



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 08:15 AM UTC

PDB ID : 8J3Z / pdb_00008j3z
EMDB ID : EMD-35968
Title : Cryo-EM structure of ATP-U46619-bound ABCC4
Authors : Chen, Y.; Wang, L.; Hou, W.T.; Zhou, C.Z.; Chen, Y.; Li, Q.
Deposited on : 2023-04-18
Resolution : 3.17 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

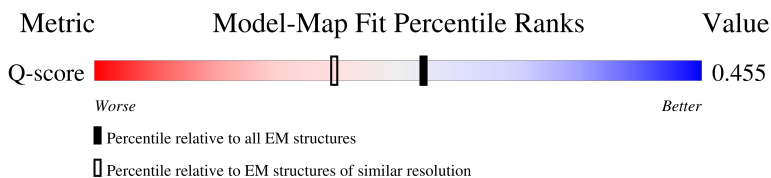
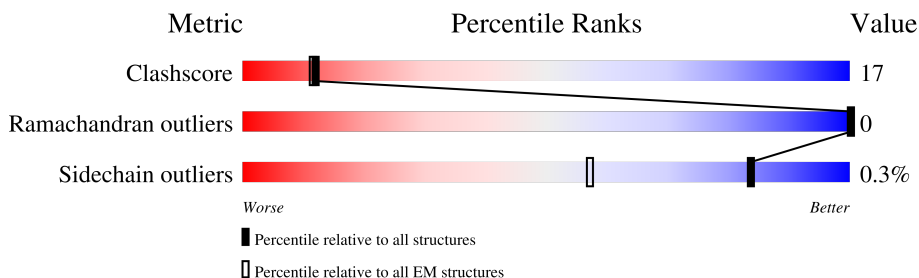
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.17 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14465 (2.67 - 3.67)

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	1325	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ATP	A	1405	-	-	X	-
4	PUC	A	1403	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9814 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.

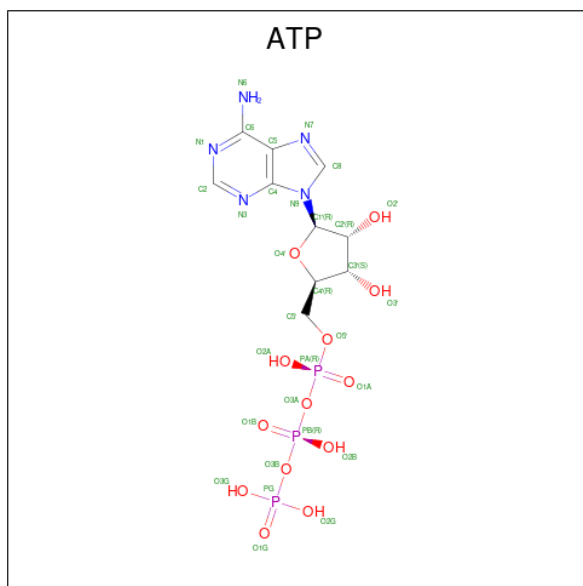
- Molecule 1 is a protein called ATP-binding cassette sub-family C member 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1218	9725	6315	1637	1730	43	0	1

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1202	GLN	GLU	conflict	UNP O15439

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

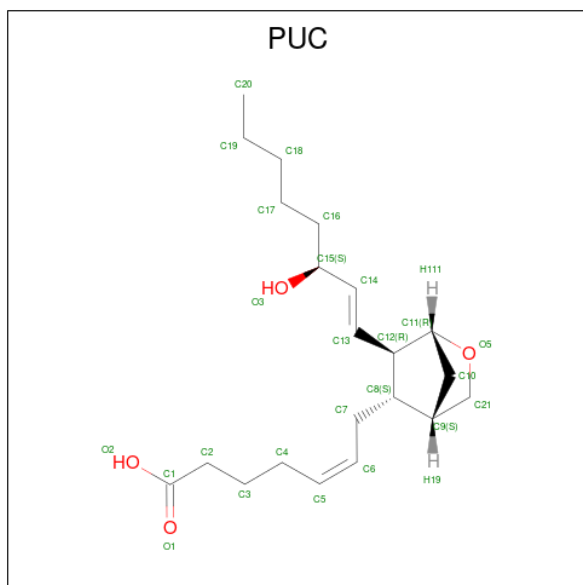


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	31	10	5	13	3	0
2	A	1	31	10	5	13	3	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is (5Z)-7-[(1R,4S,5S,6R)-6-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-2-oxabicyclo[2.2.1]hept-5-yl]hept-5-enoic acid (CCD ID: PUC) (formula: C₂₁H₃₄O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			25	21	4	

3 Residue-property plots

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

- Molecule 1: ATP-binding cassette sub-family C member 4



THR	VAL	ASN	GLY	GLY	GLY	ASN	VAL	T756	E757	K758	L759	Y768	T772	T775	V776	I780	A781	S782	S783	L784	Y788	W792	S793	S794	M801	I805	P809	V810	F813	I818	L822	F825	S826	K827	L832	D833	D834	L835	T846	L847	L848	O849	V850	V853	V860	I861	P862	W863	I866	P867	F875	D888	R891	L892	T896	R897	S898	P899	L904	L908	L911	R915	C923	L926	H930	Q931	D932	L940	R946	A949	A957	M958	F959	V963	A964	L970	L974	V979	L983	S984	Y985	T988	M990	W995	C996	V997	Q999	V1003	E1004	N1005	M1006	M1007	I1008	S1009	V1010	E1011	I1014	E1015	Y1016	T1017	D1018	L1019	E1022	E1026	Y1027	Q1028	K1029	R1030	P1031	P1032	P1033	A1034	H1037	E1038	I1042	F1043	D1044	N1045	V1046	N1047	F1048	S1051	P1052	L1056	V1057	L1058	K1059	H1060	L1061	T1062	A1063	L1064	I1065	K1066	K1070	V1071	G1072	I1073	V1074	G1075	R1076	T1077	G1080	L1084	I1085	L1088	L1091	K1097	I1098	W1099	I1100	D1101	L1104	I1108	G1109	L1110	H1111	D1112	L1113	R1114	M1117	S1118	I1119	I1120	P1121	Q1122	E1123	P1124	V1125	L1126	F1127	T1128	G1129	M1131	R1132	K1133	N1134	L1135	D1136	P1137	F1138	H1139	E1140	H1141	T1142	D1143	E1144	E1145	L1146	W1147	N1148	A1149	L1150	Q1151	E1152	V1153	Q1154	L1155	K1156	E1157	E1160	D1161	L1162	P1163	G1164	K1165	M1166	D1167	T1168	E1169	L1170	A1171	E1172	S1173	G1174	S1175	N1176	V1179	G1180	Q1181	R1182	Q1183	L1184	V1185	C1186	L1187	A1188	R1189	A1190	I1191	L1192	Q1196	T1199	I1199	I1200	T1204	A1205	N1206	V1207	D1208	P1209	R1210	T1211	D1212	E1213	L1214	K1217	K1218	I1219	R1220	E1221	K1222	F1223	T1227	V1228	L1229	T1230	I1231	A1232	H1233	R1234	L1235	N1236	T1237	I1238	T1239	D1240	S1241	D1242	K1243	L1247	D1248	R1251	L1252	K1253	E1254	Y1255	D1256	E1257	P1258	Y1259	V1260	L1261	L1262	Q1263	N1264	K1265	E1266	S1267	L1268	F1269	Y1270	K1271	M1272	V1273	Q1274	Q1275	L1276	G1277	K1278	A1279	E1280	A1281	A1282	A1283	L1284	T1285	E1286	Q1290	V1291	Y1292	F1293	K1294	R1295	N1296	Y1297	P1298	HIS	ILE	GLY	HIS	THR	ASP	HIS	MET	VAL	THR	THR	ASN	THR	SER	ASN	GLY	GLN	PRO	SER	THR	THR	LEU	THR	ILE	PHE	GLU	THR	ALA	LEU
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	170531	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.182	Depositor
Minimum map value	-0.905	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.143	Depositor
Map size (Å)	246.0, 246.0, 246.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	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: ATP, MG, PUC

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	0.34	0/9934	0.50	2/13460 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	93	LEU	N-CA-C	-8.18	103.13	113.43
1	A	306	GLU	N-CA-C	-5.39	106.76	113.55

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	9725	0	9988	342	0
2	A	62	0	24	10	0
3	A	2	0	0	0	0
4	A	25	0	33	15	0
All	All	9814	0	10045	343	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 17.

