw map



X Index: 125



Y Index: 136

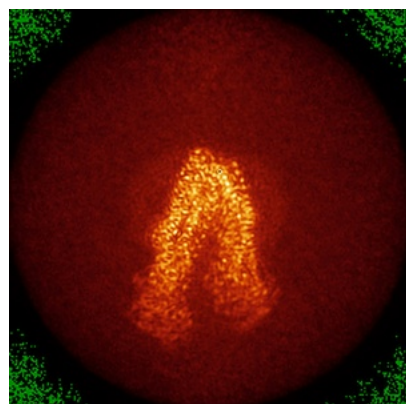


Z Index: 112

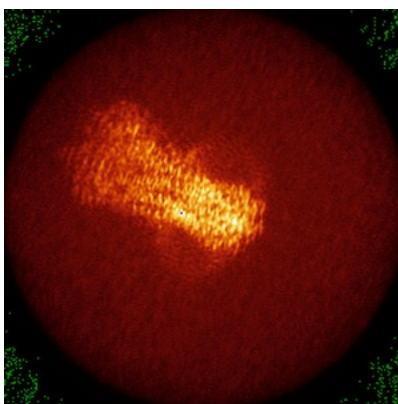
The images above show the largest variance slices of the map in three orthogonal directions.

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

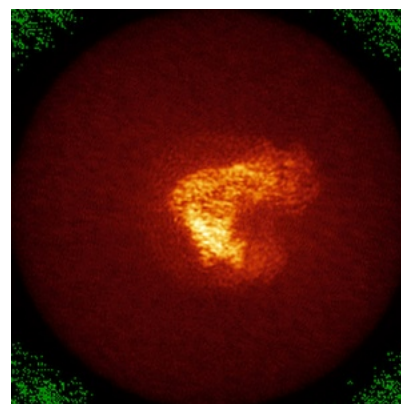
6.4.1 Primary map



X

