



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 12:36 PM UTC

PDB ID : 7CU3 / pdb_00007cu3
EMDB ID : EMD-30470
Title : Structure of mammalian NALCN-FAM155A complex at 2.65 angstrom
Authors : Chen, L.; Kang, Y.
Deposited on : 2020-08-20
Resolution : 2.65 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 EMDB 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

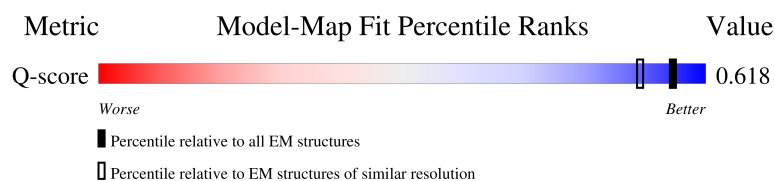
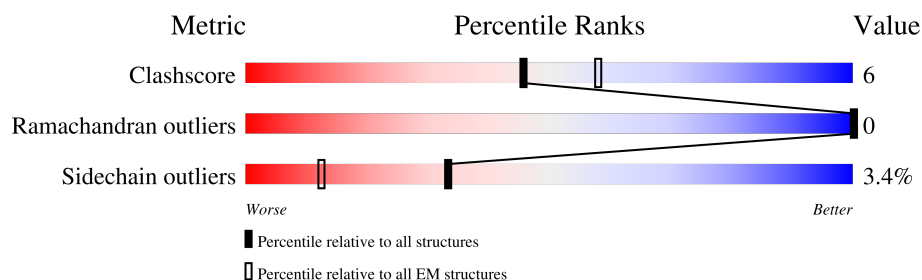
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.65 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	9050 (2.15 - 3.15)

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	1738	11% 59% 14% 27%
2	B	467	11% 29% 8% 63%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12209 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 Sodium leak channel non-selective protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1277	Total	C	N	O	S	4	0
			10353	6844	1693	1736	80		

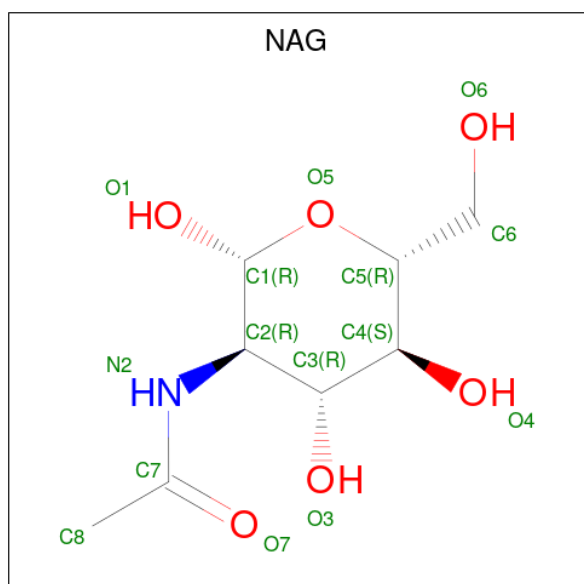
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	52	SER	PRO	conflict	UNP Q6Q760
A	748	ALA	THR	conflict	UNP Q6Q760

- Molecule 2 is a protein called Transmembrane protein FAM155A.

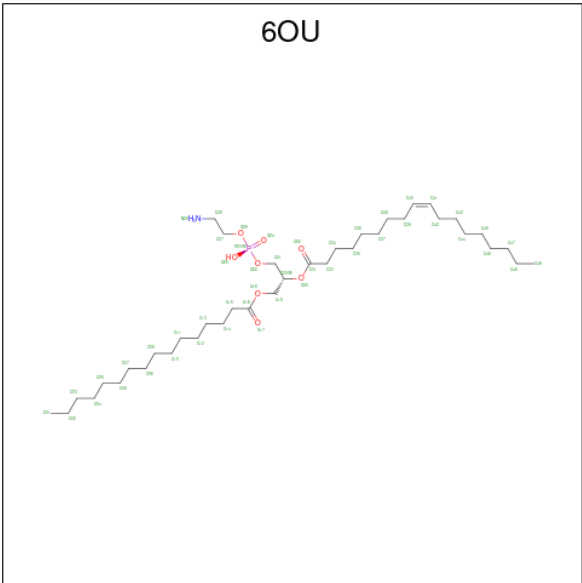
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	173	Total	C	N	O	S	0	0
			1379	875	213	275	16		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 4 is [(2 {R})-1-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-3-hexadecanoyloxy-p ropan-2-yl] ({Z})-octadec-9-enoate (CCD ID: 6OU) (formula: C₃₉H₇₆NO₈P) (labeled as "Ligand of Interest" by depositor).



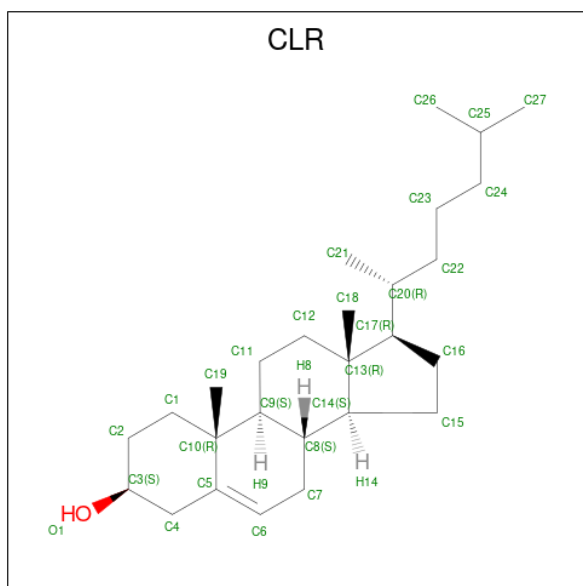
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			36	26	1	8	1	
4	A	1	Total	C	O	P		0
			46	37	8	1		
4	A	1	Total	C	O	P		0
			46	37	8	1		
4	A	1	Total	C	N	O	P	0
			37	27	1	8	1	
4	A	1	Total	C	O			0
			20	18	2			
4	A	1	Total	C	N	O	P	0
			42	32	1	8	1	
4	A	1	Total	C	O			0
			18	16	2			
4	A	1	Total	C	O			0
			18	16	2			

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Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	O		0
			20	18	2		
4	A	1	Total	C	O	P	0
			27	18	8	1	
4	A	1	Total	C	N	O	P
			38	28	1	8	1
4	A	1	Total	C	O	P	0
			31	22	8	1	

- Molecule 5 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$) (labeled as "Ligand of Interest" by depositor).

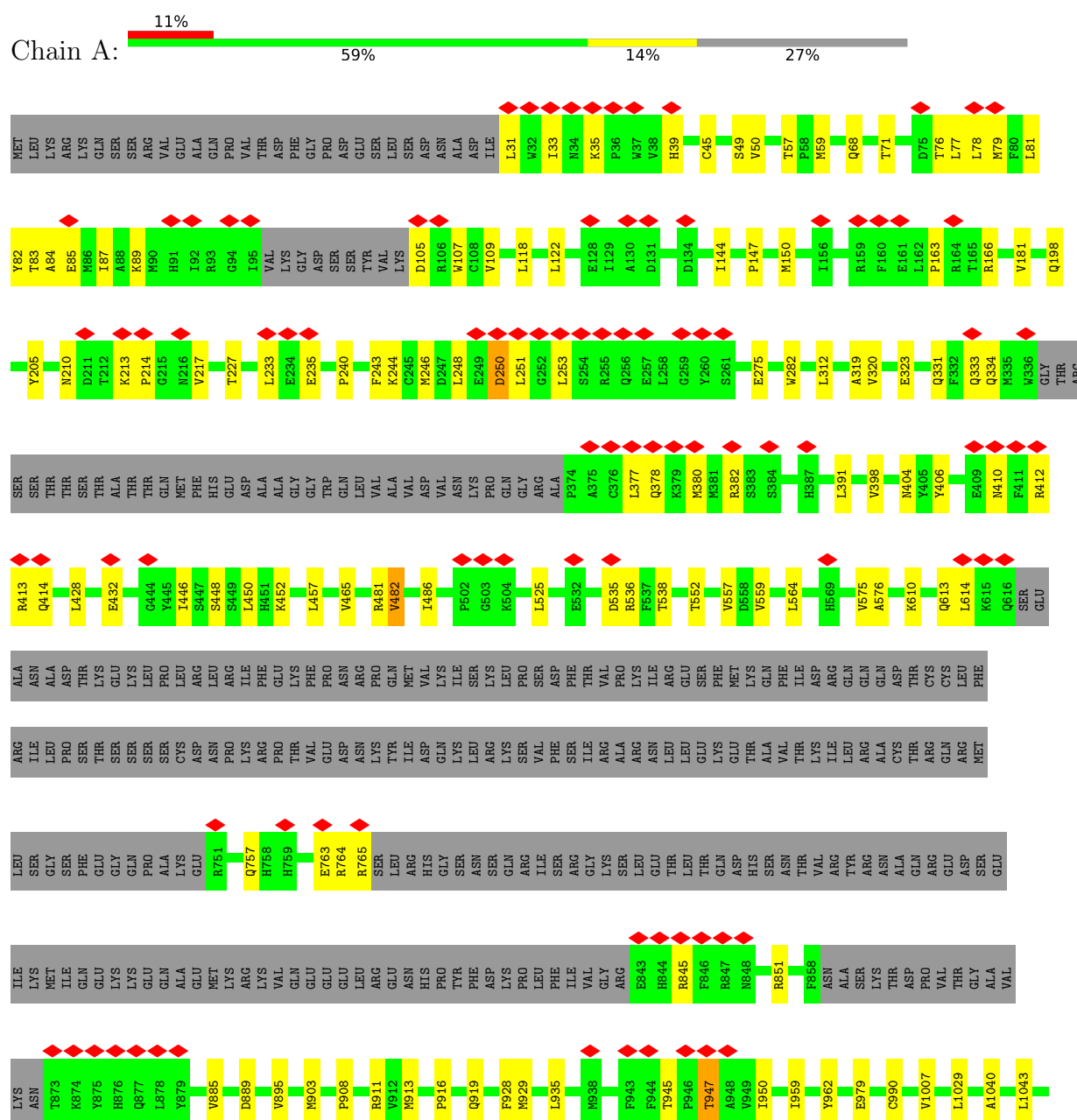


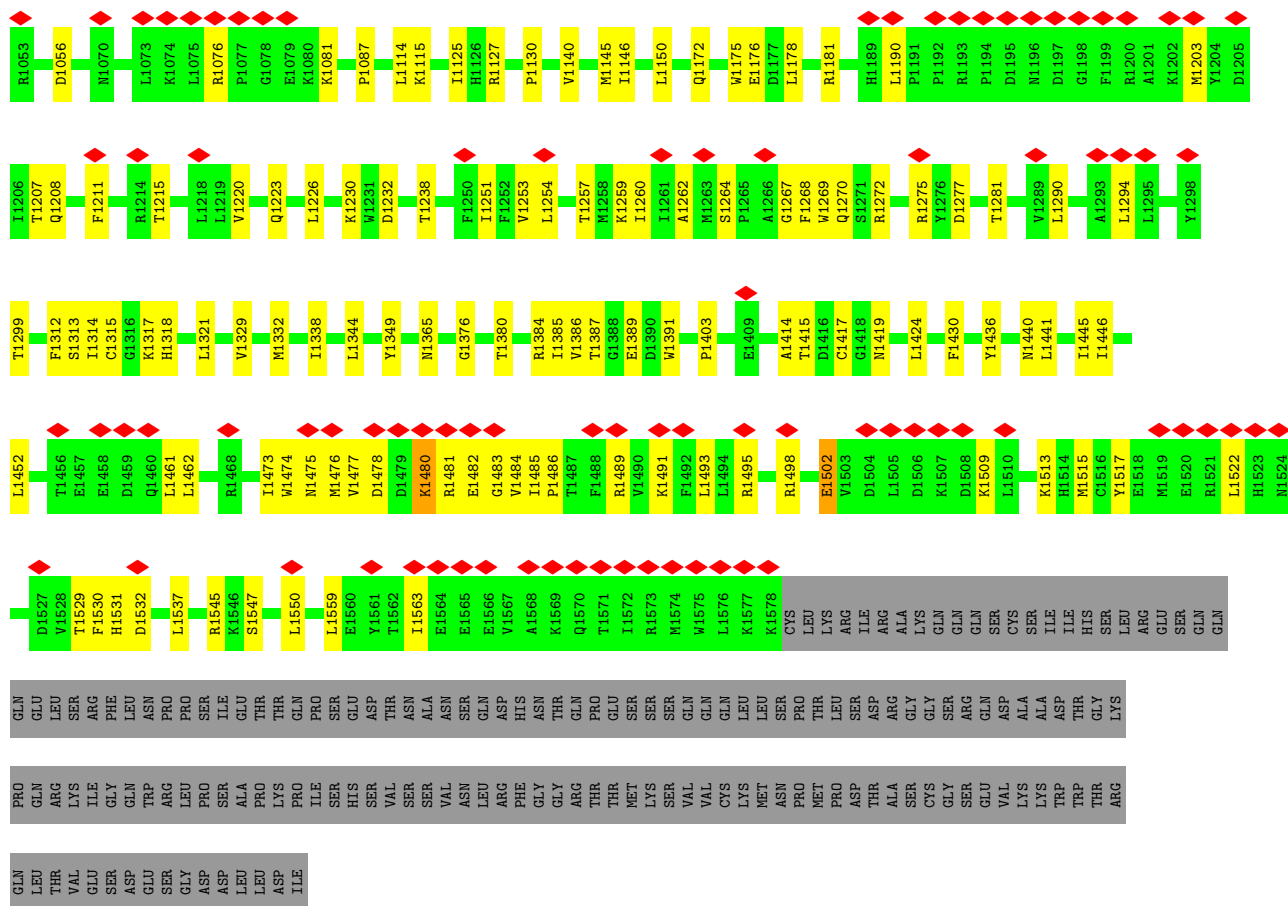
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	O		0
			28	27	1		
5	A	1	Total	C	O		0
			28	27	1		

