



Full wwPDB EM Validation Report ⓘ

Aug 27, 2024 – 04:14 PM JST

PDB ID : 8XOK
EMDB ID : EMD-38532
Title : Cryo-EM structure of human ABCC4
Authors : Zhang, P.F.; Liu, Z.
Deposited on : 2024-01-01
Resolution : 2.84 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.dev112
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) : 2.38.2

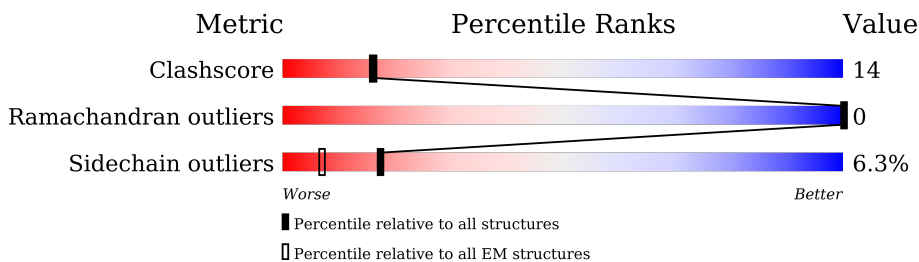
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.84 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	1325	

2 Entry composition i

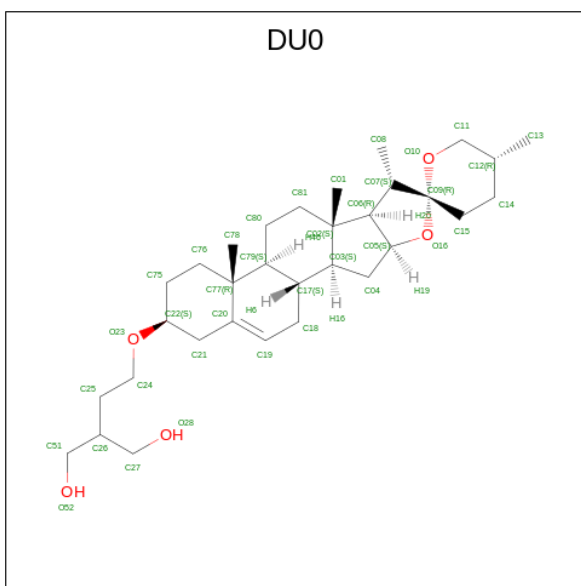
There are 3 unique types of molecules in this entry. The entry contains 10152 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	1206	9616	6237	1620	1716	43	0	0

- Molecule 2 is 2-[2-[(1 {S},2 {S},4 {S},5' {R},6 {R},7 {S},8 {R},9 {S},12 {S},13 {R},16 {S})]-5',7,9,13-tetramethylspiro[5-oxapentacyclo[10.8.0.0^{2,9}.0^{4,8}.0^{13,18}]]icos-18-ene-6,2'-oxane]-16-yl]oxyethyl]propane-1,3-diol (three-letter code: DU0) (formula: C₃₂H₅₂O₅).



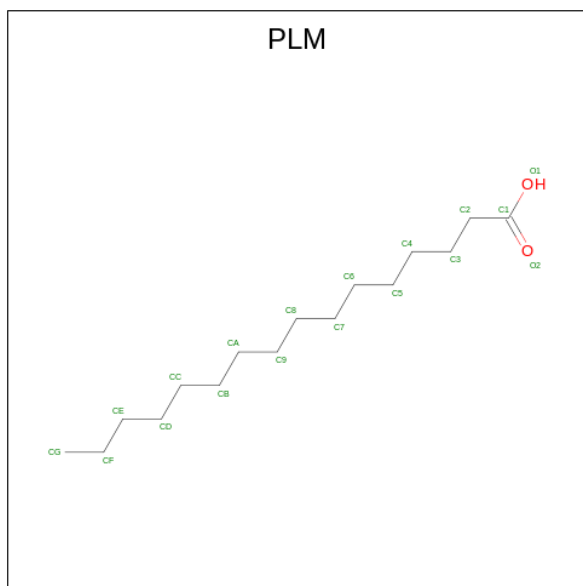
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
2	A	1	37	32	5	0
2	A	1	37	32	5	0
2	A	1	37	32	5	0
2	A	1	37	32	5	0
2	A	1	37	32	5	0

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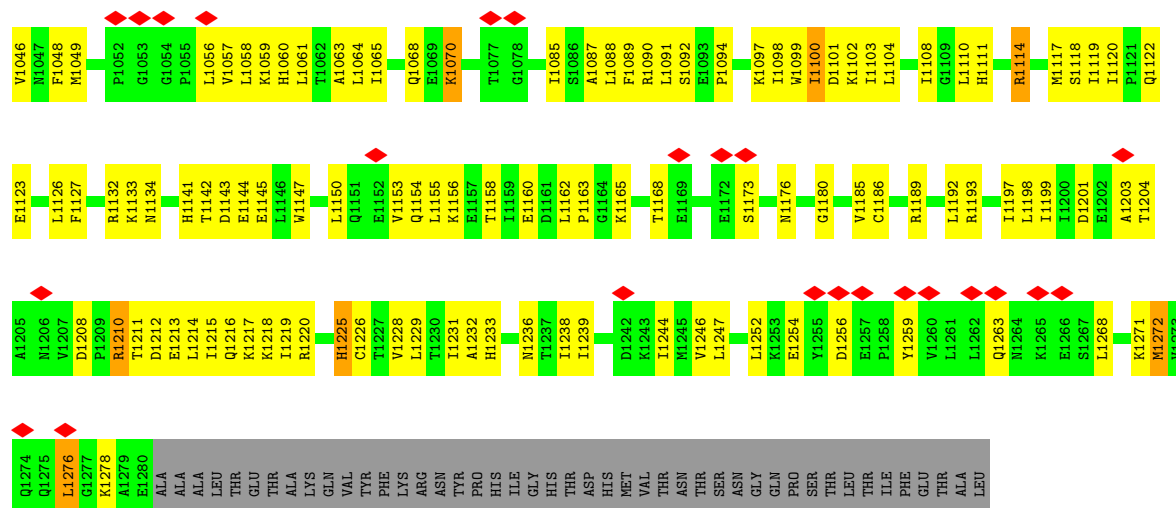
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Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	C	O	0
			37	32	5	
2	A	1	Total	C	O	0
			37	32	5	
2	A	1	Total	C	O	0
			37	32	5	
2	A	1	Total	C	O	0
			37	32	5	
2	A	1	Total	C	O	0
			37	32	5	
2	A	1	Total	C	O	0
			37	32	5	
2	A	1	Total	C	O	0
			37	32	5	
2	A	1	Total	C	O	0
			37	32	5	

- Molecule 3 is PALMITIC ACID (three-letter code: PLM) (formula: C₁₆H₃₂O₂).



Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			18	16	2	



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1487898	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 ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.477	Depositor
Minimum map value	-0.246	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.053	Depositor
Map size (\AA)	212.48, 212.48, 212.48	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.83, 0.83, 0.83	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: PLM, DU0

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	0.30	0/9821	0.54	1/13311 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	834	ASP	CB-CG-OD1	5.41	123.17	118.30