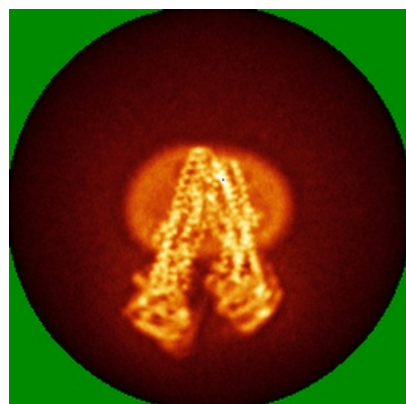


Y

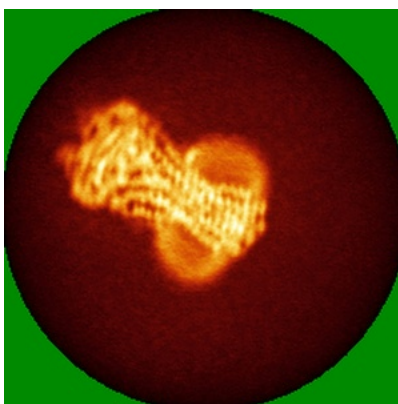


Z

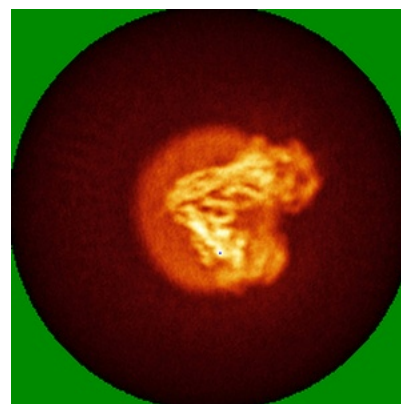
6.4.2 Raw map



X



Y

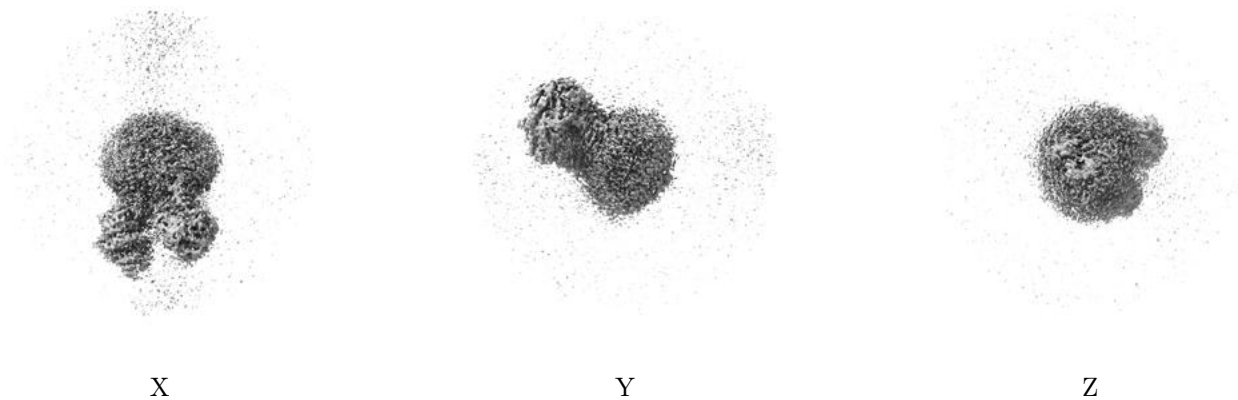


Z

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.

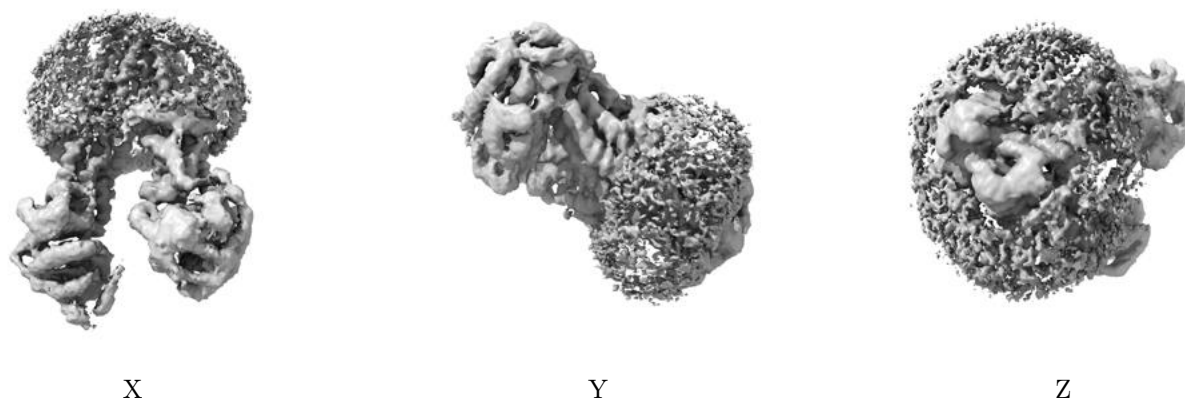
6.5 Orthogonal surface views [i](#)

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.