3 Residue-property plots

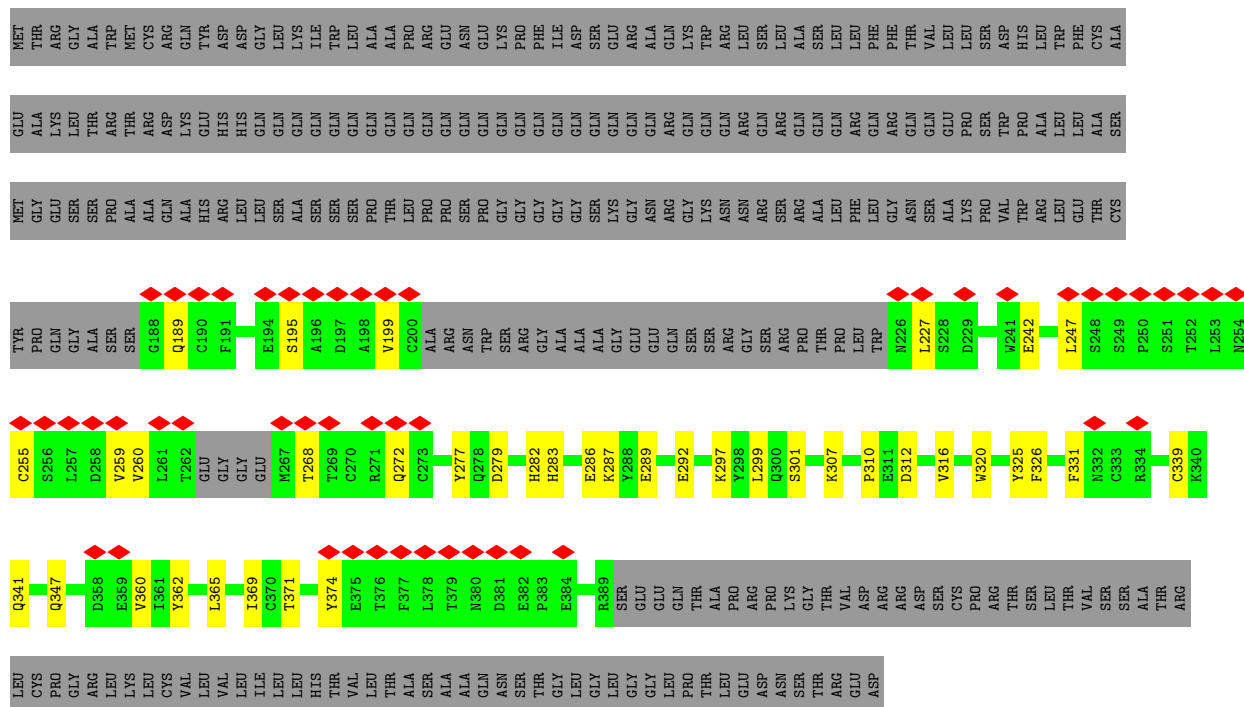
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Sodium leak channel non-selective protein





• Molecule 2: Transmembrane protein FAM155A



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	135043	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.217	Depositor
Minimum map value	-0.120	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.05	Depositor
Map size ($\text{\AA}$)	250.79999, 250.79999, 250.79999	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.045, 1.045, 1.045	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: 6OU, CLR, NAG

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	0.25	0/10620	0.38	0/14410
2	B	0.29	0/1411	0.46	0/1915
All	All	0.26	0/12031	0.39	0/16325

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10353	0	10457	133	0
2	B	1379	0	1254	24	0
3	A	42	0	39	2	0
4	A	379	0	0	0	0
5	A	56	0	92	2	0
All	All	12209	0	11842	149	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 6.

All (149) 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:250:ASP:N	1:A:250:ASP:OD1	2.21	0.73
1:A:404:ASN:O	1:A:413:ARG:NH2	2.24	0.70
1:A:1115:LYS:HE2	1:A:1389[B]:GLU:O	1.92	0.70
2:B:287:LYS:HE3	2:B:325:TYR:OH	1.93	0.69
1:A:916:PRO:HB3	5:A:2016:CLR:H41	1.75	0.69
1:A:895:VAL:HG21	1:A:928:PHE:HD2	1.57	0.68
1:A:1318:HIS:HB3	1:A:1321:LEU:HB2	1.75	0.68
1:A:76:THR:HA	1:A:122:LEU:HD11	1.77	0.66
1:A:1267:GLY:HA2	1:A:1270:GLN:HG3	1.78	0.65
1:A:1264:SER:HB3	1:A:1267:GLY:H	1.61	0.65
1:A:950:ILE:HD11	1:A:959:ILE:HG13	1.79	0.64
1:A:398:VAL:HG11	1:A:482:VAL:HG12	1.79	0.64
2:B:227:LEU:HD11	2:B:260:VAL:HG11	1.80	0.64
1:A:31:LEU:O	1:A:35:LYS:NZ	2.30	0.64
1:A:947:THR:O	1:A:947:THR:OG1	2.20	0.60
1:A:1190:LEU:O	1:A:1481:ARG:NH2	2.30	0.60
1:A:1338:ILE:HD12	1:A:1445:ILE:HD11	1.83	0.59
1:A:945:THR:HG22	1:A:947:THR:H	1.67	0.58
1:A:166:ARG:HH12	1:A:334:GLN:HE21	1.52	0.58
2:B:199:VAL:O	2:B:199:VAL:HG23	2.04	0.57
1:A:1125:ILE:HG23	1:A:1130:PRO:HA	1.87	0.56
1:A:205:TYR:HA	1:A:246:MET:O	2.05	0.56
2:B:283:HIS:O	2:B:287:LYS:HG3	2.05	0.56
1:A:552:THR:HG22	1:A:1145:MET:HE1	1.88	0.56
1:A:33:ILE:O	1:A:39:HIS:NE2	2.39	0.56
1:A:81:LEU:O	1:A:84:ALA:HB3	2.06	0.56
1:A:227:THR:HG21	2:B:299:LEU:HD12	1.88	0.55
1:A:1115:LYS:CE	1:A:1389[B]:GLU:O	2.54	0.55
1:A:49:SER:HB2	1:A:78:LEU:HD13	1.89	0.54
1:A:1415:THR:HG23	1:A:1417:CYS:H	1.72	0.54
1:A:1329:VAL:HA	1:A:1332:MET:HE3	1.90	0.54
1:A:82:TYR:O	1:A:85:GLU:HG3	2.08	0.54
1:A:214:PRO:HA	1:A:251:LEU:HD22	1.90	0.54
1:A:457:LEU:HD13	1:A:481:ARG:HG2	1.90	0.53
1:A:564:LEU:HD21	1:A:576:ALA:HB2	1.91	0.53
1:A:1087:PRO:HG2	2:B:369:ILE:O	2.09	0.52
1:A:210:ASN:HA	1:A:244:LYS:HG2	1.89	0.52
2:B:268:THR:O	2:B:272:GLN:HG3	2.09	0.52
1:A:1486:PRO:HG2	1:A:1489:ARG:HG2	1.90	0.52
1:A:333:GLN:OE1	1:A:610:LYS:NZ	2.33	0.52
1:A:1043:LEU:O	1:A:1127:ARG:NH1	2.37	0.51
1:A:166:ARG:NH1	1:A:331:GLN:OE1	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1081:LYS:NZ	3:A:2002:NAG:H61	2.26	0.51
1:A:1207:THR:OG1	1:A:1208:GLN:OE1	2.26	0.51
1:A:1386:VAL:HG23	1:A:1387[A]:THR:HG23	1.93	0.51
2:B:282:HIS:O	2:B:286:GLU:HG2	2.10	0.51
1:A:1076:ARG:NH2	3:A:2002:NAG:O6	2.44	0.50
1:A:979:GLU:HG2	1:A:1419:ASN:ND2	2.27	0.50
1:A:1338:ILE:HD13	1:A:1441:LEU:HB3	1.94	0.49
1:A:1175:TRP:HB2	1:A:1547:SER:HB3	1.94	0.49
2:B:247:LEU:HD23	2:B:277:TYR:CE1	2.48	0.49
1:A:1314:ILE:HD12	1:A:1317:LYS:HD2	1.93	0.49
1:A:1436:TYR:O	1:A:1440:ASN:ND2	2.46	0.48
1:A:929:MET:HE2	1:A:962:TYR:HB2	1.94	0.48
1:A:928:PHE:HE1	5:A:2016:CLR:H273	1.78	0.48
1:A:1477:VAL:O	1:A:1489:ARG:NH2	2.46	0.48
2:B:195:SER:O	2:B:199:VAL:HG22	2.14	0.48
1:A:50:VAL:HG21	1:A:150:MET:HB2	1.95	0.47
1:A:410:ASN:N	1:A:410:ASN:OD1	2.45	0.47
1:A:198:GLN:O	1:A:1230:LYS:NZ	2.47	0.47
1:A:1277:ASP:O	1:A:1281:THR:OG1	2.30	0.47
2:B:301:SER:HB2	2:B:310:PRO:HG3	1.96	0.47
1:A:57:THR:HG21	1:A:525:LEU:HD11	1.96	0.47
1:A:916:PRO:HA	1:A:919:GLN:HG3	1.97	0.47
1:A:1473:ILE:HG22	1:A:1493:LEU:HG	1.96	0.47
1:A:412:ARG:HB3	1:A:414:GLN:HG2	1.97	0.47
2:B:242:GLU:HG2	2:B:331:PHE:CD2	2.50	0.47
1:A:1480:LYS:HB2	1:A:1482:GLU:OE2	2.15	0.47
1:A:1517:TYR:HD2	1:A:1563:ILE:HG23	1.79	0.46
1:A:903:MET:HE1	1:A:990:CYS:HA	1.96	0.46
1:A:1253:VAL:O	1:A:1257:THR:HG23	2.16	0.46
1:A:1515:MET:HE1	1:A:1537:LEU:HD23	1.97	0.46
1:A:1491:LYS:HZ1	1:A:1495:ARG:HH11	1.64	0.46
1:A:144:ILE:O	1:A:147:PRO:HD2	2.16	0.46
1:A:1403:PRO:HG2	2:B:347:GLN:NE2	2.31	0.45
1:A:1272:ARG:HA	1:A:1275:ARG:HD3	1.98	0.45
1:A:68:GLN:O	1:A:71:THR:HG22	2.15	0.45
1:A:248:LEU:O	1:A:253:LEU:HB2	2.17	0.45
1:A:845:ARG:HD2	1:A:845:ARG:HA	1.81	0.45
1:A:1146:ILE:O	1:A:1150:LEU:HG	2.16	0.45
1:A:1259:LYS:HE3	1:A:1268:PHE:HE1	1.82	0.45
1:A:1114:LEU:HD21	1:A:1140:VAL:HG13	1.99	0.45
1:A:1480:LYS:HD2	1:A:1480:LYS:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:ARG:HD3	1:A:559:VAL:HG13	1.99	0.45
1:A:59:MET:HG3	1:A:538:THR:HB	1.98	0.45
1:A:406:TYR:HB2	1:A:1040:ALA:HB1	1.98	0.45
2:B:312:ASP:O	2:B:316:VAL:HG22	2.17	0.44
1:A:1386:VAL:HG23	1:A:1387[B]:THR:HG23	1.97	0.44
1:A:1232:ASP:O	1:A:1238:THR:HG21	2.18	0.44
1:A:885:VAL:HB	1:A:889:ASP:HB2	1.99	0.44
1:A:448:SER:C	1:A:450:LEU:H	2.26	0.44
1:A:240:PRO:HG3	2:B:299:LEU:HD22	2.00	0.44
1:A:613:GLN:HB3	1:A:1550:LEU:HD21	2.00	0.44
1:A:764:ARG:HH11	1:A:765:ARG:HH21	1.65	0.44
1:A:1403:PRO:HG2	2:B:347:GLN:HE22	1.81	0.44
1:A:1178:LEU:HD22	1:A:1461:LEU:HG	2.00	0.44
1:A:105:ASP:C	1:A:107:TRP:H	2.26	0.43
1:A:378:GLN:O	1:A:382:ARG:HG2	2.18	0.43
1:A:1522:LEU:HD23	1:A:1532:ASP:HB3	2.00	0.43
1:A:1251:ILE:O	1:A:1254:LEU:HG	2.19	0.43
1:A:1260:ILE:HG12	1:A:1268:PHE:CG	2.53	0.43
1:A:312:LEU:HD22	1:A:1446:ILE:HD11	2.00	0.43
1:A:1223:GLN:O	1:A:1226:LEU:HB2	2.19	0.43
1:A:1485:ILE:HD12	1:A:1489:ARG:HB2	2.01	0.43
1:A:1529:THR:C	1:A:1531:HIS:H	2.27	0.43
1:A:163:PRO:HD2	1:A:166:ARG:HD2	2.01	0.43
1:A:319:ALA:O	1:A:323:GLU:HG2	2.19	0.42
1:A:33:ILE:HD12	1:A:89:LYS:HE3	1.99	0.42
1:A:213:LYS:HA	1:A:213:LYS:HD3	1.74	0.42
1:A:1220:VAL:HB	1:A:1314:ILE:HD13	2.00	0.42
1:A:1389[B]:GLU:N	1:A:1389[B]:GLU:OE2	2.53	0.42
1:A:391:LEU:HD23	1:A:391:LEU:HA	1.91	0.42
1:A:1181:ARG:HD3	1:A:1452:LEU:O	2.20	0.42
1:A:1376:GLY:O	1:A:1380:THR:HG23	2.19	0.42
1:A:1498:ARG:NH2	1:A:1502:GLU:OE1	2.38	0.42
1:A:1509:LYS:O	1:A:1513:LYS:HG3	2.20	0.42
1:A:535:ASP:OD1	1:A:535:ASP:N	2.46	0.42
1:A:1172:GLN:O	1:A:1176:GLU:HG2	2.19	0.42
1:A:79:MET:HE3	1:A:79:MET:HB3	1.88	0.42
1:A:122:LEU:HA	1:A:122:LEU:HD23	1.76	0.41
1:A:377:LEU:HD23	1:A:377:LEU:HA	1.86	0.41
1:A:1290:LEU:O	1:A:1294:LEU:N	2.38	0.41
2:B:247:LEU:HD22	2:B:326:PHE:HD1	1.85	0.41
1:A:275:GLU:HG3	1:A:557:VAL:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:TRP:NE1	1:A:1387[A]:THR:O	2.38	0.41
1:A:908:PRO:O	1:A:911:ARG:NH2	2.48	0.41
1:A:1474:TRP:CZ2	1:A:1530:PHE:HB2	2.56	0.41
1:A:1478:ASP:OD2	1:A:1483:GLY:N	2.44	0.41
2:B:362:TYR:HB3	2:B:365:LEU:HB2	2.01	0.41
1:A:1349:TYR:CE2	1:A:1430:PHE:HB2	2.55	0.41
1:A:446:ILE:O	1:A:452:LYS:HE3	2.21	0.41
1:A:913:MET:HE2	1:A:913:MET:HB2	1.96	0.41
1:A:1203:MET:HB3	1:A:1262:ALA:HB2	2.02	0.41
1:A:1414:ALA:O	2:B:307:LYS:HD3	2.21	0.41
2:B:189:GLN:H	2:B:189:GLN:CD	2.28	0.41
1:A:45:CYS:HB3	1:A:78:LEU:HD22	2.03	0.40
1:A:83:THR:O	1:A:87:ILE:HG12	2.21	0.40
1:A:181:VAL:HG21	1:A:320:VAL:HG21	2.03	0.40
1:A:1384:ARG:O	1:A:1389[B]:GLU:HB3	2.20	0.40
2:B:289:GLU:HA	2:B:292:GLU:HG2	2.03	0.40
1:A:764:ARG:HD2	1:A:1545:ARG:HD3	2.02	0.40
1:A:1087:PRO:HD3	2:B:320:TRP:CZ2	2.55	0.40
1:A:1211:PHE:O	1:A:1215:THR:OG1	2.32	0.40
2:B:255:CYS:SG	2:B:259:VAL:HG21	2.61	0.40
1:A:243:PHE:HZ	2:B:297:LYS:HA	1.86	0.40
1:A:1389[B]:GLU:HG3	1:A:1391:TRP:HD1	1.85	0.40
1:A:89:LYS:HE3	1:A:89:LYS:HB2	1.76	0.40
1:A:1269:TRP:CD2	1:A:1275:ARG:HG2	2.57	0.40
1:A:59:MET:HE3	1:A:59:MET:HB3	1.98	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	1269/1738 (73%)	1217 (96%)	52 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	167/467 (36%)	152 (91%)	15 (9%)	0	100	100
All	All	1436/2205 (65%)	1369 (95%)	67 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	1124/1572 (72%)	1086 (97%)	38 (3%)	32	53
2	B	157/409 (38%)	151 (96%)	6 (4%)	29	49
All	All	1281/1981 (65%)	1237 (97%)	44 (3%)	33	53