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	9616	0	9868	282	0
2	A	518	0	0	1	0
3	A	18	0	31	1	0
All	All	10152	0	9899	283	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 (283) 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:515:LYS:HE2	1:A:515:LYS:H	1.43	0.84
1:A:27:LEU:HD22	1:A:943:THR:HG22	1.67	0.76
1:A:474:ARG:NH2	1:A:551:GLN:O	2.22	0.72
1:A:571:ARG:HH11	1:A:574:PHE:HB3	1.54	0.72
1:A:198:LEU:HD22	1:A:904:LEU:HD22	1.73	0.70
1:A:1259:TYR:O	1:A:1263:GLN:NE2	2.24	0.70
1:A:555:ILE:HA	1:A:586:ILE:HB	1.71	0.69
1:A:404:SER:HA	1:A:407:LYS:HE3	1.72	0.69
1:A:1025:TRP:HA	1:A:1110:LEU:HB2	1.73	0.69
1:A:275:THR:HB	1:A:299:ILE:HD11	1.74	0.69
1:A:510:ALA:O	1:A:572:HIS:NE2	2.21	0.68
1:A:194:ILE:HG22	1:A:904:LEU:HD21	1.75	0.68
1:A:520:LEU:HD22	1:A:526:THR:HG21	1.77	0.67
1:A:1153:VAL:HG23	1:A:1218:LYS:HE2	1.77	0.66
1:A:1236:ASN:HA	1:A:1239:ILE:HD12	1.77	0.66
1:A:461:GLU:OE2	1:A:915:ARG:NH1	2.29	0.65
1:A:1048:PHE:HZ	1:A:1092:SER:HB3	1.61	0.65
1:A:742:GLN:HG2	1:A:759:LEU:HD22	1.77	0.65
1:A:458:VAL:HG11	1:A:557:LEU:HD21	1.79	0.65
1:A:1144:GLU:N	1:A:1144:GLU:OE1	2.31	0.64
1:A:474:ARG:H	1:A:554:ASP:HB2	1.63	0.63
1:A:92:TYR:OH	1:A:209:THR:O	2.17	0.62
1:A:1247:LEU:HD13	1:A:1252:LEU:HD13	1.81	0.62
1:A:581:ILE:HG22	1:A:582:LEU:HD23	1.81	0.61
1:A:708:GLY:O	1:A:792:ASN:ND2	2.32	0.61
1:A:1210:ARG:NH1	1:A:1214:LEU:HB2	2.15	0.61
1:A:1246:VAL:HB	1:A:1254:GLU:HB2	1.82	0.61
1:A:596:TYR:HA	1:A:599:ALA:HB3	1.82	0.60
1:A:794:SER:OG	1:A:833:ASP:OD1	2.15	0.60
1:A:853:VAL:HG11	1:A:989:LEU:HB2	1.83	0.60
1:A:183:ASN:ND2	1:A:461:GLU:O	2.34	0.60
1:A:26:TRP:CH2	1:A:943:THR:HG21	2.36	0.60
1:A:288:MET:HG3	1:A:1089:PHE:HE1	1.67	0.60
1:A:731:GLN:HE21	1:A:772:THR:HB	1.65	0.60
1:A:537:GLY:HA2	1:A:540:LYS:HD2	1.83	0.60
1:A:560:ASP:OD2	1:A:592:HIS:ND1	2.29	0.60
1:A:262:ARG:NH1	1:A:262:ARG:HB2	2.17	0.59
1:A:142:THR:HA	1:A:145:THR:HG22	1.84	0.59
1:A:1238:ILE:HG21	1:A:1244:ILE:HD13	1.84	0.59
1:A:577:CYS:HA	1:A:581:ILE:HB	1.85	0.58
1:A:993:PHE:HE1	3:A:1415:PLM:HE2	1.67	0.58
1:A:265:THR:HG22	1:A:309:LYS:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:LEU:HB2	1:A:589:LEU:HD23	1.86	0.58
1:A:1155:LEU:HD22	1:A:1158:THR:HB	1.85	0.58
1:A:1165:LYS:O	1:A:1168:THR:OG1	2.22	0.58
1:A:38:ARG:NH1	1:A:40:GLU:OE2	2.37	0.57
1:A:498:LYS:O	1:A:550:TYR:OH	2.21	0.57
1:A:1213:GLU:O	1:A:1217:LYS:HG2	2.05	0.57
1:A:1117:MET:HA	1:A:1197:ILE:HD11	1.85	0.57
1:A:1144:GLU:HA	1:A:1147:TRP:HD1	1.69	0.57
1:A:1141:HIS:NE2	1:A:1192:LEU:O	2.30	0.57
1:A:1150:LEU:HG	1:A:1155:LEU:HB3	1.87	0.57
1:A:284:ARG:NH1	1:A:814:ASP:OD1	2.38	0.57
1:A:621:LEU:H	1:A:621:LEU:HD23	1.69	0.57
1:A:574:PHE:O	1:A:579:CYS:N	2.38	0.56
1:A:1143:ASP:OD1	1:A:1147:TRP:NE1	2.38	0.56
1:A:1198:LEU:O	1:A:1228:VAL:HA	2.06	0.56
1:A:262:ARG:HB2	1:A:262:ARG:HH11	1.70	0.56
1:A:183:ASN:OD1	1:A:183:ASN:N	2.38	0.56
1:A:604:LEU:HB2	1:A:614:LYS:HZ1	1.70	0.56
1:A:292:GLU:OE1	1:A:1111:HIS:NE2	2.38	0.56
1:A:842:ASP:OD2	1:A:999:GLN:NE2	2.28	0.56
1:A:493:ILE:HG21	1:A:504:TYR:CE1	2.41	0.56
1:A:1070:LYS:HG3	1:A:1228:VAL:HG22	1.87	0.56
1:A:558:LEU:HB3	1:A:561:PRO:HG3	1.88	0.55
1:A:1150:LEU:HB3	1:A:1156:LYS:HG2	1.88	0.55
1:A:167:ARG:NH1	1:A:206:ASP:OD2	2.33	0.55
1:A:1199:ILE:HD12	1:A:1229:LEU:HB2	1.88	0.55
1:A:336:PHE:O	1:A:340:VAL:HG23	2.05	0.55
1:A:1118:SER:HB3	1:A:1198:LEU:HD23	1.89	0.55
1:A:853:VAL:HG22	1:A:985:TYR:HB3	1.87	0.55
1:A:1035:TRP:HZ2	1:A:1100:ILE:HD11	1.71	0.55
1:A:1048:PHE:H	1:A:1058:LEU:HB2	1.72	0.55
1:A:717:LEU:HD13	1:A:785:LEU:HD23	1.88	0.55
1:A:500:GLU:HG2	1:A:503:ARG:HB3	1.88	0.54
1:A:1214:LEU:O	1:A:1218:LYS:HG2	2.07	0.54
1:A:484:VAL:HG13	1:A:492:ASN:ND2	2.23	0.54
1:A:594:LEU:O	1:A:598:LYS:NZ	2.30	0.54
1:A:616:THR:OG1	1:A:617:TYR:N	2.41	0.54
1:A:1035:TRP:CZ2	1:A:1100:ILE:HD11	2.42	0.54
1:A:280:ILE:HG22	1:A:818:ILE:HD12	1.90	0.54
1:A:746:ASN:HA	1:A:749:VAL:HG22	1.90	0.54
1:A:288:MET:HG3	1:A:1089:PHE:CE1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:LYS:HE2	1:A:515:LYS:N	2.17	0.54
1:A:839:THR:HG22	1:A:1003:VAL:HG23	1.90	0.54
1:A:1057:VAL:O	1:A:1058:LEU:HD23	2.08	0.53
1:A:605:ILE:HG13	1:A:613:GLN:HE22	1.74	0.53
1:A:1132:ARG:NH2	1:A:1143:ASP:OD2	2.41	0.53
1:A:443:VAL:HA	1:A:604:LEU:O	2.08	0.53
1:A:702:LYS:O	1:A:706:ARG:HG2	2.09	0.53
1:A:170:MET:HG3	1:A:205:PHE:CE2	2.44	0.53
1:A:485:PHE:H	1:A:485:PHE:HD1	1.57	0.53
2:A:1414:DU0:O28	2:A:1414:DU0:O52	2.26	0.53
1:A:1043:PHE:HD2	1:A:1063:ALA:HB3	1.75	0.52
1:A:1201:ASP:HA	1:A:1231:ILE:HG13	1.89	0.52
1:A:562:LEU:HA	1:A:565:VAL:HG22	1.90	0.52
1:A:782:ARG:HG3	1:A:783:SER:N	2.24	0.52
1:A:1031:PRO:HG3	1:A:1108:ILE:HG23	1.91	0.52
1:A:1162:LEU:HD13	1:A:1163:PRO:HD2	1.92	0.52
1:A:975:ASP:OD1	1:A:978:GLN:NE2	2.27	0.52
1:A:1180:GLY:HA2	1:A:1211:THR:HG21	1.92	0.51
1:A:1123:GLU:N	1:A:1123:GLU:OE2	2.44	0.51
1:A:428:LEU:HD11	1:A:431:LEU:HD12	1.92	0.51
1:A:717:LEU:HD11	1:A:786:VAL:HG23	1.91	0.51
1:A:177:LYS:NZ	1:A:394:GLU:OE1	2.44	0.51
1:A:402:LEU:HD12	1:A:404:SER:H	1.75	0.51
1:A:408:LYS:HG2	1:A:437:PRO:HG3	1.92	0.51
1:A:965:PHE:O	1:A:969:ILE:HG12	2.11	0.51
1:A:1211:THR:O	1:A:1215:ILE:HG13	2.11	0.51
1:A:428:LEU:HD21	1:A:431:LEU:HB2	1.93	0.50
1:A:1122:GLN:HB2	1:A:1123:GLU:OE2	2.11	0.50
1:A:577:CYS:O	1:A:582:LEU:N	2.27	0.50
1:A:1210:ARG:HH12	1:A:1214:LEU:HB2	1.76	0.50
1:A:1144:GLU:HA	1:A:1147:TRP:CD1	2.47	0.50
1:A:570:SER:O	1:A:573:LEU:HG	2.12	0.50
1:A:1042:ILE:HG22	1:A:1064:LEU:HA	1.94	0.50
1:A:1119:ILE:HG13	1:A:1199:ILE:HB	1.93	0.49
1:A:289:TYR:HA	1:A:1193:ARG:HH22	1.78	0.49
1:A:531:ARG:NH2	1:A:902:SER:O	2.46	0.49
1:A:1215:ILE:O	1:A:1219:ILE:HG13	2.12	0.49
1:A:1120:ILE:HD12	1:A:1198:LEU:HD21	1.95	0.49
1:A:475:ILE:HD13	1:A:555:ILE:HD13	1.96	0.48
1:A:214:PHE:HA	1:A:217:ALA:HB3	1.95	0.48
1:A:1232:ALA:HB3	1:A:1238:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1098:ILE:O	1:A:1104:LEU:HD23	2.13	0.48
1:A:1156:LYS:HE3	1:A:1156:LYS:HA	1.94	0.48
1:A:1162:LEU:HD12	1:A:1168:THR:HG21	1.95	0.48
1:A:1198:LEU:HD22	1:A:1199:ILE:H	1.78	0.48
1:A:1186:CYS:SG	1:A:1189:ARG:NH1	2.85	0.47
1:A:416:THR:HB	1:A:418:PHE:HE1	1.77	0.47
1:A:824:ARG:CZ	1:A:1012:ARG:HD2	2.44	0.47
1:A:12:PRO:HG2	1:A:26:TRP:CE3	2.48	0.47
1:A:742:GLN:OE1	1:A:746:ASN:ND2	2.47	0.47
1:A:1097:LYS:HE2	1:A:1099:TRP:HH2	1.79	0.47
1:A:1024:PRO:HG2	1:A:1027:TYR:HE2	1.78	0.47
1:A:1065:ILE:HD13	1:A:1229:LEU:HD21	1.97	0.47
1:A:74:ASP:OD2	1:A:76:GLN:HG3	2.13	0.47
1:A:340:VAL:HG11	1:A:761:LEU:HD11	1.96	0.47
1:A:12:PRO:HG2	1:A:26:TRP:HE3	1.80	0.47
1:A:555:ILE:HG22	1:A:557:LEU:HD23	1.97	0.47
1:A:729:VAL:HG22	1:A:985:TYR:HE2	1.80	0.47
1:A:336:PHE:CZ	1:A:351:VAL:HA	2.50	0.47
1:A:96:GLY:O	1:A:99:THR:HG22	2.15	0.46
1:A:455:LEU:HD22	1:A:557:LEU:HD13	1.97	0.46
1:A:1091:LEU:HA	1:A:1114:ARG:HH21	1.79	0.46
1:A:497:LYS:NZ	1:A:550:TYR:O	2.34	0.46
1:A:503:ARG:HA	1:A:506:LYS:HG2	1.98	0.46
1:A:614:LYS:HA	1:A:614:LYS:HE2	1.98	0.46
1:A:244:LEU:HD21	1:A:362:ARG:HG3	1.98	0.46
1:A:1254:GLU:OE2	1:A:1268:LEU:N	2.49	0.46
1:A:546:ALA:HA	1:A:549:VAL:HG12	1.97	0.45
1:A:329:LYS:HD3	1:A:728:TYR:CE2	2.52	0.45
1:A:602:GLN:HG3	1:A:614:LYS:NZ	2.31	0.45
1:A:606:LEU:HD21	1:A:609:GLY:H	1.79	0.45
1:A:594:LEU:HA	1:A:597:LEU:HD13	1.98	0.45
1:A:1198:LEU:HD22	1:A:1199:ILE:N	2.32	0.45
1:A:11:ASN:HD22	1:A:48:LEU:HG	1.82	0.45
1:A:745:LEU:HD11	1:A:757:GLU:O	2.16	0.45
1:A:602:GLN:HG3	1:A:614:LYS:HZ2	1.82	0.45
1:A:610:LYS:HA	1:A:610:LYS:HD3	1.64	0.45
1:A:1085:ILE:HD13	1:A:1231:ILE:HD13	1.98	0.45
1:A:1212:ASP:O	1:A:1215:ILE:HD12	2.17	0.45
1:A:1126:LEU:HD21	1:A:1185:VAL:HG11	1.99	0.45
1:A:177:LYS:NZ	1:A:394:GLU:HB3	2.31	0.45
1:A:507:VAL:O	1:A:511:CYS:CB	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:ILE:HD13	1:A:285:ILE:HA	1.87	0.45
1:A:484:VAL:HG13	1:A:492:ASN:HD21	1.80	0.45
1:A:528:ILE:HG12	1:A:535:LEU:HD11	1.98	0.45
1:A:244:LEU:HD23	1:A:244:LEU:HA	1.80	0.45
1:A:570:SER:OG	1:A:596:TYR:HE2	2.00	0.45
1:A:1046:VAL:HG23	1:A:1061:LEU:HB3	1.99	0.45
1:A:1024:PRO:HG2	1:A:1027:TYR:CE2	2.51	0.45
1:A:510:ALA:C	1:A:572:HIS:HE2	2.12	0.44
1:A:293:LYS:HE2	1:A:293:LYS:HB2	1.83	0.44
1:A:974:LEU:HD23	1:A:979:VAL:HG22	1.98	0.44
1:A:1212:ASP:O	1:A:1216:GLN:HG3	2.17	0.44
1:A:745:LEU:HD21	1:A:757:GLU:HB3	2.00	0.44
1:A:30:LEU:O	1:A:33:ILE:HG12	2.17	0.44
1:A:1272:MET:O	1:A:1276:LEU:HD22	2.18	0.44
1:A:1041:ILE:HD11	1:A:1065:ILE:HD12	1.98	0.44
1:A:1127:PHE:O	1:A:1134:ASN:ND2	2.49	0.44
1:A:1100:ILE:O	1:A:1103:ILE:HG12	2.18	0.44
1:A:1208:ASP:OD2	1:A:1211:THR:OG1	2.31	0.44
1:A:1271:LYS:HB3	1:A:1272:MET:HE1	2.00	0.44
1:A:100:LEU:HB2	1:A:216:TRP:HH2	1.83	0.44
1:A:489:LEU:HD12	1:A:528:ILE:HD11	1.99	0.43
1:A:1268:LEU:HG	1:A:1272:MET:SD	2.58	0.43
1:A:31:PHE:HZ	1:A:944:THR:HG1	1.60	0.43
1:A:109:GLN:HB2	1:A:144:CYS:SG	2.58	0.43
1:A:284:ARG:O	1:A:288:MET:HB2	2.18	0.43
1:A:735:LEU:HD23	1:A:735:LEU:HA	1.83	0.43
1:A:1098:ILE:O	1:A:1104:LEU:HA	2.19	0.43
1:A:1176:ASN:OD1	1:A:1176:ASN:N	2.49	0.43
1:A:184:MET:SD	1:A:185:ALA:N	2.92	0.43
1:A:248:LEU:HD23	1:A:248:LEU:HA	1.80	0.43
1:A:554:ASP:O	1:A:586:ILE:N	2.52	0.43
1:A:883:LEU:HD23	1:A:883:LEU:HA	1.87	0.43
1:A:1068:GLN:OE1	1:A:1068:GLN:HA	2.18	0.43
1:A:1142:THR:N	1:A:1145:GLU:OE1	2.48	0.43
1:A:143:PHE:HD1	1:A:143:PHE:O	2.01	0.43
1:A:418:PHE:HA	1:A:427:THR:HB	2.01	0.43
1:A:571:ARG:HA	1:A:574:PHE:HB2	2.00	0.43
1:A:1215:ILE:HD12	1:A:1216:GLN:N	2.33	0.43
1:A:261:LEU:O	1:A:265:THR:HG23	2.19	0.43
1:A:1225:HIS:O	1:A:1225:HIS:ND1	2.51	0.43
1:A:1268:LEU:HD12	1:A:1271:LYS:HE2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ALA:HB2	1:A:990:MET:HE1	2.00	0.43
1:A:157:TYR:HB2	1:A:946:ARG:HG3	2.01	0.43
1:A:1133:LYS:HE3	1:A:1133:LYS:HB3	1.92	0.43
1:A:765:LEU:HD12	1:A:765:LEU:HA	1.73	0.43
1:A:1210:ARG:O	1:A:1213:GLU:HG3	2.19	0.43
1:A:12:PRO:HB2	1:A:26:TRP:HB2	2.00	0.42
1:A:407:LYS:HD3	1:A:409:MET:HB3	2.00	0.42
1:A:297:ASN:OD1	1:A:298:LEU:N	2.52	0.42
1:A:1038:GLU:HB3	1:A:1040:VAL:HG22	2.01	0.42
1:A:180:ARG:O	1:A:395:ILE:HG22	2.19	0.42
1:A:439:GLU:OE1	1:A:601:SER:OG	2.24	0.42
1:A:556:TYR:HB3	1:A:558:LEU:HD21	2.01	0.42
1:A:744:MET:O	1:A:748:THR:HG23	2.19	0.42
1:A:824:ARG:HD2	1:A:1016:TYR:CE1	2.54	0.42
1:A:854:VAL:HG13	1:A:868:LEU:HD21	2.01	0.42
1:A:70:ARG:HH12	1:A:82:ARG:HD3	1.85	0.42
1:A:85:ILE:O	1:A:89:TRP:HB3	2.20	0.42
1:A:307:ILE:HD12	1:A:307:ILE:HA	1.81	0.42
1:A:827:LYS:HB3	1:A:827:LYS:NZ	2.34	0.42
1:A:1101:ASP:OD1	1:A:1102:LYS:NZ	2.52	0.42
1:A:1142:THR:O	1:A:1145:GLU:HB2	2.20	0.42
1:A:524:ASP:OD1	1:A:524:ASP:N	2.53	0.42
1:A:940:LEU:HD23	1:A:940:LEU:HA	1.80	0.42
1:A:807:LYS:HE2	1:A:1025:TRP:CE2	2.55	0.42
1:A:1048:PHE:HD2	1:A:1087:ALA:HB2	1.85	0.42
1:A:1090:ARG:HA	1:A:1094:PRO:HD3	2.02	0.42
1:A:405:ASP:OD1	1:A:405:ASP:N	2.53	0.42
1:A:504:TYR:HD2	1:A:504:TYR:O	2.03	0.42
1:A:1156:LYS:O	1:A:1160:GLU:HB2	2.20	0.42
1:A:138:ALA:O	1:A:142:THR:HG22	2.20	0.42
1:A:287:LYS:NZ	1:A:1022:GLU:OE2	2.34	0.42
1:A:120:PHE:CE2	1:A:979:VAL:HG21	2.55	0.41
1:A:197:LEU:HA	1:A:201:ASP:HB3	2.02	0.41
1:A:761:LEU:HD12	1:A:761:LEU:HA	1.76	0.41
1:A:1013:VAL:O	1:A:1017:THR:HG23	2.19	0.41
1:A:1216:GLN:O	1:A:1219:ILE:HD12	2.20	0.41
1:A:1097:LYS:HE3	1:A:1097:LYS:HB2	1.65	0.41
1:A:312:ARG:HE	1:A:312:ARG:HB2	1.72	0.41
1:A:508:ILE:HD12	1:A:508:ILE:HA	1.84	0.41
1:A:113:LEU:HD13	1:A:983:LEU:HB3	2.02	0.41
1:A:562:LEU:HD13	1:A:570:SER:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:THR:OG1	1:A:306:GLU:OE2	2.24	0.41
1:A:477:TYR:HA	1:A:557:LEU:HB2	2.03	0.41
1:A:495:PHE:HB3	1:A:551:GLN:NE2	2.35	0.41
1:A:829:ILE:HD13	1:A:829:ILE:HA	1.88	0.41
1:A:1226:CYS:O	1:A:1228:VAL:HG13	2.20	0.41
1:A:1150:LEU:HB3	1:A:1156:LYS:HD2	2.01	0.41
1:A:378:GLU:O	1:A:381:VAL:HG12	2.20	0.41
1:A:1088:LEU:HD23	1:A:1088:LEU:HA	1.82	0.41
1:A:107:VAL:O	1:A:110:PRO:HD2	2.21	0.41
1:A:1089:PHE:CE2	1:A:1117:MET:HB3	2.56	0.41
1:A:47:VAL:HG11	1:A:935:SER:HB2	2.02	0.41
1:A:106:LYS:HG3	1:A:148:LEU:HD21	2.03	0.41
1:A:229:LEU:HB3	1:A:237:CYS:HB2	2.02	0.41
1:A:541:ALA:O	1:A:545:LEU:HD12	2.21	0.41
1:A:892:LEU:HA	1:A:892:LEU:HD12	1.80	0.41
1:A:1056:LEU:HB3	1:A:1059:LYS:HE3	2.03	0.41
1:A:1122:GLN:CD	1:A:1203:ALA:HB3	2.41	0.41
1:A:329:LYS:HG3	1:A:775:THR:HG21	2.01	0.41
1:A:472:HIS:O	1:A:555:ILE:HD11	2.21	0.41
1:A:952:LEU:HD12	1:A:952:LEU:HA	1.93	0.41
1:A:37:ARG:HH22	1:A:43:ASP:CG	2.24	0.40
1:A:326:SER:OG	1:A:776:VAL:HG22	2.22	0.40
1:A:576:LEU:HD13	1:A:580:GLN:OE1	2.21	0.40
1:A:900:VAL:HG13	1:A:927:PHE:CE1	2.56	0.40
1:A:255:GLY:O	1:A:258:PHE:HB3	2.21	0.40
1:A:474:ARG:CZ	1:A:553:ALA:HA	2.51	0.40
1:A:1150:LEU:HA	1:A:1153:VAL:HG12	2.03	0.40
1:A:502:GLU:H	1:A:502:GLU:CD	2.25	0.40
1:A:1041:ILE:HG22	1:A:1100:ILE:HB	2.02	0.40
1:A:421:LYS:O	1:A:421:LYS:NZ	2.33	0.40
1:A:824:ARG:HD2	1:A:1016:TYR:CD1	2.57	0.40
1:A:1043:PHE:HZ	1:A:1088:LEU:HG	1.86	0.40
1:A:1147:TRP:CZ3	1:A:1156:LYS:HE2	2.57	0.40
1:A:1210:ARG:NH2	1:A:1211:THR:HA	2.37	0.40
1:A:455:LEU:O	1:A:458:VAL:HG22	2.21	0.40
1:A:868:LEU:HD12	1:A:868:LEU:HA	1.83	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	1202/1325 (91%)	1150 (96%)	52 (4%)	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	1052/1159 (91%)	986 (94%)	66 (6%)	15 30