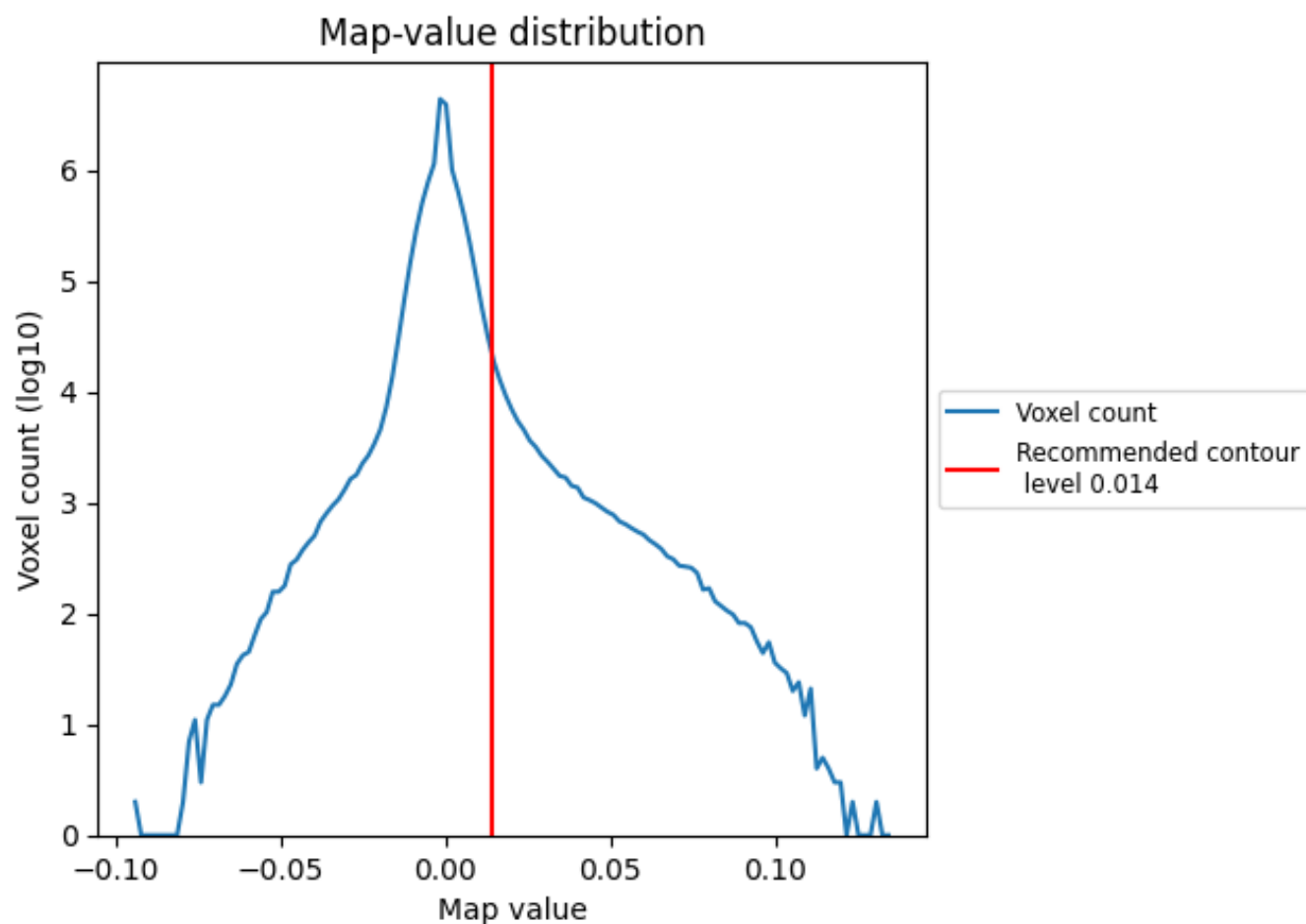
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

