Full wwPDB EM Validation Report ⓘ

Mar 31, 2025 – 02:27 PM JST

PDB ID	:	8ZBU / pdb_00008zbu
EMDB ID	:	EMD-39911
Title	:	Cryo-EM structure of nanodisc-reconstituted human MRP4 withE1202Q mutation (in complex with lapatinib)
Authors	:	Xie, Z.; Long, F.
Deposited on	:	2024-04-27
Resolution	:	3.28 Å(reported)
Based on initial model	:	.

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 ①) were used in the production of this report:

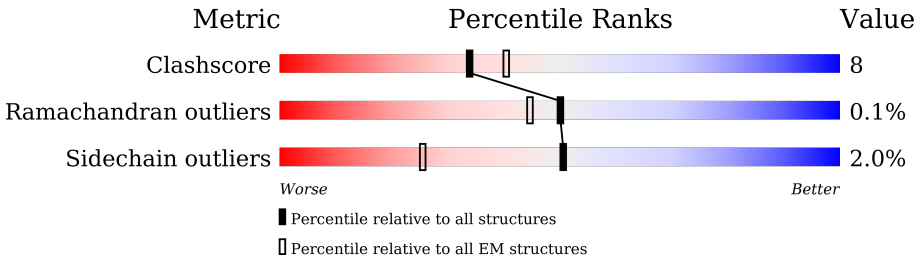
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.28 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 <=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	1344	21% 71% 19% • 9%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9831 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.

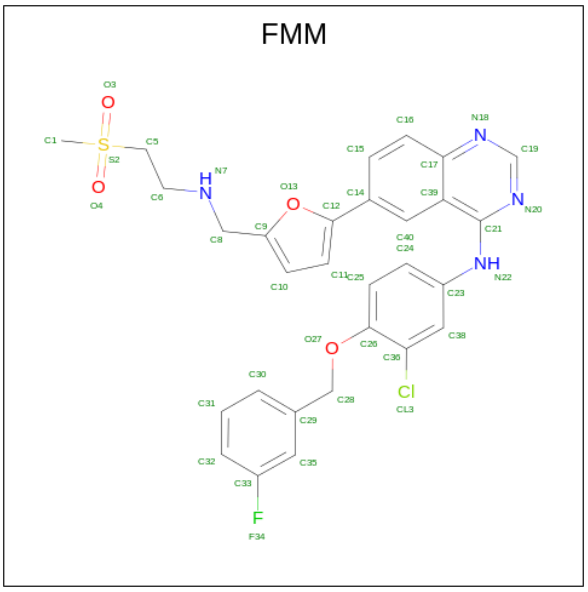
- Molecule 1 is a protein called ATP-binding cassette sub-family C member 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1218	9727	6316	1638	1730	43	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	initiating methionine	UNP O15439
A	-9	HIS	-	expression tag	UNP O15439
A	-8	HIS	-	expression tag	UNP O15439
A	-7	HIS	-	expression tag	UNP O15439
A	-6	HIS	-	expression tag	UNP O15439
A	-5	HIS	-	expression tag	UNP O15439
A	-4	HIS	-	expression tag	UNP O15439
A	-3	HIS	-	expression tag	UNP O15439
A	-2	HIS	-	expression tag	UNP O15439
A	-1	HIS	-	expression tag	UNP O15439
A	0	HIS	-	expression tag	UNP O15439
A	1202	GLN	GLU	engineered mutation	UNP O15439
A	1326	ASP	-	expression tag	UNP O15439
A	1327	TYR	-	expression tag	UNP O15439
A	1328	LYS	-	expression tag	UNP O15439
A	1329	ASP	-	expression tag	UNP O15439
A	1330	ASP	-	expression tag	UNP O15439
A	1331	ASP	-	expression tag	UNP O15439
A	1332	ASP	-	expression tag	UNP O15439
A	1333	LYS	-	expression tag	UNP O15439

- Molecule 2 is N-{3-CHLORO-4-[(3-FLUOROBENZYL)OXY]PHENYL}-6-[5-({[2-(METHYLSULFONYL)ETHYL]AMINO}METHYL)-2-FURYL]-4-QUINAZOLINAMINE (CCD ID: FMM) (formula: $C_{29}H_{26}ClFN_4O_4S$) (labeled as "Ligand of Interest" by depositor).

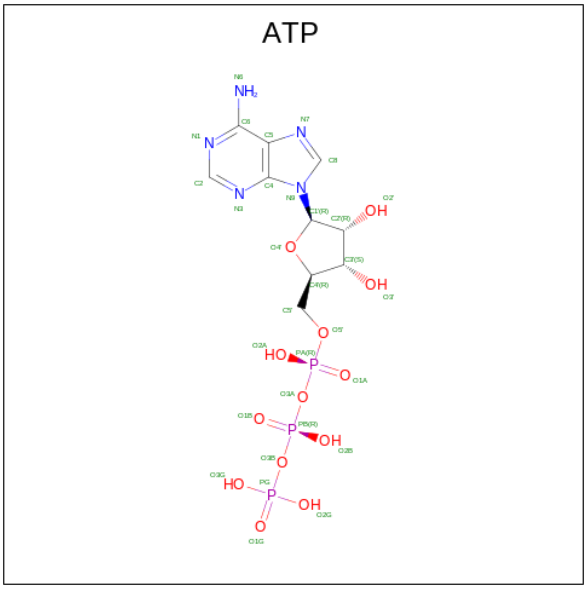


Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	Cl	F	N	O	S	0
			40	29	1	1	4	4	1	

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



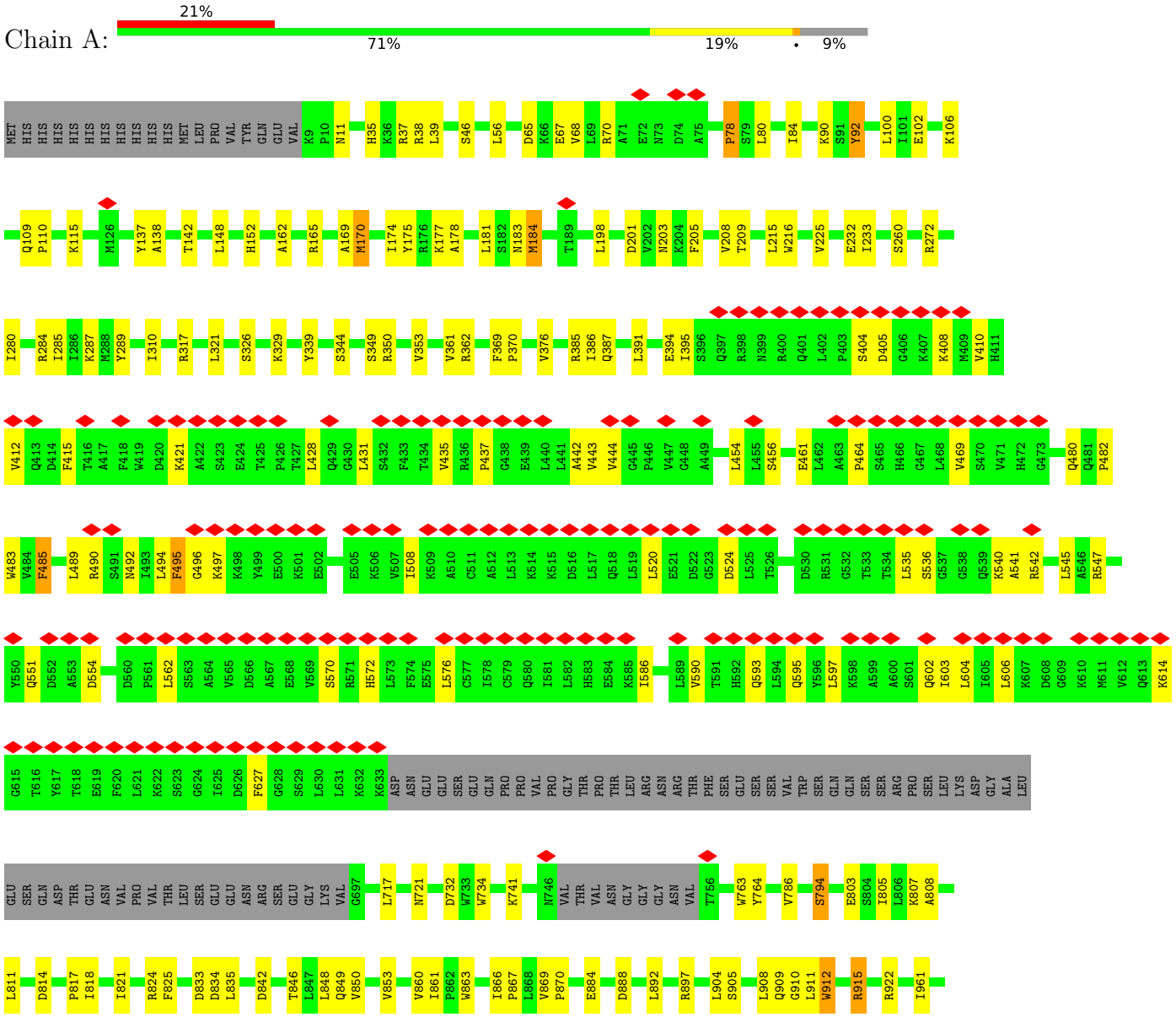
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