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	LEU
1	A	109	VAL
1	A	118	LEU
1	A	217	VAL
1	A	233	LEU
1	A	235	GLU
1	A	250	ASP
1	A	380	MET
1	A	428	LEU
1	A	432	GLU
1	A	465	VAL
1	A	482	VAL
1	A	486	ILE
1	A	575	VAL
1	A	614	LEU
1	A	757	GLN
1	A	763	GLU
1	A	851	ARG

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Mol	Chain	Res	Type
1	A	935	LEU
1	A	947	THR
1	A	1007	VAL
1	A	1029	LEU
1	A	1056	ASP
1	A	1299	THR
1	A	1312	PHE
1	A	1313	SER
1	A	1315	CYS
1	A	1344	LEU
1	A	1365	ASN
1	A	1385	ILE
1	A	1424	LEU
1	A	1462	LEU
1	A	1475	ASN
1	A	1476	MET
1	A	1480	LYS
1	A	1484	VAL
1	A	1502	GLU
1	A	1559	LEU
2	B	279	ASP
2	B	339	CYS
2	B	341	GLN
2	B	360	VAL
2	B	371	THR
2	B	374	TYR

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	334	GLN
1	A	1037	GLN
1	A	1449	ASN

5.3.3 RNA ⓘ

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](#)

17 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
4	6OU	A	2006	-	45,45,48	1.37	6 (13%)	48,50,53	1.12	2 (4%)
4	6OU	A	2012	-	19,19,48	1.18	2 (10%)	19,19,53	1.06	1 (5%)
4	6OU	A	2004	-	35,35,48	1.37	4 (11%)	38,40,53	1.18	3 (7%)
4	6OU	A	2015	-	30,30,48	1.53	6 (20%)	33,35,53	1.26	2 (6%)
3	NAG	A	2002	1	14,14,15	0.49	0	17,19,21	0.39	0
5	CLR	A	2016	-	31,31,31	0.75	0	48,48,48	1.07	2 (4%)
5	CLR	A	2017	-	31,31,31	0.72	0	48,48,48	1.21	4 (8%)
4	6OU	A	2014	-	37,37,48	1.38	4 (10%)	40,42,53	1.09	2 (5%)
4	6OU	A	2013	-	26,26,48	1.62	5 (19%)	29,31,53	1.25	2 (6%)
3	NAG	A	2001	1	14,14,15	0.29	0	17,19,21	0.70	0
4	6OU	A	2011	-	17,17,48	1.39	2 (11%)	17,17,53	1.11	1 (5%)
3	NAG	A	2003	1	14,14,15	0.27	0	17,19,21	0.54	0
4	6OU	A	2007	-	36,36,48	1.37	4 (11%)	39,41,53	1.13	2 (5%)
4	6OU	A	2008	-	19,19,48	1.22	2 (10%)	19,19,53	1.04	0
4	6OU	A	2005	-	45,45,48	1.33	6 (13%)	48,50,53	1.17	2 (4%)
4	6OU	A	2009	-	41,41,48	1.33	4 (9%)	44,46,53	1.15	2 (4%)
4	6OU	A	2010	-	17,17,48	2.13	4 (23%)	17,17,53	1.16	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	6OU	A	2006	-	-	27/47/47/52	-
4	6OU	A	2012	-	-	10/17/17/52	-
4	6OU	A	2004	-	-	20/39/39/52	-
4	6OU	A	2015	-	-	16/32/32/52	-
3	NAG	A	2002	1	-	2/6/23/26	0/1/1/1
5	CLR	A	2016	-	-	5/10/68/68	0/4/4/4
5	CLR	A	2017	-	-	2/10/68/68	0/4/4/4
4	6OU	A	2014	-	-	19/41/41/52	-
4	6OU	A	2013	-	-	13/28/28/52	-
3	NAG	A	2001	1	-	2/6/23/26	0/1/1/1
4	6OU	A	2011	-	-	11/15/15/52	-
3	NAG	A	2003	1	-	0/6/23/26	0/1/1/1
4	6OU	A	2007	-	-	20/40/40/52	-
4	6OU	A	2008	-	-	8/17/17/52	-
4	6OU	A	2005	-	-	26/47/47/52	-
4	6OU	A	2009	-	-	23/45/45/52	-
4	6OU	A	2010	-	-	11/15/15/52	-

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2010	6OU	O17-C16	5.99	1.41	1.22
4	A	2010	6OU	O18-C16	-3.86	1.18	1.30
4	A	2011	6OU	O18-C16	3.56	1.42	1.30
4	A	2010	6OU	C08-C07	-3.56	1.34	1.51
4	A	2008	6OU	O30-C31	3.39	1.42	1.30
4	A	2005	6OU	P23-O26	3.35	1.67	1.54
4	A	2004	6OU	O30-C20	-3.35	1.38	1.46
4	A	2013	6OU	P23-O26	3.33	1.67	1.54
4	A	2006	6OU	P23-O26	3.32	1.67	1.54
4	A	2014	6OU	O30-C20	-3.31	1.38	1.46
4	A	2013	6OU	O30-C20	-3.30	1.38	1.46
4	A	2012	6OU	O30-C31	3.27	1.41	1.30
4	A	2009	6OU	O30-C20	-3.26	1.38	1.46
4	A	2006	6OU	O18-C16	3.25	1.42	1.33
4	A	2015	6OU	P23-O26	3.22	1.66	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2013	6OU	O18-C16	3.21	1.42	1.33
4	A	2007	6OU	O30-C20	-3.18	1.39	1.46
4	A	2007	6OU	O18-C16	3.18	1.42	1.33
4	A	2014	6OU	O18-C16	3.17	1.42	1.33
4	A	2005	6OU	O18-C16	3.16	1.42	1.33
4	A	2015	6OU	O18-C16	3.15	1.42	1.33
4	A	2015	6OU	O30-C20	-3.12	1.39	1.46
4	A	2005	6OU	O30-C20	-3.09	1.39	1.46
4	A	2009	6OU	O18-C16	3.08	1.42	1.33
4	A	2004	6OU	O18-C16	3.05	1.42	1.33
4	A	2006	6OU	O30-C20	-3.04	1.39	1.46
4	A	2006	6OU	O30-C31	2.81	1.42	1.34
4	A	2015	6OU	O30-C31	2.78	1.42	1.34
4	A	2007	6OU	O30-C31	2.73	1.42	1.34
4	A	2005	6OU	O30-C31	2.72	1.42	1.34
4	A	2011	6OU	C15-C16	2.71	1.56	1.50
4	A	2014	6OU	O30-C31	2.66	1.41	1.34
4	A	2009	6OU	O30-C31	2.62	1.41	1.34
4	A	2013	6OU	O30-C31	2.58	1.41	1.34
4	A	2004	6OU	O30-C31	2.56	1.41	1.34
4	A	2006	6OU	P23-O22	2.36	1.67	1.60
4	A	2005	6OU	P23-O22	2.32	1.67	1.60
4	A	2015	6OU	P23-O22	2.20	1.67	1.60
4	A	2014	6OU	C15-C16	2.20	1.57	1.50
4	A	2008	6OU	C33-C31	2.18	1.55	1.50
4	A	2006	6OU	C15-C16	2.16	1.57	1.50
4	A	2013	6OU	P23-O22	2.15	1.67	1.60
4	A	2010	6OU	C15-C16	2.14	1.55	1.50
4	A	2005	6OU	C15-C16	2.09	1.56	1.50
4	A	2009	6OU	P23-O26	2.08	1.67	1.59
4	A	2015	6OU	C15-C16	2.08	1.56	1.50
4	A	2012	6OU	C33-C31	2.06	1.55	1.50
4	A	2004	6OU	P23-O26	2.02	1.67	1.59
4	A	2007	6OU	C15-C16	2.02	1.56	1.50

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2015	6OU	O30-C31-C33	4.15	120.45	111.48
4	A	2004	6OU	O30-C31-C33	4.11	120.37	111.48
4	A	2005	6OU	O30-C31-C33	4.09	120.34	111.48
4	A	2006	6OU	O30-C31-C33	4.08	120.31	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2009	6OU	O30-C31-C33	3.94	120.00	111.48
4	A	2013	6OU	O30-C31-C33	3.79	119.67	111.48
4	A	2007	6OU	O30-C31-C33	3.75	119.58	111.48
4	A	2014	6OU	O30-C31-C33	3.70	119.50	111.48
5	A	2017	CLR	C8-C7-C6	-3.61	107.75	112.76
4	A	2006	6OU	O18-C16-C15	2.95	120.82	111.83
4	A	2013	6OU	O18-C16-C15	2.88	120.62	111.83
4	A	2014	6OU	O18-C16-C15	2.86	120.57	111.83
4	A	2004	6OU	O18-C16-C15	2.84	120.49	111.83
4	A	2007	6OU	O18-C16-C15	2.78	120.32	111.83
4	A	2015	6OU	O18-C16-C15	2.71	120.11	111.83
4	A	2009	6OU	O18-C16-C15	2.69	120.05	111.83
5	A	2017	CLR	C9-C10-C5	2.66	113.54	109.65
4	A	2005	6OU	O18-C16-C15	2.54	119.59	111.83
5	A	2017	CLR	C3-C4-C5	-2.39	108.24	112.05
5	A	2017	CLR	C13-C14-C8	-2.35	111.07	114.41
5	A	2016	CLR	C4-C5-C10	2.26	119.31	116.42
4	A	2011	6OU	O18-C16-C15	2.11	120.67	114.00
5	A	2016	CLR	C4-C5-C6	-2.06	117.77	120.57
4	A	2012	6OU	O30-C31-C33	2.00	120.33	114.00
4	A	2004	6OU	C20-O30-C31	-2.00	113.00	117.80

There are no chirality outliers.