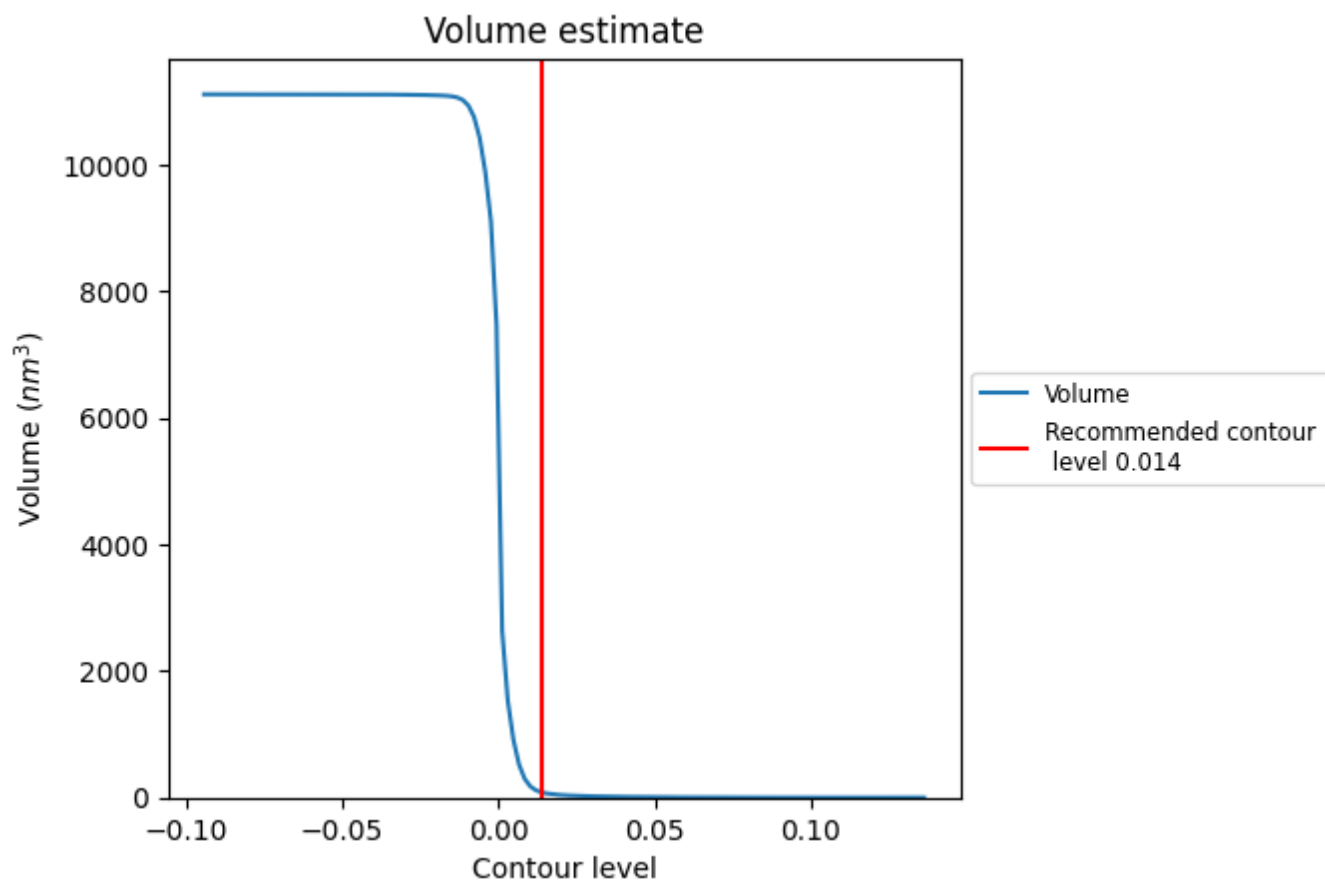
This section contains the results of statistical analysis of the map.

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.