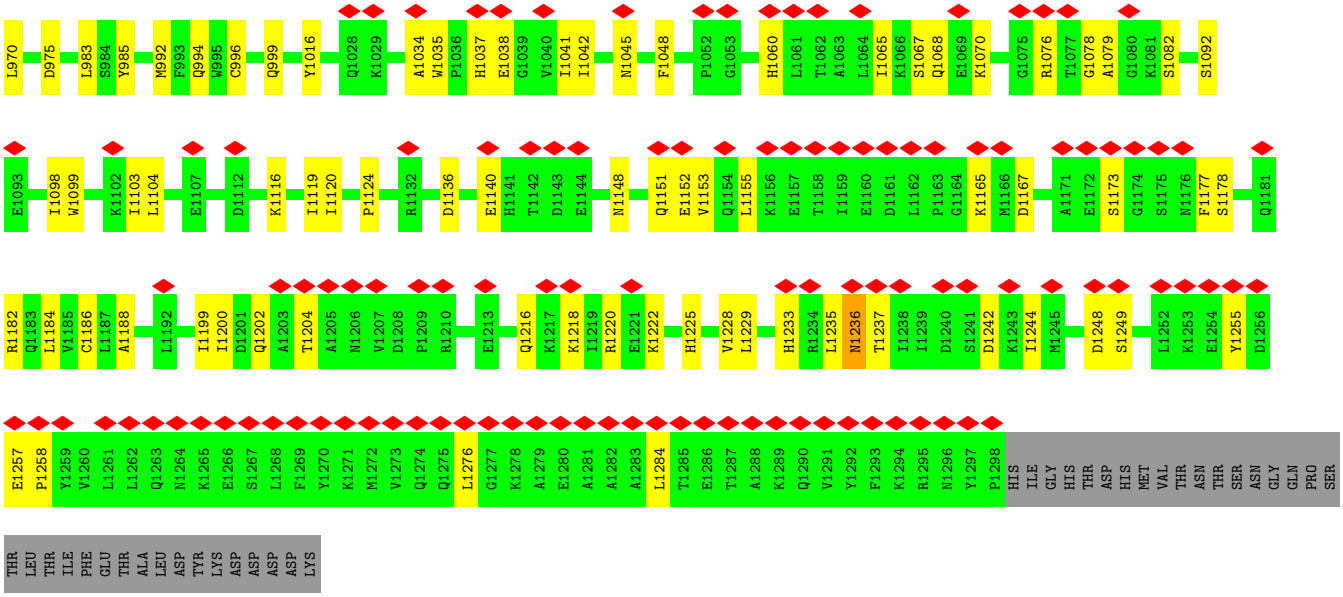
3 Residue-property plots (i)

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: ATP-binding cassette sub-family C member 4

Chain A:




L970 D975 L983 S984 Y985 M992 F993 Q994 W995 C996 Q999 Y1016 Q1028 K1029 A1034 W1035 P1036 H1037 E1038 G1039 V1040 I1041 I1042 N1045 F1048 P1052 G1053 H1060 L1061 T1062 A1063 L1064 I1065 K1066 S1067 Q1068 E1069 K1070 G1075 R1076 T1077 G1078 A1079 G1080 K1081 S1082 S1092
E1093 I1098 W1099 K1102 I1103 L1104 E1107 D1112 K1116 I1119 I1120 P1124 R1132 D1136 E1140 H1141 T1142 D1143 E1144 N1148 Q1151 E1152 V1153 Q1154 L1155 K1156 E1157 T1158 I1159 E1160 D1161 L1162 P1163 G1164 K1165 M1166 D1167 A1171 E1172 S1173 G1174 S1175 N1176 F1177 S1178 Q1181
R1182 Q1183 L1184 V1185 C1186 L1187 A1188 L1192 I1199 I1200 D1201 Q1202 A1203 T1204 A1205 N1206 V1207 D1208 P1209 R1210 E1213 Q1216 K1217 K1218 I1219 R1220 E1221 K1222 H1225 V1228 L1229 H1233 R1234 L1235 N1236 T1237 I1238 I1239 D1240 S1241 D1242 K1243 I1244 M1245 D1248 S1249 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 T1287 A1288 K1289 Q1290 V1291 Y1292 F1293 K1294 R1295 N1296 Y1297 P1298 HIS ILE GLY HIS THR ASP HIS MET VAL THR ASN THR SER ASN GLY GLN PRO SER
THR LEU THR ILE PHE GLU THR ALA LEU ASP TYR LYS ASP ASP ASP ASP LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	334794	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.399	Depositor
Minimum map value	-1.146	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.11	Depositor
Map size (Å)	215.04, 215.04, 215.04	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, FMM, MG

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	0.28	0/9936	0.47	0/13463

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	9727	0	9990	157	0
2	A	40	0	26	4	0
3	A	2	0	0	0	0
4	A	62	0	24	2	0
All	All	9831	0	10040	158	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 8.