All (215) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2004	6OU	C21-O22-P23-O24
4	A	2004	6OU	C21-O22-P23-O26
4	A	2004	6OU	C27-O26-P23-O22
4	A	2004	6OU	C27-O26-P23-O24
4	A	2005	6OU	C15-C16-O18-C19
4	A	2005	6OU	O17-C16-O18-C19
4	A	2006	6OU	C21-O22-P23-O25
4	A	2006	6OU	C21-O22-P23-O26
4	A	2006	6OU	C33-C31-O30-C20
4	A	2007	6OU	O26-C27-C28-N29
4	A	2009	6OU	C27-O26-P23-O22
4	A	2009	6OU	C28-C27-O26-P23
4	A	2009	6OU	O26-C27-C28-N29
4	A	2013	6OU	O18-C19-C20-O30
4	A	2013	6OU	C21-O22-P23-O25
4	A	2013	6OU	C21-O22-P23-O26

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Mol	Chain	Res	Type	Atoms
4	A	2014	6OU	O26-C27-C28-N29
4	A	2015	6OU	C21-O22-P23-O25
4	A	2015	6OU	C21-O22-P23-O26
4	A	2015	6OU	O32-C31-O30-C20
4	A	2015	6OU	C33-C31-O30-C20
4	A	2014	6OU	O17-C16-O18-C19
4	A	2006	6OU	O32-C31-O30-C20
4	A	2014	6OU	O32-C31-O30-C20
4	A	2007	6OU	C15-C16-O18-C19
4	A	2014	6OU	C15-C16-O18-C19
4	A	2014	6OU	C33-C31-O30-C20
5	A	2017	CLR	C21-C20-C22-C23
4	A	2015	6OU	C15-C16-O18-C19
4	A	2007	6OU	O17-C16-O18-C19
4	A	2015	6OU	O17-C16-O18-C19
4	A	2010	6OU	C06-C07-C08-C09
5	A	2017	CLR	C17-C20-C22-C23
4	A	2012	6OU	C36-C37-C38-C39
4	A	2004	6OU	C15-C16-O18-C19
4	A	2004	6OU	O17-C16-O18-C19
4	A	2005	6OU	O30-C20-C21-O22
4	A	2005	6OU	C33-C31-O30-C20
3	A	2001	NAG	C8-C7-N2-C2
3	A	2001	NAG	O7-C7-N2-C2
5	A	2016	CLR	C17-C20-C22-C23
4	A	2007	6OU	C13-C14-C15-C16
4	A	2005	6OU	C31-C33-C34-C35
4	A	2006	6OU	C31-C33-C34-C35
4	A	2008	6OU	C31-C33-C34-C35
4	A	2012	6OU	C31-C33-C34-C35
4	A	2009	6OU	C13-C14-C15-C16
4	A	2006	6OU	C13-C14-C15-C16
4	A	2015	6OU	C10-C11-C12-C13
4	A	2006	6OU	C15-C16-O18-C19
5	A	2016	CLR	C21-C20-C22-C23
4	A	2005	6OU	O32-C31-O30-C20
4	A	2011	6OU	C13-C14-C15-C16
4	A	2009	6OU	C31-C33-C34-C35
3	A	2002	NAG	C4-C5-C6-O6
4	A	2006	6OU	O17-C16-O18-C19
4	A	2004	6OU	C13-C14-C15-C16
5	A	2016	CLR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
5	A	2016	CLR	C23-C24-C25-C27
4	A	2006	6OU	C12-C13-C14-C15
4	A	2011	6OU	C03-C04-C05-C06
4	A	2005	6OU	C12-C13-C14-C15
4	A	2007	6OU	C36-C37-C38-C39
4	A	2012	6OU	C43-C44-C45-C46
4	A	2015	6OU	C13-C14-C15-C16
4	A	2014	6OU	C06-C07-C08-C09
4	A	2013	6OU	C31-C33-C34-C35
4	A	2015	6OU	C09-C10-C11-C12
4	A	2006	6OU	C08-C09-C10-C11
4	A	2011	6OU	C09-C10-C11-C12
4	A	2004	6OU	C34-C35-C36-C37
4	A	2006	6OU	C02-C03-C04-C05
4	A	2010	6OU	C03-C04-C05-C06
4	A	2012	6OU	C34-C35-C36-C37
4	A	2013	6OU	C35-C36-C37-C38
4	A	2012	6OU	C45-C46-C47-C48
4	A	2011	6OU	C06-C07-C08-C09
4	A	2010	6OU	C10-C11-C12-C13
4	A	2006	6OU	C10-C11-C12-C13
4	A	2008	6OU	C42-C43-C44-C45
4	A	2010	6OU	C08-C09-C10-C11
4	A	2011	6OU	C08-C09-C10-C11
4	A	2005	6OU	C36-C37-C38-C39
4	A	2014	6OU	C08-C09-C10-C11
4	A	2006	6OU	C35-C36-C37-C38
4	A	2013	6OU	C15-C16-O18-C19
4	A	2009	6OU	C12-C13-C14-C15
4	A	2005	6OU	C45-C46-C47-C48
4	A	2009	6OU	C03-C04-C05-C06
4	A	2015	6OU	C12-C13-C14-C15
4	A	2004	6OU	C36-C37-C38-C39
4	A	2009	6OU	C06-C07-C08-C09
4	A	2012	6OU	C35-C36-C37-C38
4	A	2005	6OU	C35-C36-C37-C38
4	A	2007	6OU	C33-C31-O30-C20
4	A	2007	6OU	O32-C31-O30-C20
4	A	2007	6OU	C37-C38-C39-C40
4	A	2008	6OU	C36-C37-C38-C39
4	A	2009	6OU	C36-C37-C38-C39
4	A	2005	6OU	C44-C45-C46-C47

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Mol	Chain	Res	Type	Atoms
4	A	2006	6OU	C36-C37-C38-C39
4	A	2014	6OU	C04-C05-C06-C07
4	A	2014	6OU	C31-C33-C34-C35
4	A	2007	6OU	C12-C13-C14-C15
4	A	2006	6OU	C06-C07-C08-C09
4	A	2009	6OU	O18-C19-C20-O30
3	A	2002	NAG	O5-C5-C6-O6
4	A	2007	6OU	C35-C36-C37-C38
4	A	2005	6OU	C08-C09-C10-C11
4	A	2007	6OU	C33-C34-C35-C36
4	A	2007	6OU	C31-C33-C34-C35
4	A	2007	6OU	C34-C35-C36-C37
4	A	2013	6OU	O17-C16-O18-C19
4	A	2005	6OU	C06-C07-C08-C09
4	A	2006	6OU	C45-C46-C47-C48
4	A	2005	6OU	C19-C20-C21-O22
4	A	2014	6OU	C19-C20-C21-O22
4	A	2010	6OU	C05-C06-C07-C08
4	A	2015	6OU	C36-C37-C38-C39
4	A	2012	6OU	C33-C34-C35-C36
4	A	2004	6OU	C41-C42-C43-C44
4	A	2006	6OU	C03-C04-C05-C06
4	A	2009	6OU	C10-C11-C12-C13
4	A	2014	6OU	C13-C14-C15-C16
4	A	2009	6OU	C08-C09-C10-C11
4	A	2006	6OU	C21-O22-P23-O24
4	A	2015	6OU	C21-O22-P23-O24
4	A	2014	6OU	C03-C04-C05-C06
4	A	2005	6OU	C46-C47-C48-C49
4	A	2007	6OU	O30-C20-C21-O22
4	A	2013	6OU	O30-C20-C21-O22
4	A	2006	6OU	C11-C12-C13-C14
4	A	2008	6OU	C34-C35-C36-C37
4	A	2004	6OU	O18-C19-C20-O30
4	A	2006	6OU	O18-C19-C20-O30
4	A	2014	6OU	C34-C35-C36-C37
4	A	2009	6OU	C34-C35-C36-C37
4	A	2010	6OU	C04-C05-C06-C07
4	A	2011	6OU	C01-C02-C03-C04
4	A	2006	6OU	O18-C19-C20-C21
4	A	2009	6OU	O18-C19-C20-C21
4	A	2014	6OU	O18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
4	A	2013	6OU	C10-C11-C12-C13
4	A	2007	6OU	C06-C07-C08-C09
4	A	2010	6OU	C01-C02-C03-C04
4	A	2007	6OU	C07-C08-C09-C10
4	A	2005	6OU	C34-C35-C36-C37
4	A	2005	6OU	O18-C19-C20-O30
4	A	2005	6OU	C33-C34-C35-C36
4	A	2009	6OU	C09-C10-C11-C12
4	A	2014	6OU	C35-C36-C37-C38
4	A	2009	6OU	C05-C06-C07-C08
4	A	2015	6OU	C34-C35-C36-C37
4	A	2006	6OU	C46-C47-C48-C49
4	A	2013	6OU	O18-C19-C20-C21
4	A	2008	6OU	C37-C38-C39-C40
4	A	2005	6OU	C09-C10-C11-C12
4	A	2011	6OU	C10-C11-C12-C13
4	A	2011	6OU	C02-C03-C04-C05
4	A	2006	6OU	C42-C43-C44-C45
4	A	2013	6OU	C19-C20-C21-O22
4	A	2009	6OU	C33-C34-C35-C36
4	A	2004	6OU	O30-C20-C21-O22
4	A	2014	6OU	O30-C20-C21-O22
4	A	2004	6OU	C12-C13-C14-C15
4	A	2014	6OU	O18-C19-C20-O30
4	A	2005	6OU	O18-C19-C20-C21
4	A	2004	6OU	C27-O26-P23-O25
4	A	2007	6OU	C21-O22-P23-O24
4	A	2009	6OU	C27-O26-P23-O24
4	A	2005	6OU	C05-C06-C07-C08
4	A	2008	6OU	C44-C45-C46-C47
4	A	2004	6OU	C19-C20-C21-O22
4	A	2007	6OU	C19-C20-C21-O22
4	A	2007	6OU	C08-C09-C10-C11
4	A	2005	6OU	C13-C14-C15-C16
4	A	2005	6OU	O30-C31-C33-C34
4	A	2006	6OU	C34-C35-C36-C37
4	A	2004	6OU	C33-C34-C35-C36
4	A	2015	6OU	O30-C20-C21-O22
4	A	2007	6OU	C20-C21-O22-P23
4	A	2010	6OU	C11-C12-C13-C14
4	A	2014	6OU	C01-C02-C03-C04
4	A	2011	6OU	C14-C15-C16-O17

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Mol	Chain	Res	Type	Atoms
4	A	2009	6OU	C02-C03-C04-C05
4	A	2010	6OU	C02-C03-C04-C05
4	A	2010	6OU	C14-C15-C16-O18
4	A	2011	6OU	C14-C15-C16-O18
4	A	2004	6OU	O18-C19-C20-C21
4	A	2015	6OU	C19-C20-C21-O22
4	A	2012	6OU	C40-C41-C42-C43
4	A	2005	6OU	C43-C44-C45-C46
4	A	2004	6OU	C40-C41-C42-C43
4	A	2004	6OU	C35-C36-C37-C38
4	A	2012	6OU	O30-C31-C33-C34
4	A	2010	6OU	C14-C15-C16-O17
4	A	2012	6OU	O32-C31-C33-C34
4	A	2008	6OU	O30-C31-C33-C34
4	A	2014	6OU	C02-C03-C04-C05
4	A	2009	6OU	O17-C16-O18-C19
4	A	2006	6OU	C07-C08-C09-C10
4	A	2009	6OU	C01-C02-C03-C04
4	A	2008	6OU	O32-C31-C33-C34
4	A	2009	6OU	C15-C16-O18-C19
4	A	2004	6OU	C11-C12-C13-C14
4	A	2011	6OU	C04-C05-C06-C07
4	A	2006	6OU	O30-C31-C33-C34
5	A	2016	CLR	C22-C23-C24-C25
4	A	2013	6OU	O30-C31-C33-C34
4	A	2005	6OU	C03-C04-C05-C06
4	A	2006	6OU	O32-C31-C33-C34
4	A	2015	6OU	C07-C08-C09-C10
4	A	2005	6OU	C11-C12-C13-C14
4	A	2013	6OU	C20-C21-O22-P23
4	A	2009	6OU	C19-C20-C21-O22