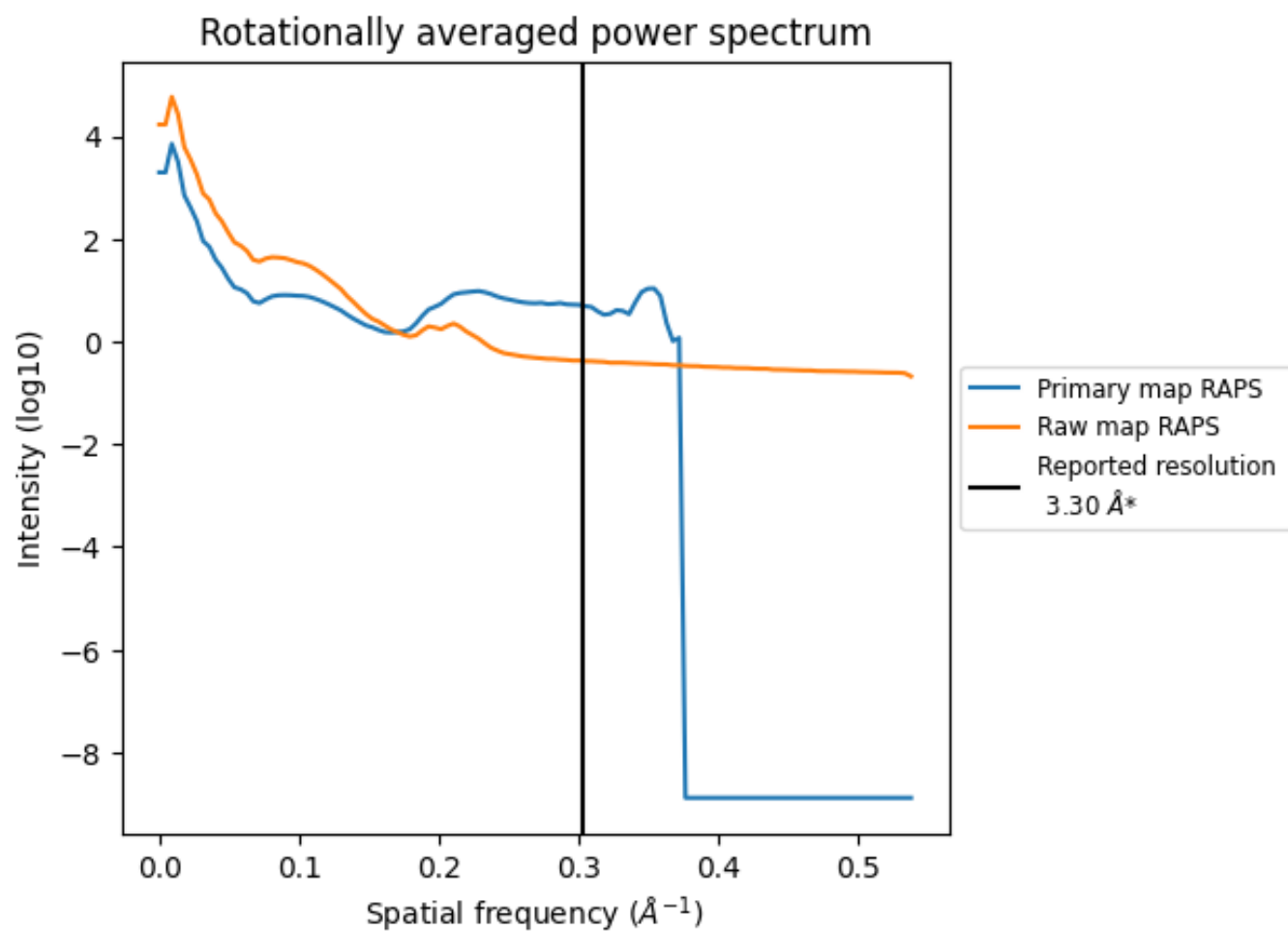
7.2 Volume estimate [i](#)