All (158) 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:1035:TRP:HB3	1:A:1116:LYS:HZ3	1.55	0.72
1:A:1235:LEU:O	1:A:1237:THR:N	2.23	0.71
1:A:362:ARG:NH2	2:A:1401:FMM:O4	2.25	0.70
1:A:287:LYS:NZ	1:A:808:ALA:O	2.28	0.67
1:A:860:VAL:HG12	1:A:861:ILE:HG13	1.76	0.67
1:A:395:ILE:HD13	1:A:915:ARG:HH11	1.60	0.67
1:A:824:ARG:HH11	1:A:824:ARG:HG3	1.62	0.65
1:A:177:LYS:NZ	1:A:394:GLU:OE1	2.29	0.64
1:A:198:LEU:HD13	1:A:904:LEU:HD22	1.80	0.64
1:A:102:GLU:OE2	1:A:152:HIS:ND1	2.30	0.63
1:A:1235:LEU:HD13	1:A:1276:LEU:HD11	1.82	0.62
1:A:1076:ARG:HH12	1:A:1248:ASP:HA	1.65	0.62
1:A:184:MET:SD	1:A:184:MET:N	2.72	0.62
1:A:1244:ILE:HG12	1:A:1258:PRO:HG3	1.83	0.59
1:A:203:ASN:OD1	1:A:897:ARG:NH2	2.36	0.58
1:A:106:LYS:HG2	1:A:148:LEU:HD21	1.85	0.58
1:A:1152:GLU:O	1:A:1218:LYS:NZ	2.25	0.57
1:A:1120:ILE:HD13	1:A:1200:ILE:HG22	1.87	0.57
1:A:142:THR:HG22	1:A:961:ILE:HG12	1.87	0.57
1:A:496:GLY:HA3	1:A:922:ARG:HG2	1.87	0.56
1:A:1041:ILE:HB	1:A:1065:ILE:HB	1.87	0.56
1:A:717:LEU:HD21	1:A:786:VAL:HG22	1.88	0.56
1:A:992:MET:HB2	2:A:1401:FMM:H81	1.88	0.56
1:A:1148:ASN:OD1	1:A:1151:GLN:NE2	2.37	0.56
1:A:482:PRO:HB2	1:A:540:LYS:HE3	1.87	0.56
1:A:803:GLU:O	1:A:807:LYS:NZ	2.39	0.56
1:A:905:SER:O	1:A:909:GLN:HG2	2.07	0.55
1:A:1173:SER:O	1:A:1182:ARG:NH1	2.40	0.55
1:A:1155:LEU:HD13	1:A:1184:LEU:HD23	1.88	0.55
1:A:339:TYR:O	1:A:344:SER:OG	2.23	0.55
1:A:1257:GLU:OE1	1:A:1258:PRO:HD2	2.06	0.55
1:A:497:LYS:HE3	1:A:551:GLN:HA	1.88	0.54
1:A:280:ILE:HG22	1:A:818:ILE:HD12	1.90	0.54
1:A:232:GLU:HB3	1:A:233:ILE:HD12	1.90	0.54
1:A:215:LEU:HD11	1:A:376:VAL:HG21	1.89	0.53
1:A:284:ARG:NH2	1:A:814:ASP:OD1	2.42	0.53
1:A:56:LEU:HD21	1:A:165:ARG:HD2	1.90	0.53
1:A:593:GLN:OE1	1:A:595:GLN:NE2	2.43	0.52
1:A:494:LEU:O	1:A:497:LYS:NZ	2.35	0.52
1:A:1216:GLN:O	1:A:1220:ARG:HG2	2.09	0.52
1:A:483:TRP:CE2	1:A:910:GLY:HA3	2.45	0.52
1:A:602:GLN:HB3	1:A:614:LYS:HE2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:ASN:ND2	1:A:46:SER:O	2.36	0.51
1:A:35:HIS:ND1	1:A:884:GLU:OE1	2.38	0.51
1:A:721:ASN:HB3	1:A:848:LEU:HD11	1.92	0.51
1:A:485:PHE:HE1	1:A:492:ASN:HA	1.76	0.50
1:A:1068:GLN:NE2	1:A:1225:HIS:O	2.35	0.50
1:A:520:LEU:HD11	1:A:535:LEU:HD21	1.94	0.50
1:A:37:ARG:NH1	1:A:38:ARG:O	2.45	0.50
1:A:541:ALA:O	1:A:545:LEU:HG	2.12	0.49
1:A:201:ASP:OD2	1:A:385:ARG:NH1	2.46	0.49
1:A:536:SER:O	1:A:540:LYS:HG2	2.13	0.49
1:A:911:LEU:HD22	1:A:915:ARG:HH21	1.77	0.49
1:A:817:PRO:O	1:A:821:ILE:HG12	2.13	0.49
1:A:1216:GLN:OE1	1:A:1220:ARG:NH2	2.46	0.48
1:A:1035:TRP:CD1	1:A:1103:ILE:HD12	2.48	0.48
1:A:272:ARG:NH2	1:A:825:PHE:O	2.47	0.48
1:A:310:ILE:HD13	1:A:833:ASP:HB3	1.96	0.48
1:A:1202:GLN:HB3	1:A:1233:HIS:H	1.78	0.48
1:A:404:SER:OG	1:A:405:ASP:N	2.47	0.48
1:A:994:GLN:OE1	2:A:1401:FMM:F34	2.22	0.47
1:A:410:VAL:HB	1:A:435:VAL:HG12	1.96	0.47
1:A:1045:ASN:OD1	1:A:1060:HIS:ND1	2.44	0.47
1:A:109:GLN:HG2	1:A:110:PRO:HD3	1.96	0.47
1:A:1124:PRO:HB3	1:A:1186:CYS:SG	2.54	0.47
1:A:1178:SER:O	1:A:1182:ARG:HG3	2.15	0.47
1:A:80:LEU:O	1:A:84:ILE:HG12	2.14	0.47
1:A:483:TRP:CZ2	1:A:485:PHE:HB3	2.49	0.47
1:A:1034:ALA:O	1:A:1037:HIS:HB3	2.15	0.47
1:A:174:ILE:HD11	1:A:386:ILE:HD13	1.96	0.46
1:A:562:LEU:HD13	1:A:570:SER:HB2	1.98	0.46
1:A:794:SER:OG	1:A:833:ASP:OD1	2.29	0.46
1:A:489:LEU:HD22	1:A:524:ASP:HA	1.98	0.46
1:A:1070:LYS:HD2	1:A:1228:VAL:HB	1.96	0.46
1:A:170:MET:HG2	1:A:205:PHE:HE2	1.81	0.46
1:A:443:VAL:HB	1:A:590:VAL:HG22	1.98	0.46
1:A:848:LEU:HD23	1:A:848:LEU:HA	1.81	0.46
1:A:56:LEU:HB3	1:A:169:ALA:HB2	1.98	0.46
1:A:805:ILE:HG21	1:A:825:PHE:HZ	1.80	0.46
1:A:1218:LYS:O	1:A:1222:LYS:HB2	2.17	0.45
1:A:442:ALA:HB3	1:A:603:ILE:HG12	1.97	0.45
1:A:90:LYS:HE2	1:A:90:LYS:HB3	1.64	0.45
1:A:1202:GLN:O	1:A:1204:THR:N	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:908:LEU:HD12	1:A:911:LEU:HD12	1.98	0.45
1:A:138:ALA:O	1:A:142:THR:HG23	2.16	0.45
2:A:1401:FMM:N20	2:A:1401:FMM:H38	2.32	0.45
1:A:391:LEU:HD23	1:A:391:LEU:HA	1.86	0.45
1:A:863:TRP:HD1	1:A:970:LEU:HD21	1.81	0.45
1:A:1042:ILE:HB	1:A:1099:TRP:HB2	1.99	0.45
1:A:1136:ASP:OD2	1:A:1140:GLU:N	2.50	0.44
1:A:67:GLU:OE2	1:A:70:ARG:NH2	2.51	0.44
1:A:454:LEU:HD11	1:A:606:LEU:HD22	1.99	0.44
1:A:1177:PHE:O	1:A:1182:ARG:NH2	2.50	0.44
1:A:408:LYS:HD3	1:A:554:ASP:HB3	2.00	0.44
1:A:456:SER:HA	1:A:461:GLU:OE1	2.18	0.44
1:A:604:LEU:HB2	1:A:614:LYS:HG3	1.99	0.44
1:A:842:ASP:OD2	1:A:999:GLN:NE2	2.50	0.44
1:A:92:TYR:OH	1:A:209:THR:HB	2.17	0.43
1:A:369:PHE:HB3	1:A:370:PRO:HD3	2.00	0.43
1:A:983:LEU:HD12	1:A:983:LEU:HA	1.79	0.43
1:A:39:LEU:HB2	1:A:888:ASP:OD1	2.18	0.43
1:A:1199:ILE:HG12	1:A:1229:LEU:HB2	2.00	0.43
1:A:285:ILE:HG23	1:A:289:TYR:CE2	2.53	0.43
1:A:846:THR:HG22	1:A:996:CYS:HB2	2.01	0.43
1:A:1244:ILE:CG1	1:A:1258:PRO:HG3	2.47	0.43
1:A:1038:GLU:HG2	1:A:1067:SER:HB2	2.00	0.43
1:A:415:PHE:CE1	1:A:464:PRO:HB3	2.54	0.43
1:A:428:LEU:HD22	1:A:431:LEU:HD11	2.00	0.43
1:A:1124:PRO:HB2	1:A:1182:ARG:HB3	2.00	0.43
1:A:1165:LYS:HD3	1:A:1165:LYS:HA	1.85	0.42
1:A:495:PHE:CD1	1:A:547:ARG:HD3	2.54	0.42
1:A:1148:ASN:O	1:A:1151:GLN:HG3	2.18	0.42
1:A:1048:PHE:CE1	1:A:1092:SER:HB2	2.54	0.42
1:A:205:PHE:HA	1:A:208:VAL:HG12	2.01	0.42
1:A:68:VAL:HG23	1:A:78:PRO:HG3	2.02	0.42
1:A:329:LYS:NZ	1:A:732:ASP:OD2	2.52	0.42
1:A:437:PRO:HA	1:A:586:ILE:HG12	2.02	0.42
1:A:869:VAL:HB	1:A:870:PRO:HD3	2.01	0.42
1:A:1244:ILE:O	1:A:1255:TYR:HA	2.20	0.42
1:A:183:ASN:ND2	1:A:912:TRP:HZ2	2.18	0.42
1:A:444:VAL:HG11	1:A:597:LEU:HD11	2.01	0.42
1:A:490:ARG:NH2	1:A:524:ASP:OD2	2.53	0.42
1:A:115:LYS:HD3	1:A:137:TYR:CZ	2.55	0.42
1:A:178:ALA:HA	1:A:181:LEU:CD2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:835:LEU:HD12	1:A:835:LEU:HA	1.87	0.42
1:A:1070:LYS:O	1:A:1242:ASP:N	2.53	0.41
1:A:1098:ILE:O	1:A:1104:LEU:HD12	2.20	0.41
1:A:1119:ILE:HA	1:A:1199:ILE:O	2.19	0.41
1:A:572:HIS:NE2	1:A:576:LEU:HD12	2.35	0.41
1:A:597:LEU:HB3	1:A:603:ILE:HD11	2.01	0.41
1:A:975:ASP:OD1	1:A:975:ASP:N	2.53	0.41
1:A:1078:GLY:H	4:A:1403:ATP:PB	2.43	0.41
1:A:1236:ASN:HB3	1:A:1284:LEU:HD21	2.01	0.41
1:A:866:ILE:HB	1:A:867:PRO:HD3	2.02	0.41
1:A:225:VAL:HG11	1:A:361:VAL:HB	2.03	0.41
1:A:317:ARG:NH1	1:A:834:ASP:O	2.54	0.41
1:A:849:GLN:HB3	1:A:992:MET:SD	2.61	0.41
1:A:1184:LEU:HD12	1:A:1184:LEU:HA	1.87	0.41
1:A:92:TYR:HE1	1:A:162:ALA:HB1	1.85	0.41
1:A:100:LEU:HB2	1:A:216:TRP:HH2	1.85	0.41
1:A:175:TYR:HD1	1:A:904:LEU:HD13	1.85	0.41
1:A:562:LEU:HB3	1:A:570:SER:HB2	2.01	0.41
1:A:853:VAL:HG22	1:A:985:TYR:HD2	1.86	0.41
1:A:1038:GLU:O	1:A:1067:SER:OG	2.38	0.41
1:A:1079:ALA:HB1	1:A:1249:SER:H	1.85	0.41
1:A:1082:SER:N	4:A:1403:ATP:O2A	2.54	0.41
1:A:811:LEU:HD12	1:A:811:LEU:HA	1.89	0.41
1:A:421:LYS:HD2	1:A:421:LYS:HA	1.88	0.41
1:A:349:SER:O	1:A:353:VAL:HG23	2.20	0.41
1:A:1276:LEU:HD23	1:A:1276:LEU:HA	1.97	0.41
1:A:321:LEU:HD23	1:A:321:LEU:HA	1.89	0.40
1:A:412:VAL:HG22	1:A:469:VAL:HG22	2.02	0.40
1:A:850:VAL:HG23	1:A:992:MET:HG2	2.03	0.40
1:A:892:LEU:HD23	1:A:892:LEU:HA	1.95	0.40
1:A:1153:VAL:HG21	1:A:1188:ALA:HB2	2.02	0.40
1:A:508:ILE:HD13	1:A:508:ILE:HA	1.96	0.40
1:A:911:LEU:HD22	1:A:915:ARG:NH2	2.37	0.40
1:A:734:TRP:HZ2	1:A:764:TYR:HA	1.86	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	1212/1344 (90%)	1167 (96%)	44 (4%)	1 (0%)	48 77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1236	ASN

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	1062/1178 (90%)	1041 (98%)	21 (2%)	50 71

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	ASP
1	A	78	PRO
1	A	92	TYR
1	A	170	MET
1	A	184	MET
1	A	260	SER
1	A	326	SER
1	A	350	ARG
1	A	387	GLN
1	A	480	GLN

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Mol	Chain	Res	Type
1	A	485	PHE
1	A	495	PHE
1	A	542	ARG
1	A	627	PHE
1	A	741	LYS
1	A	763	TRP
1	A	794	SER
1	A	912	TRP
1	A	915	ARG
1	A	1016	TYR
1	A	1167	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	481	GLN
1	A	1195	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	ATP	A	1403	3	26,33,33	0.60	0	31,52,52	0.73	2 (6%)
4	ATP	A	1405	3	26,33,33	0.60	0	31,52,52	0.74	2 (6%)
2	FMM	A	1401	-	41,44,44	0.87	2 (4%)	54,62,62	0.73	2 (3%)

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	ATP	A	1403	3	-	8/18/38/38	0/3/3/3
4	ATP	A	1405	3	-	6/18/38/38	0/3/3/3
2	FMM	A	1401	-	-	4/15/21/21	0/5/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1401	FMM	C10-C9	-3.83	1.34	1.39
2	A	1401	FMM	C8-C9	-2.34	1.49	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1401	FMM	C8-C9-C10	2.55	133.24	129.01
4	A	1405	ATP	C5-C6-N6	2.31	123.86	120.35
4	A	1403	ATP	C5-C6-N6	2.30	123.85	120.35
2	A	1401	FMM	O27-C26-C36	2.27	119.20	116.40
4	A	1405	ATP	PB-O3B-PG	2.03	139.81	132.83
4	A	1403	ATP	PB-O3B-PG	2.02	139.76	132.83

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1403	ATP	PB-O3B-PG-O2G
4	A	1403	ATP	C5'-O5'-PA-O3A
4	A	1405	ATP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
4	A	1405	ATP	C5'-O5'-PA-O2A
4	A	1405	ATP	C5'-O5'-PA-O3A
4	A	1405	ATP	O4'-C4'-C5'-O5'
4	A	1403	ATP	O4'-C4'-C5'-O5'
4	A	1403	ATP	C3'-C4'-C5'-O5'
4	A	1405	ATP	C3'-C4'-C5'-O5'
2	A	1401	FMM	C36-C26-O27-C28
4	A	1403	ATP	PA-O3A-PB-O3B
2	A	1401	FMM	C25-C26-O27-C28
2	A	1401	FMM	C39-C21-N22-C23
2	A	1401	FMM	C5-C6-N7-C8
4	A	1405	ATP	PA-O3A-PB-O1B
4	A	1403	ATP	PB-O3B-PG-O1G
4	A	1403	ATP	PG-O3B-PB-O2B
4	A	1403	ATP	C5'-O5'-PA-O1A

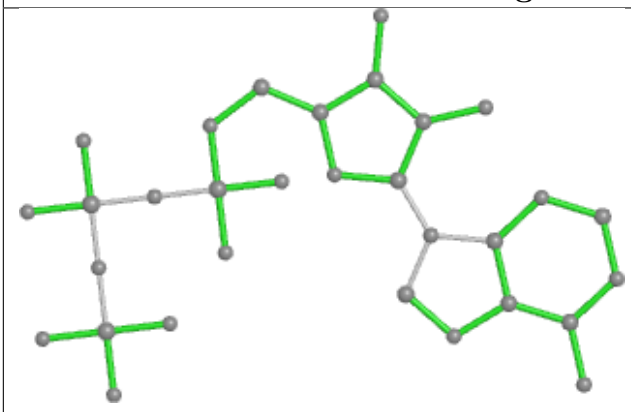
There are no ring outliers.