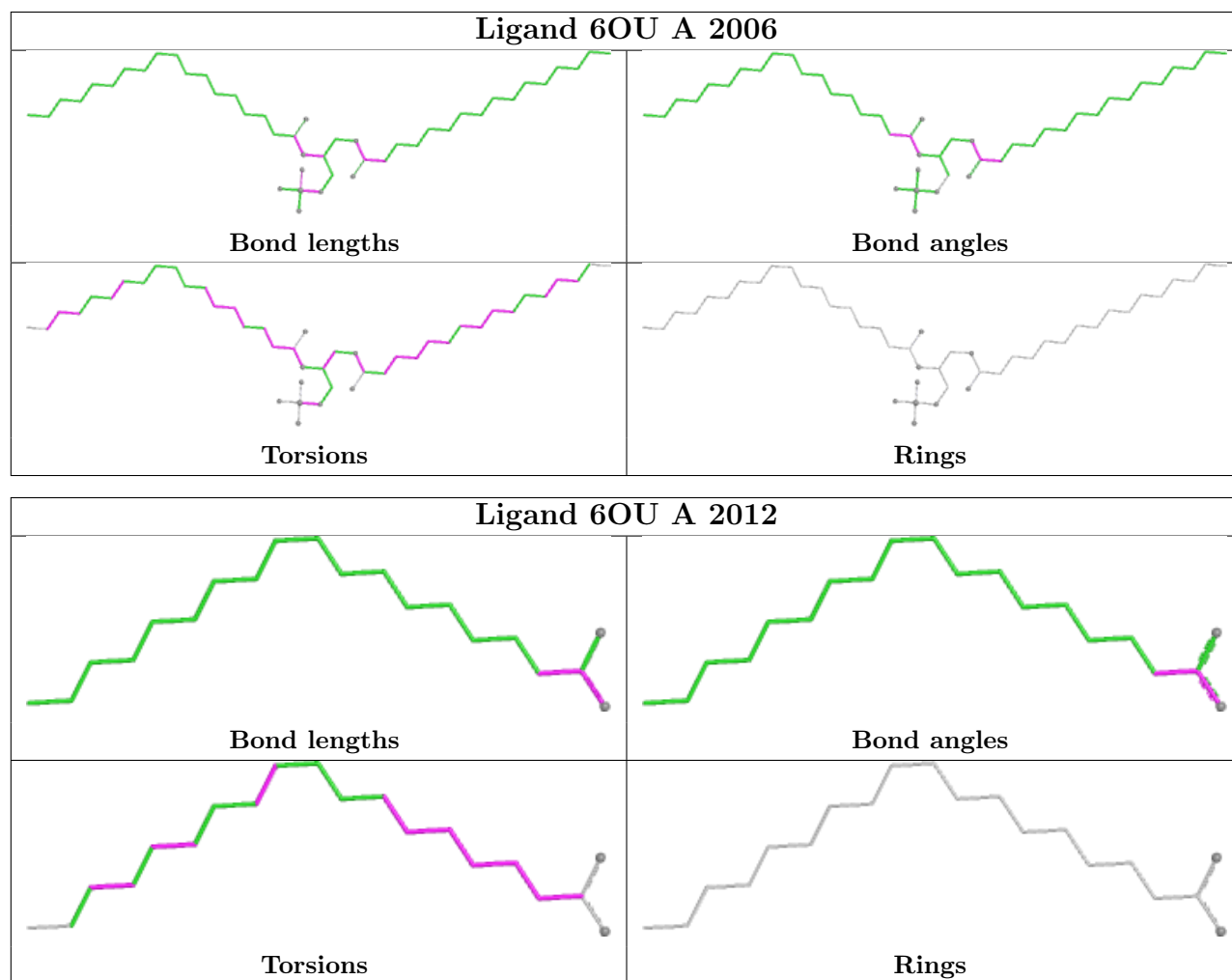
There are no ring outliers.

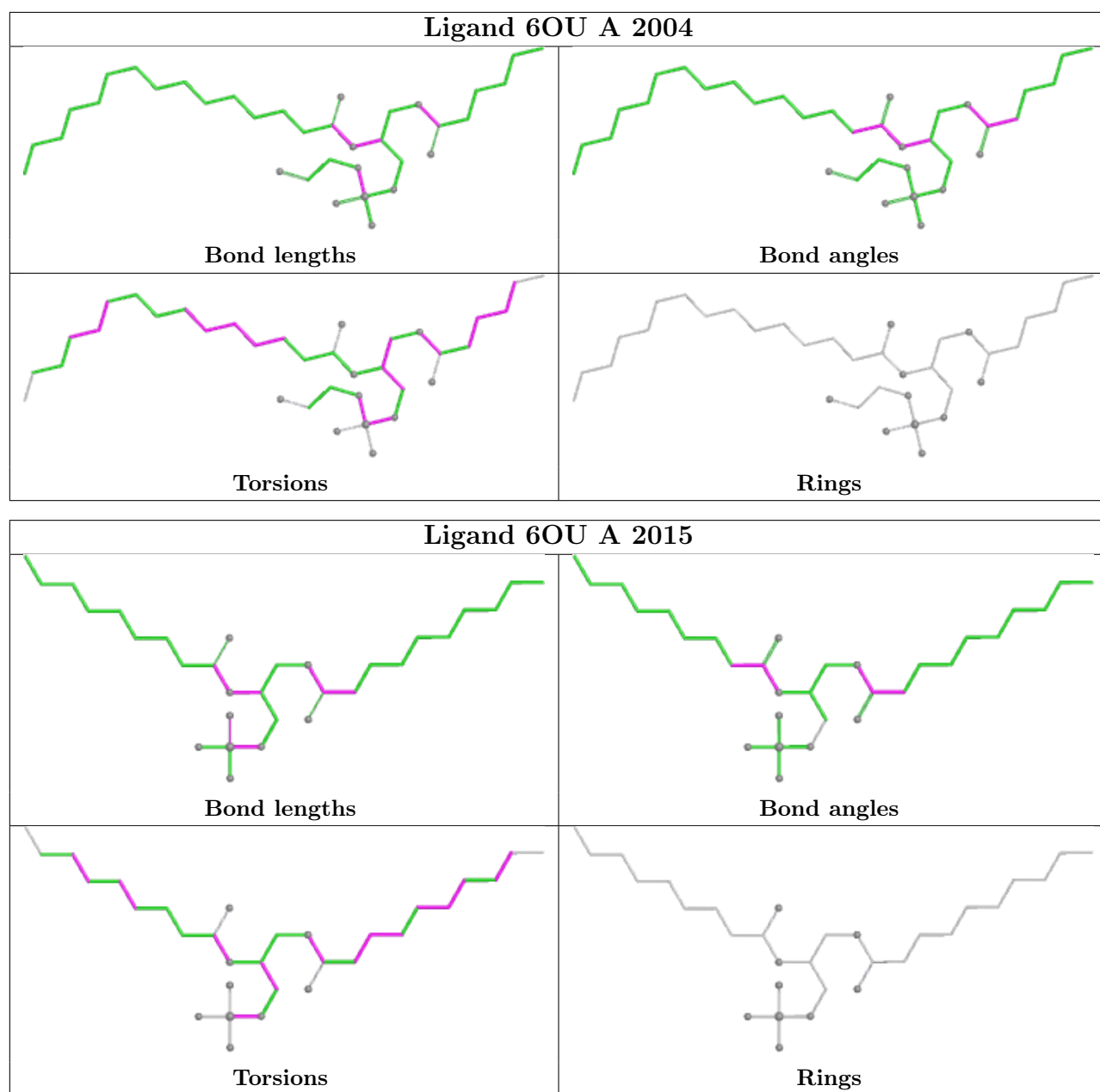
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2002	NAG	2	0
5	A	2016	CLR	2	0

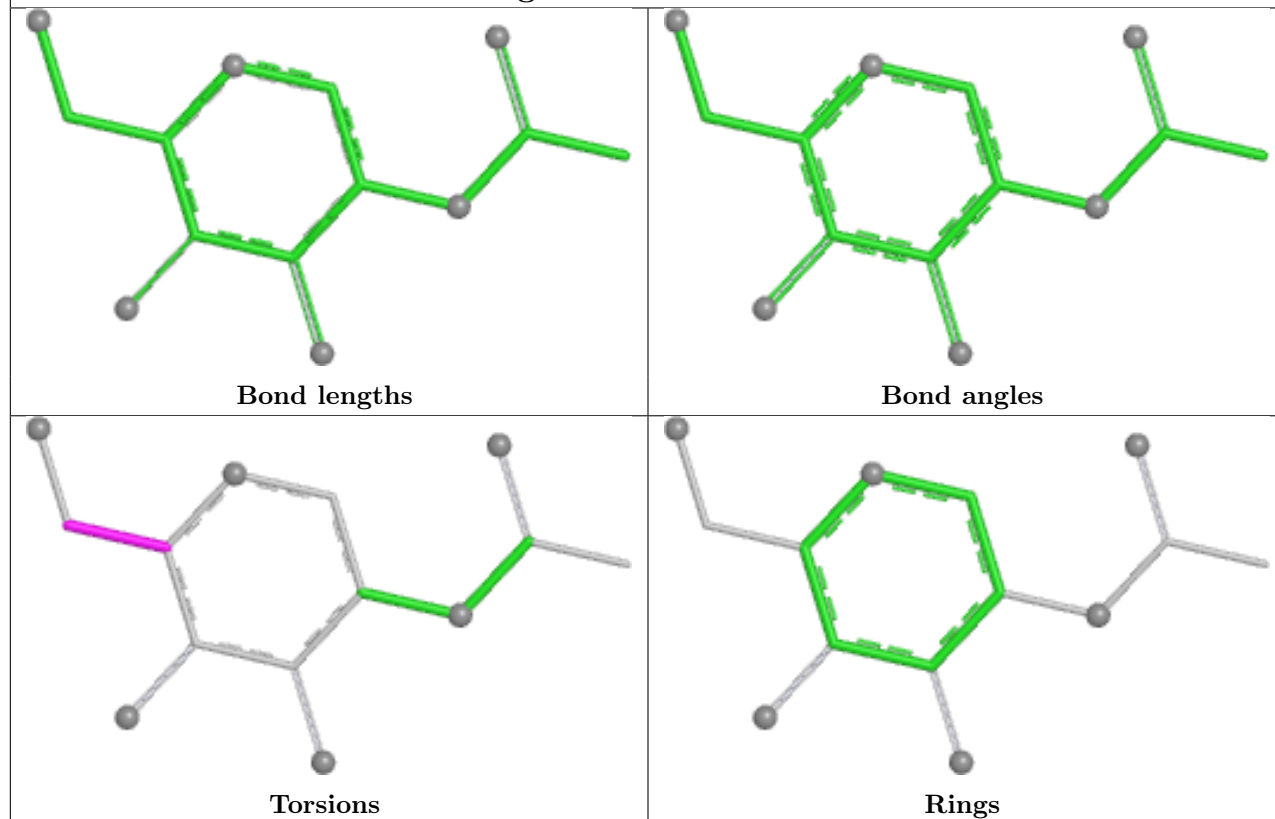
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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