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LEU
1	A	92	TYR
1	A	143	PHE
1	A	152	HIS
1	A	155	TYR
1	A	184	MET
1	A	202	VAL
1	A	206	ASP
1	A	252	SER
1	A	377	SER
1	A	382	SER
1	A	397	GLN
1	A	407	LYS

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Mol	Chain	Res	Type
1	A	418	PHE
1	A	419	TRP
1	A	451	LYS
1	A	479	SER
1	A	485	PHE
1	A	492	ASN
1	A	498	LYS
1	A	499	TYR
1	A	502	GLU
1	A	504	TYR
1	A	509	LYS
1	A	515	LYS
1	A	557	LEU
1	A	583	HIS
1	A	596	TYR
1	A	611	MET
1	A	619	GLU
1	A	623	SER
1	A	696	VAL
1	A	758	LYS
1	A	787	PHE
1	A	805	ILE
1	A	824	ARG
1	A	840	PHE
1	A	845	GLN
1	A	894	SER
1	A	920	GLU
1	A	958	MET
1	A	984	SER
1	A	990	MET
1	A	998	ARG
1	A	1002	GLU
1	A	1006	MET
1	A	1016	TYR
1	A	1035	TRP
1	A	1037	HIS
1	A	1040	VAL
1	A	1049	MET
1	A	1060	HIS
1	A	1070	LYS
1	A	1100	ILE
1	A	1114	ARG

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Mol	Chain	Res	Type
1	A	1154	GLN
1	A	1173	SER
1	A	1204	THR
1	A	1210	ARG
1	A	1220	ARG
1	A	1225	HIS
1	A	1233	HIS
1	A	1256	ASP
1	A	1272	MET
1	A	1276	LEU
1	A	1278	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	746	ASN
1	A	1122	GLN

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](#)

15 ligands are modelled in this entry.

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
2	DU0	A	1409	-	42,42,42	0.49	0	66,66,66	0.48	0
2	DU0	A	1404	-	42,42,42	0.50	0	66,66,66	0.48	0
2	DU0	A	1402	-	42,42,42	0.48	0	66,66,66	0.54	0
2	DU0	A	1405	-	42,42,42	0.53	0	66,66,66	0.65	0
2	DU0	A	1410	-	42,42,42	0.51	0	66,66,66	0.64	0
2	DU0	A	1413	-	42,42,42	0.50	0	66,66,66	0.84	3 (4%)
3	PLM	A	1415	-	17,17,17	0.65	0	17,17,17	0.64	0
2	DU0	A	1401	-	42,42,42	0.46	0	66,66,66	0.52	0
2	DU0	A	1407	-	42,42,42	0.53	0	66,66,66	0.96	3 (4%)
2	DU0	A	1406	-	42,42,42	0.56	0	66,66,66	0.81	1 (1%)
2	DU0	A	1414	-	42,42,42	0.49	0	66,66,66	0.66	1 (1%)
2	DU0	A	1403	-	42,42,42	0.48	0	66,66,66	0.47	0
2	DU0	A	1411	-	42,42,42	0.50	0	66,66,66	1.33	7 (10%)
2	DU0	A	1412	-	42,42,42	0.47	0	66,66,66	0.78	3 (4%)
2	DU0	A	1408	-	42,42,42	0.50	0	66,66,66	1.12	3 (4%)

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
2	DU0	A	1409	-	-	0/10/98/98	0/6/6/6
2	DU0	A	1404	-	-	5/10/98/98	0/6/6/6
2	DU0	A	1402	-	-	7/10/98/98	0/6/6/6
2	DU0	A	1405	-	-	1/10/98/98	0/6/6/6
2	DU0	A	1410	-	-	3/10/98/98	0/6/6/6
2	DU0	A	1413	-	-	1/10/98/98	0/6/6/6
3	PLM	A	1415	-	-	4/15/15/15	-
2	DU0	A	1401	-	-	6/10/98/98	0/6/6/6
2	DU0	A	1407	-	-	5/10/98/98	0/6/6/6
2	DU0	A	1406	-	-	2/10/98/98	0/6/6/6
2	DU0	A	1414	-	-	8/10/98/98	0/6/6/6
2	DU0	A	1403	-	-	6/10/98/98	0/6/6/6
2	DU0	A	1411	-	-	6/10/98/98	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DU0	A	1412	-	-	3/10/98/98	0/6/6/6
2	DU0	A	1408	-	-	6/10/98/98	0/6/6/6

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1411	DU0	O10-C09-C15	6.24	116.58	110.77
2	A	1408	DU0	O10-C09-C15	5.80	116.17	110.77
2	A	1406	DU0	C78-C77-C79	-3.94	106.99	111.68
2	A	1408	DU0	C14-C15-C09	3.90	118.67	111.93
2	A	1407	DU0	C03-C04-C05	-3.79	95.07	102.37
2	A	1411	DU0	C14-C15-C09	3.63	118.20	111.93
2	A	1412	DU0	O10-C09-C15	3.06	113.62	110.77
2	A	1411	DU0	C11-O10-C09	2.83	119.08	113.72
2	A	1408	DU0	C11-O10-C09	2.81	119.04	113.72
2	A	1407	DU0	O16-C09-C07	2.76	108.56	104.47
2	A	1411	DU0	O16-C09-C07	-2.70	100.46	104.47
2	A	1413	DU0	O16-C09-C07	2.60	108.33	104.47
2	A	1411	DU0	C09-C07-C06	-2.33	99.58	103.37
2	A	1414	DU0	C77-C79-C17	-2.24	109.38	112.73
2	A	1407	DU0	O16-C05-C06	2.21	108.34	105.07
2	A	1412	DU0	C15-C09-C07	-2.18	111.20	115.69
2	A	1413	DU0	O16-C05-C06	2.13	108.21	105.07
2	A	1412	DU0	C14-C15-C09	2.10	115.56	111.93
2	A	1413	DU0	C03-C04-C05	-2.09	98.35	102.37
2	A	1411	DU0	C22-C21-C20	2.08	114.74	111.52
2	A	1411	DU0	C04-C03-C02	-2.04	101.19	103.91

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1402	DU0	C21-C22-O23-C24
2	A	1402	DU0	C24-C25-C26-C27
2	A	1402	DU0	C25-C26-C27-O28
2	A	1402	DU0	C51-C26-C27-O28
2	A	1403	DU0	C21-C22-O23-C24
2	A	1403	DU0	C24-C25-C26-C51
2	A	1403	DU0	C27-C26-C51-O52
2	A	1404	DU0	C75-C22-O23-C24

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Mol	Chain	Res	Type	Atoms
2	A	1407	DU0	C25-C26-C51-O52
2	A	1408	DU0	C75-C22-O23-C24
2	A	1408	DU0	C24-C25-C26-C51
2	A	1410	DU0	C25-C24-O23-C22
2	A	1411	DU0	C21-C22-O23-C24
2	A	1413	DU0	C25-C24-O23-C22
2	A	1414	DU0	C25-C24-O23-C22
2	A	1414	DU0	C24-C25-C26-C27
2	A	1414	DU0	C25-C26-C27-O28
2	A	1414	DU0	C25-C26-C51-O52
2	A	1408	DU0	O23-C24-C25-C26
2	A	1414	DU0	O23-C24-C25-C26
2	A	1411	DU0	O23-C24-C25-C26
2	A	1407	DU0	C21-C22-O23-C24
2	A	1407	DU0	C75-C22-O23-C24
2	A	1412	DU0	C21-C22-O23-C24
2	A	1412	DU0	C75-C22-O23-C24
2	A	1404	DU0	C24-C25-C26-C51
2	A	1406	DU0	C24-C25-C26-C51
2	A	1408	DU0	C24-C25-C26-C27
2	A	1401	DU0	O23-C24-C25-C26
2	A	1401	DU0	C21-C22-O23-C24
2	A	1411	DU0	C27-C26-C51-O52
2	A	1403	DU0	C25-C26-C51-O52
2	A	1408	DU0	C25-C26-C27-O28
2	A	1411	DU0	C25-C26-C51-O52
2	A	1401	DU0	C24-C25-C26-C27
2	A	1401	DU0	C24-C25-C26-C51
2	A	1402	DU0	C24-C25-C26-C51
2	A	1406	DU0	C24-C25-C26-C27
2	A	1410	DU0	C24-C25-C26-C51
2	A	1414	DU0	C24-C25-C26-C51
2	A	1403	DU0	O23-C24-C25-C26
2	A	1404	DU0	O23-C24-C25-C26
2	A	1405	DU0	O23-C24-C25-C26
3	A	1415	PLM	CC-CD-CE-CF
2	A	1401	DU0	C75-C22-O23-C24
2	A	1408	DU0	C21-C22-O23-C24
2	A	1404	DU0	C25-C24-O23-C22
2	A	1403	DU0	C24-C25-C26-C27
2	A	1411	DU0	C24-C25-C26-C51
2	A	1411	DU0	C25-C24-O23-C22