All (343) 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:152:HIS:HE1	4:A:1403:PUC:H121	1.34	0.92
1:A:92:TYR:OH	1:A:212:LEU:HB3	1.72	0.87
1:A:266:ALA:O	1:A:269:THR:HG22	1.73	0.87
1:A:1126:LEU:HB3	1:A:1170:LEU:HD21	1.57	0.85
1:A:152:HIS:CE1	4:A:1403:PUC:C21	2.62	0.83
1:A:157:TYR:HB2	1:A:946:ARG:HG2	1.59	0.83
1:A:152:HIS:HE1	4:A:1403:PUC:C21	1.91	0.82
1:A:87:CYS:O	1:A:87:CYS:SG	2.38	0.80
1:A:152:HIS:CE1	4:A:1403:PUC:H221	2.17	0.79
1:A:558:LEU:HD12	1:A:561:PRO:HG3	1.66	0.77
1:A:111:ILE:HD11	1:A:228:LEU:HD11	1.67	0.77
1:A:266:ALA:HA	1:A:269:THR:HG22	1.65	0.77
1:A:448:GLY:HA2	2:A:1405:ATP:O1A	1.85	0.76
1:A:198:LEU:HD22	1:A:904:LEU:HD22	1.69	0.74
1:A:544:ASN:OD1	1:A:547:ARG:NH1	2.21	0.73
1:A:446:PRO:HD2	1:A:449:ALA:HB2	1.67	0.73
1:A:266:ALA:C	1:A:269:THR:HG22	2.13	0.73
1:A:412:VAL:O	1:A:432:SER:HA	1.89	0.72
1:A:178:ALA:HA	1:A:181:LEU:HD22	1.71	0.71
1:A:167:ARG:HG2	1:A:202:VAL:HG12	1.73	0.71
2:A:1405:ATP:O1A	2:A:1405:ATP:H4'	1.91	0.71
1:A:93:LEU:O	1:A:96:GLY:N	2.20	0.71
1:A:411:HIS:NE2	1:A:413:GLN:OE1	2.24	0.71
1:A:717:LEU:O	1:A:721:ASN:ND2	2.19	0.70
1:A:191:THR:HG23	1:A:908:LEU:HD23	1.73	0.70
1:A:211:PHE:HZ	4:A:1403:PUC:H113	1.55	0.70
1:A:447:VAL:HA	2:A:1405:ATP:O1G	1.91	0.70
1:A:1211:THR:HA	1:A:1214:LEU:HG	1.73	0.70
1:A:52:ARG:NH2	1:A:932:ASP:OD2	2.24	0.70
1:A:181:LEU:HA	1:A:394:GLU:HA	1.74	0.70
1:A:218:GLY:HA2	1:A:364:THR:HG22	1.74	0.69
1:A:474:ARG:NH2	1:A:552:ASP:O	2.23	0.69
1:A:266:ALA:HA	1:A:269:THR:CG2	2.22	0.69
1:A:39:LEU:HB2	1:A:888:ASP:HB3	1.75	0.69
1:A:211:PHE:HZ	4:A:1403:PUC:C13	2.06	0.68
1:A:284:ARG:O	1:A:288:MET:HG3	1.94	0.68
1:A:1207:VAL:HG11	1:A:1211:THR:HB	1.75	0.68
1:A:327:ALA:HB2	1:A:366:THR:HG21	1.76	0.68
1:A:1186:CYS:HA	1:A:1189:ARG:HD2	1.76	0.67
1:A:805:ILE:HD12	1:A:825:PHE:HE1	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1016:TYR:HA	1:A:1019:LEU:HG	1.76	0.67
1:A:266:ALA:CA	1:A:269:THR:HG22	2.24	0.66
1:A:846:THR:CG2	4:A:1403:PUC:H22	2.25	0.66
1:A:251:GLN:NE2	1:A:366:THR:O	2.29	0.66
1:A:1048:PHE:HB3	1:A:1058:LEU:HB2	1.76	0.66
1:A:196:ASN:ND2	1:A:270:ASP:OD2	2.29	0.66
1:A:324:PHE:HA	1:A:366:THR:CG2	2.26	0.65
1:A:109:GLN:HG2	1:A:110:PRO:HD3	1.77	0.65
1:A:846:THR:HG21	4:A:1403:PUC:H22	1.78	0.65
1:A:336:PHE:CZ	1:A:351:VAL:HA	2.32	0.65
1:A:1070:LYS:HG2	1:A:1228:VAL:HB	1.78	0.65
1:A:1209:PRO:HA	1:A:1212:ASP:HB3	1.80	0.64
1:A:1162:LEU:HD13	1:A:1168:THR:HG21	1.79	0.64
1:A:13:LEU:HD23	1:A:48:LEU:HD11	1.78	0.64
1:A:51:ASP:OD2	1:A:165:ARG:NH1	2.31	0.64
1:A:483:TRP:O	1:A:547:ARG:NH2	2.24	0.64
1:A:245:ILE:O	1:A:249:PRO:HD2	1.97	0.63
1:A:1153:VAL:HB	1:A:1184:LEU:HB3	1.81	0.63
1:A:447:VAL:HG23	2:A:1405:ATP:O1G	1.98	0.62
1:A:448:GLY:C	2:A:1405:ATP:O1A	2.42	0.62
1:A:20:SER:HB2	1:A:25:TRP:HB3	1.81	0.62
1:A:995:TRP:CE3	4:A:1403:PUC:H210	2.34	0.62
1:A:398:ARG:NH2	1:A:915:ARG:O	2.32	0.62
1:A:1164:GLY:O	1:A:1168:THR:N	2.32	0.62
1:A:92:TYR:HE1	1:A:159:VAL:HG23	1.64	0.61
1:A:211:PHE:CZ	4:A:1403:PUC:H113	2.35	0.61
1:A:1184:LEU:O	1:A:1187:LEU:HG	2.01	0.61
1:A:248:LEU:HD21	1:A:365:VAL:HG13	1.82	0.61
1:A:448:GLY:N	2:A:1405:ATP:O1G	2.31	0.61
1:A:92:TYR:CE2	1:A:212:LEU:HD23	2.35	0.60
1:A:106:LYS:HG3	1:A:148:LEU:HD11	1.83	0.60
1:A:794:SER:OG	1:A:833:ASP:OD1	2.20	0.60
1:A:167:ARG:NH1	1:A:206:ASP:OD2	2.34	0.60
1:A:737:TYR:OH	1:A:741:LYS:NZ	2.34	0.60
1:A:810:VAL:HG11	1:A:1091:LEU:HB3	1.83	0.60
1:A:266:ALA:O	1:A:269:THR:CG2	2.49	0.60
1:A:1186:CYS:O	1:A:1189:ARG:HB2	2.01	0.60
1:A:1219:ILE:O	1:A:1223:PHE:N	2.30	0.60
1:A:448:GLY:CA	2:A:1405:ATP:O1A	2.49	0.60
1:A:327:ALA:HB3	1:A:362:ARG:HG3	1.84	0.60
1:A:329:LYS:HG3	1:A:775:THR:HG21	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:ALA:HA	1:A:351:VAL:HG12	1.84	0.60
1:A:324:PHE:CD1	1:A:367:LEU:HB2	2.37	0.59
1:A:336:PHE:HA	1:A:339:TYR:HB3	1.84	0.59
1:A:307:ILE:HD13	1:A:310:ILE:HD12	1.84	0.59
1:A:1150:LEU:HA	1:A:1153:VAL:HG22	1.83	0.59
1:A:1204:THR:O	1:A:1234:ARG:NH1	2.36	0.59
1:A:56:LEU:HB3	1:A:169:ALA:HB2	1.85	0.58
1:A:70:ARG:HH12	1:A:77:LYS:HE2	1.67	0.58
1:A:358:TYR:HA	1:A:361:VAL:HG12	1.84	0.58
1:A:446:PRO:O	1:A:451:LYS:NZ	2.35	0.58
1:A:1008:ILE:HA	1:A:1011:GLU:HG2	1.84	0.58
1:A:194:ILE:HG22	1:A:904:LEU:HD21	1.85	0.57
1:A:324:PHE:HA	1:A:366:THR:HG22	1.86	0.57
1:A:1141:HIS:ND1	1:A:1145:GLU:OE2	2.37	0.57
1:A:545:LEU:HD13	1:A:558:LEU:HD11	1.85	0.57
1:A:211:PHE:CZ	4:A:1403:PUC:C13	2.88	0.57
1:A:758:LYS:HG3	1:A:759:LEU:H	1.68	0.57
1:A:303:ARG:NH2	1:A:794:SER:O	2.36	0.57
1:A:613:GLN:HB3	1:A:620:PHE:HE1	1.70	0.57
1:A:416:THR:O	1:A:465:SER:N	2.37	0.57
1:A:517:LEU:HD13	1:A:524:ASP:HB3	1.87	0.57
1:A:267:THR:HG23	1:A:268:PHE:HD1	1.70	0.56
1:A:272:ARG:NH2	1:A:825:PHE:O	2.37	0.56
1:A:580:GLN:O	1:A:583:HIS:ND1	2.36	0.56
1:A:1047:ASN:OD1	1:A:1060:HIS:N	2.20	0.55
1:A:201:ASP:OD2	1:A:385:ARG:NE	2.40	0.55
1:A:805:ILE:HD12	1:A:825:PHE:CE1	2.41	0.55
1:A:1210:ARG:O	1:A:1213:GLU:HG3	2.07	0.55
1:A:633:LYS:HD3	1:A:1210:ARG:HE	1.71	0.55
1:A:500:GLU:CD	1:A:503:ARG:HH21	2.16	0.54
1:A:238:LEU:O	1:A:242:ALA:N	2.36	0.54
1:A:1132:ARG:NH1	1:A:1143:ASP:OD1	2.40	0.54
1:A:152:HIS:CE1	4:A:1403:PUC:H121	2.23	0.54
1:A:328:SER:H	1:A:362:ARG:HD3	1.72	0.54
1:A:702:LYS:HG3	1:A:711:TRP:HZ2	1.71	0.54
1:A:80:LEU:HD11	1:A:82:ARG:NE	2.22	0.54
1:A:794:SER:HB2	1:A:832:LEU:HB3	1.89	0.54
1:A:80:LEU:HD23	1:A:83:ALA:HB2	1.90	0.53
1:A:152:HIS:NE2	4:A:1403:PUC:H221	2.23	0.53
1:A:323:SER:O	1:A:327:ALA:HB2	2.09	0.53
1:A:324:PHE:HA	1:A:366:THR:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:VAL:HG22	1:A:295:PHE:HD2	1.74	0.53
1:A:371:SER:O	1:A:375:ARG:HG2	2.08	0.53
1:A:995:TRP:CZ3	4:A:1403:PUC:H210	2.44	0.53
1:A:1199:ILE:HG12	1:A:1229:LEU:HD12	1.91	0.53
1:A:278:GLU:OE1	1:A:1127:PHE:HD1	1.91	0.53
1:A:1124:PRO:HG3	1:A:1183:GLN:HG3	1.91	0.53
1:A:443:VAL:N	1:A:589:LEU:O	2.28	0.53
1:A:504:TYR:HB2	1:A:550:TYR:HE2	1.74	0.52
1:A:285:ILE:HG23	1:A:289:TYR:CE2	2.43	0.52
1:A:268:PHE:HE2	1:A:305:LYS:HE3	1.73	0.52
1:A:415:PHE:O	1:A:430:GLY:N	2.43	0.52
1:A:926:LEU:O	1:A:930:HIS:ND1	2.39	0.52
1:A:832:LEU:HD11	1:A:1010:VAL:HG22	1.92	0.52
1:A:44:MET:HG2	1:A:940:LEU:HD12	1.92	0.52
1:A:542:ARG:HH11	1:A:569:VAL:HG11	1.73	0.52
1:A:598:LYS:HG2	1:A:617:TYR:CE2	2.45	0.52
1:A:809:PRO:HD3	1:A:1022:GLU:N	2.25	0.52
1:A:1138:PHE:CD2	1:A:1140:GLU:HB2	2.45	0.51
1:A:329:LYS:NZ	1:A:732:ASP:OD1	2.43	0.51
1:A:455:LEU:HD22	1:A:557:LEU:HB3	1.92	0.51
1:A:959:PHE:O	1:A:963:VAL:HG23	2.11	0.51
1:A:1005:ASN:O	1:A:1008:ILE:HG22	2.09	0.51
1:A:572:HIS:CE1	1:A:576:LEU:HD12	2.45	0.51
1:A:1043:PHE:O	1:A:1062:THR:HA	2.10	0.51
1:A:1135:LEU:HD11	1:A:1150:LEU:HD21	1.93	0.51
1:A:1120:ILE:HD13	1:A:1200:ILE:HG12	1.92	0.50
1:A:39:LEU:O	1:A:891:ARG:NH2	2.39	0.50
1:A:229:LEU:HD13	1:A:357:LEU:HD12	1.93	0.50
1:A:283:ILE:HG12	1:A:813:PHE:CE2	2.47	0.50
1:A:489:LEU:HD12	1:A:528:ILE:HD11	1.93	0.50
1:A:1179:VAL:HA	1:A:1182:ARG:NH2	2.27	0.50
1:A:1207:VAL:CG1	1:A:1211:THR:HB	2.42	0.50
1:A:275:THR:O	1:A:279:VAL:HG23	2.12	0.50
1:A:279:VAL:HG22	1:A:295:PHE:CD2	2.46	0.50
1:A:1073:ILE:HB	1:A:1231:ILE:HG12	1.92	0.50
1:A:1181:GLN:HA	1:A:1184:LEU:HD13	1.93	0.49
1:A:11:ASN:HD22	1:A:48:LEU:HD21	1.77	0.49
1:A:120:PHE:CE1	1:A:979:VAL:HG11	2.47	0.49
1:A:482:PRO:HA	1:A:544:ASN:ND2	2.27	0.49
1:A:1014:ILE:HA	1:A:1017:THR:HG22	1.95	0.49
1:A:365:VAL:O	1:A:370:PRO:HD3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:594:LEU:HD11	1:A:631:LEU:HD12	1.95	0.49
1:A:721:ASN:HA	1:A:782:ARG:HD3	1.94	0.49
1:A:190:THR:HG21	1:A:1172:GLU:OE2	2.13	0.49
1:A:594:LEU:HD21	1:A:631:LEU:HD11	1.94	0.49
1:A:1084:LEU:O	1:A:1088:LEU:HG	2.13	0.49
1:A:287:LYS:HG2	1:A:292:GLU:OE2	2.13	0.48
1:A:288:MET:SD	1:A:1119:ILE:HD13	2.52	0.48
1:A:194:ILE:HD12	1:A:908:LEU:HD21	1.95	0.48
1:A:308:SER:O	1:A:312:ARG:HG3	2.12	0.48