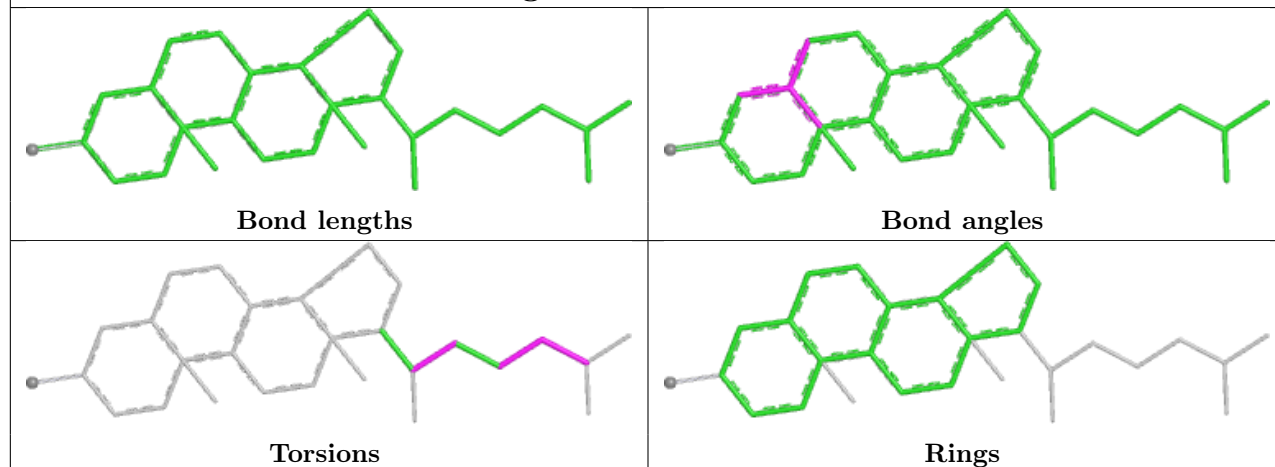


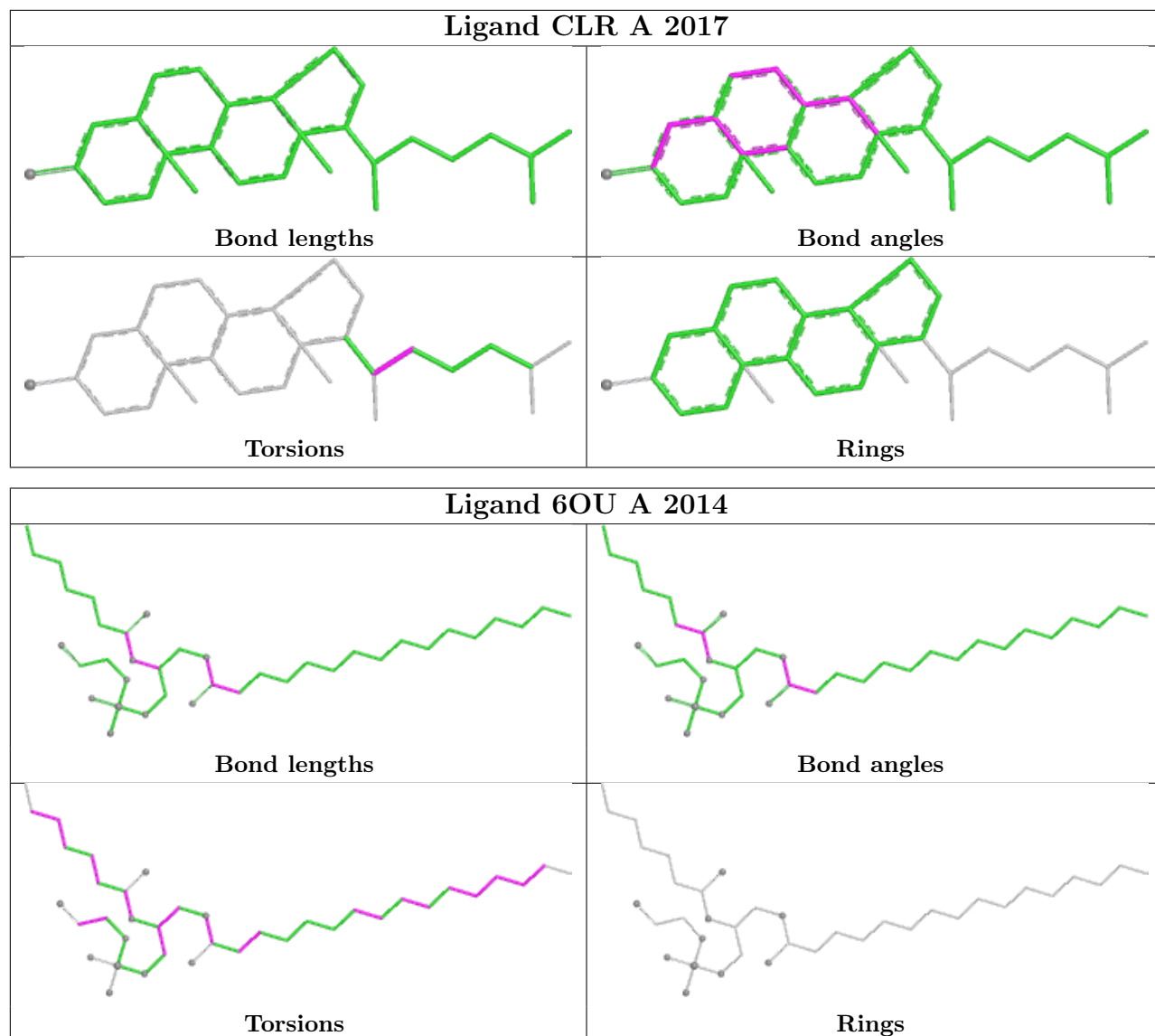


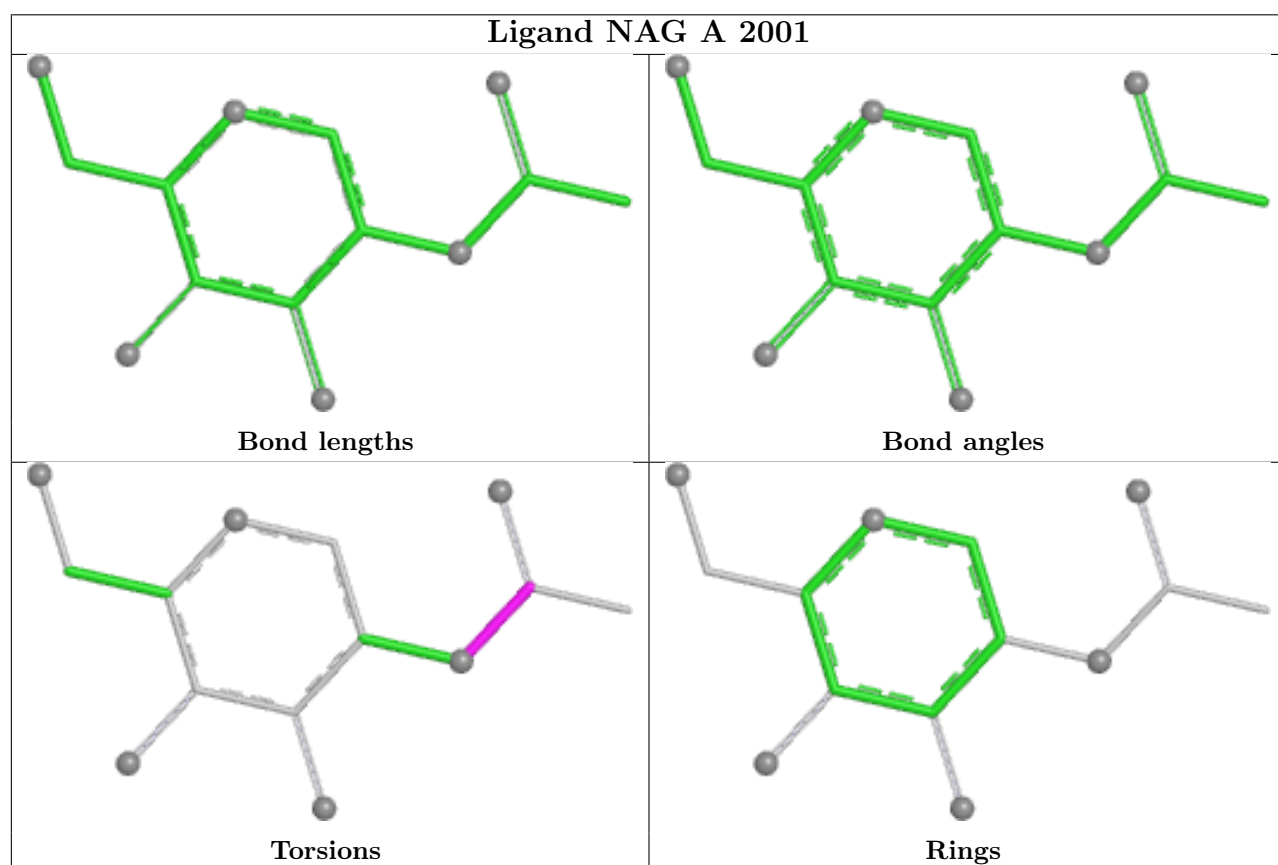
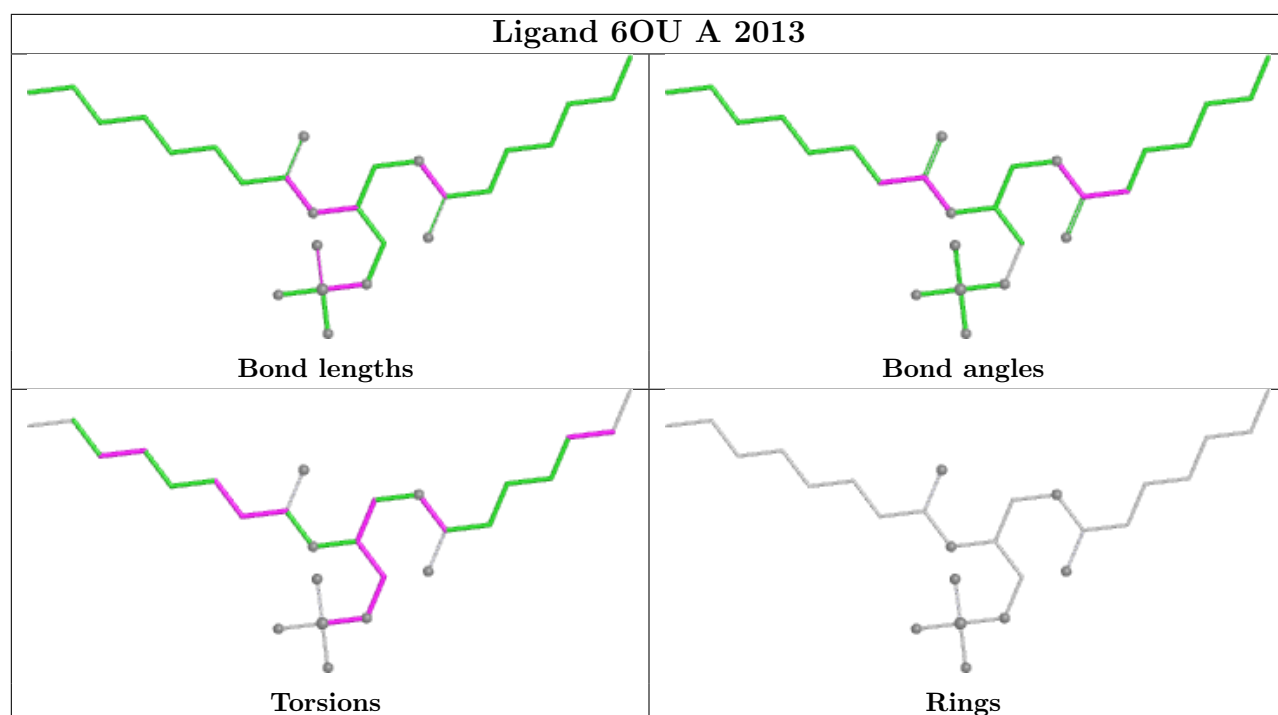
Ligand NAG A 2002

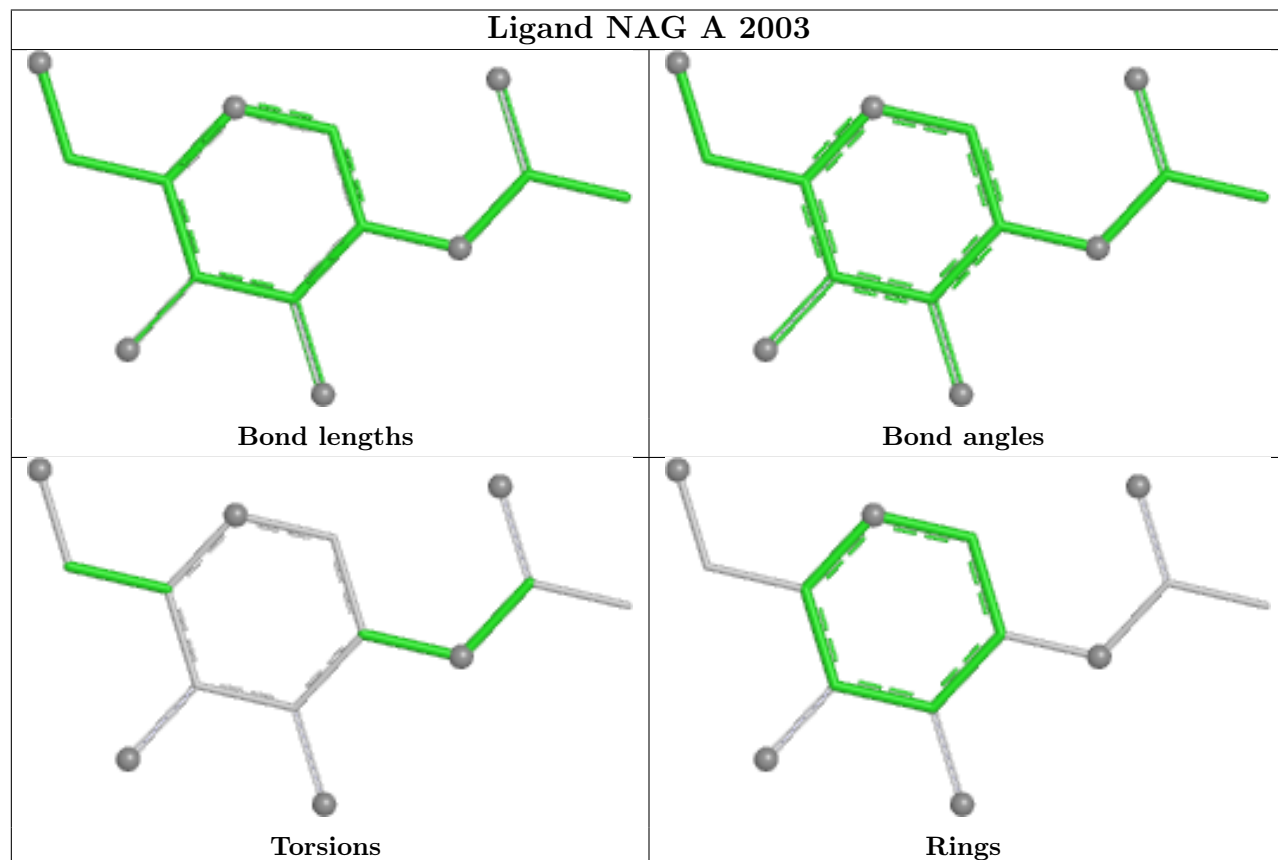
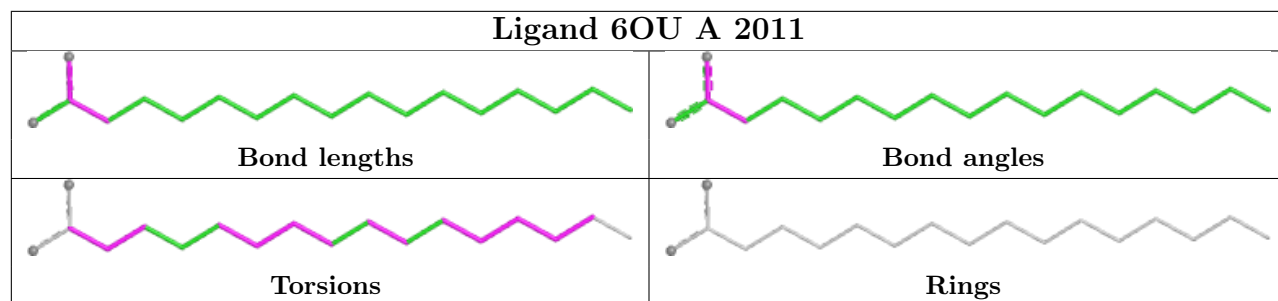