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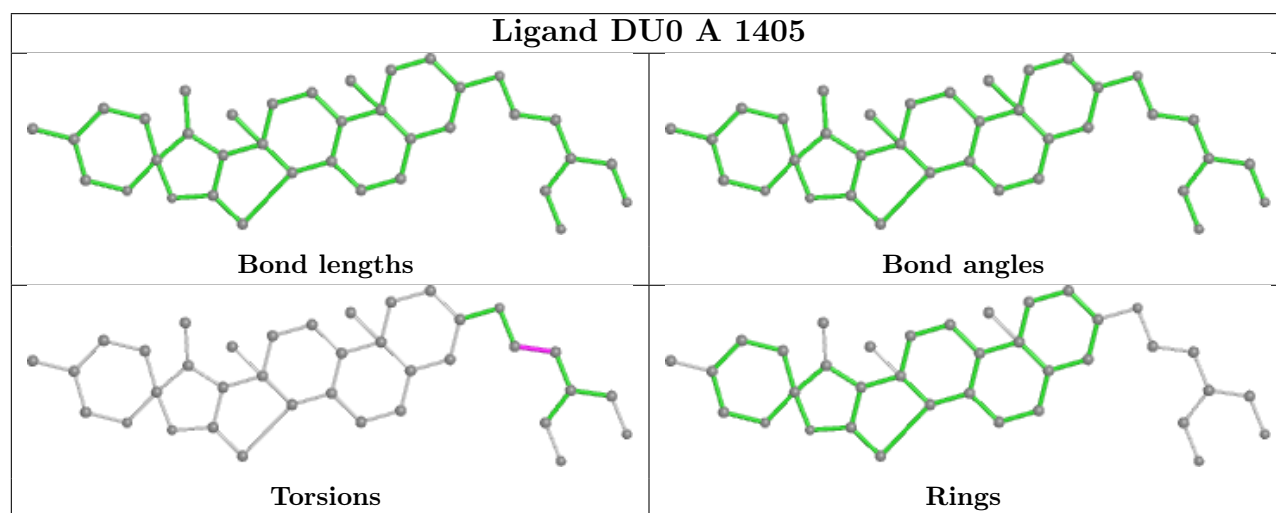
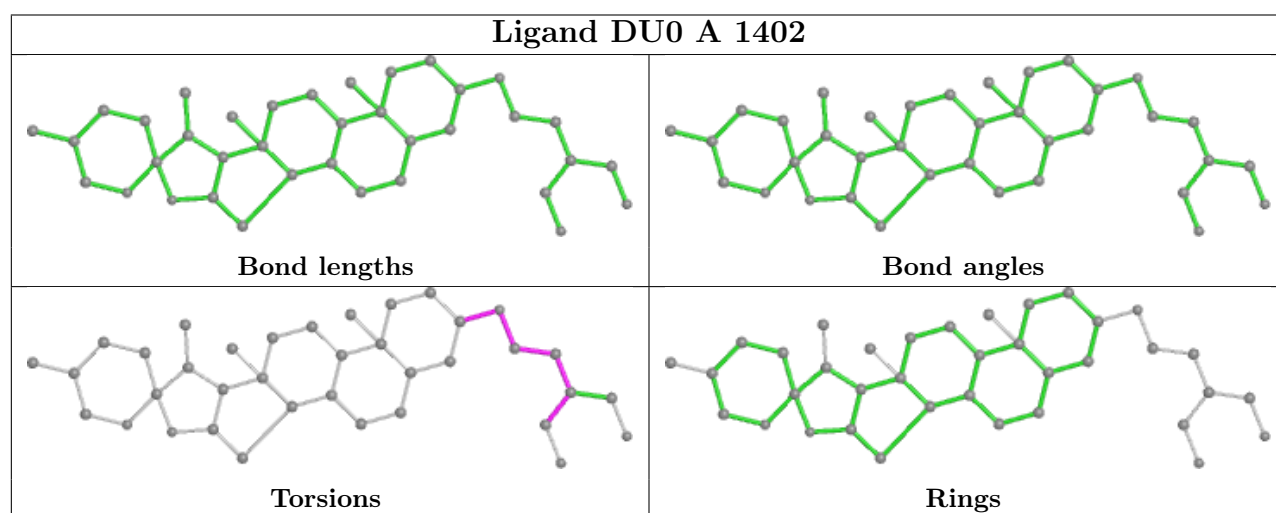
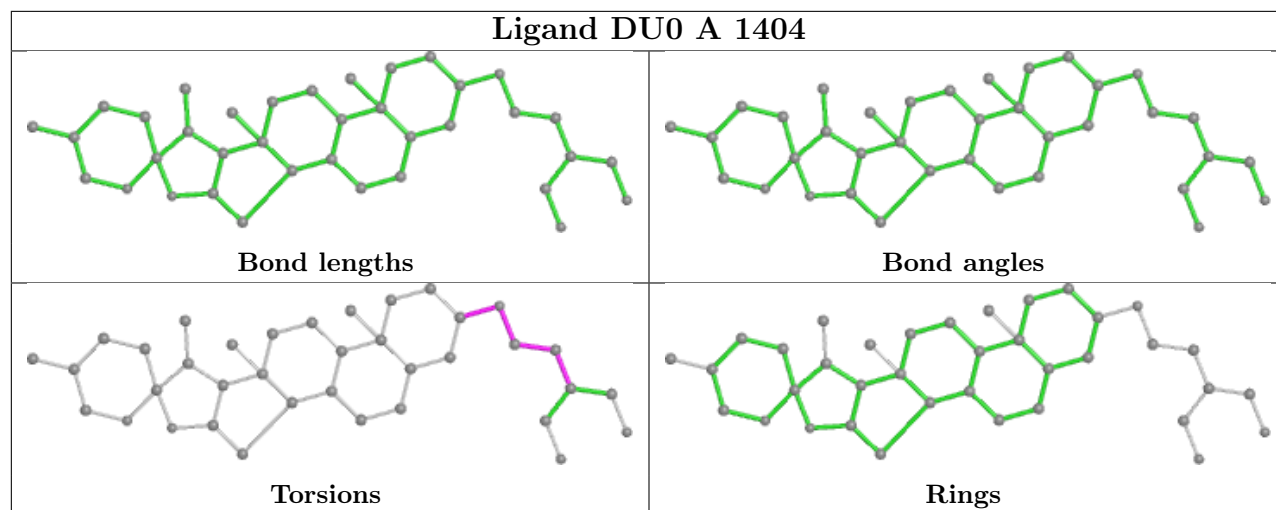
Mol	Chain	Res	Type	Atoms
2	A	1412	DU0	C25-C24-O23-C22
2	A	1407	DU0	C27-C26-C51-O52
2	A	1414	DU0	C51-C26-C27-O28
2	A	1414	DU0	C27-C26-C51-O52
3	A	1415	PLM	O2-C1-C2-C3
3	A	1415	PLM	C3-C4-C5-C6
2	A	1410	DU0	O23-C24-C25-C26
3	A	1415	PLM	O1-C1-C2-C3
2	A	1401	DU0	C25-C24-O23-C22
2	A	1402	DU0	C25-C24-O23-C22
2	A	1407	DU0	C25-C24-O23-C22
2	A	1404	DU0	C24-C25-C26-C27
2	A	1402	DU0	O23-C24-C25-C26

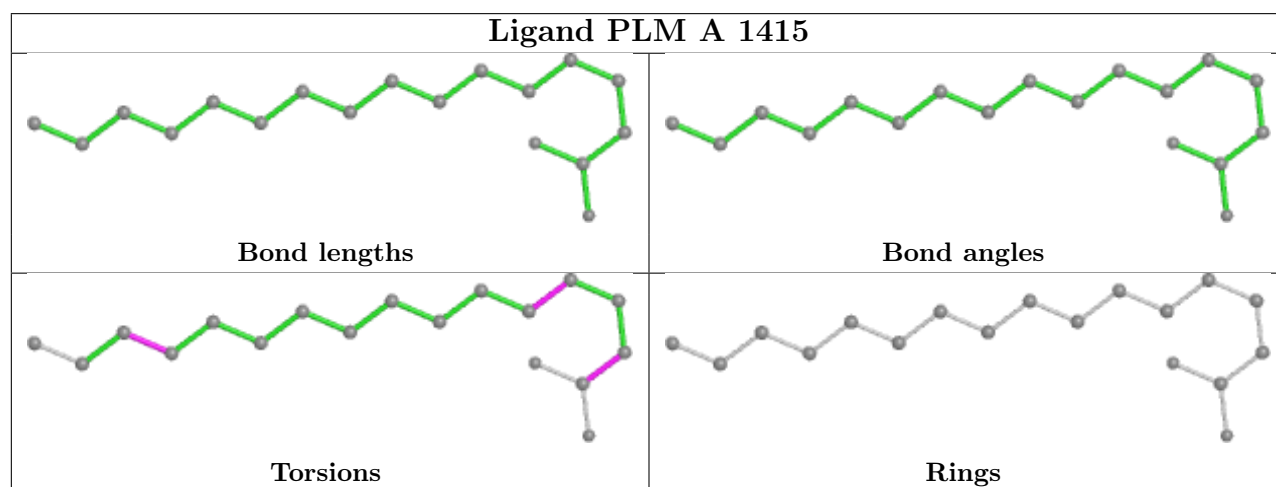
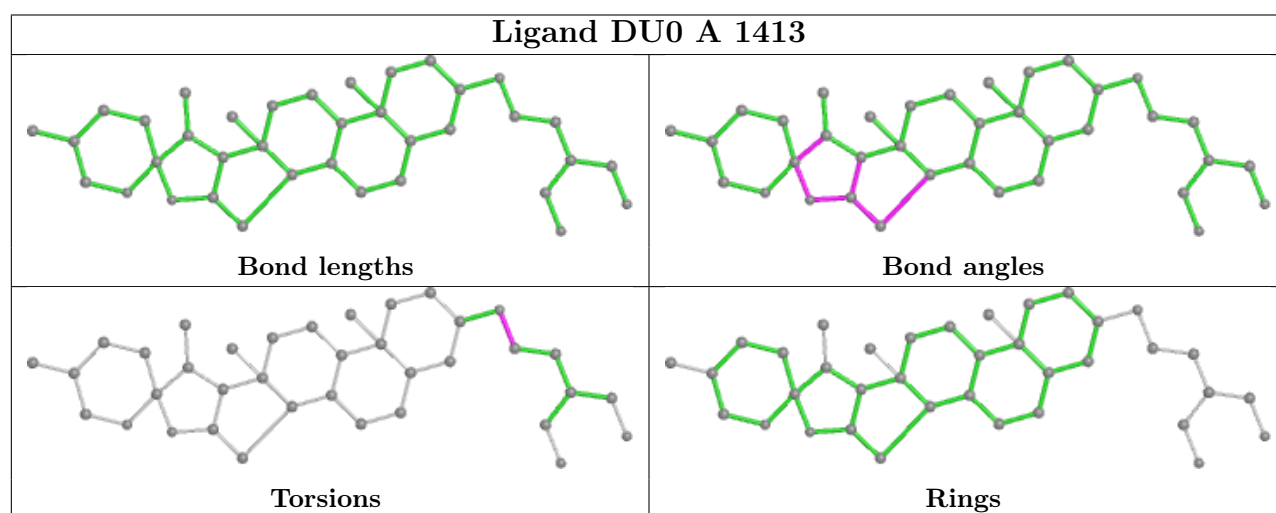
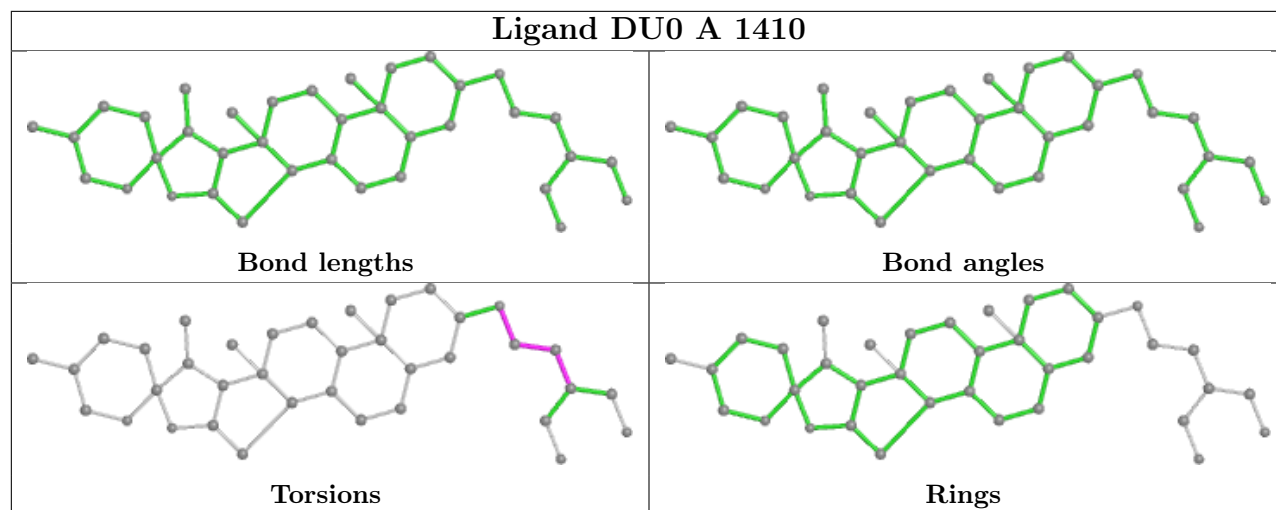
There are no ring outliers.