2 monomers are involved in 6 short contacts:

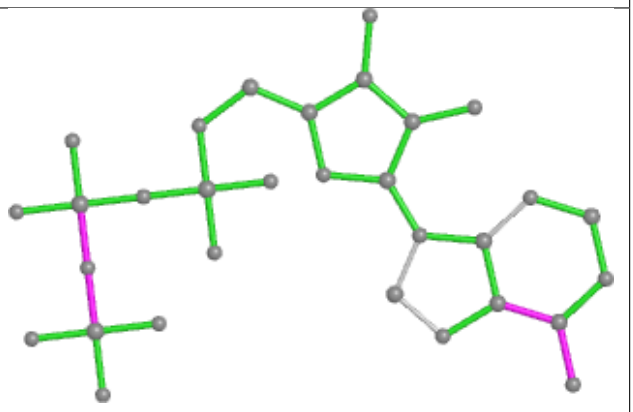
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1403	ATP	2	0
2	A	1401	FMM	4	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

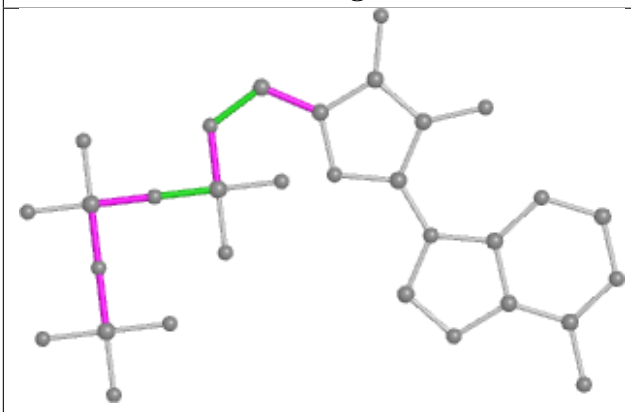
Ligand ATP A 1403



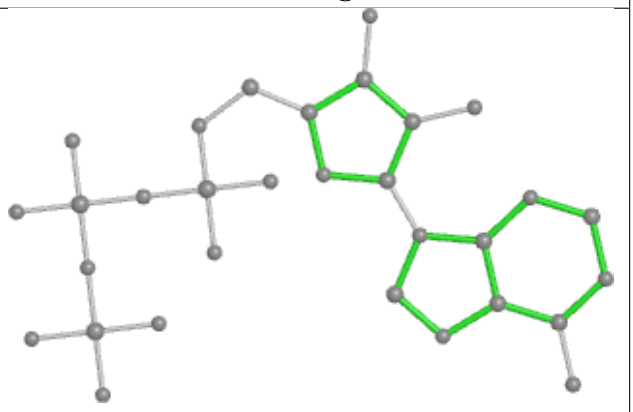
Bond lengths



Bond angles

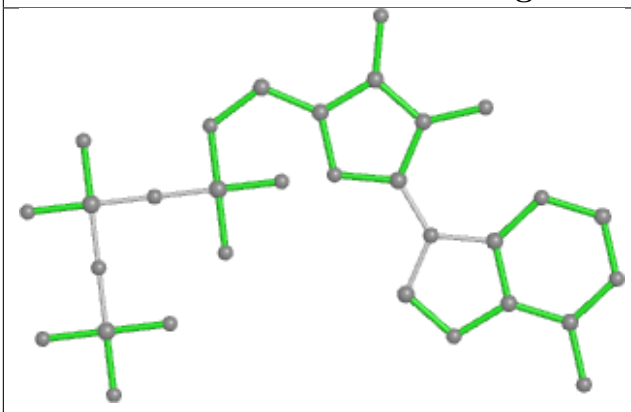


Torsions

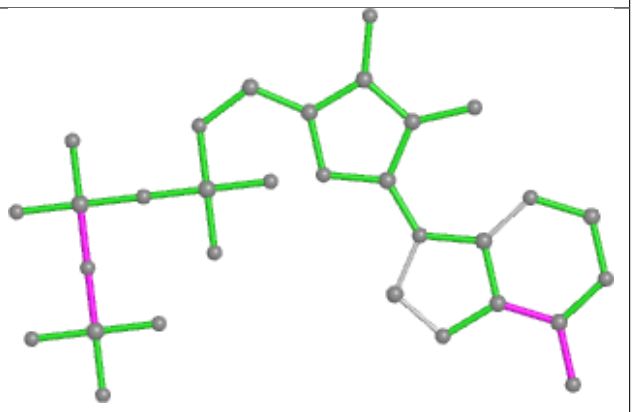


Rings

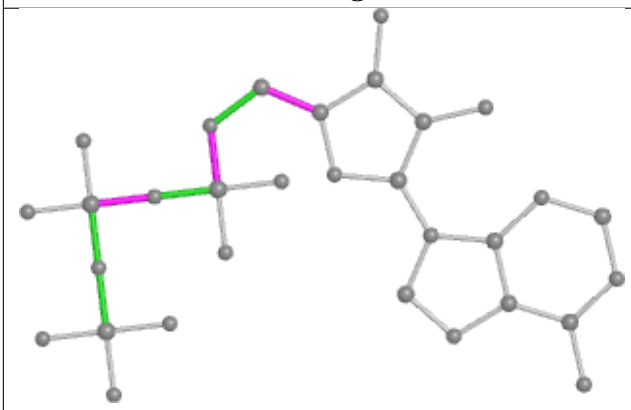
Ligand ATP A 1405



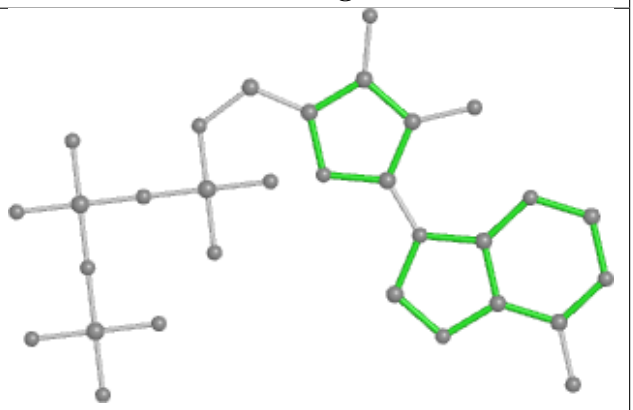
Bond lengths



Bond angles

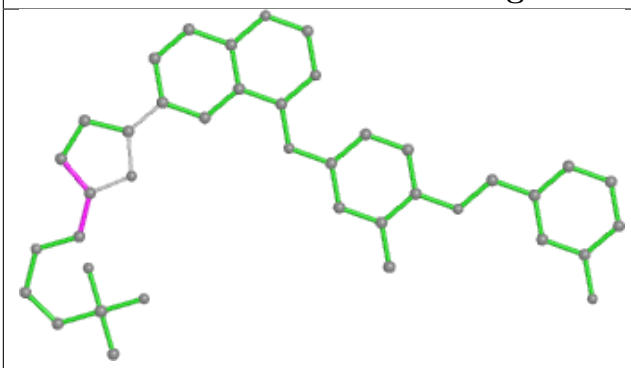


Torsions

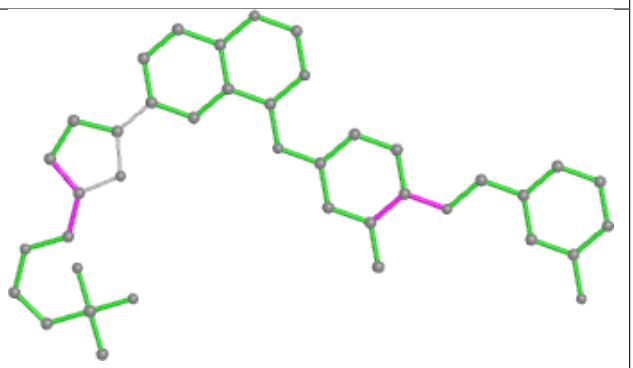


Rings

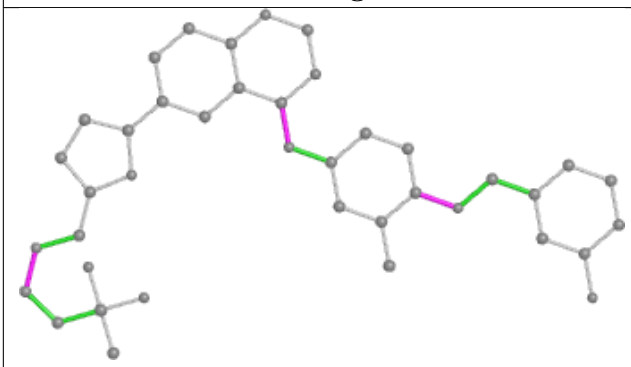
Ligand FMM A 1401



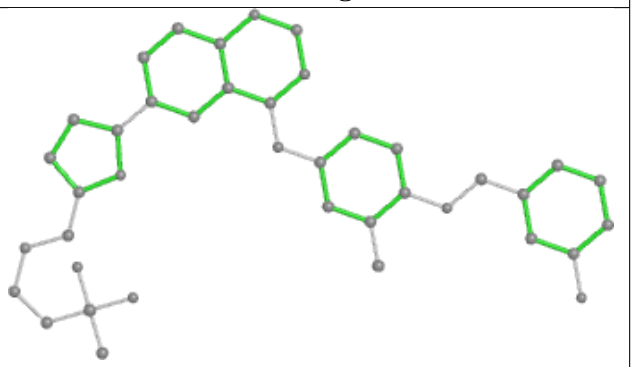
Bond lengths



Bond angles



Torsions



Rings

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.

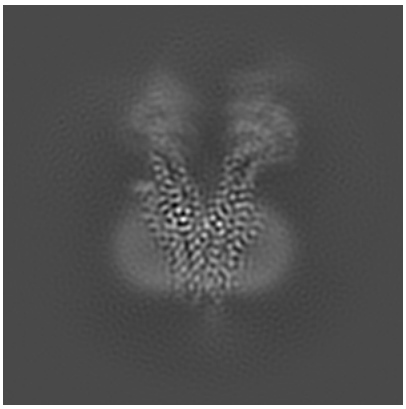
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-39911. These allow visual inspection of the internal detail of the map and identification of artifacts.