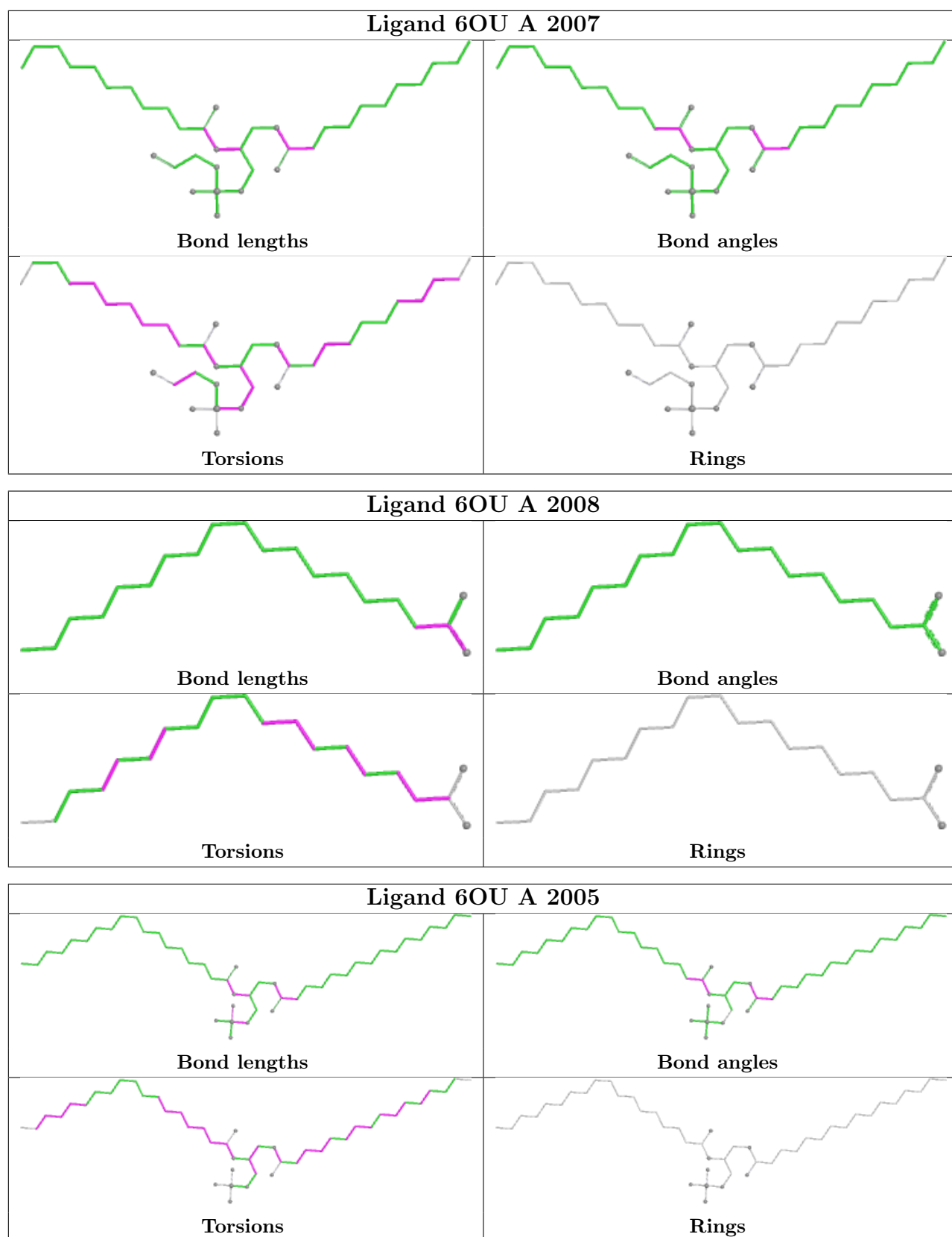
Ligand CLR A 2016

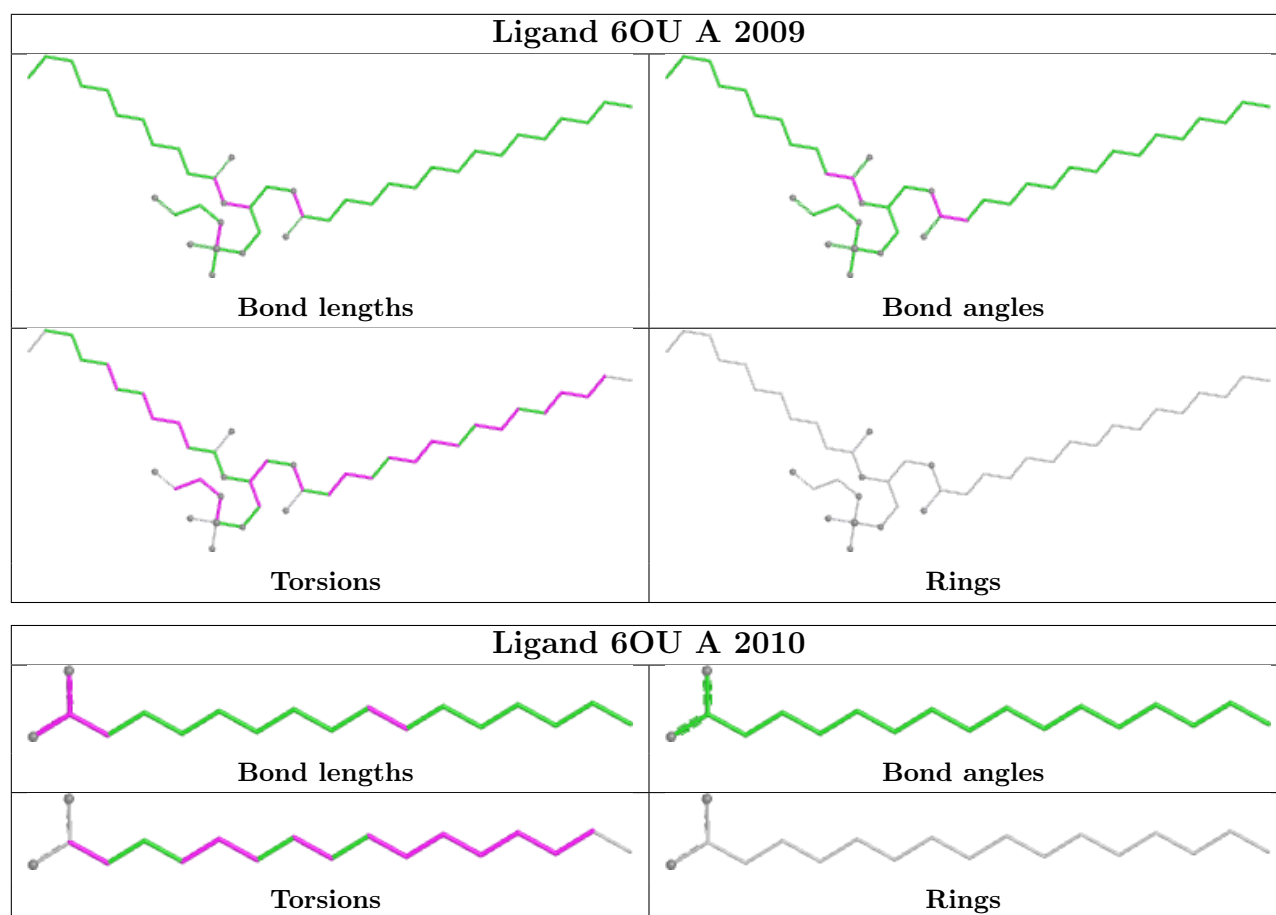












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

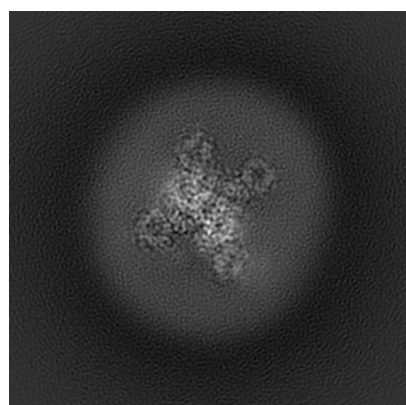
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30470. These allow visual inspection of the internal detail of the map and identification of artifacts.

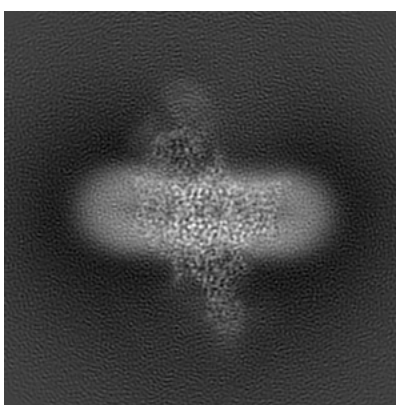
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

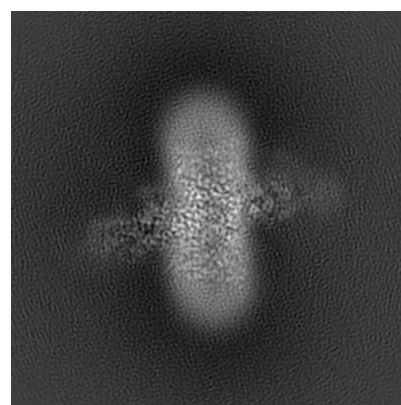
6.1.1 Primary map



X



Y

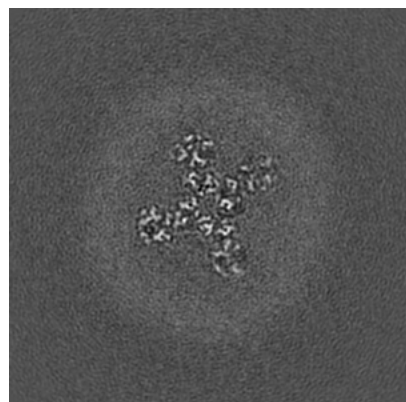


Z

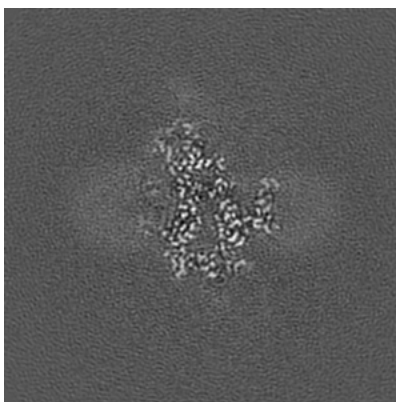
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

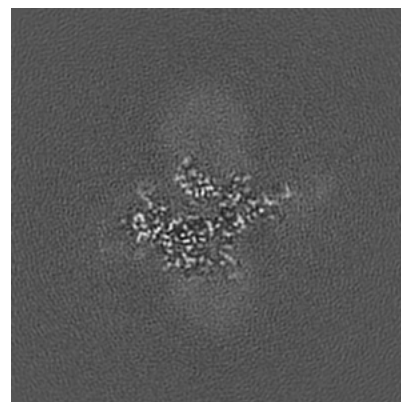
6.2.1 Primary map



X Index: 120



Y Index: 120

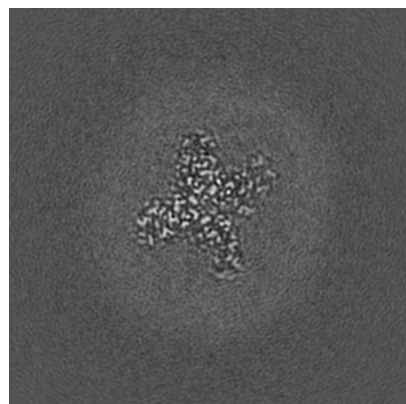


Z Index: 120

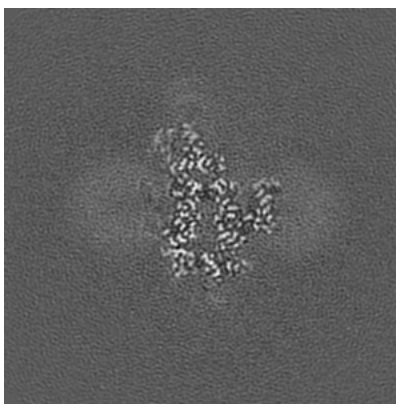
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

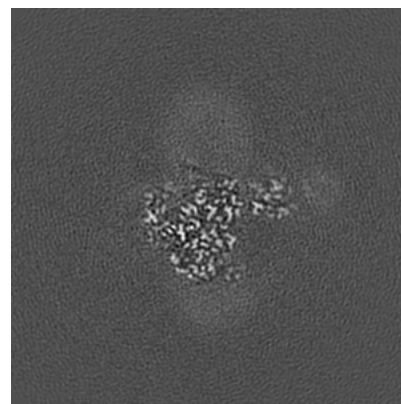
6.3.1 Primary map



X Index: 110



Y Index: 119

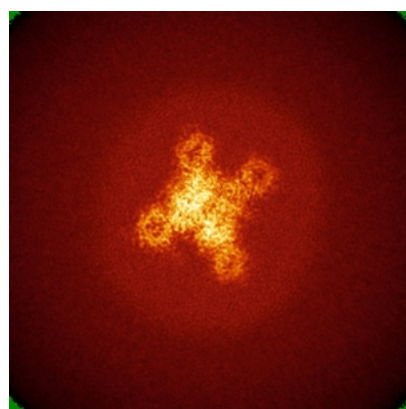


Z Index: 113

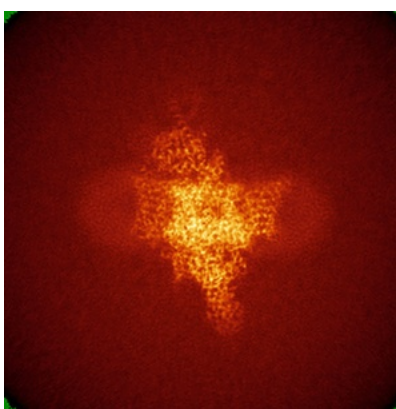
The images above show the largest variance slices of the map in three orthogonal directions.