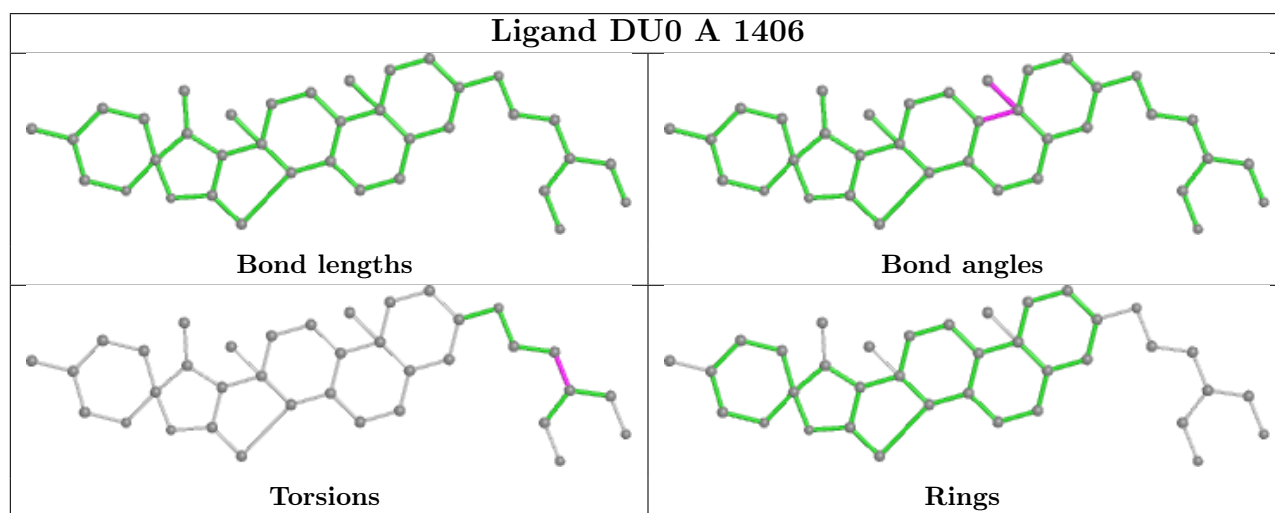
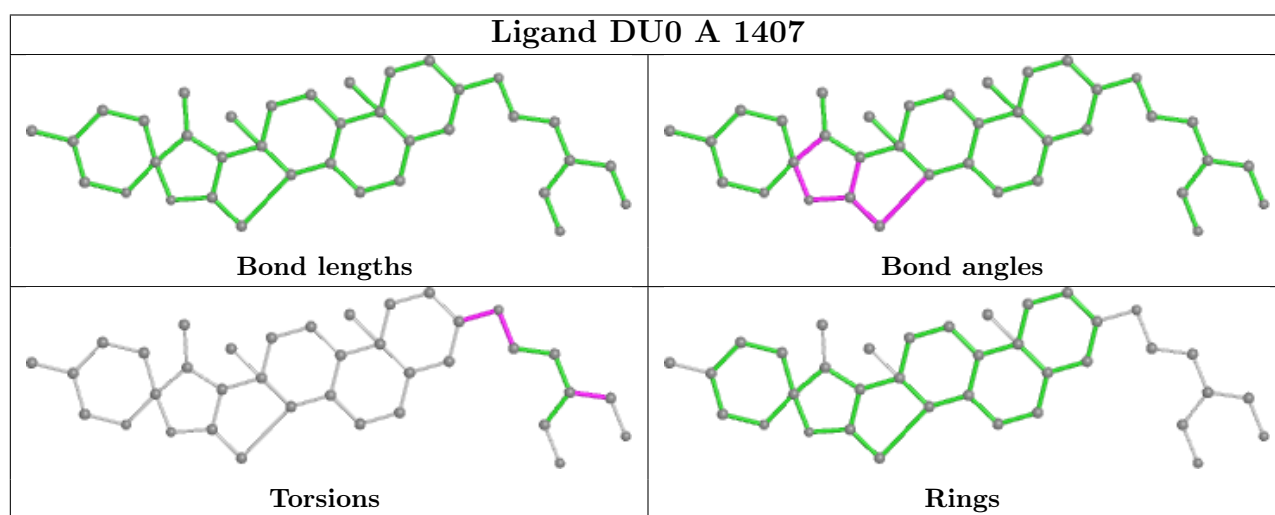
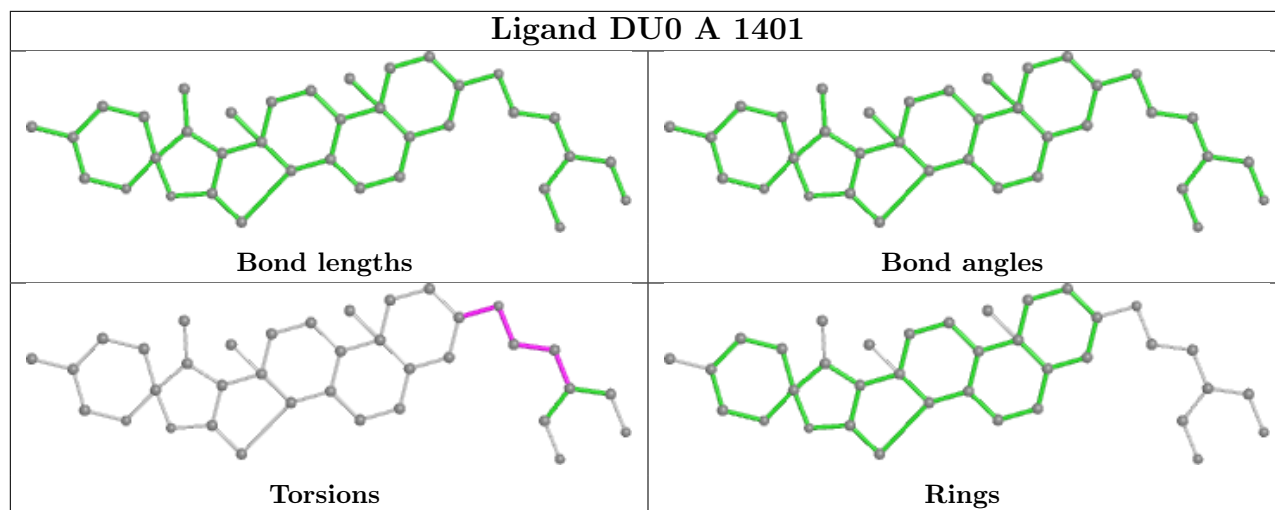
2 monomers are involved in 2 short contacts:

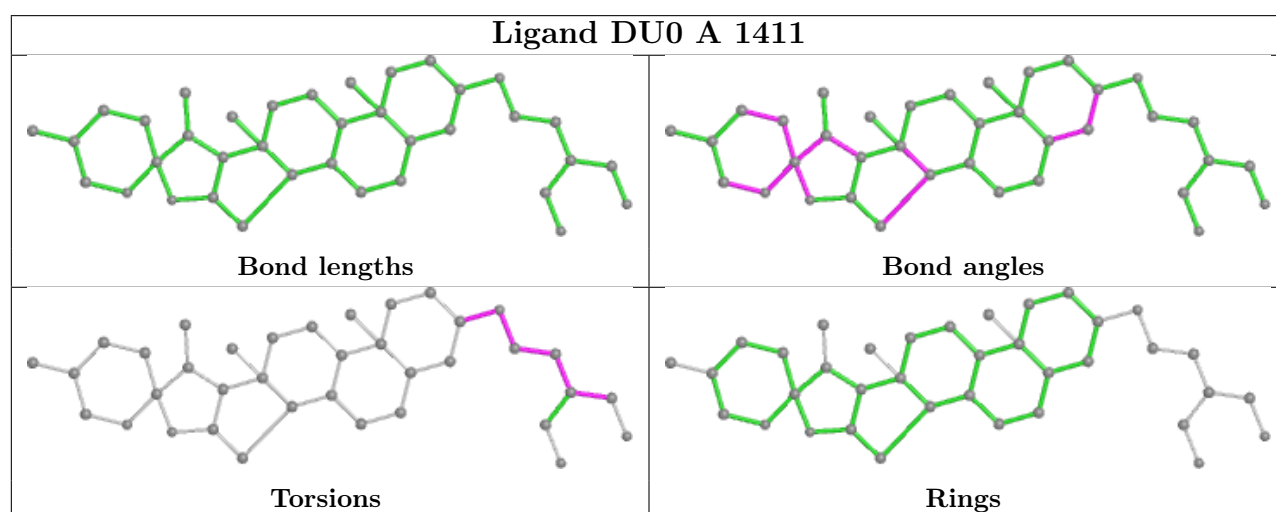
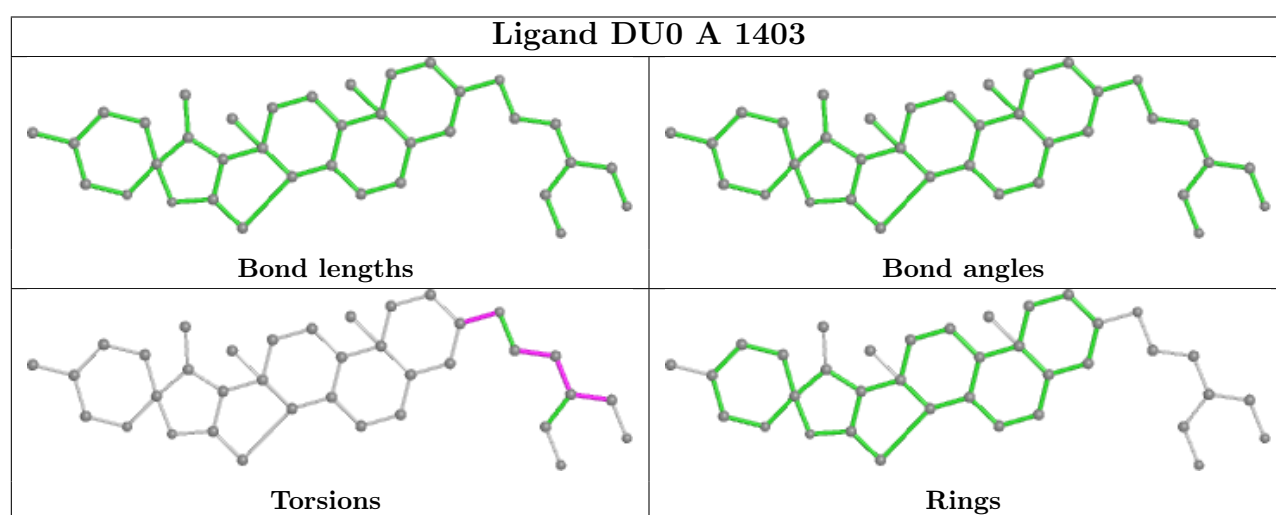
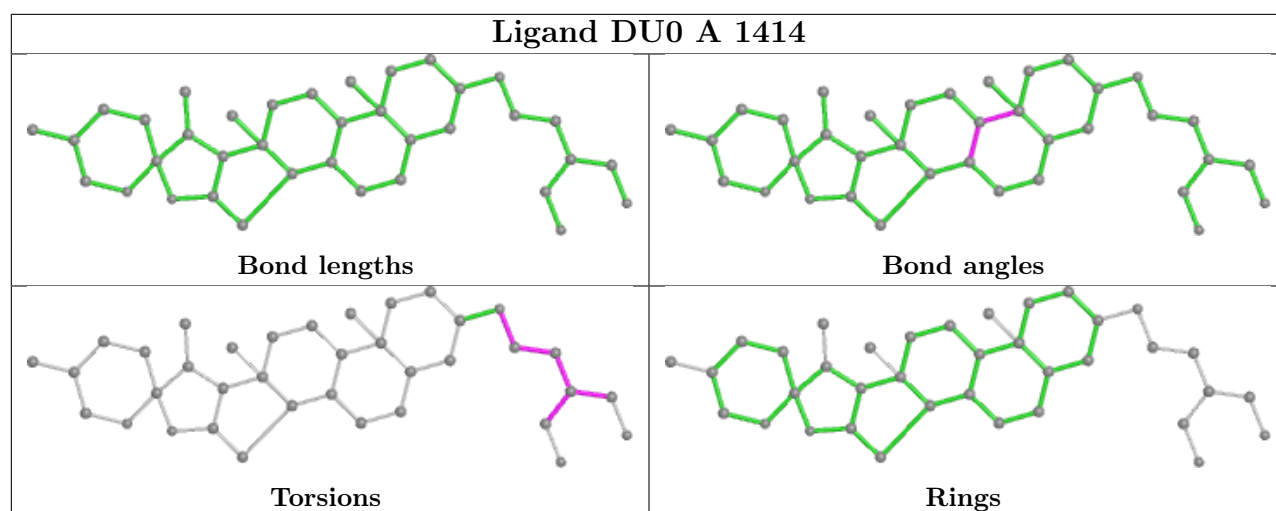
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1415	PLM	1	0
2	A	1414	DU0	1	0

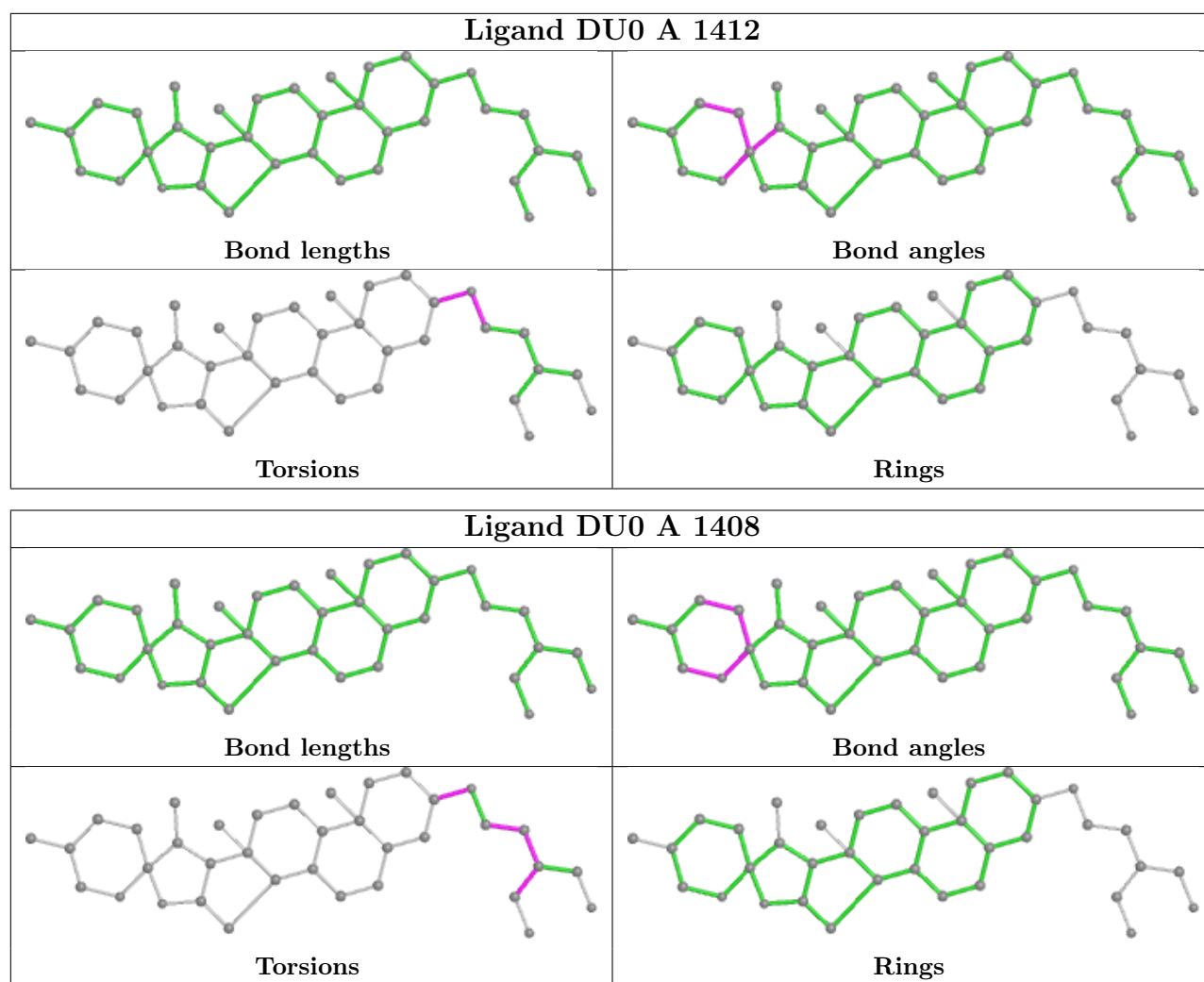
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

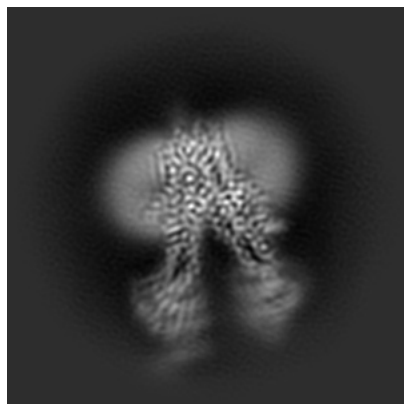
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38532. These allow visual inspection of the internal detail of the map and identification of artifacts.