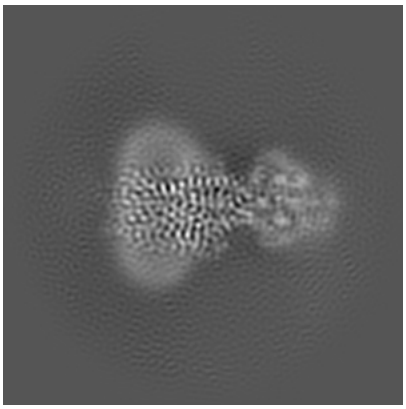
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

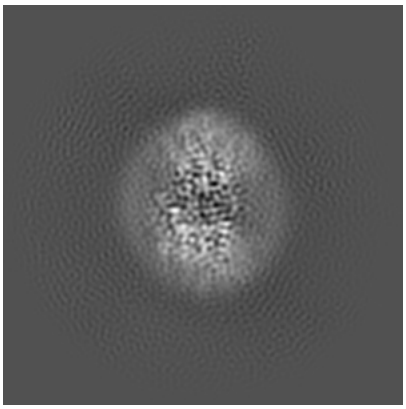
6.1.1 Primary map



X

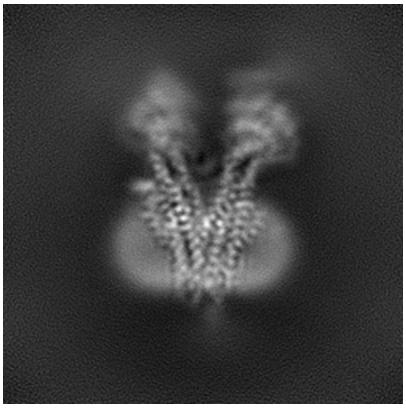


Y

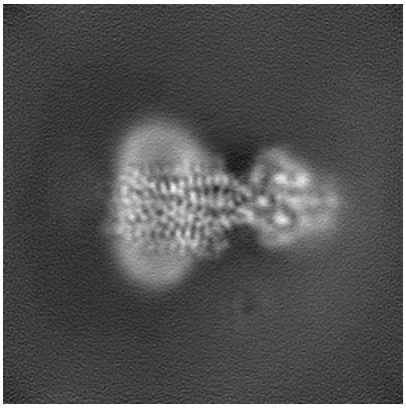


Z

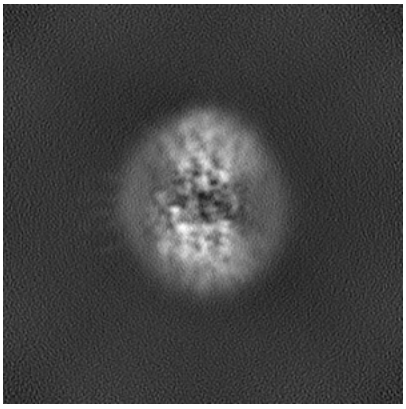
6.1.2 Raw map



X



Y

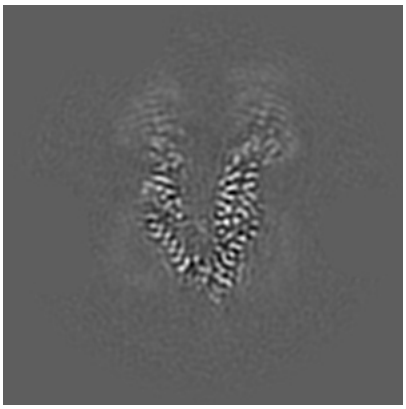


Z

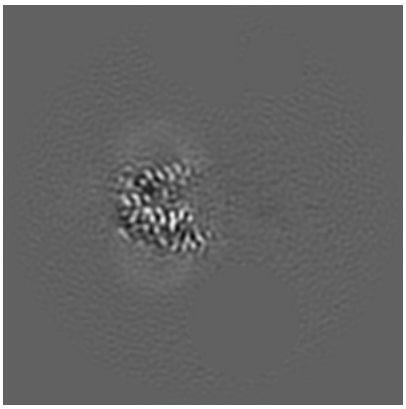
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

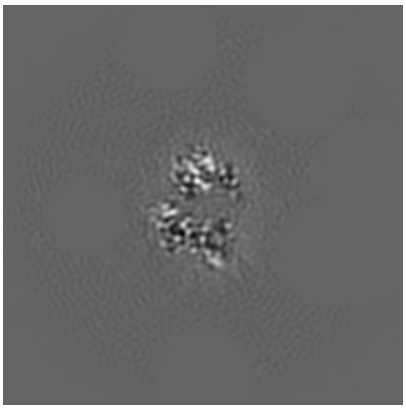
6.2.1 Primary map



X Index: 128

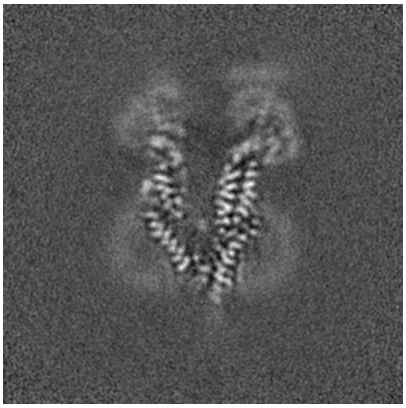


Y Index: 128

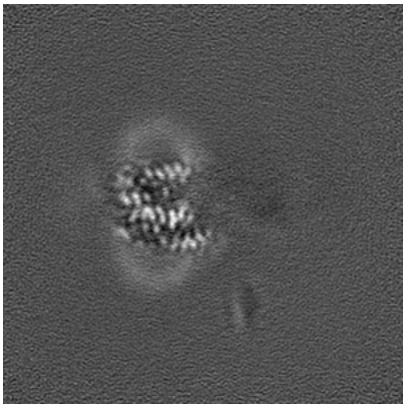


Z Index: 128

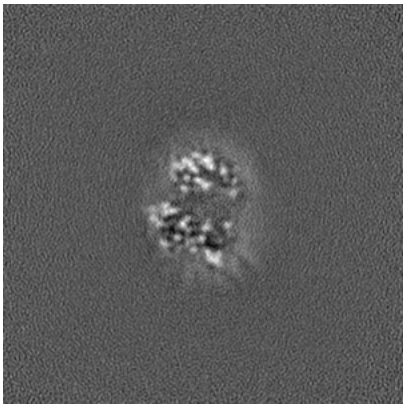
6.2.2 Raw map



X Index: 128



Y Index: 128

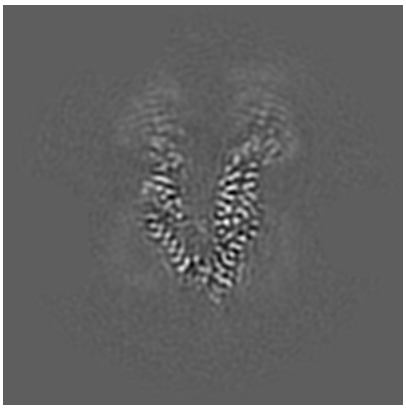


Z Index: 128

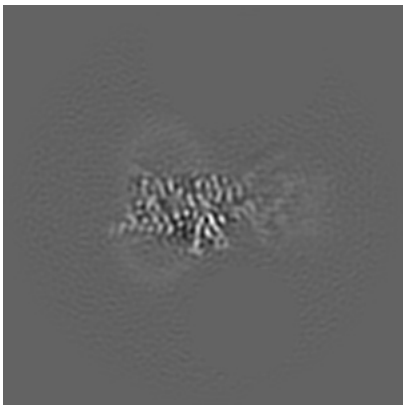
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

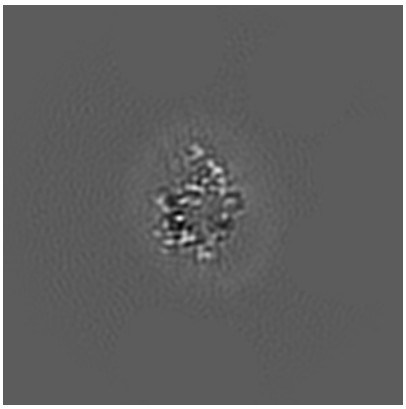
6.3.1 Primary map



X Index: 128

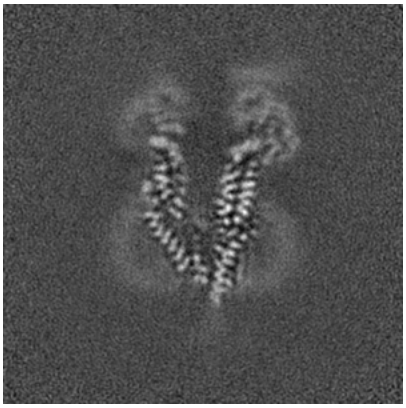


Y Index: 112

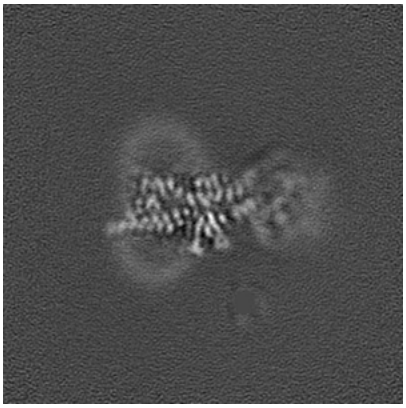


Z Index: 115

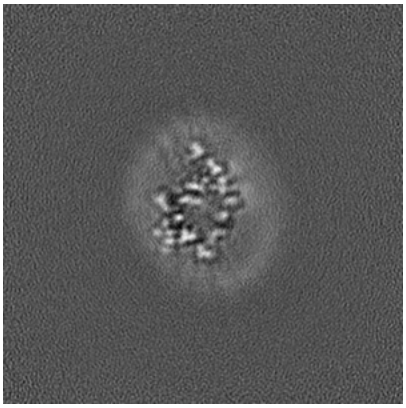
6.3.2 Raw map



X Index: 129



Y Index: 112

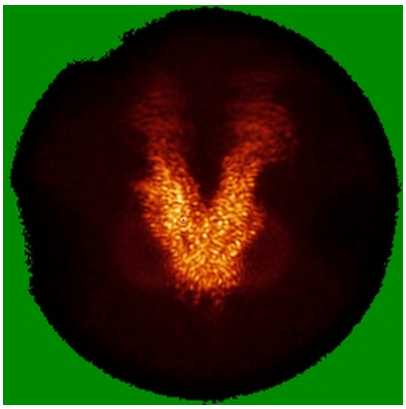


Z Index: 115

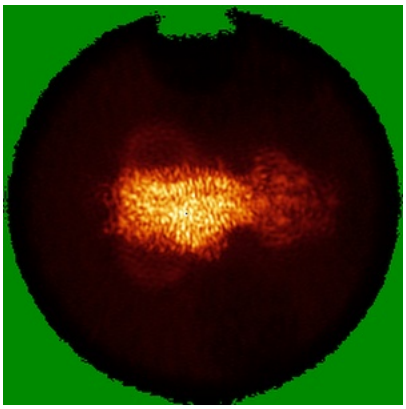
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