1:A:572:HIS:NE2	1:A:576:LEU:HD12	2.28	0.48
1:A:995:TRP:CE3	4:A:1403:PUC:C10	2.97	0.48
1:A:1127:PHE:N	1:A:1134:ASN:OD1	2.46	0.48
1:A:303:ARG:NH2	1:A:833:ASP:OD1	2.42	0.48
1:A:911:LEU:HD21	1:A:915:ARG:HH12	1.77	0.48
1:A:336:PHE:HZ	1:A:351:VAL:HA	1.78	0.48
1:A:1282:ALA:O	1:A:1286:GLU:OE1	2.32	0.48
1:A:80:LEU:HG	1:A:82:ARG:HG2	1.96	0.48
1:A:553:ALA:N	1:A:556:TYR:OH	2.46	0.48
1:A:1131:MET:HE1	1:A:1170:LEU:HD13	1.95	0.48
1:A:115:LYS:HD3	1:A:137:TYR:CZ	2.49	0.48
1:A:447:VAL:CA	2:A:1405:ATP:O1G	2.60	0.47
1:A:574:PHE:HA	1:A:578:ILE:HD12	1.95	0.47
1:A:721:ASN:HB3	1:A:848:LEU:CD1	2.44	0.47
1:A:1043:PHE:CZ	1:A:1084:LEU:HD11	2.49	0.47
1:A:827:LYS:HB2	1:A:827:LYS:HE2	1.74	0.47
1:A:269:THR:HG23	1:A:270:ASP:N	2.30	0.47
1:A:1059:LYS:HE2	1:A:1251:ARG:HG3	1.95	0.47
1:A:117:ILE:HG21	1:A:348:ALA:O	2.15	0.47
1:A:348:ALA:HA	1:A:351:VAL:CG1	2.44	0.47
1:A:57:GLY:HA3	1:A:172:HIS:ND1	2.30	0.47
1:A:75:ALA:HB1	1:A:77:LYS:HG3	1.95	0.47
1:A:285:ILE:HG23	1:A:289:TYR:HE2	1.80	0.47
1:A:126:MET:O	1:A:126:MET:HG2	2.15	0.47
1:A:228:LEU:HD22	1:A:357:LEU:HD11	1.96	0.47
1:A:268:PHE:HE2	1:A:305:LYS:HB3	1.79	0.47
1:A:181:LEU:HD12	1:A:185:ALA:HB1	1.96	0.47
1:A:533:THR:O	2:A:1401:ATP:N6	2.48	0.47
1:A:721:ASN:HB3	1:A:848:LEU:HD11	1.96	0.47
1:A:788:TYR:O	1:A:792:ASN:HB2	2.14	0.47
1:A:853:VAL:HG22	1:A:985:TYR:HD1	1.80	0.46
1:A:330:ILE:O	1:A:334:VAL:HG23	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:HIS:HA	1:A:161:CYS:SG	2.56	0.46
1:A:444:VAL:HG21	1:A:597:LEU:HD11	1.97	0.46
1:A:44:MET:HA	1:A:940:LEU:HD11	1.98	0.46
1:A:447:VAL:CG2	2:A:1405:ATP:O1G	2.64	0.46
1:A:805:ILE:CD1	1:A:825:PHE:HE1	2.28	0.46
1:A:51:ASP:OD1	1:A:165:ARG:HD3	2.16	0.46
1:A:283:ILE:HG21	1:A:813:PHE:CG	2.51	0.46
1:A:262:ARG:HD2	1:A:262:ARG:HA	1.72	0.46
1:A:850:VAL:HG21	1:A:996:CYS:SG	2.56	0.46
1:A:861:ILE:HG12	1:A:974:LEU:HD11	1.98	0.46
1:A:985:TYR:O	1:A:988:THR:HG22	2.15	0.46
1:A:71:ALA:HB1	1:A:77:LYS:O	2.16	0.46
1:A:758:LYS:HG3	1:A:759:LEU:N	2.31	0.46
1:A:957:ALA:HB2	1:A:990:MET:HE1	1.98	0.46
1:A:1044:ASP:HB3	1:A:1097:LYS:HB2	1.97	0.46
1:A:92:TYR:CG	1:A:92:TYR:O	2.68	0.46
1:A:152:HIS:O	1:A:152:HIS:ND1	2.49	0.46
1:A:1133:LYS:HG2	1:A:1137:PRO:HA	1.97	0.46
1:A:92:TYR:O	1:A:92:TYR:CD2	2.69	0.45
1:A:93:LEU:C	1:A:95:LEU:N	2.70	0.45
1:A:1074:VAL:HG11	1:A:1238:ILE:HD13	1.98	0.45
1:A:1112:ASP:OD1	1:A:1113:LEU:N	2.49	0.45
1:A:1239:ILE:HD13	1:A:1284:LEU:HD22	1.97	0.45
1:A:225:VAL:HG21	1:A:361:VAL:HB	1.98	0.45
1:A:576:LEU:O	1:A:580:GLN:HB2	2.17	0.45
1:A:147:ILE:HG22	1:A:147:ILE:O	2.16	0.45
1:A:37:ARG:NH2	1:A:43:ASP:OD1	2.41	0.45
1:A:251:GLN:OE1	1:A:366:THR:HG23	2.17	0.45
1:A:593:GLN:HB3	1:A:595:GLN:HG2	1.99	0.45
1:A:307:ILE:HG22	1:A:307:ILE:O	2.17	0.45
1:A:780:ILE:O	1:A:784:LEU:HG	2.17	0.45
1:A:853:VAL:HG11	1:A:989:LEU:HB2	1.98	0.45
1:A:1138:PHE:HD2	1:A:1140:GLU:HB2	1.80	0.45
1:A:369:PHE:HB3	1:A:370:PRO:HD3	1.97	0.45
1:A:450:GLY:O	1:A:454:LEU:N	2.49	0.45
1:A:1022:GLU:HG2	1:A:1110:LEU:HD11	1.99	0.45
1:A:92:TYR:HE2	1:A:212:LEU:HD23	1.82	0.45
1:A:303:ARG:NH1	1:A:833:ASP:OD2	2.42	0.45
1:A:720:LEU:HD21	1:A:781:ALA:HB1	1.99	0.45
1:A:835:LEU:HG	1:A:1006:MET:HE1	1.98	0.45
1:A:1235:LEU:HA	1:A:1238:ILE:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:631:LEU:HD13	1:A:1209:PRO:HD2	1.99	0.44
1:A:863:TRP:CE3	1:A:970:LEU:HD11	2.52	0.44
1:A:451:LYS:HD2	1:A:590:VAL:HG13	1.99	0.44
1:A:1071:VAL:HG23	1:A:1243:LYS:C	2.42	0.44
1:A:1070:LYS:O	1:A:1242:ASP:N	2.51	0.44
1:A:999:GLN:O	1:A:1003:VAL:N	2.34	0.44
1:A:1014:ILE:O	1:A:1017:THR:HG22	2.18	0.44
1:A:415:PHE:HB3	1:A:431:LEU:HB2	1.98	0.44
1:A:613:GLN:HB3	1:A:620:PHE:CE1	2.52	0.44
1:A:508:ILE:HG23	1:A:513:LEU:HB2	1.99	0.43
1:A:772:THR:O	1:A:776:VAL:HG23	2.18	0.43
1:A:964:ALA:HB2	1:A:983:LEU:HD11	1.99	0.43
1:A:1153:VAL:HG23	1:A:1155:LEU:HB2	1.99	0.43
1:A:565:VAL:HG23	1:A:570:SER:HB3	2.00	0.43
1:A:597:LEU:HD22	1:A:603:ILE:HG12	2.00	0.43
1:A:734:TRP:CD1	1:A:768:TYR:HB2	2.53	0.43
1:A:892:LEU:O	1:A:896:THR:HG22	2.19	0.43
1:A:222:ALA:HB2	1:A:365:VAL:HG21	2.00	0.43
1:A:334:VAL:O	1:A:338:THR:HG23	2.17	0.43
1:A:113:LEU:HD23	1:A:356:THR:HG21	2.00	0.43
1:A:175:TYR:OH	1:A:923:CYS:HB3	2.19	0.43
1:A:500:GLU:H	1:A:550:TYR:HH	1.61	0.43
1:A:756:THR:OG1	1:A:757:GLU:N	2.51	0.43
1:A:801:MET:HG3	1:A:1016:TYR:HB2	2.00	0.43
1:A:1219:ILE:HG23	1:A:1223:PHE:HB2	1.99	0.43
1:A:275:THR:HG21	1:A:298:LEU:HD23	2.01	0.43
1:A:1243:LYS:HE3	1:A:1256:ASP:HA	2.00	0.43
1:A:256:LYS:HE3	1:A:256:LYS:HB3	1.83	0.43
1:A:107:VAL:HG12	1:A:228:LEU:HD13	2.00	0.43
1:A:285:ILE:O	1:A:289:TYR:HD2	2.01	0.43
1:A:860:VAL:HG12	1:A:861:ILE:HG13	2.00	0.43
1:A:896:THR:C	1:A:899:PRO:HD2	2.44	0.43
1:A:327:ALA:CB	1:A:366:THR:HG21	2.46	0.43
1:A:592:HIS:CE1	1:A:1208:ASP:HB3	2.53	0.43
1:A:1242:ASP:O	1:A:1257:GLU:HG3	2.19	0.43
1:A:866:ILE:HB	1:A:867:PRO:HD3	2.01	0.42
1:A:898:SER:OG	1:A:899:PRO:HD3	2.19	0.42
1:A:1146:LEU:O	1:A:1150:LEU:HD23	2.19	0.42
1:A:107:VAL:C	1:A:110:PRO:HD2	2.43	0.42
1:A:272:ARG:HG3	1:A:299:ILE:HG23	2.00	0.42
1:A:156:PHE:HA	1:A:159:VAL:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:PHE:CZ	1:A:596:TYR:HB3	2.53	0.42
1:A:949:ALA:HB2	1:A:998:ARG:HD2	2.00	0.42
1:A:98:PHE:CB	1:A:155:TYR:HB2	2.49	0.42
1:A:307:ILE:HD12	1:A:307:ILE:HG23	1.80	0.42
1:A:82:ARG:HB3	1:A:383:ILE:HG21	2.02	0.42
1:A:402:LEU:HD12	1:A:402:LEU:H	1.84	0.42
1:A:417:ALA:HB2	1:A:464:PRO:HA	2.00	0.42
1:A:1042:ILE:HB	1:A:1099:TRP:HB2	2.01	0.42
1:A:98:PHE:HB3	1:A:155:TYR:HB2	2.01	0.42
1:A:196:ASN:OD1	1:A:200:ASN:HB2	2.19	0.42
1:A:497:LYS:HD3	1:A:550:TYR:HD1	1.83	0.42
1:A:706:ARG:HH11	1:A:711:TRP:CD1	2.36	0.42
1:A:1186:CYS:SG	1:A:1189:ARG:NH1	2.93	0.42
1:A:177:LYS:NZ	1:A:394:GLU:HB3	2.35	0.42
1:A:268:PHE:CE2	1:A:305:LYS:HE3	2.54	0.42
1:A:1127:PHE:O	1:A:1134:ASN:ND2	2.36	0.42
1:A:1187:LEU:O	1:A:1191:ILE:N	2.45	0.42
1:A:1196:GLN:O	1:A:1227:THR:N	2.49	0.42
1:A:40:GLU:N	1:A:43:ASP:OD2	2.27	0.41
1:A:65:ASP:HA	1:A:68:VAL:HG22	2.01	0.41
1:A:504:TYR:CE1	1:A:508:ILE:HG13	2.56	0.41
1:A:822:LEU:HD12	1:A:822:LEU:HA	1.90	0.41
1:A:269:THR:O	1:A:273:ILE:HG12	2.19	0.41
1:A:279:VAL:HA	1:A:286:ILE:CD1	2.50	0.41
1:A:875:PHE:HE1	1:A:997:VAL:HG11	1.85	0.41
1:A:1091:LEU:HD23	1:A:1114:ARG:NH2	2.35	0.41
1:A:1128:THR:HG22	1:A:1172:GLU:HB3	2.03	0.41
1:A:1130:THR:HB	1:A:1166:MET:O	2.20	0.41
1:A:11:ASN:HD22	1:A:48:LEU:CD2	2.34	0.41
1:A:435:VAL:HG12	1:A:586:ILE:HG23	2.03	0.41
1:A:730:LEU:HD23	1:A:730:LEU:HA	1.79	0.41
1:A:805:ILE:HD11	1:A:1016:TYR:CD2	2.56	0.41
1:A:1149:ALA:HB1	1:A:1188:ALA:HB1	2.01	0.41
1:A:1016:TYR:CD1	1:A:1019:LEU:HD11	2.56	0.41
1:A:1164:GLY:O	1:A:1167:ASP:N	2.53	0.41
1:A:92:TYR:HD1	1:A:95:LEU:HD12	1.86	0.41
1:A:348:ALA:HB2	1:A:739:ALA:CB	2.50	0.41
1:A:459:LEU:HB3	1:A:461:GLU:HG2	2.01	0.41
1:A:974:LEU:HD13	1:A:979:VAL:HG22	2.03	0.41
1:A:1260:VAL:O	1:A:1263:GLN:HB2	2.21	0.41
1:A:118:ASN:HA	1:A:121:GLU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:LEU:HD23	1:A:261:LEU:HA	1.81	0.41
1:A:1026:GLU:HA	1:A:1109:GLY:HA3	2.02	0.41
1:A:431:LEU:HD22	1:A:611:MET:HB3	2.02	0.41
1:A:568:GLU:HB2	1:A:1275:GLN:OE1	2.21	0.41
1:A:1113:LEU:HD11	1:A:1117:MET:HE2	2.03	0.41
1:A:419:TRP:NE1	1:A:453:SER:OG	2.37	0.41
1:A:262:ARG:HG2	1:A:378:GLU:OE1	2.21	0.40
1:A:44:MET:HE3	1:A:44:MET:HB2	1.88	0.40
1:A:493:ILE:HD12	1:A:546:ALA:HB3	2.03	0.40
1:A:578:ILE:O	1:A:582:LEU:HB2	2.22	0.40
1:A:184:MET:HA	1:A:184:MET:HE2	2.04	0.40
1:A:280:ILE:HG22	1:A:818:ILE:HG23	2.04	0.40
1:A:287:LYS:O	1:A:1114:ARG:HD3	2.20	0.40
1:A:288:MET:HB3	1:A:1119:ILE:HG21	2.03	0.40
1:A:497:LYS:HD3	1:A:550:TYR:CD1	2.57	0.40
1:A:415:PHE:CE1	1:A:464:PRO:HB3	2.57	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	1212/1325 (92%)	1149 (95%)	63 (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	1062/1159 (92%)	1059 (100%)	3 (0%)	86	86