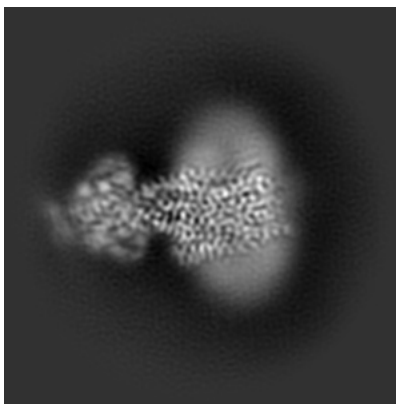
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

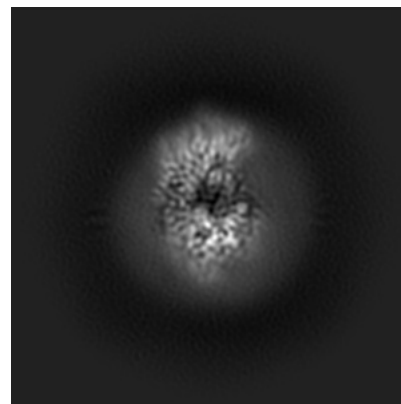
6.1.1 Primary map



X

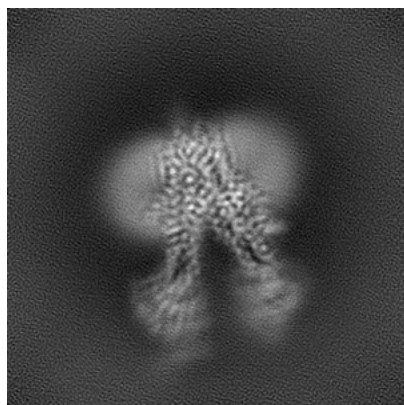


Y

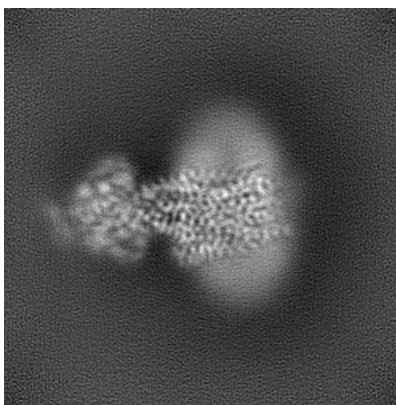


Z

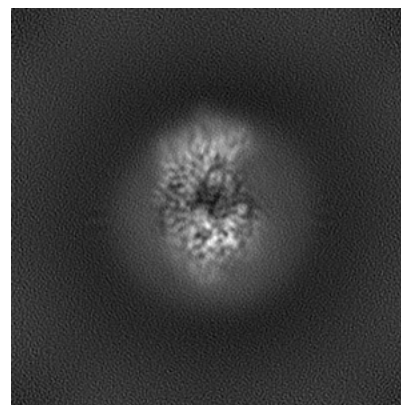
6.1.2 Raw map



X



Y

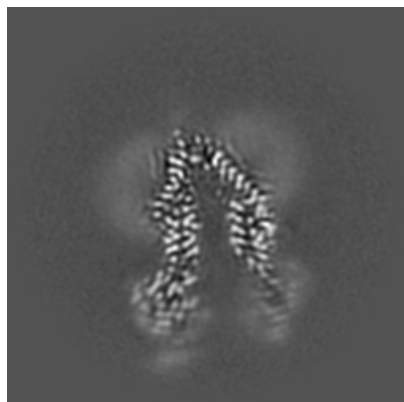


Z

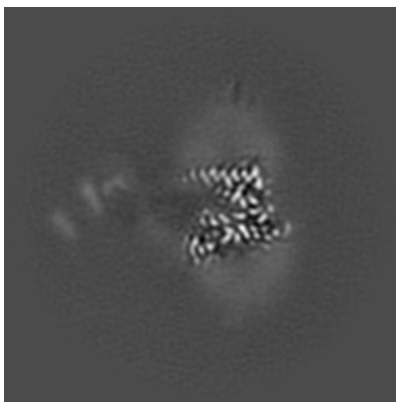
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

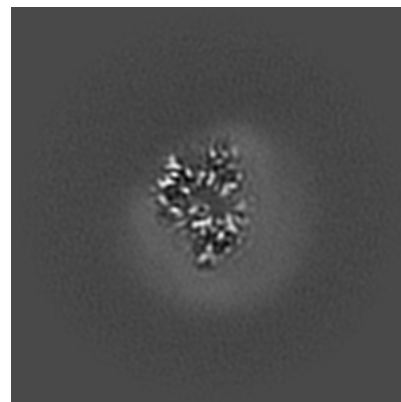
6.2.1 Primary map



X Index: 128

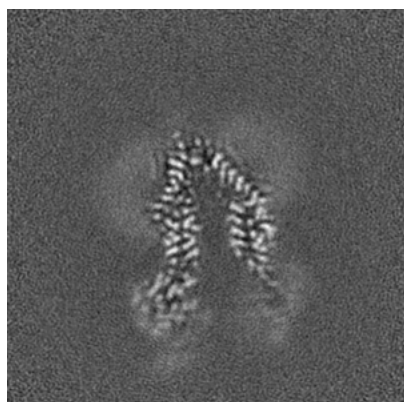


Y Index: 128

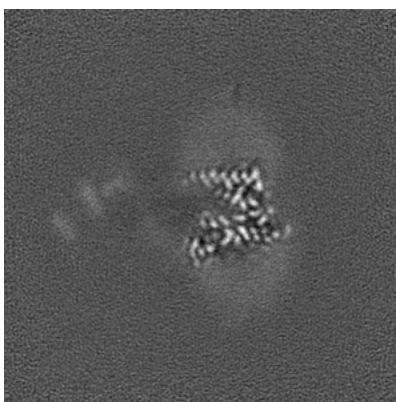


Z Index: 128

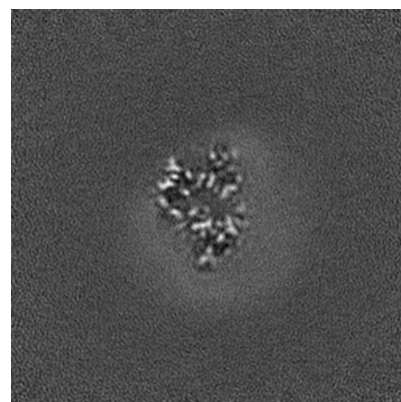
6.2.2 Raw map



X Index: 128



Y Index: 128

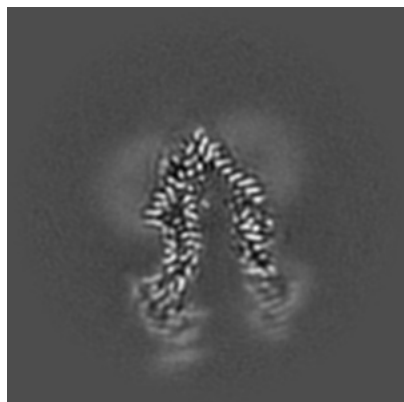


Z Index: 128

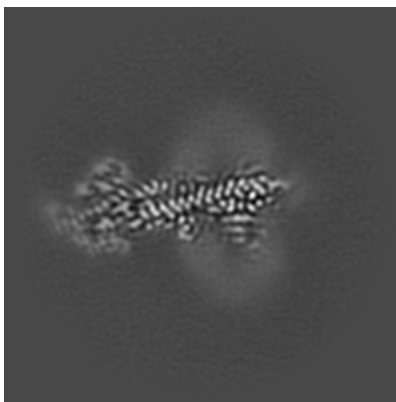
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

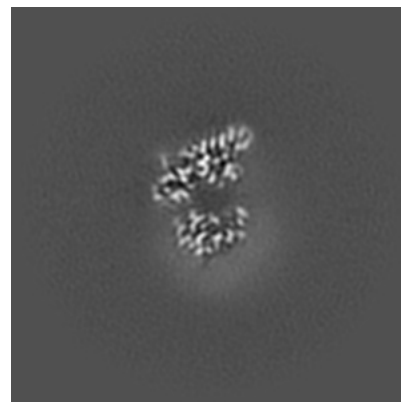
6.3.1 Primary map



X Index: 125

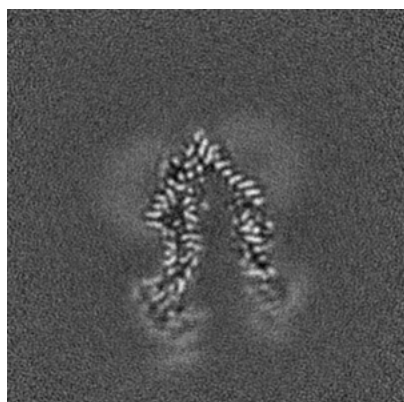


Y Index: 106

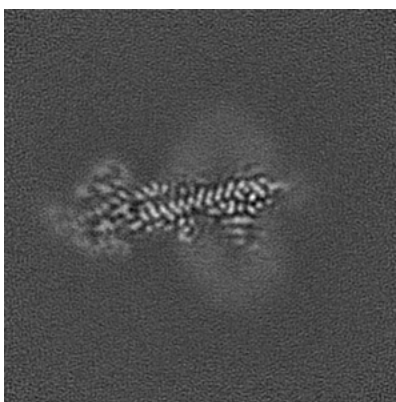


Z Index: 114

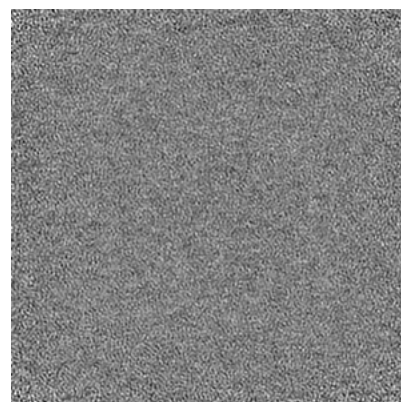
6.3.2 Raw map



X Index: 125



Y Index: 106

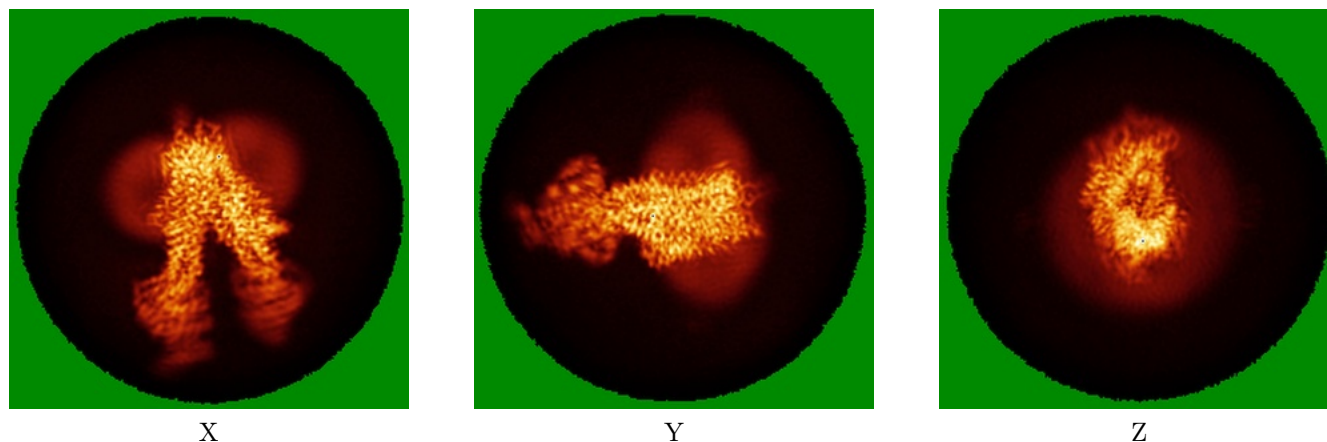


Z Index: 255

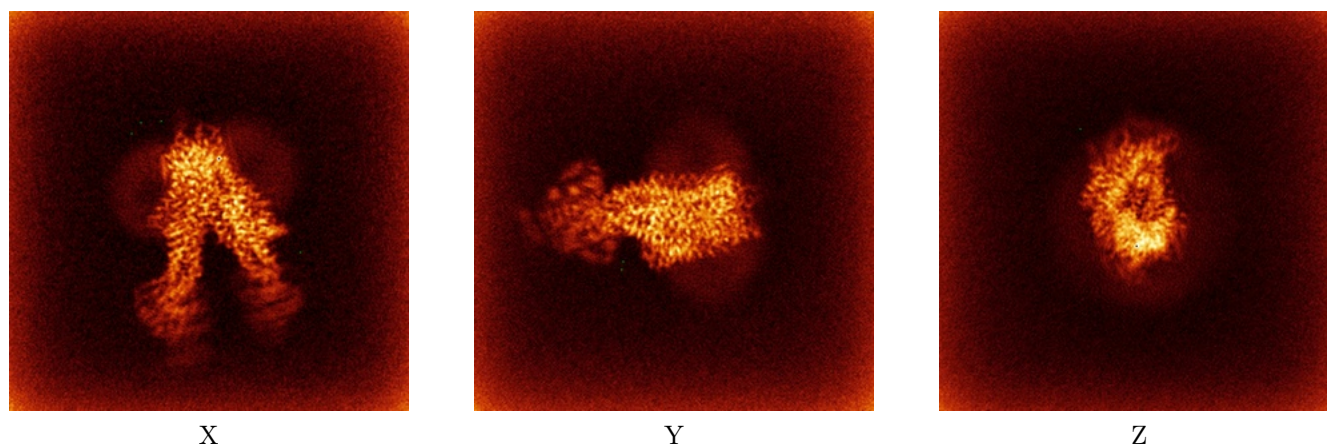
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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.