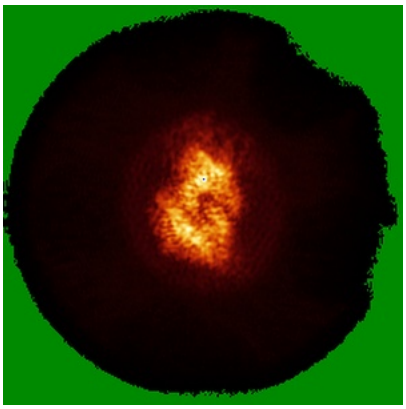
6.4.1 Primary map



X

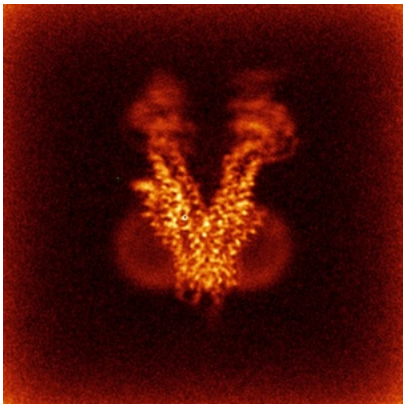


Y

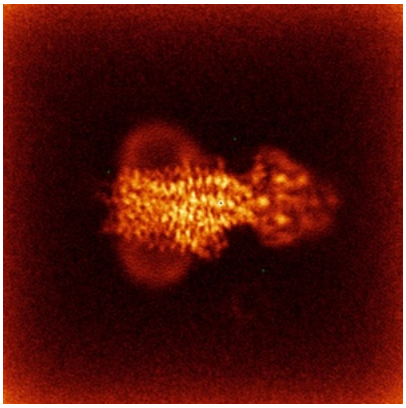


Z

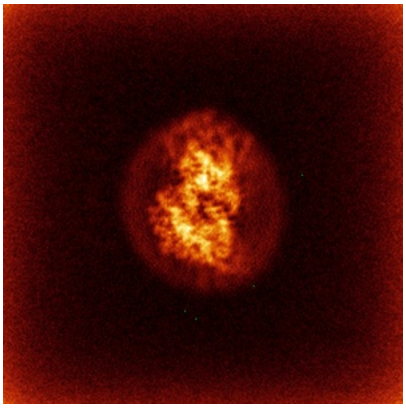
6.4.2 Raw map



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.

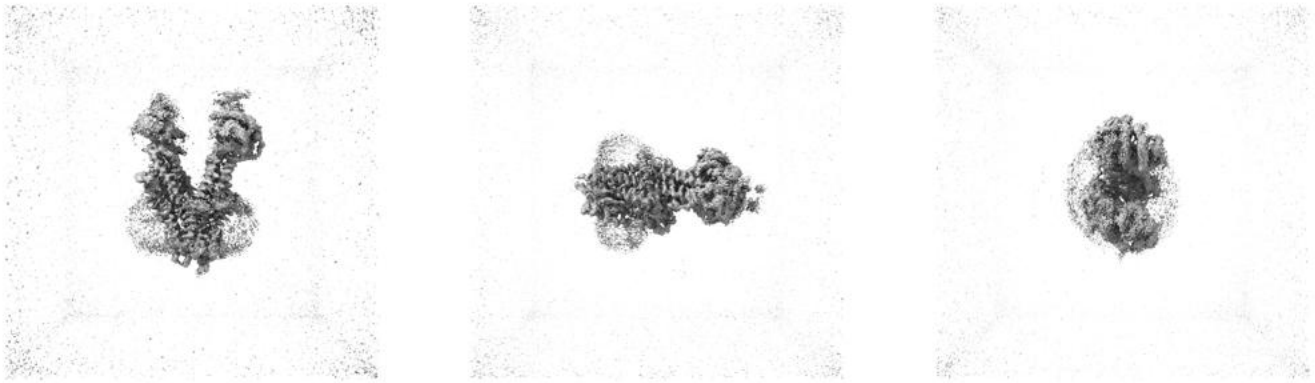
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.11. 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



X Y Z

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.

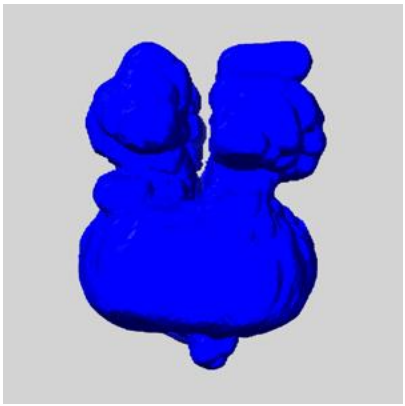
6.6 Mask visualisation (i)

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

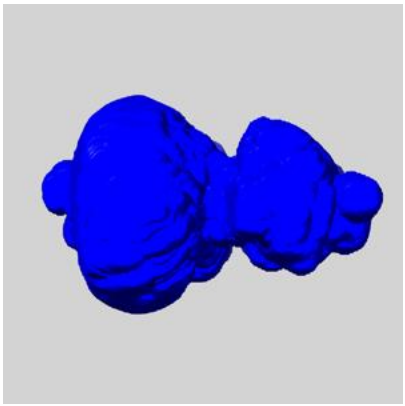
A mask typically either:

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

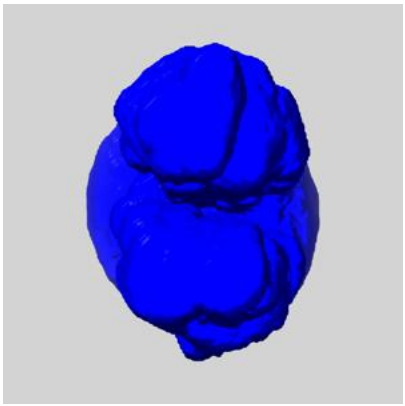
6.6.1 emd_39911_msk_1.map (i)