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

Mol	Chain	Res	Type
1	A	89	TRP
1	A	93	LEU
1	A	94	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	HIS
1	A	203	ASN
1	A	207	GLN
1	A	221	GLN
1	A	429	GLN
1	A	580	GLN
1	A	592	HIS
1	A	1005	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	PUC	A	1403	-	26,26,26	0.62	1 (3%)	28,33,33	1.69	2 (7%)
2	ATP	A	1401	3	32,33,33	1.39	5 (15%)	48,52,52	1.79	9 (18%)
2	ATP	A	1405	3	32,33,33	0.56	0	48,52,52	0.53	0

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
4	PUC	A	1403	-	-	11/19/40/40	0/3/2/2
2	ATP	A	1401	3	-	6/22/38/38	0/3/3/3
2	ATP	A	1405	3	-	9/22/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1401	ATP	C5-C4	4.48	1.47	1.39
2	A	1401	ATP	C5-C6	2.61	1.48	1.41
2	A	1401	ATP	C5-N7	-2.32	1.34	1.39
4	A	1403	PUC	O2-C1	-2.21	1.23	1.30
2	A	1401	ATP	C8-N7	2.20	1.35	1.31
2	A	1401	ATP	PB-O3A	2.17	1.61	1.59

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1403	PUC	C9-C10-C11	-7.25	92.06	103.73
2	A	1401	ATP	C5-C4-N3	-5.88	118.62	126.72
2	A	1401	ATP	N3-C4-N9	4.72	135.19	127.17
2	A	1401	ATP	C2-N3-C4	3.80	121.12	111.83
2	A	1401	ATP	C4-C5-N7	-3.42	106.68	110.58
2	A	1401	ATP	N3-C2-N1	-3.39	123.46	128.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1403	PUC	O5-C11-C10	-2.95	101.00	105.61
2	A	1401	ATP	C4-N9-C8	2.83	108.71	105.74
2	A	1401	ATP	C5-N7-C8	2.52	107.42	103.45
2	A	1401	ATP	N9-C8-N7	-2.06	111.02	113.94
2	A	1401	ATP	C6-C5-N7	2.04	136.02	132.09

There are no chirality outliers.

All (26) torsion outliers are listed below:

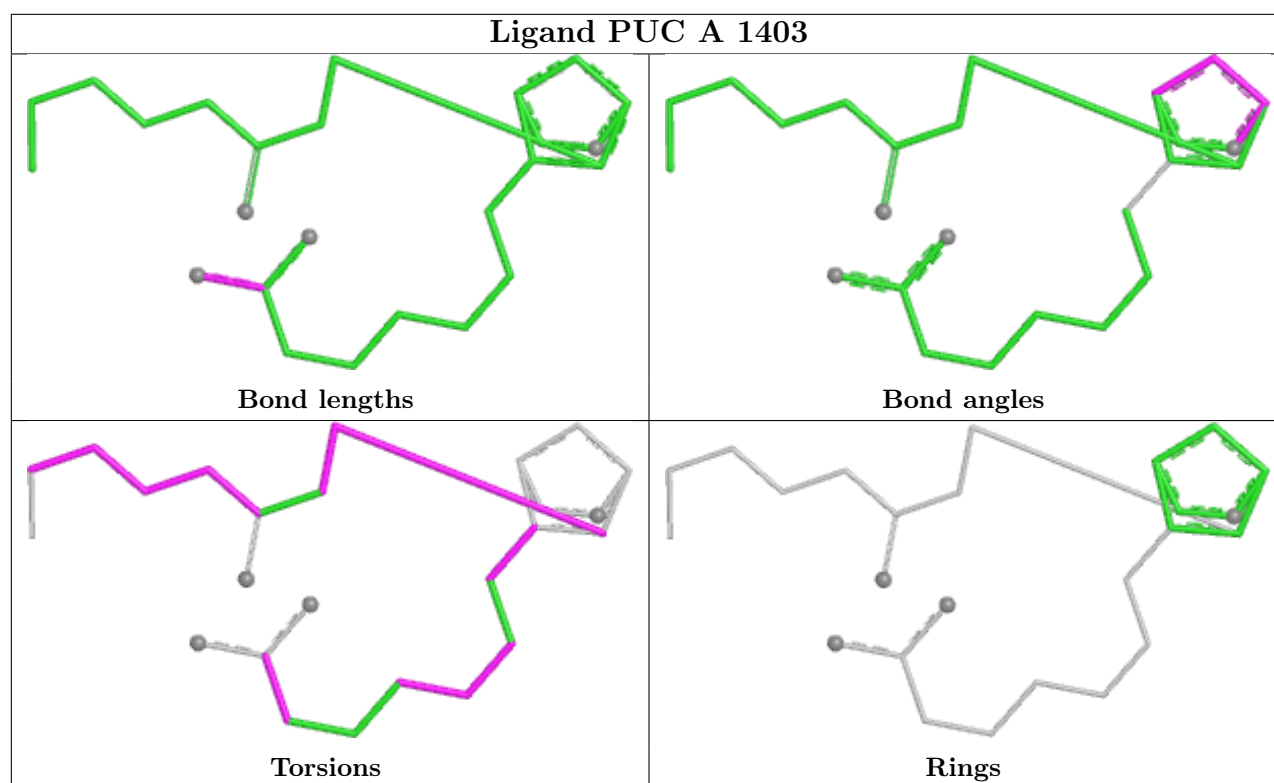
Mol	Chain	Res	Type	Atoms
2	A	1401	ATP	C5'-O5'-PA-O1A
2	A	1401	ATP	C5'-O5'-PA-O3A
2	A	1405	ATP	C5'-O5'-PA-O1A
2	A	1405	ATP	C5'-O5'-PA-O2A
2	A	1405	ATP	C5'-O5'-PA-O3A
2	A	1405	ATP	C4'-C5'-O5'-PA
2	A	1405	ATP	O4'-C1'-N9-C8
2	A	1405	ATP	O4'-C1'-N9-C4
4	A	1403	PUC	C12-C13-C14-C15
4	A	1403	PUC	O3-C15-C16-C17
4	A	1403	PUC	C14-C15-C16-C17
4	A	1403	PUC	C4-C5-C6-C7
4	A	1403	PUC	C16-C17-C18-C19
4	A	1403	PUC	C3-C4-C5-C6
2	A	1401	ATP	C2'-C1'-N9-C8
4	A	1403	PUC	C15-C16-C17-C18
2	A	1405	ATP	PG-O3B-PB-O3A
4	A	1403	PUC	C6-C7-C8-C9
2	A	1401	ATP	C2'-C1'-N9-C4
4	A	1403	PUC	C17-C18-C19-C20
2	A	1405	ATP	PG-O3B-PB-O1B
4	A	1403	PUC	C11-C12-C13-C14
2	A	1401	ATP	O4'-C1'-N9-C8
4	A	1403	PUC	O2-C1-C2-C3
2	A	1401	ATP	PB-O3A-PA-O1A
2	A	1405	ATP	PG-O3B-PB-O2B