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 ⓘ

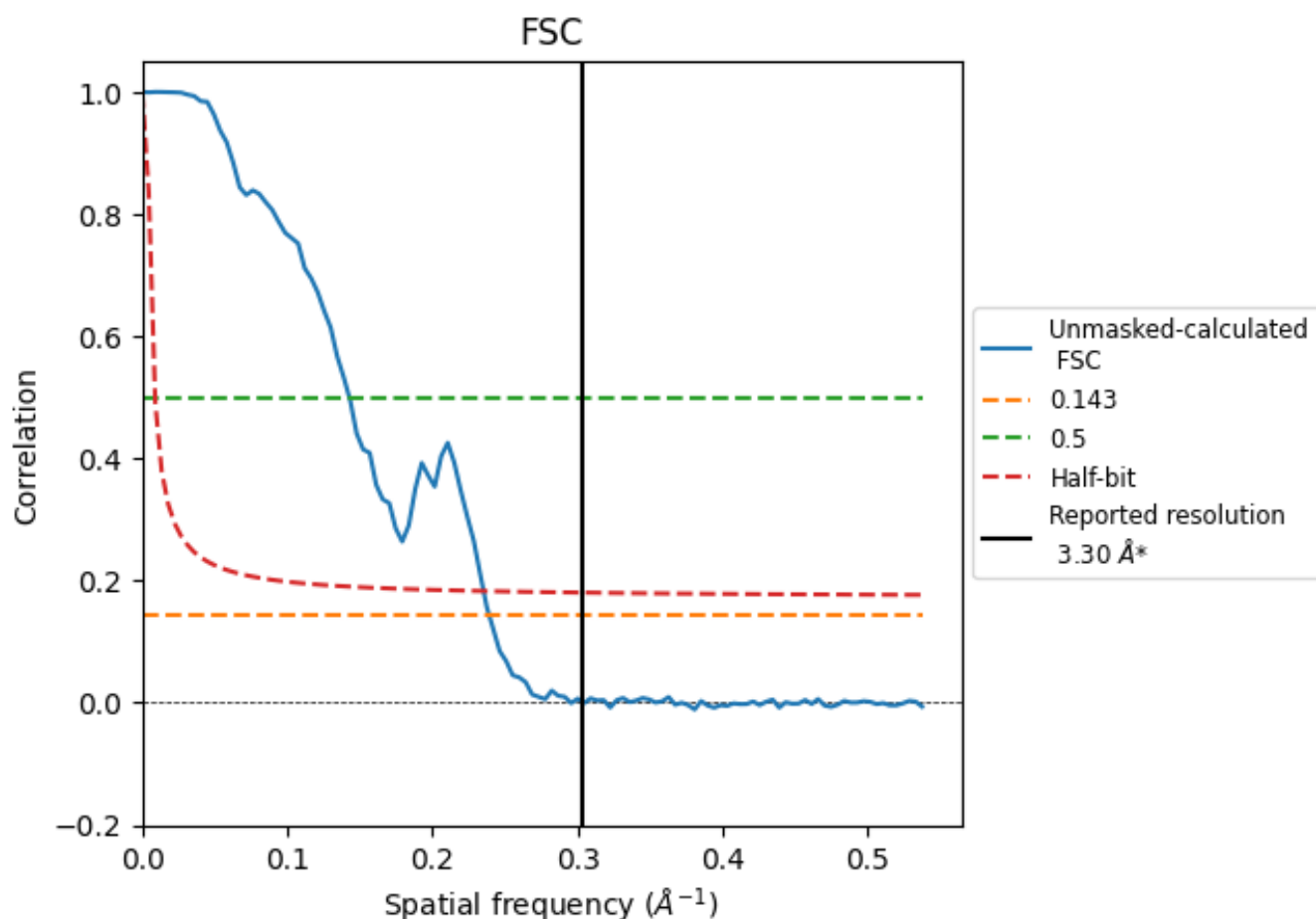


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

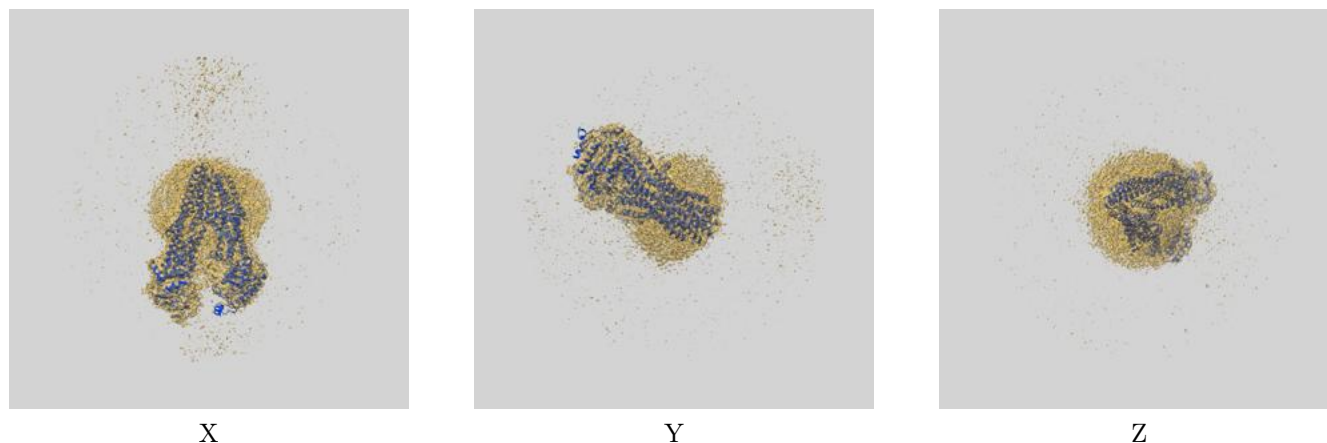
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.18	7.01	4.25