X



Y

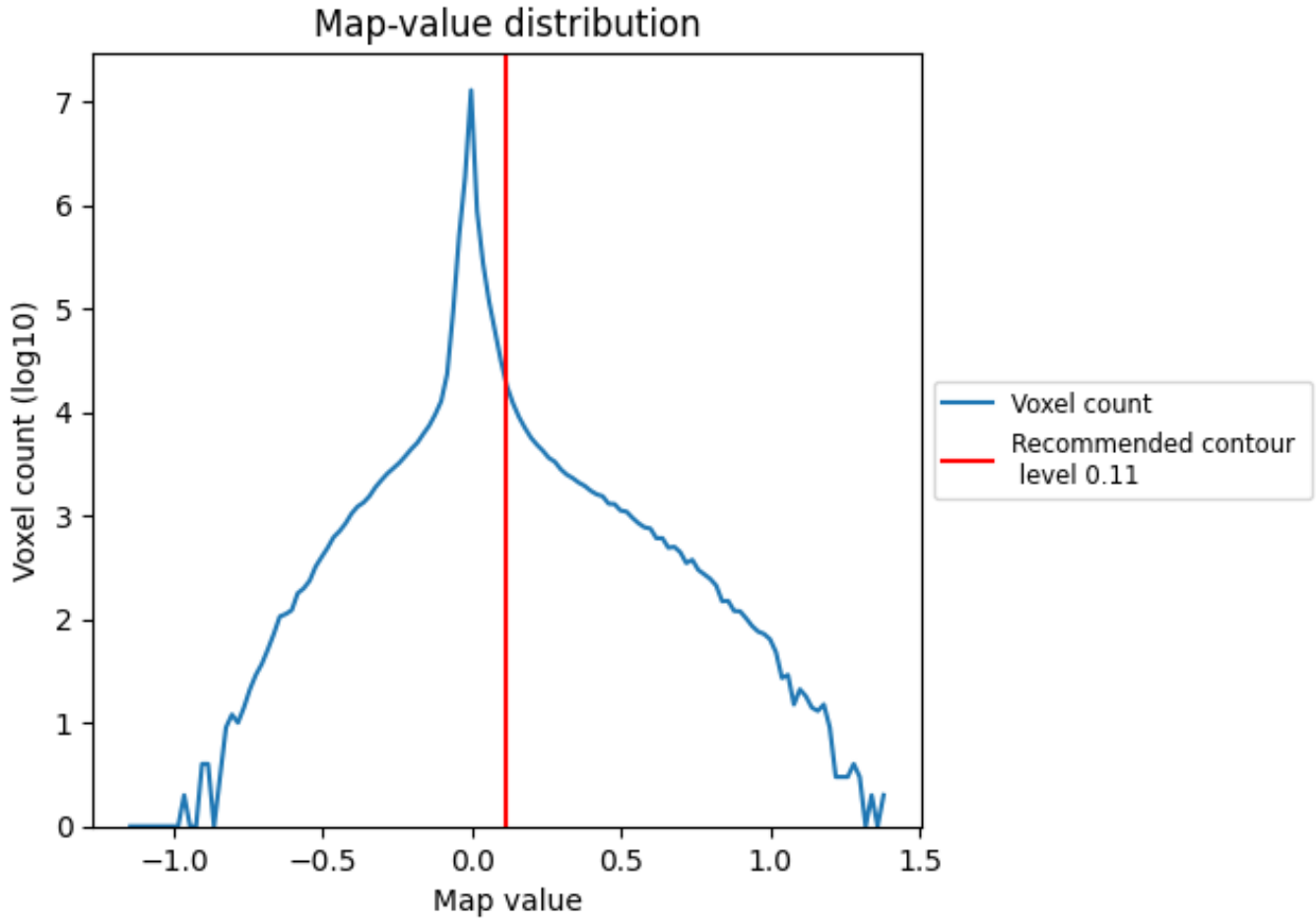


Z

7 Map analysis

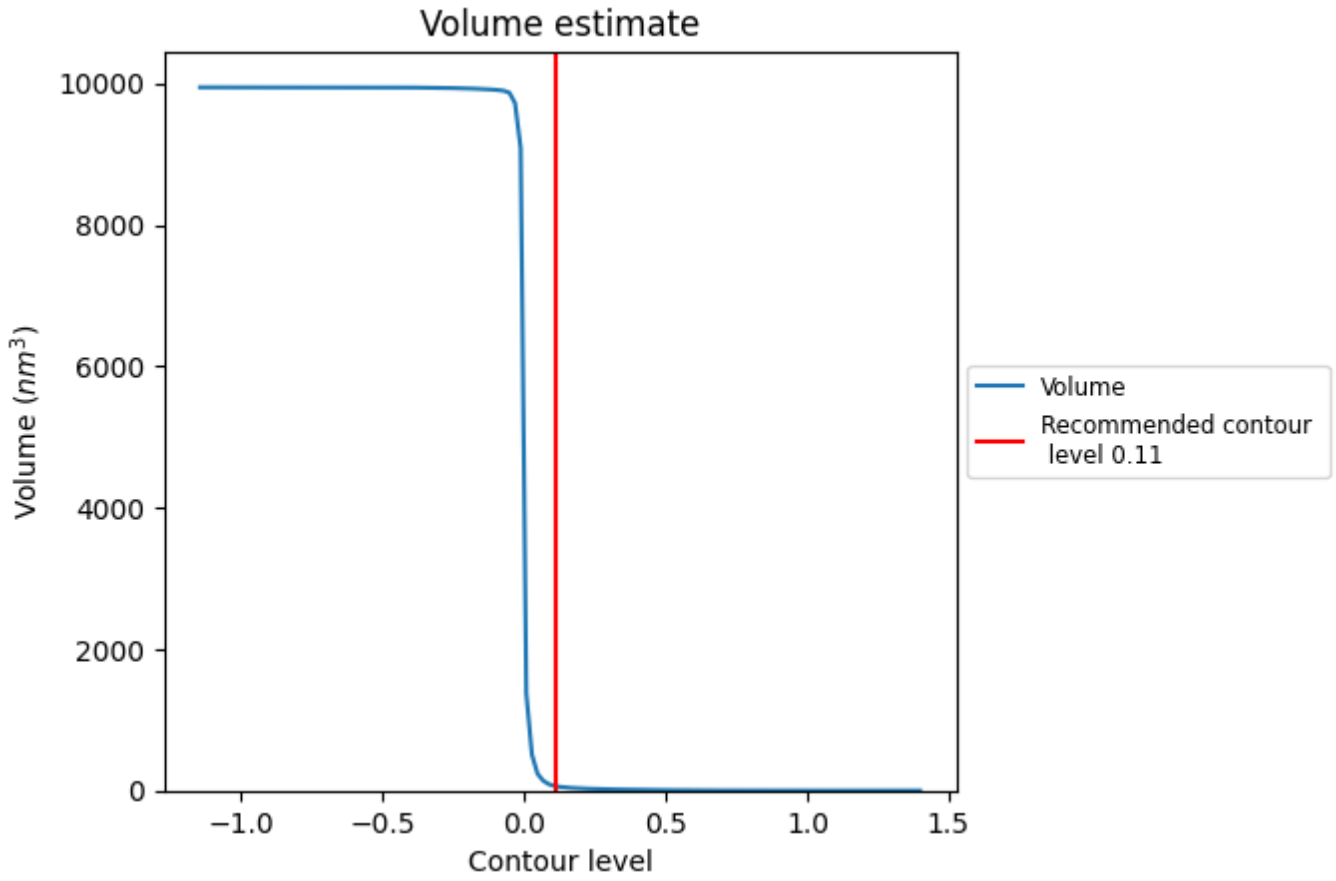
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

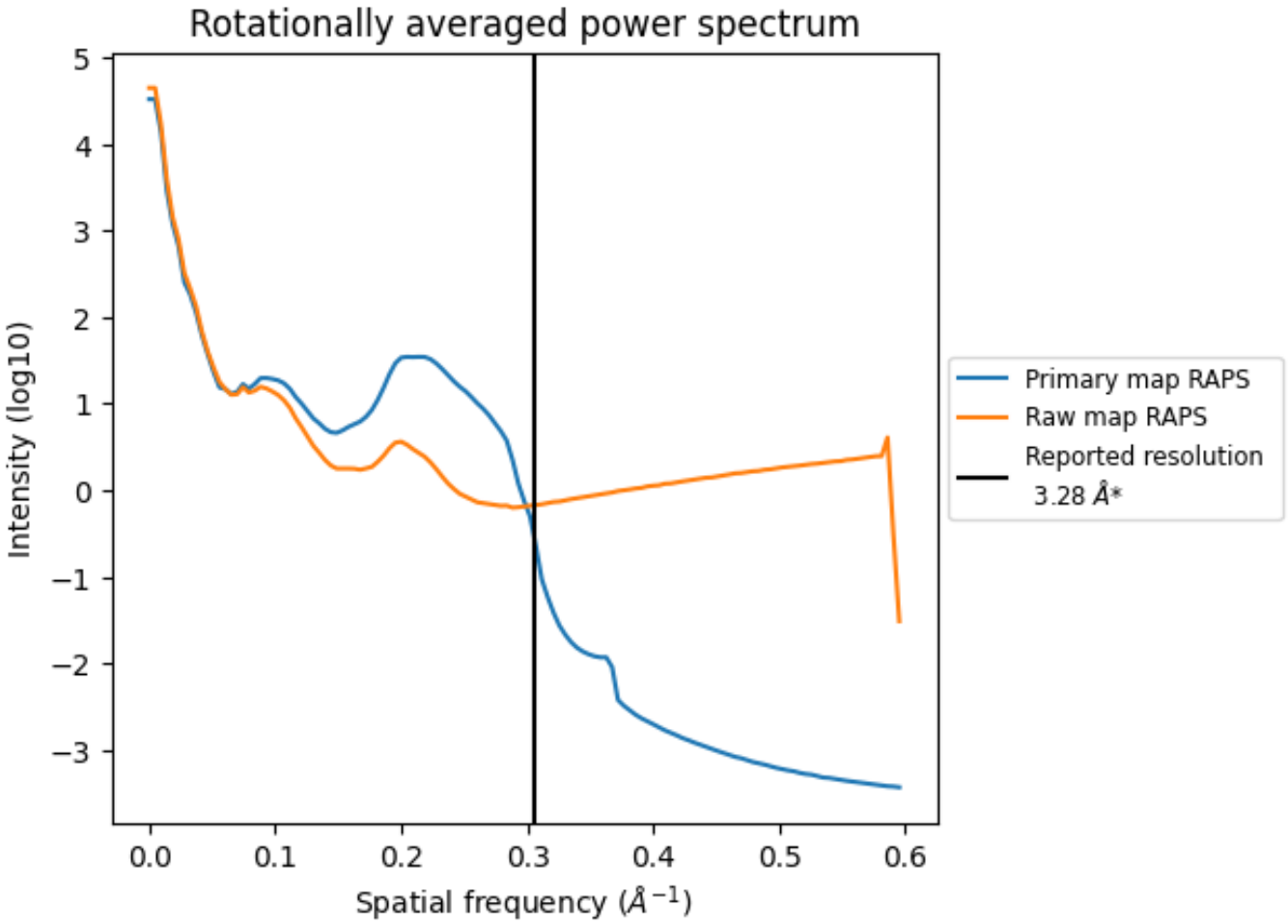
7.2 Volume estimate



The volume at the recommended contour level is 63 nm^3; this corresponds to an approximate mass of 57 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 (i)

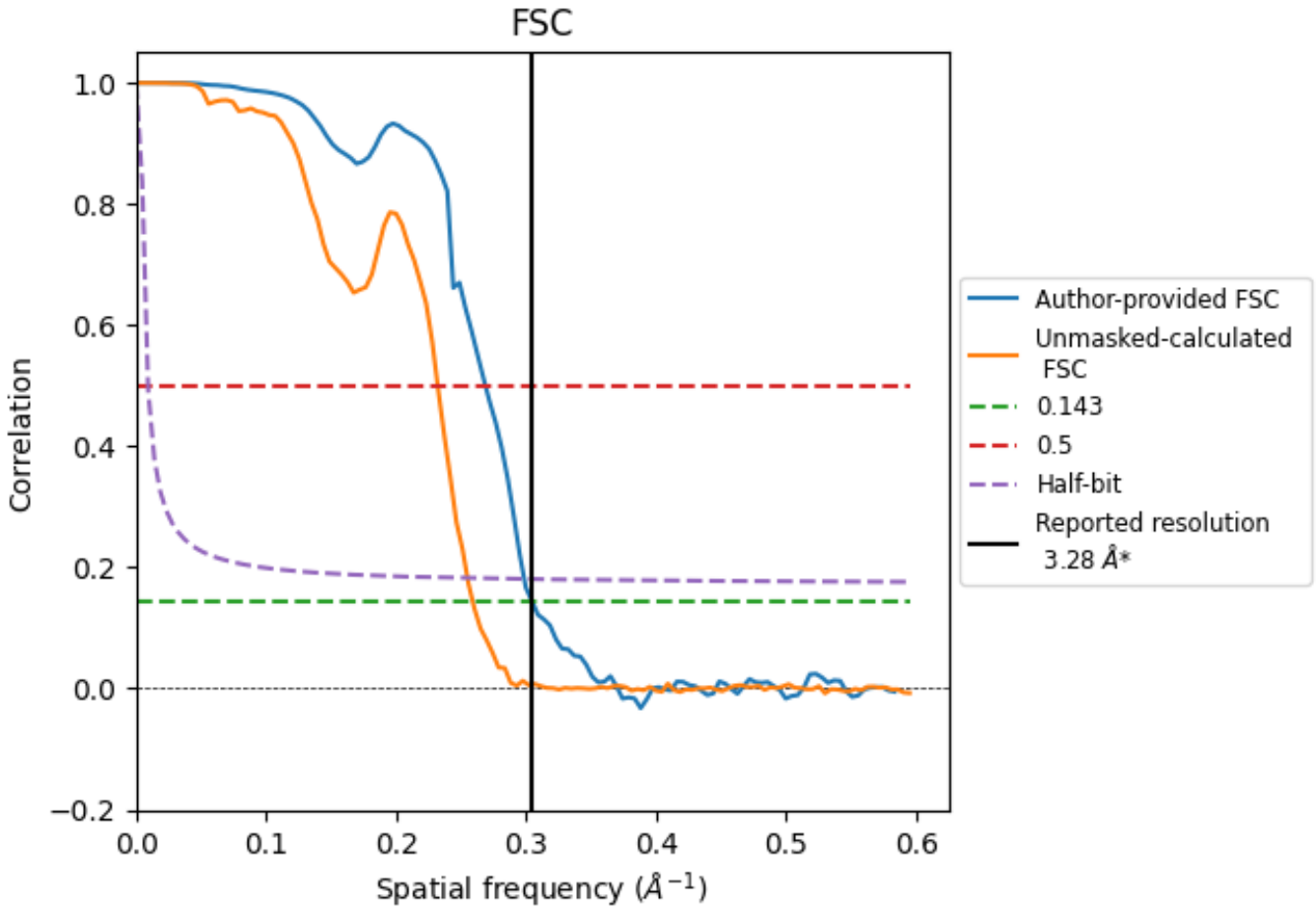


*Reported resolution corresponds to spatial frequency of 0.305 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.305 Å^{-1}