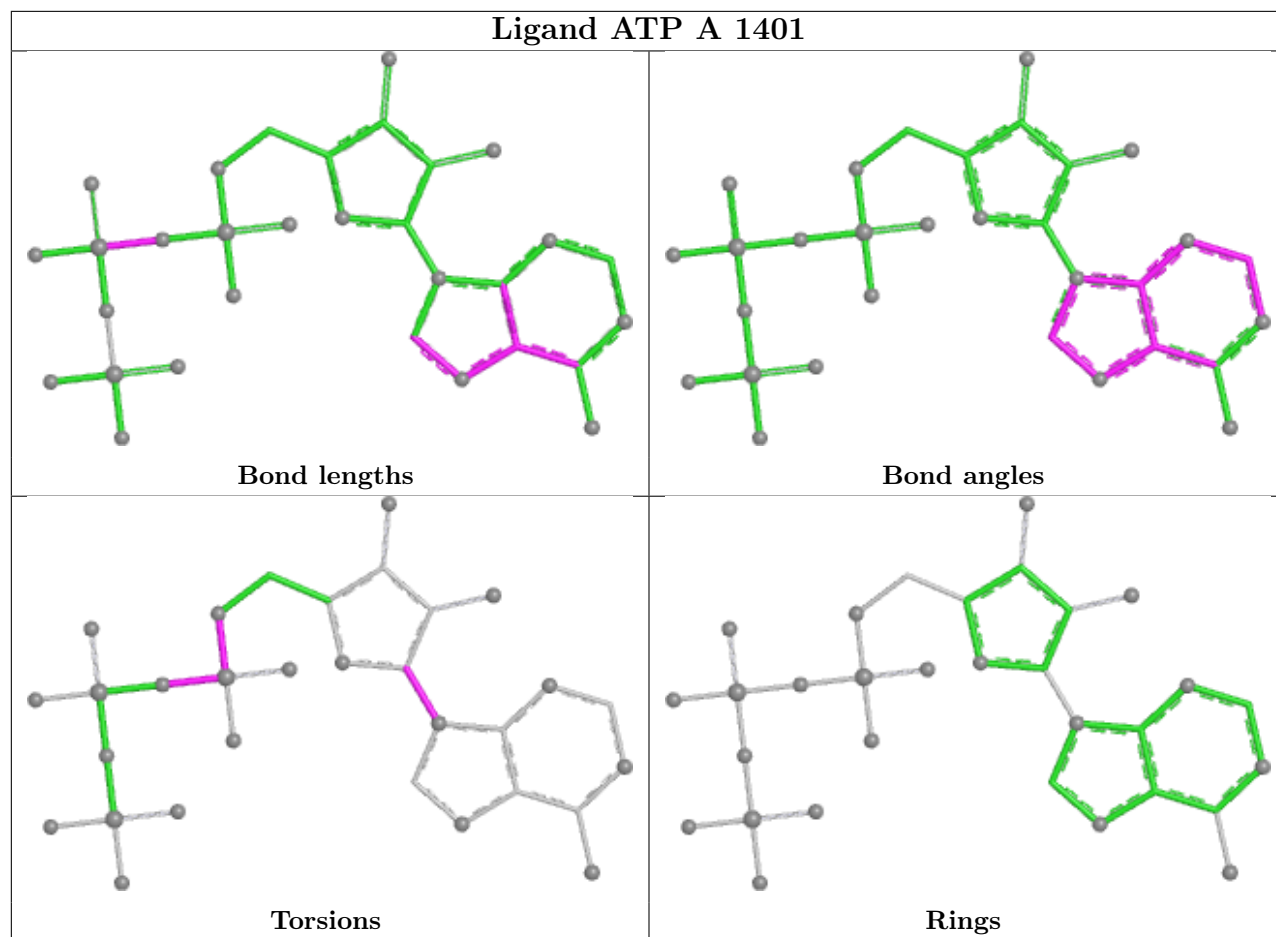
There are no ring outliers.

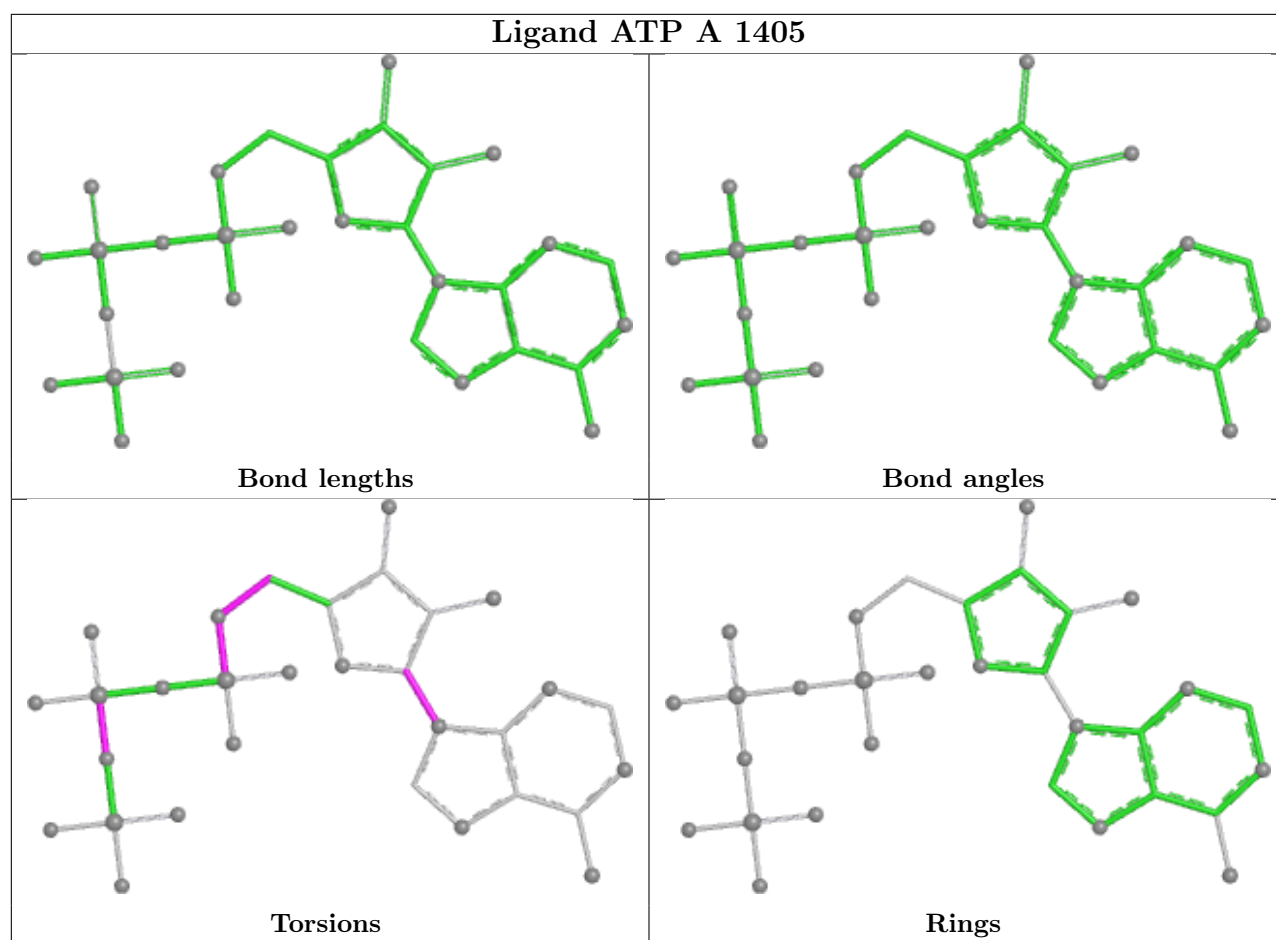
3 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1403	PUC	15	0
2	A	1401	ATP	1	0
2	A	1405	ATP	9	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.

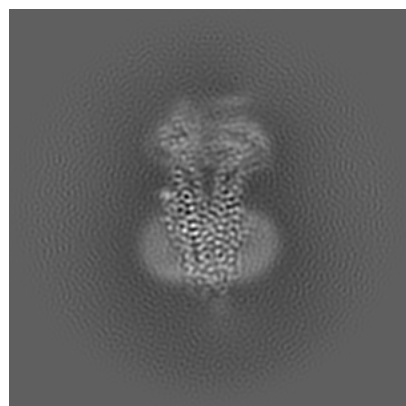
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35968. These allow visual inspection of the internal detail of the map and identification of artifacts.

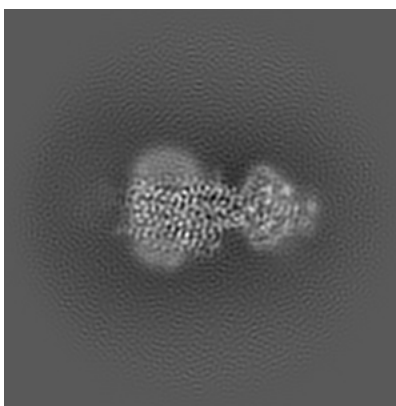
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

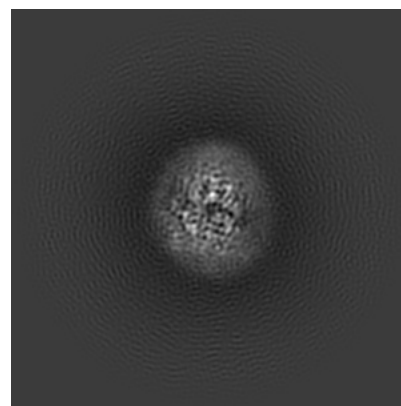
6.1.1 Primary map



X

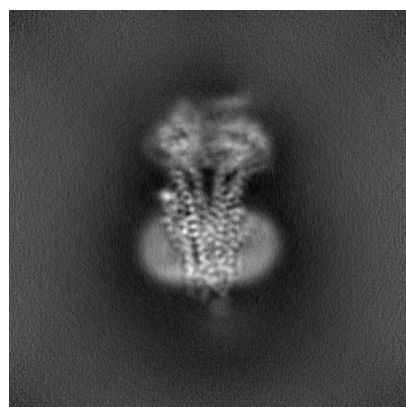


Y

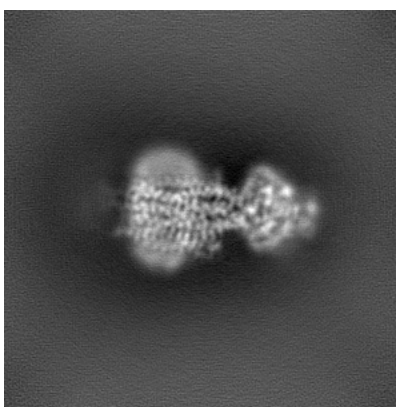


Z

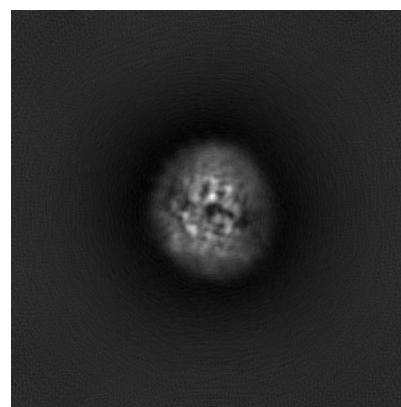
6.1.2 Raw map



X



Y

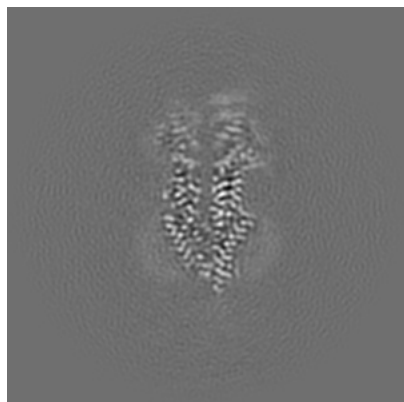


Z

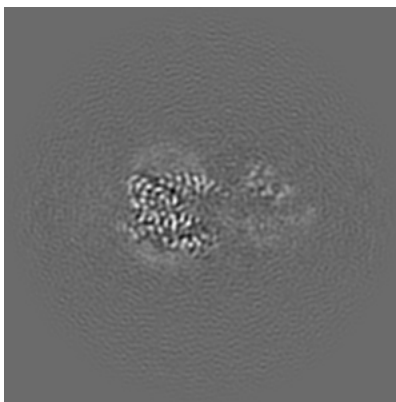
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