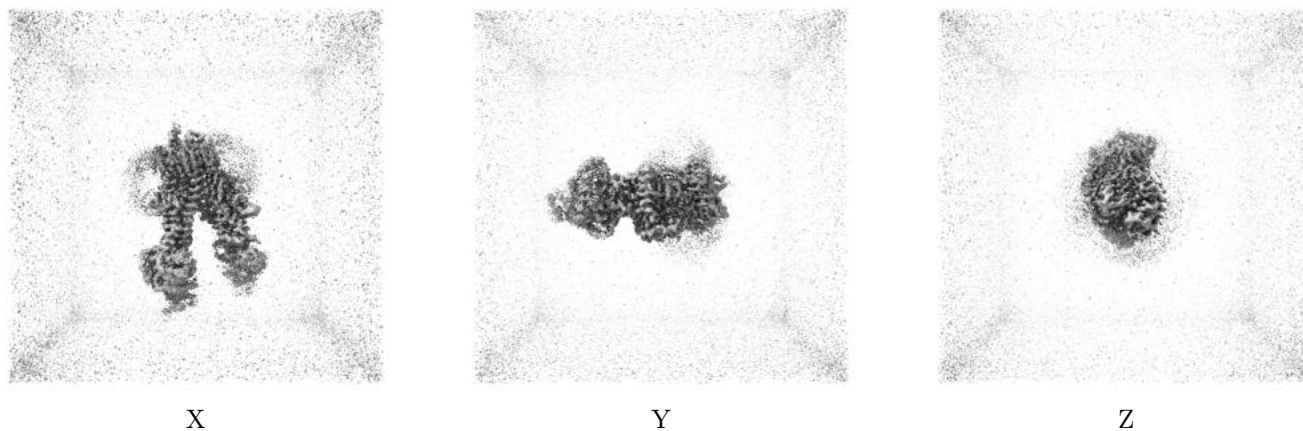
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.053. 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.

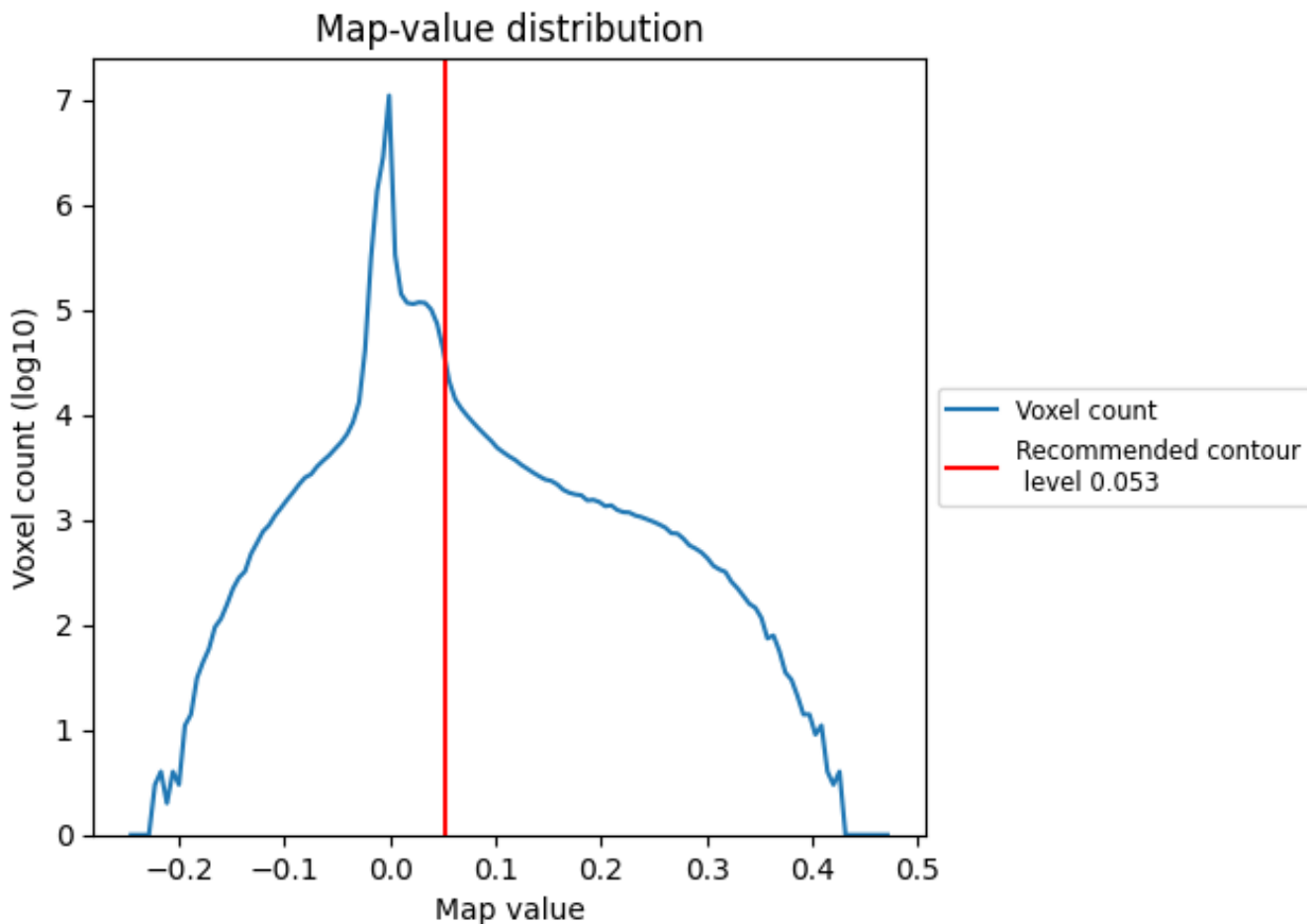
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

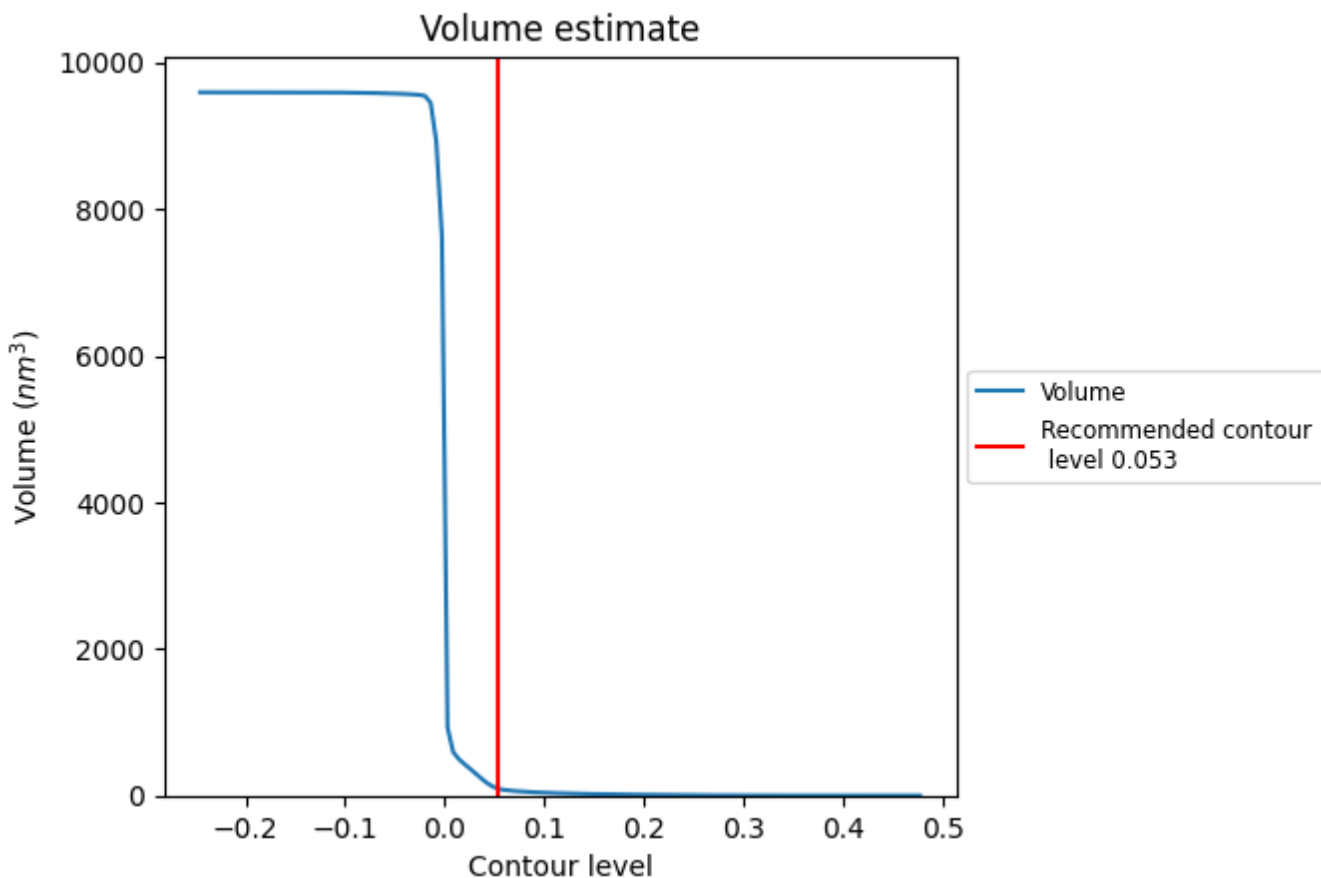
This section contains the results of statistical analysis of the map.

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.

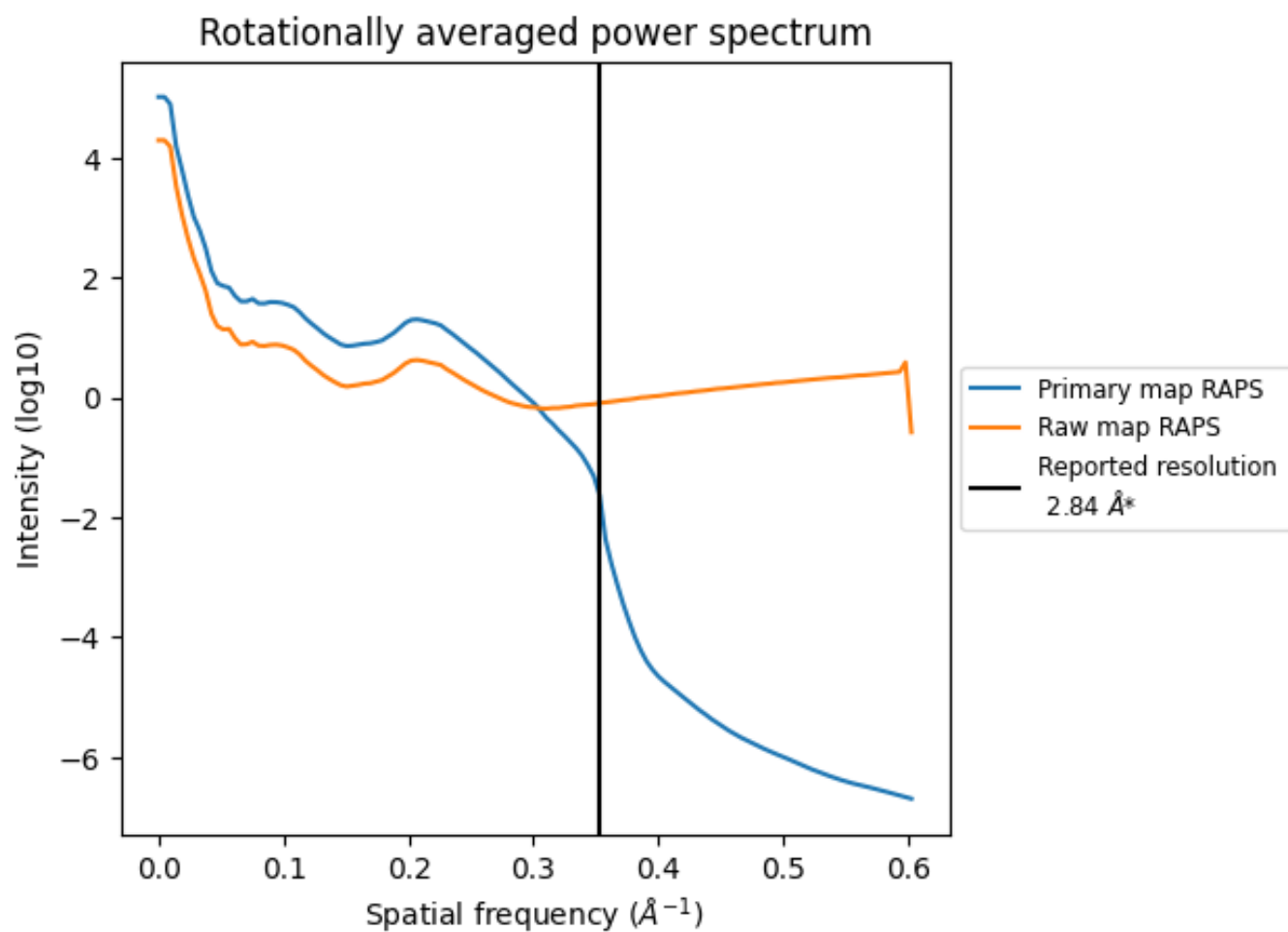
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 97 nm³; this corresponds to an approximate mass of 87 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