8.2 Resolution estimates (i)

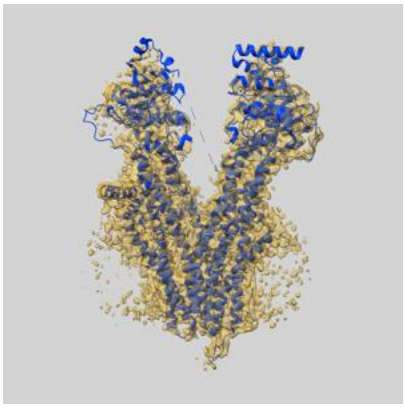
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.28	-	-
Author-provided FSC curve	3.28	3.72	3.35
Unmasked-calculated*	3.86	4.31	3.92

*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 3.86 differs from the reported value 3.28 by more than 10 %

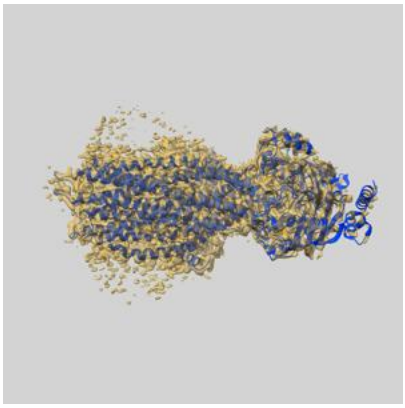
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-39911 and PDB model 8ZBU. Per-residue inclusion information can be found in section 3 on page 6.

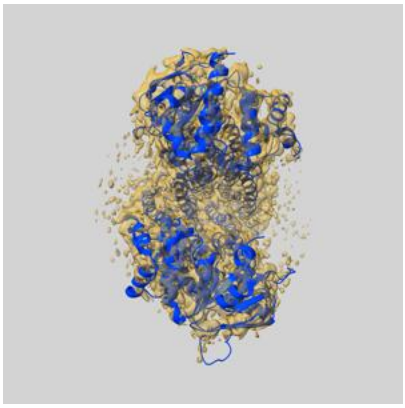
9.1 Map-model overlay



X



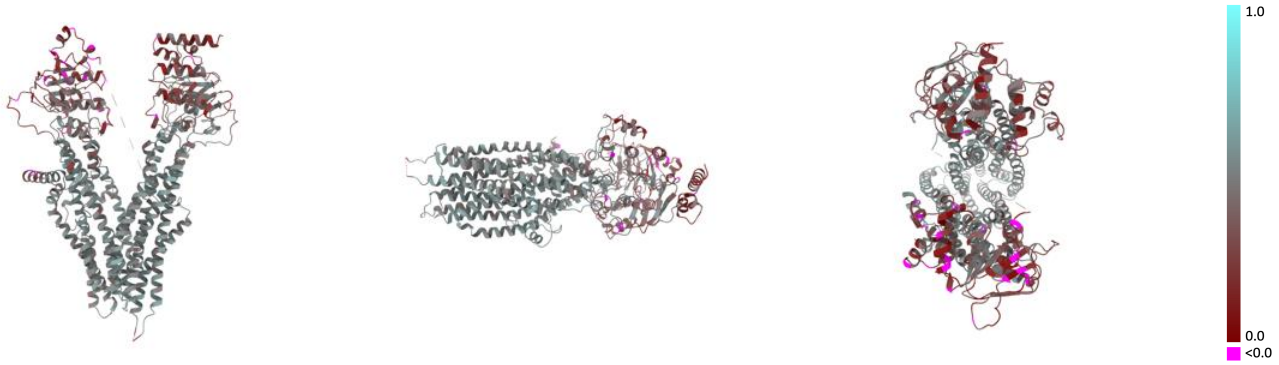
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.11 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.

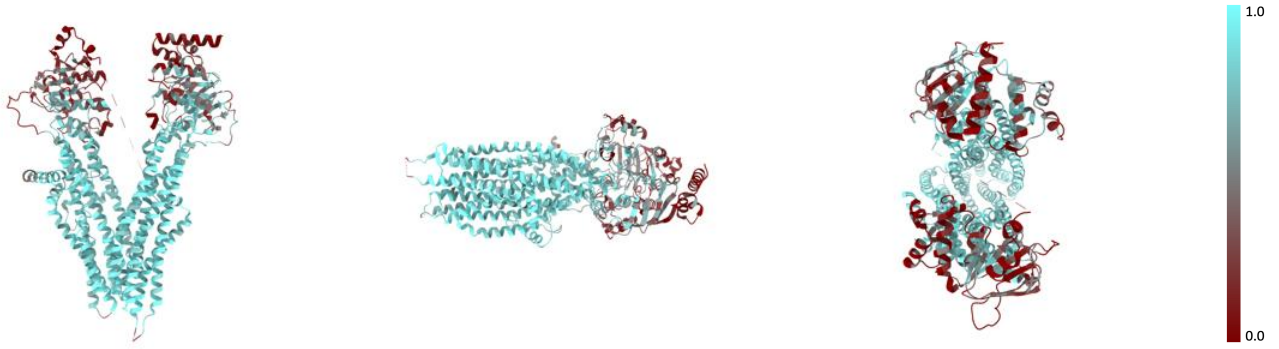
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

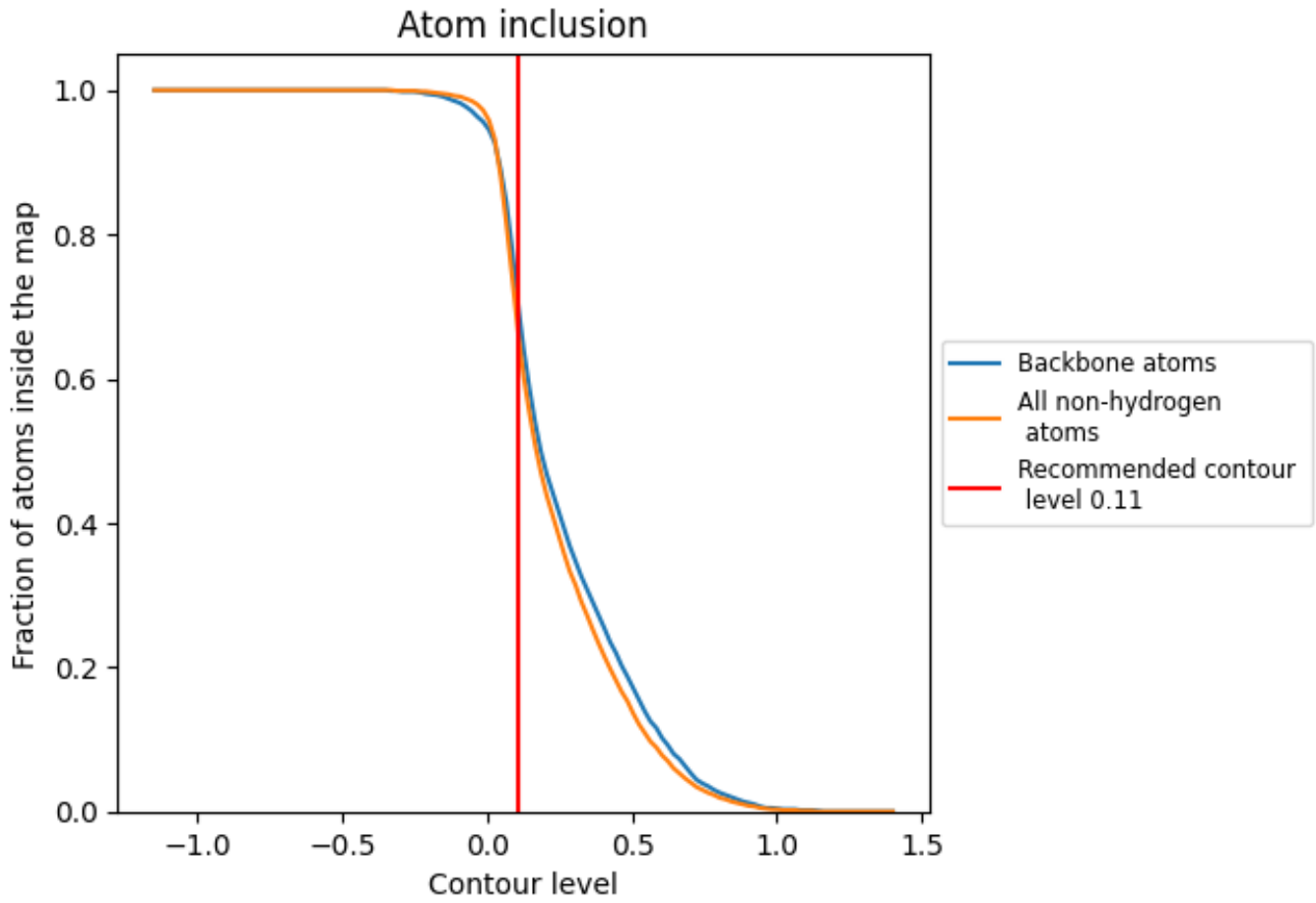
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.11).

9.4 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6560	0.4260
A	0.6560	0.4260