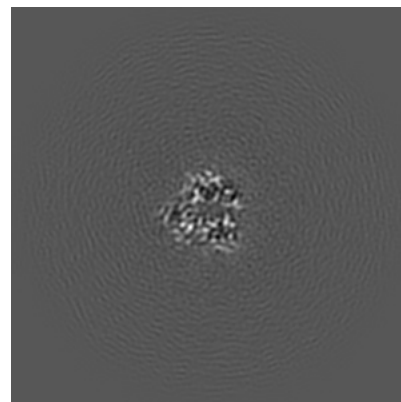
6.2.1 Primary map



X Index: 150

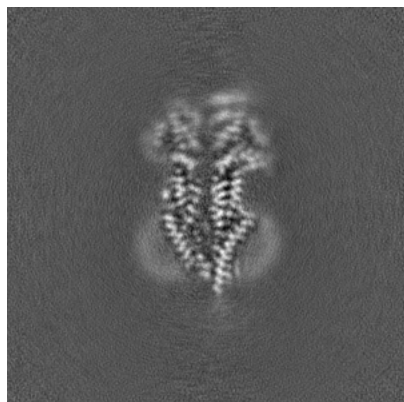


Y Index: 150

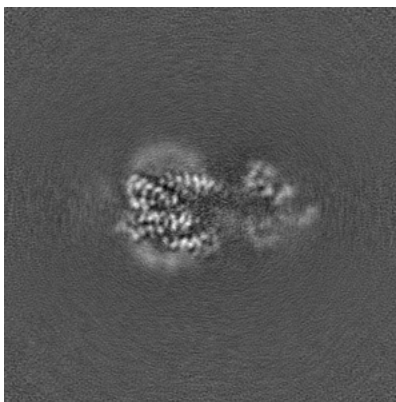


Z Index: 150

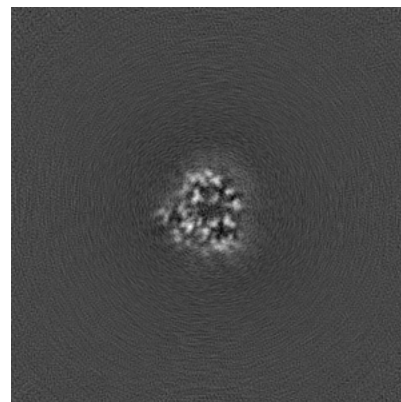
6.2.2 Raw map



X Index: 150



Y Index: 150

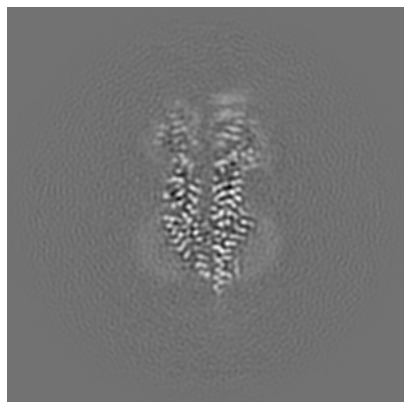


Z Index: 150

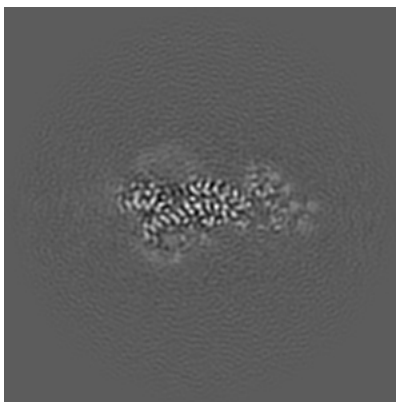
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

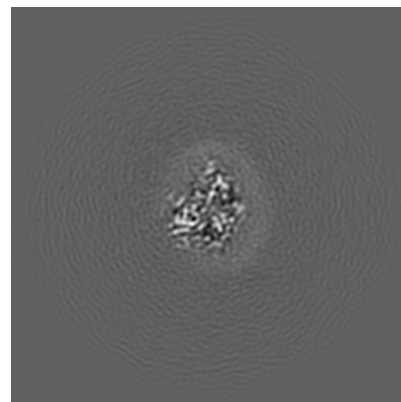
6.3.1 Primary map



X Index: 151

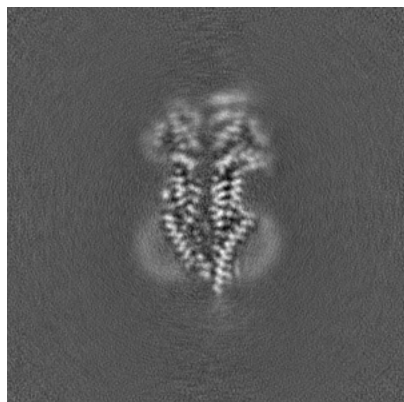


Y Index: 160

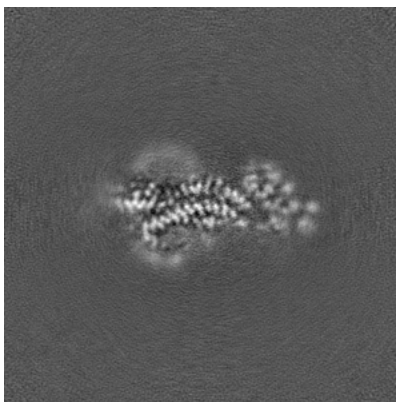


Z Index: 137

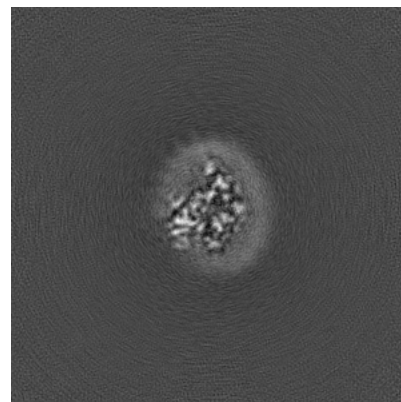
6.3.2 Raw map



X Index: 150



Y Index: 159

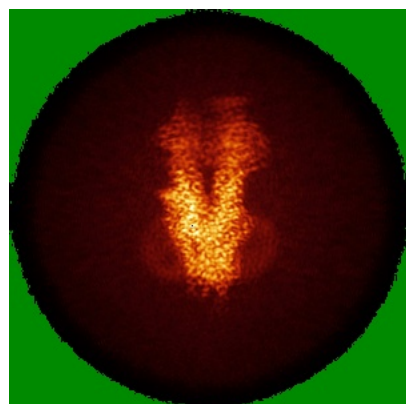


Z Index: 137

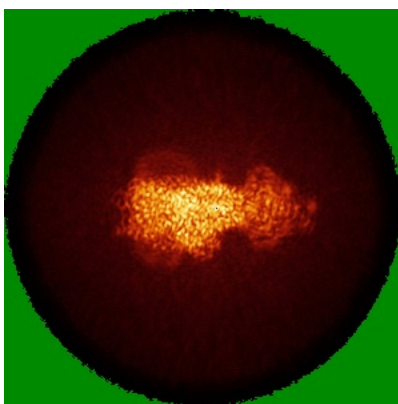
The images above show the largest variance slices of the map in three orthogonal directions.

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

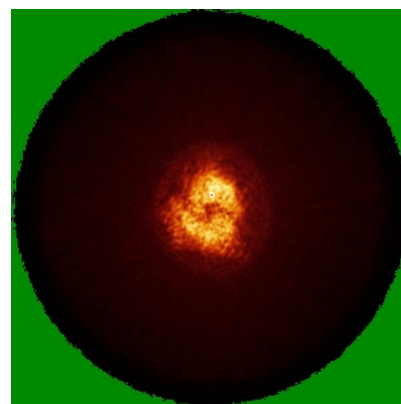
6.4.1 Primary map



X

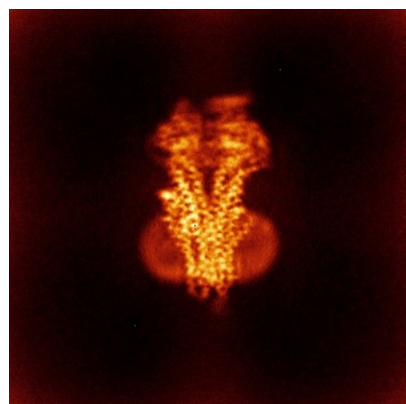


Y

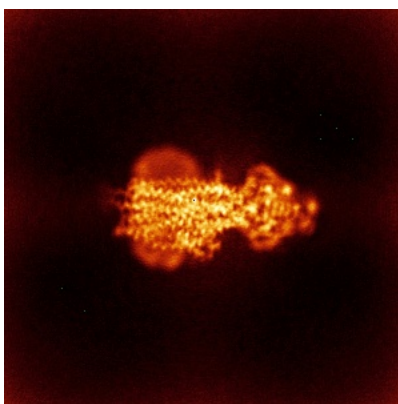


Z

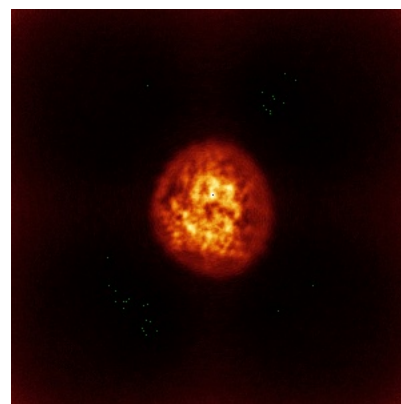
6.4.2 Raw map



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](#)

This section was not generated.

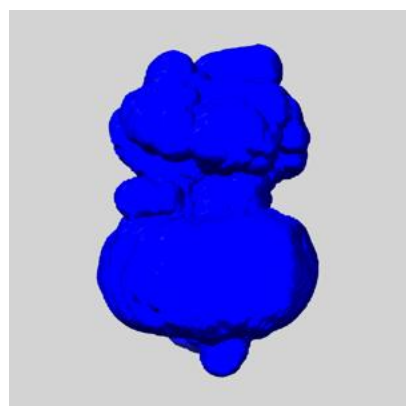
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

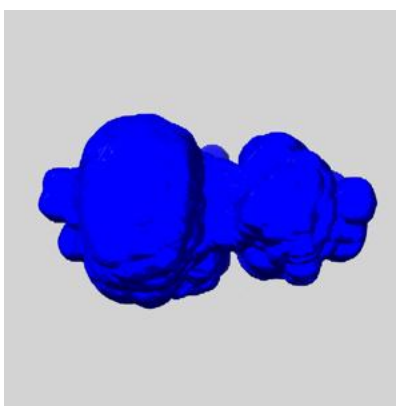
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

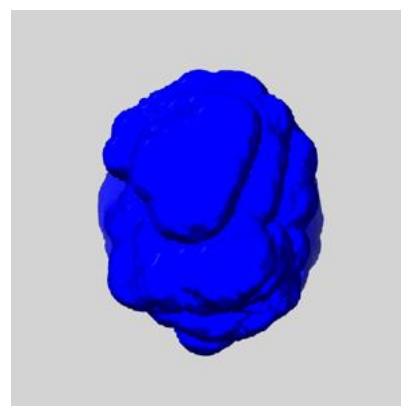
6.6.1 emd_35968_msk_1.map [i](#)