*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](#)

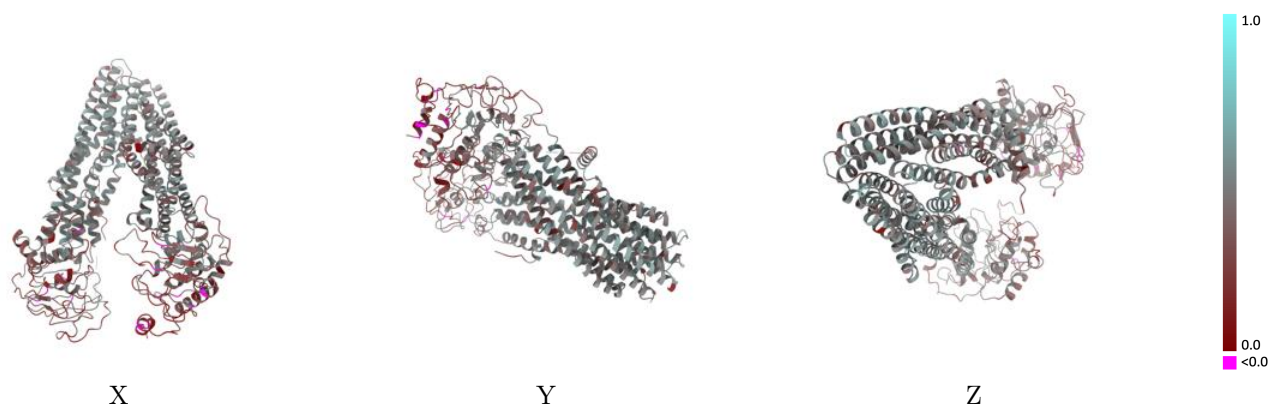
This section contains information regarding the fit between EMDB map EMD-61828 and PDB model 9JUK. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



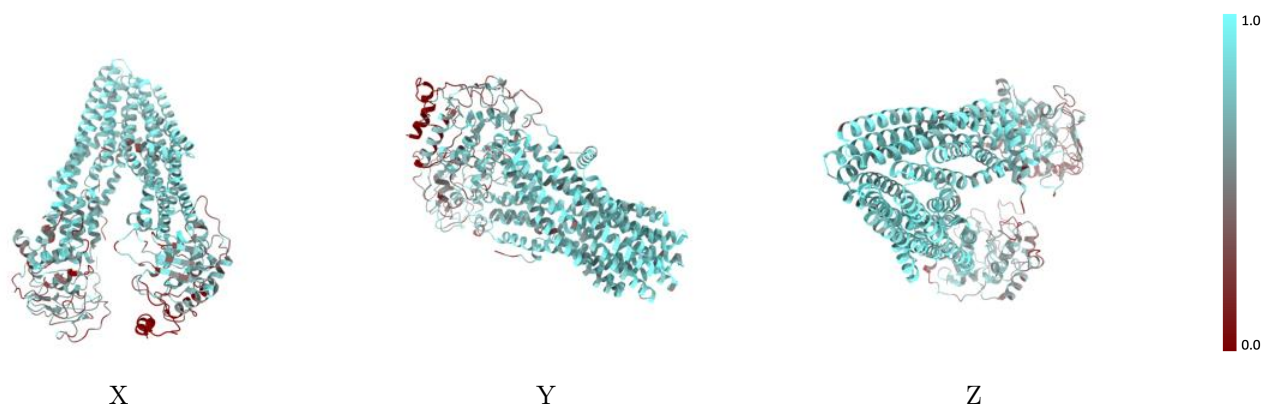
The images above show the 3D surface view of the map at the recommended contour level 0.014 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