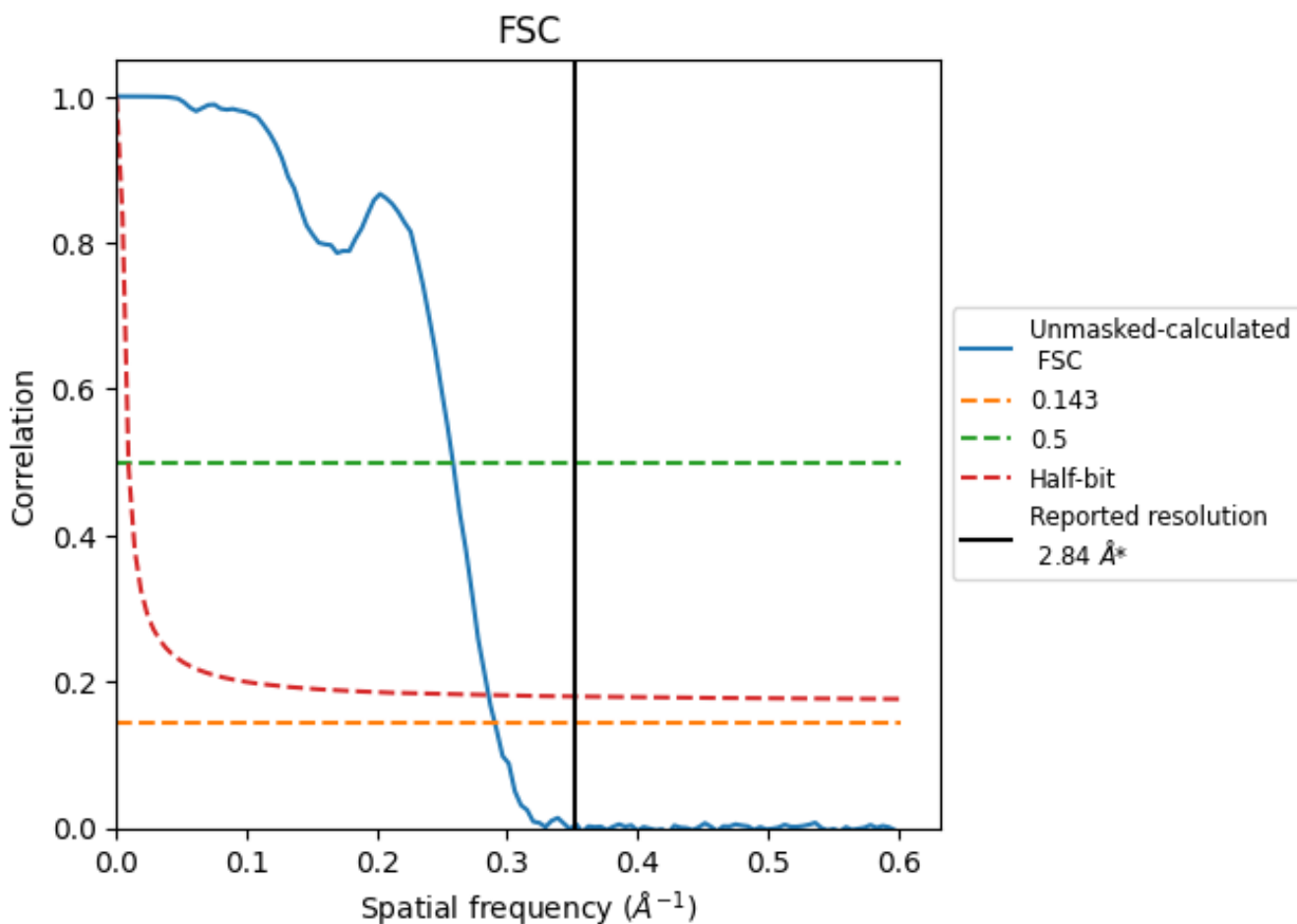


*Reported resolution corresponds to spatial frequency of 0.352 Å⁻¹

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 0.352 \AA^{-1}

8.2 Resolution estimates [i](#)

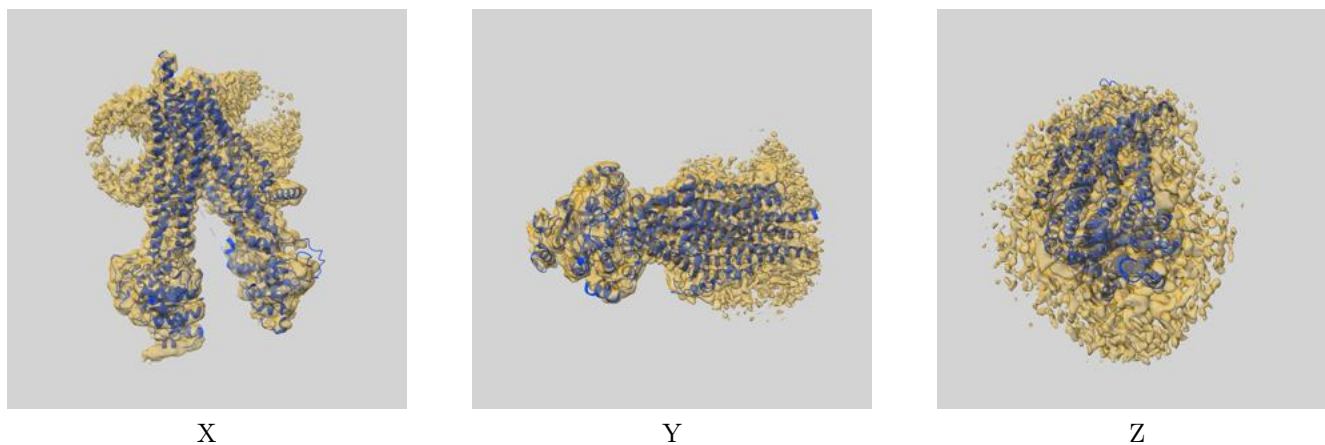
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.84	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.44	3.87	3.50

*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 3.44 differs from the reported value 2.84 by more than 10 %

9 Map-model fit [i](#)

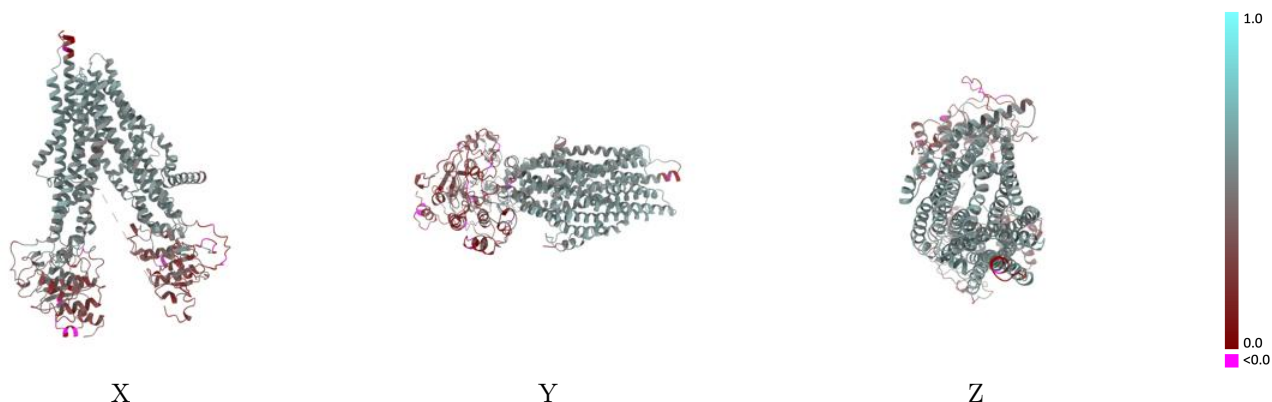
This section contains information regarding the fit between EMDB map EMD-38532 and PDB model 8XOK. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



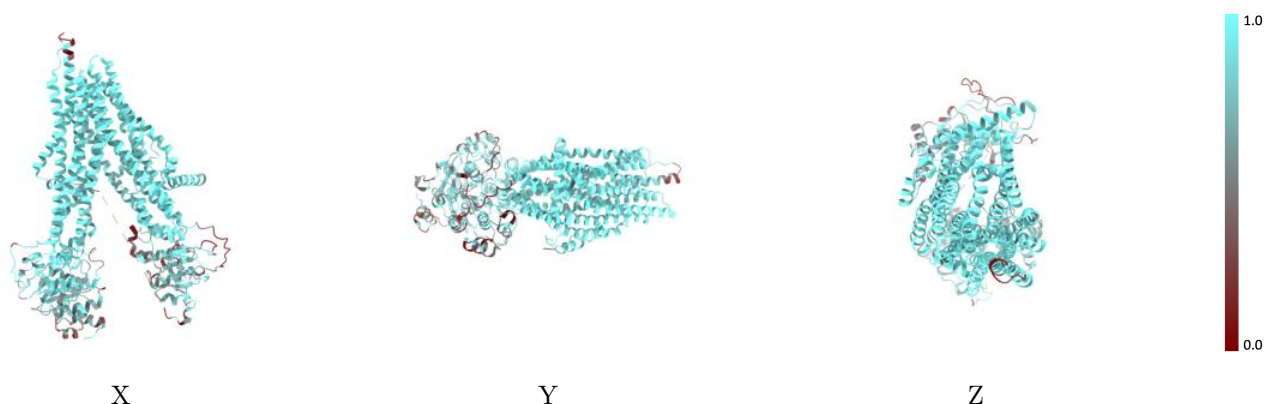
The images above show the 3D surface view of the map at the recommended contour level 0.053 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



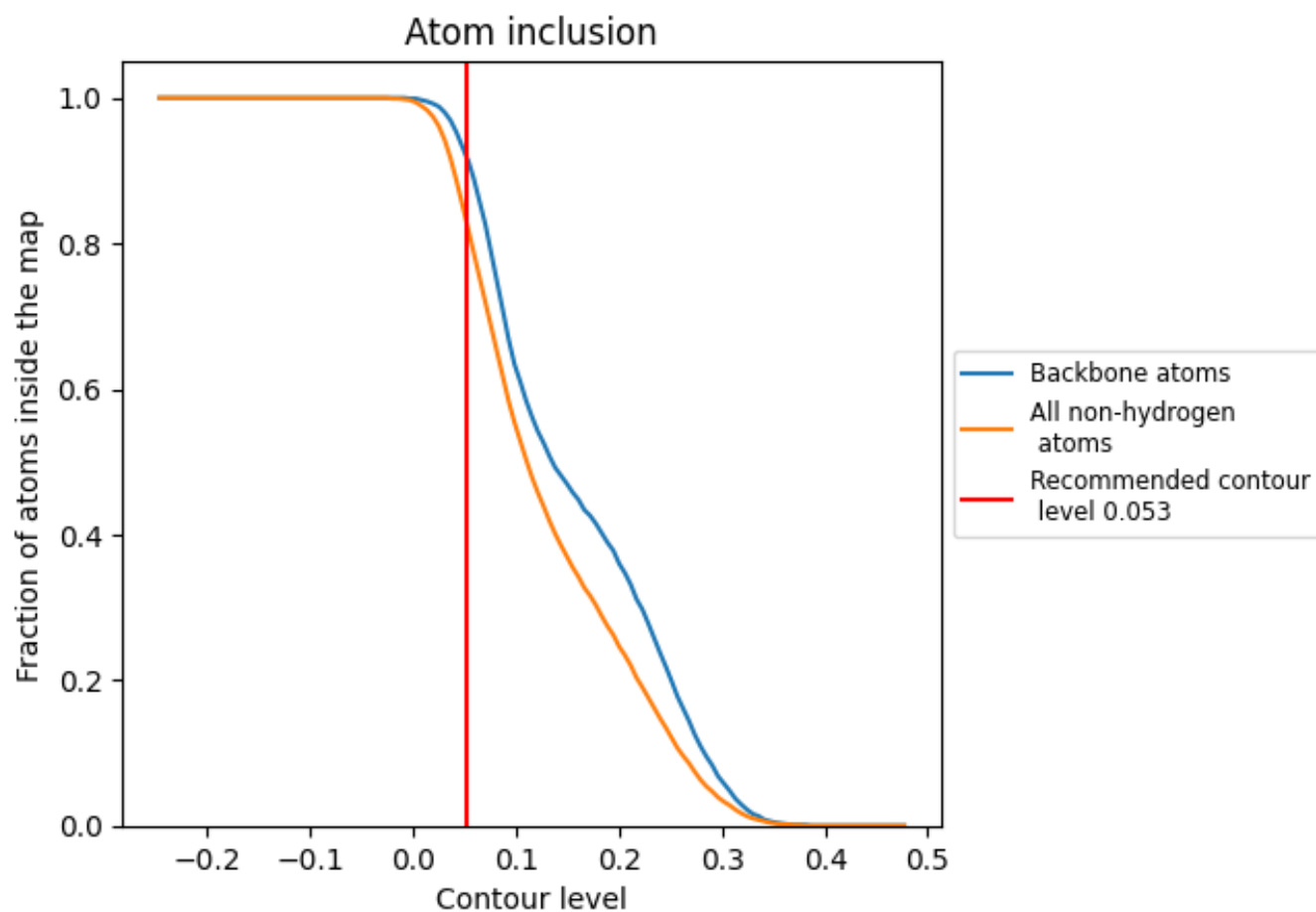
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.053).





9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 82% 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 (0.053) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8250	 0.4380
A	 0.8250	 0.4380