X



Y

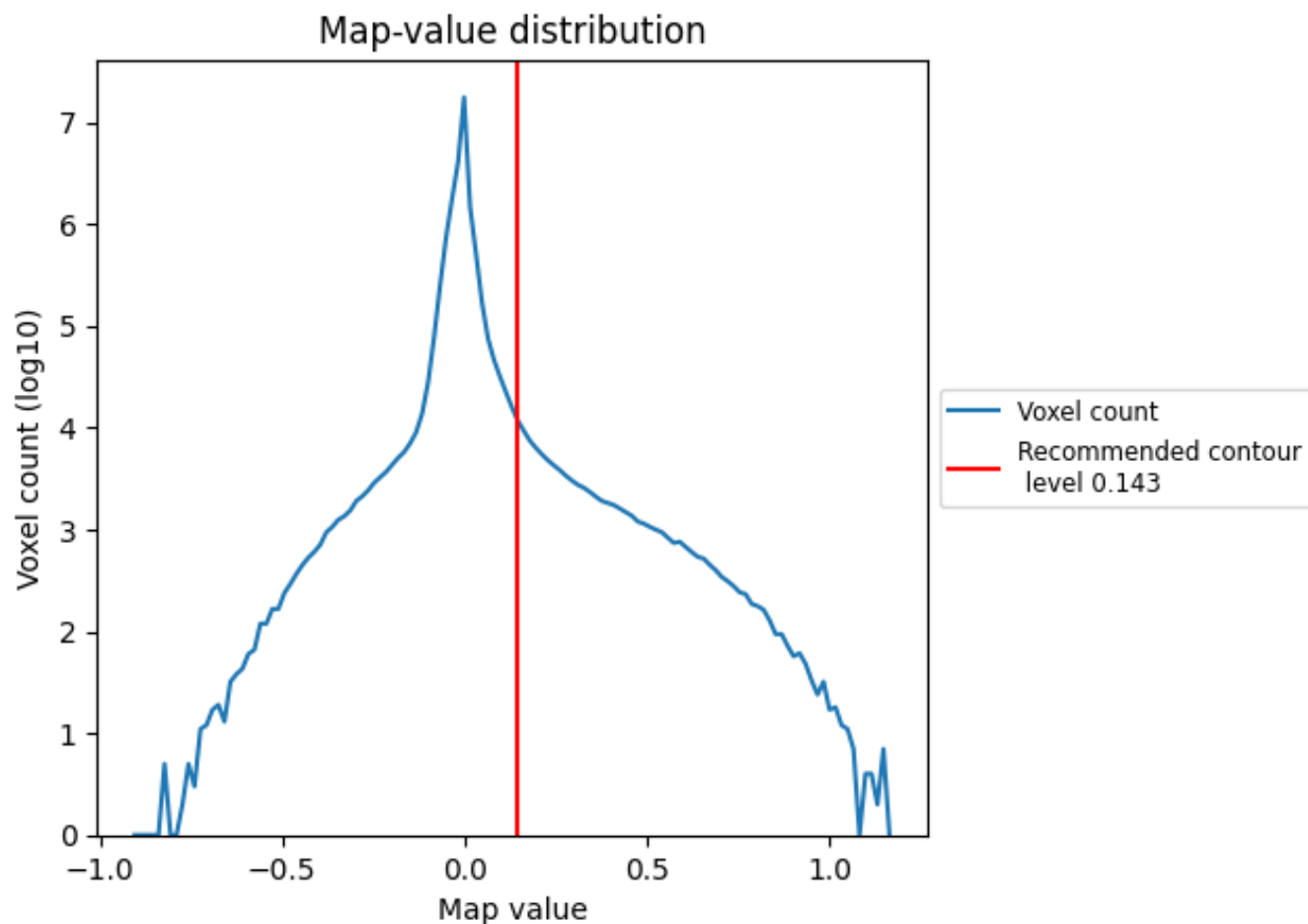


Z

7 Map analysis [i](#)

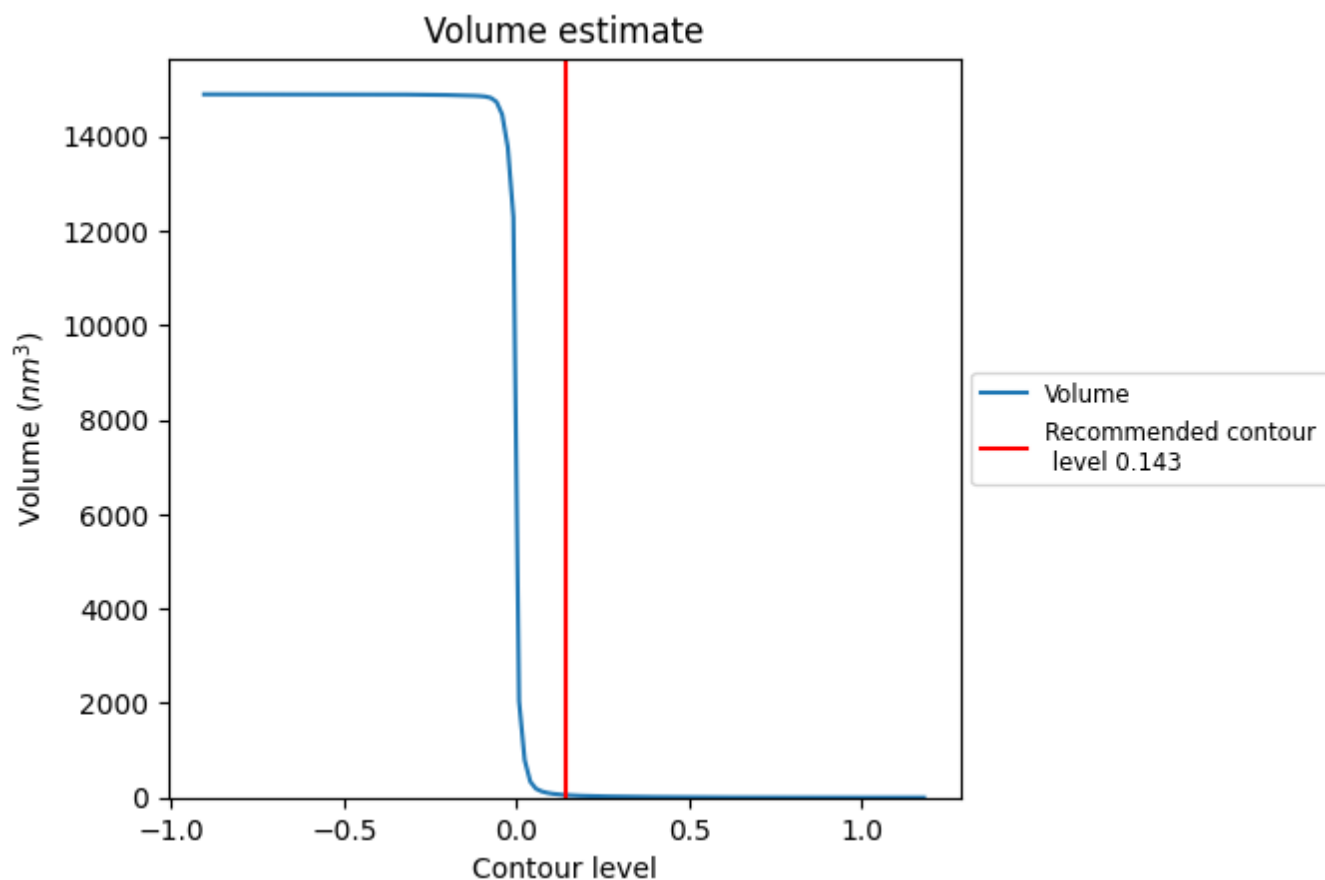
This section contains the results of statistical analysis of the map.

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.

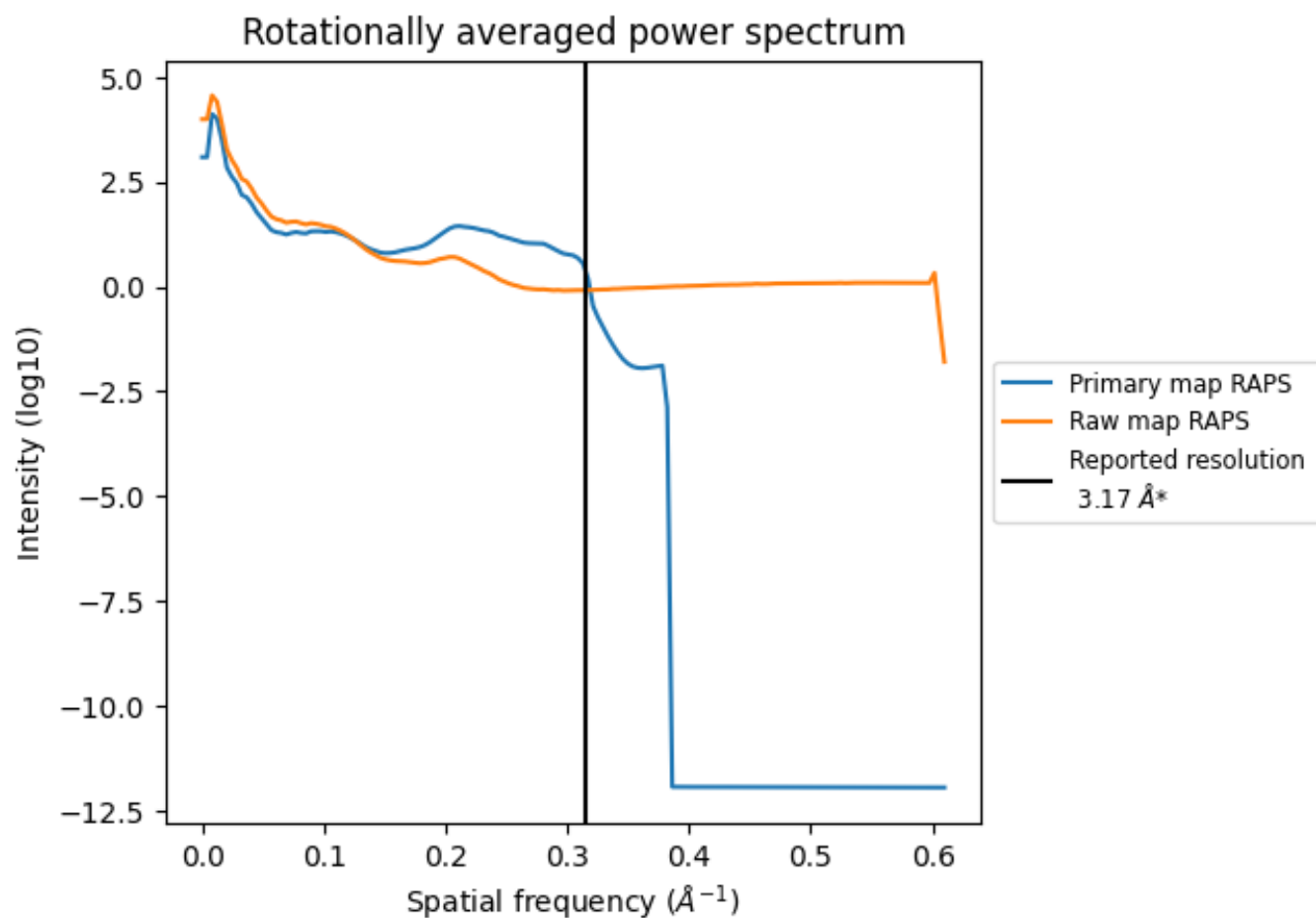
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 53 nm³; this corresponds to an approximate mass of 48 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 ⓘ