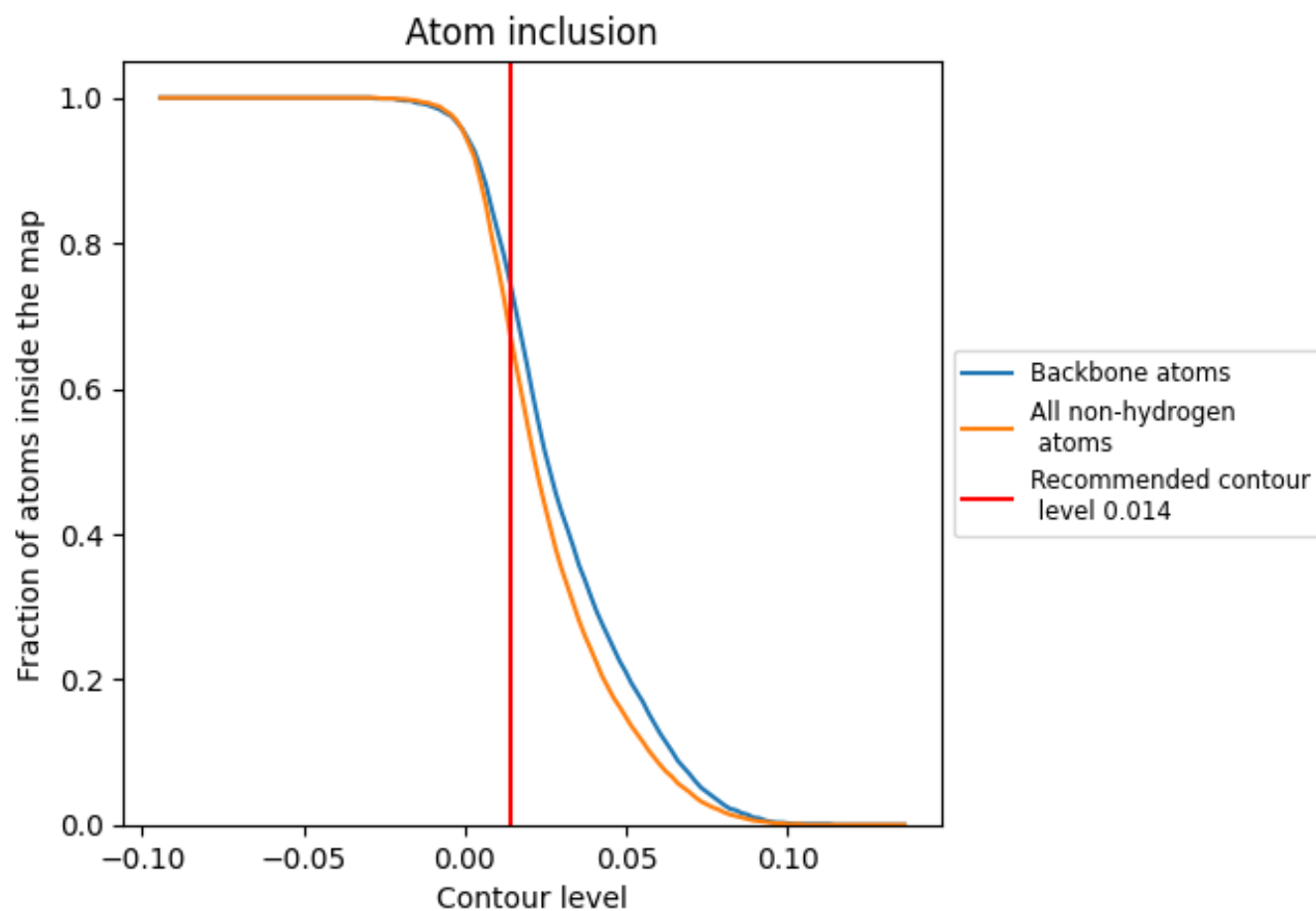
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