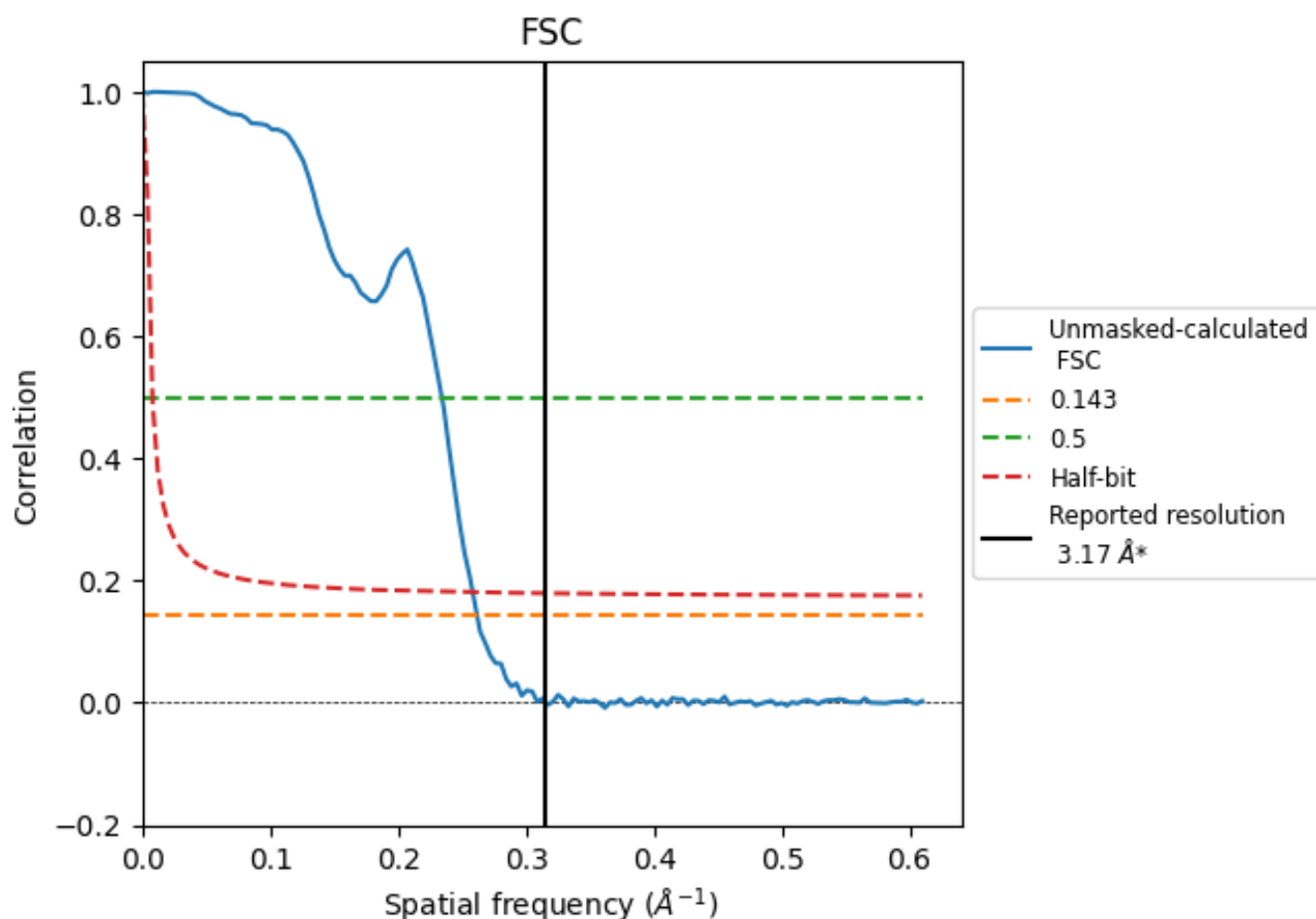


*Reported resolution corresponds to spatial frequency of 0.315 Å⁻¹

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 $0.315 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

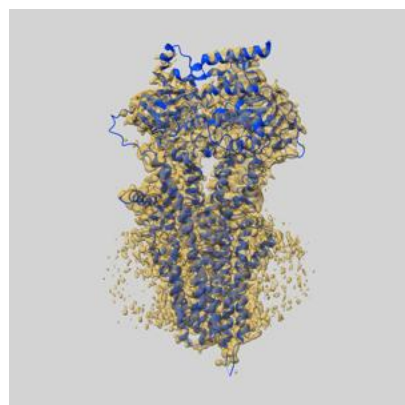
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.17	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.82	4.27	3.87

*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 3.82 differs from the reported value 3.17 by more than 10 %

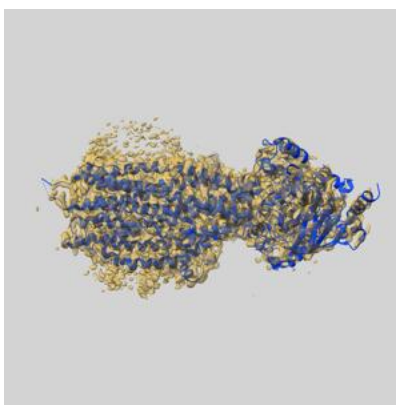
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-35968 and PDB model 8J3Z. Per-residue inclusion information can be found in section 3 on page 6.

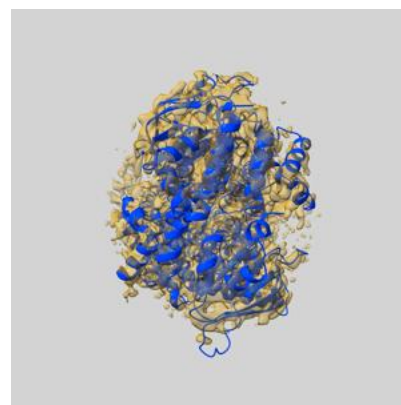
9.1 Map-model overlay [i](#)



X



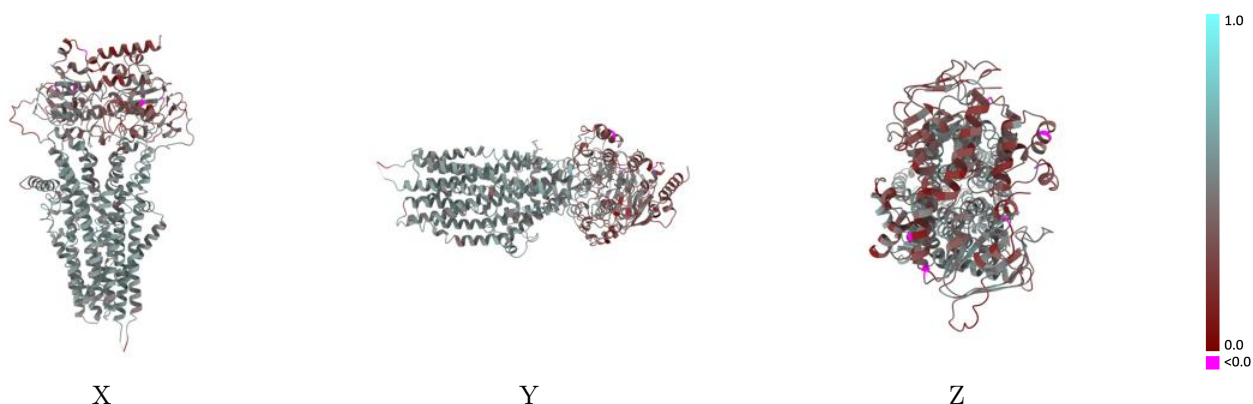
Y



Z

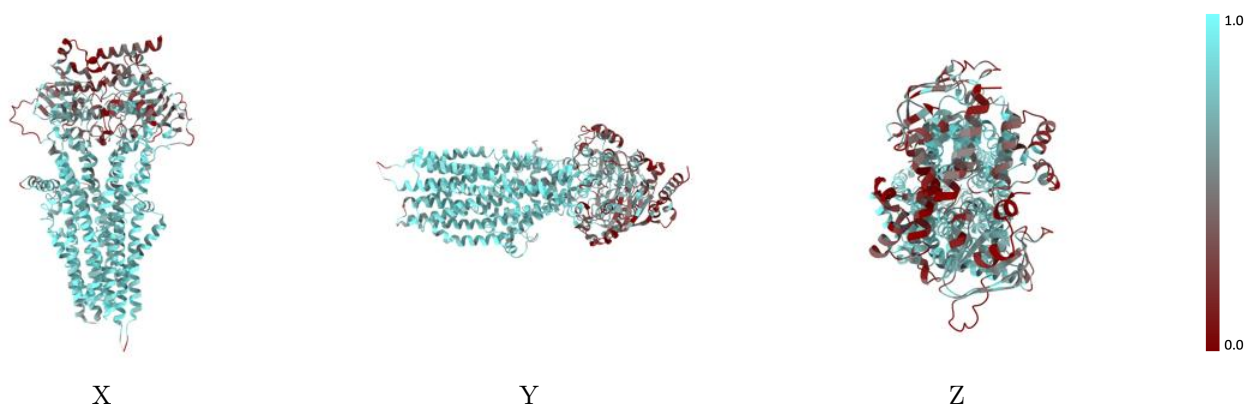
The images above show the 3D surface view of the map at the recommended contour level 0.143 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



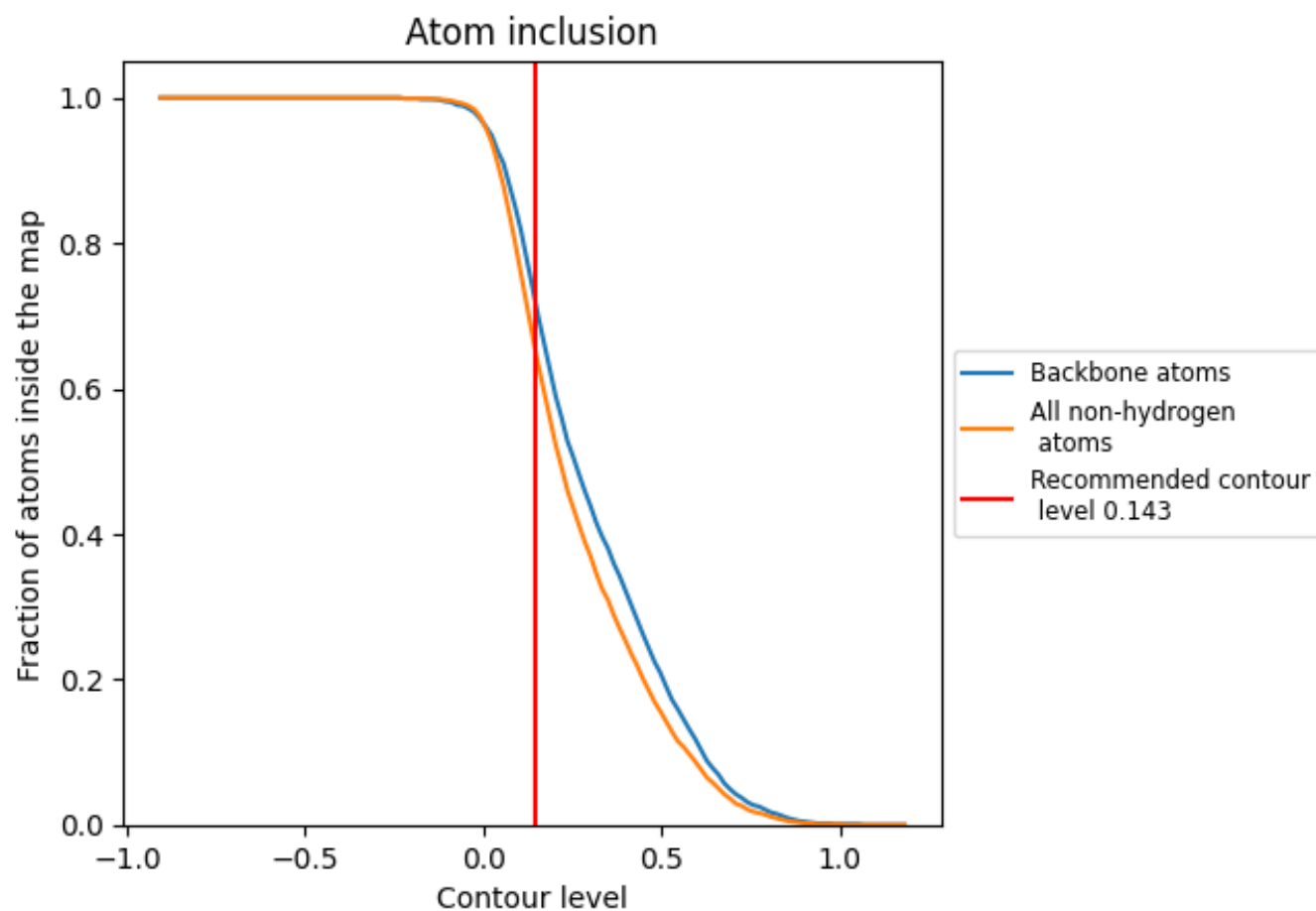
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.143).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 66% 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 (0.143) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6600	0.4550
A	0.6600	0.4550