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

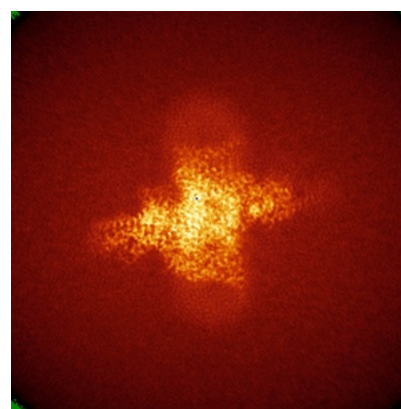
6.4.1 Primary map



X



Y



Z

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

This section was not generated.

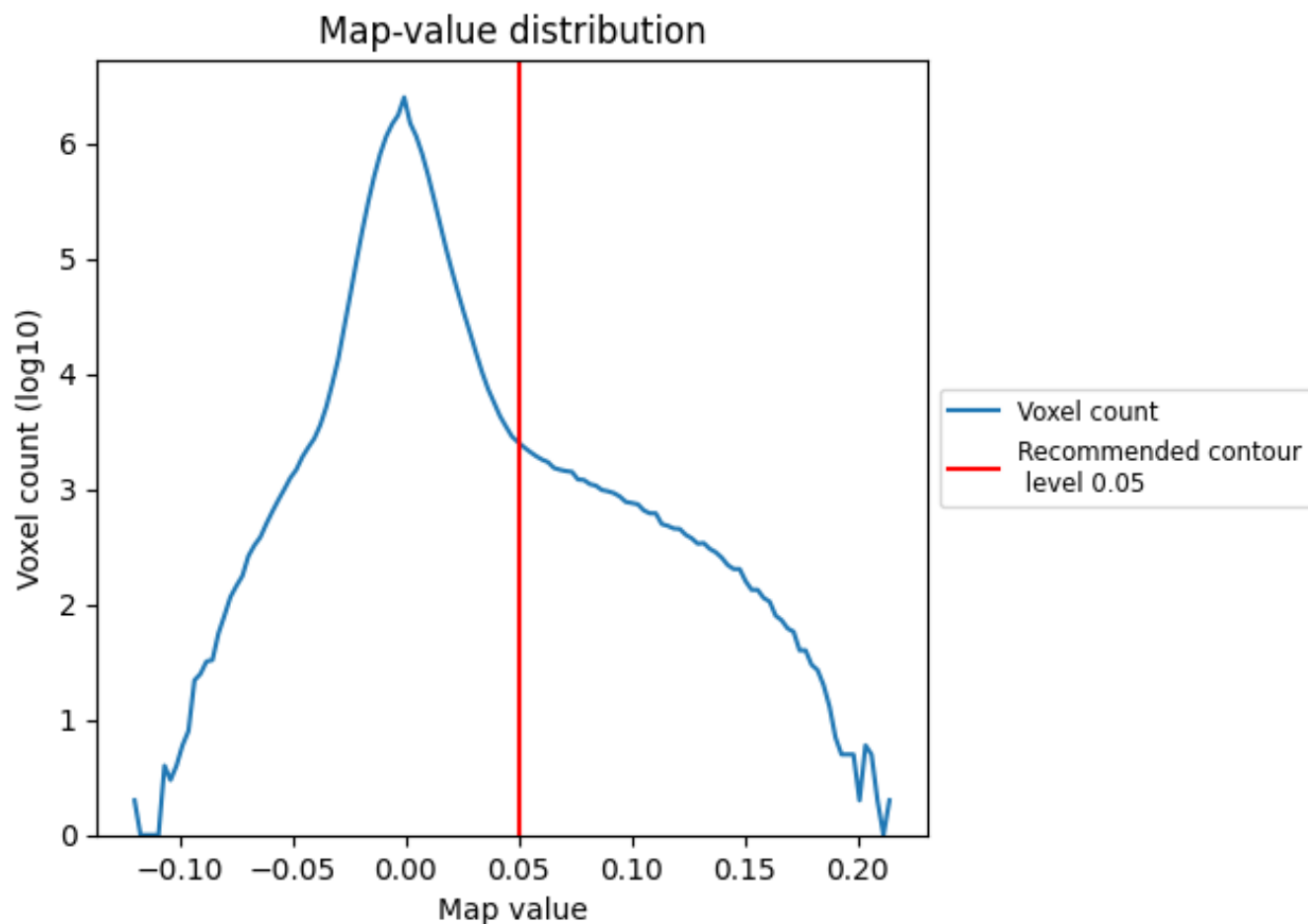
6.6 Mask visualisation

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

7 Map analysis [i](#)

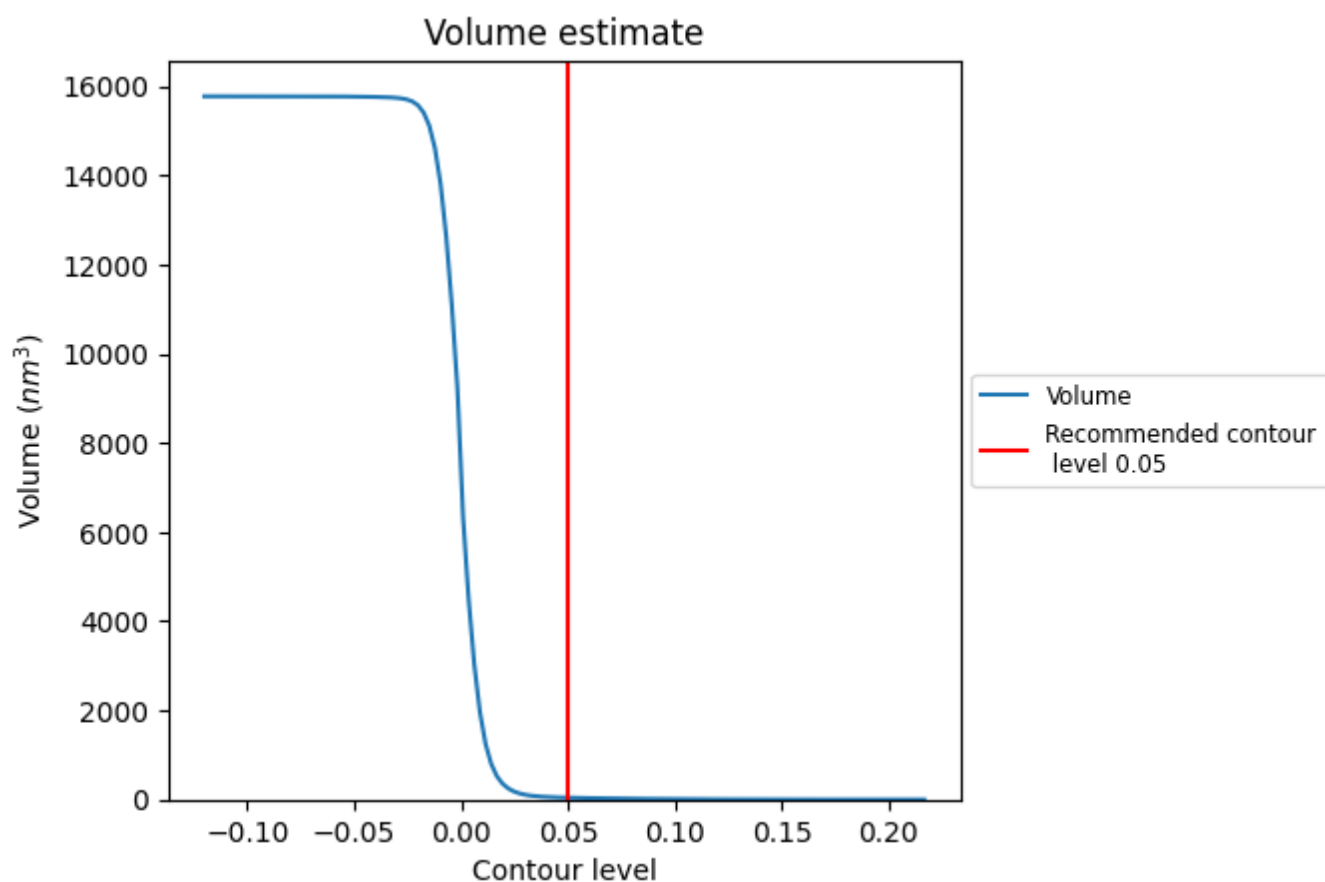
This section contains the results of statistical analysis of the map.

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.

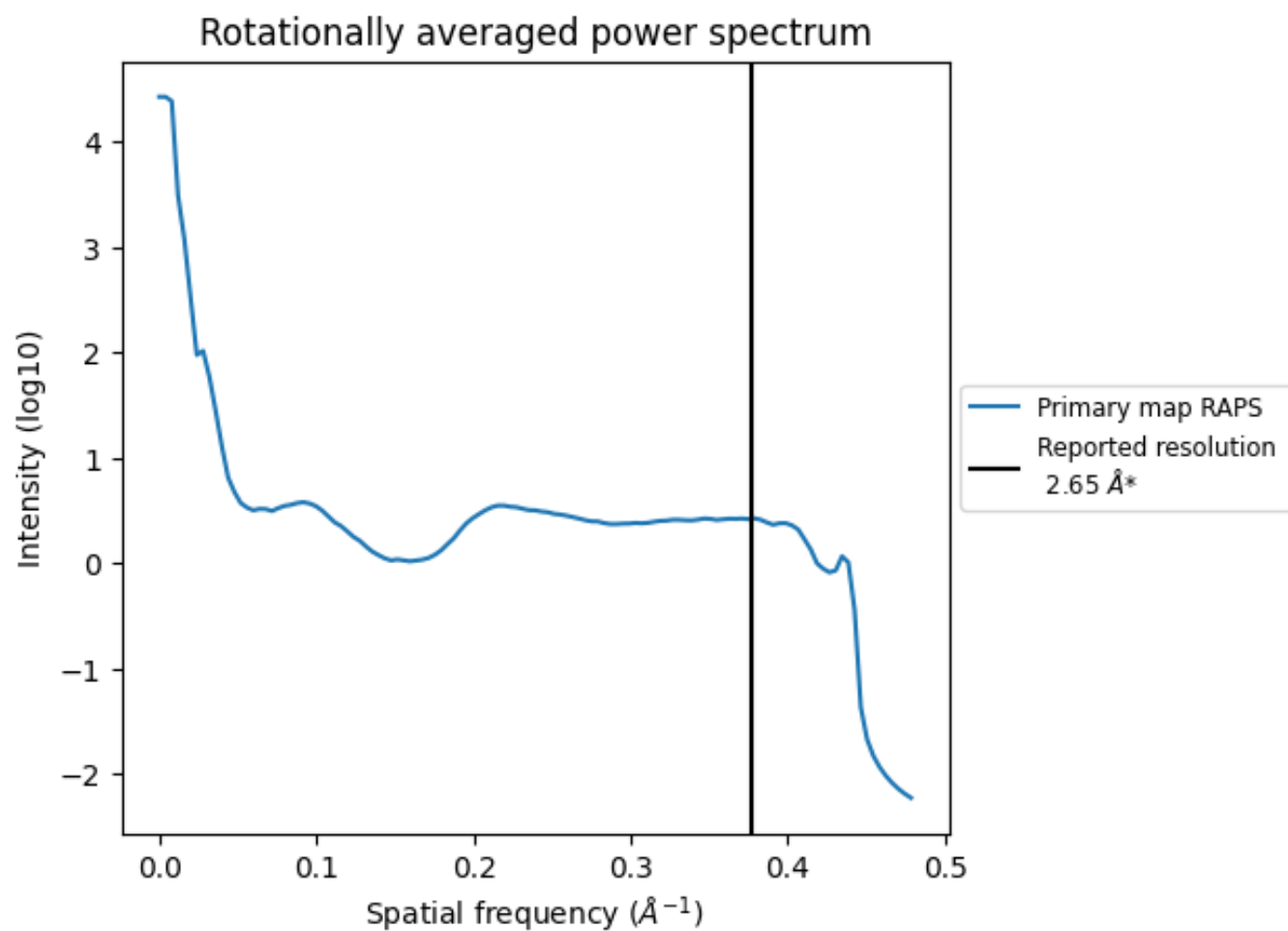
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 42 nm³; this corresponds to an approximate mass of 38 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 ⓘ

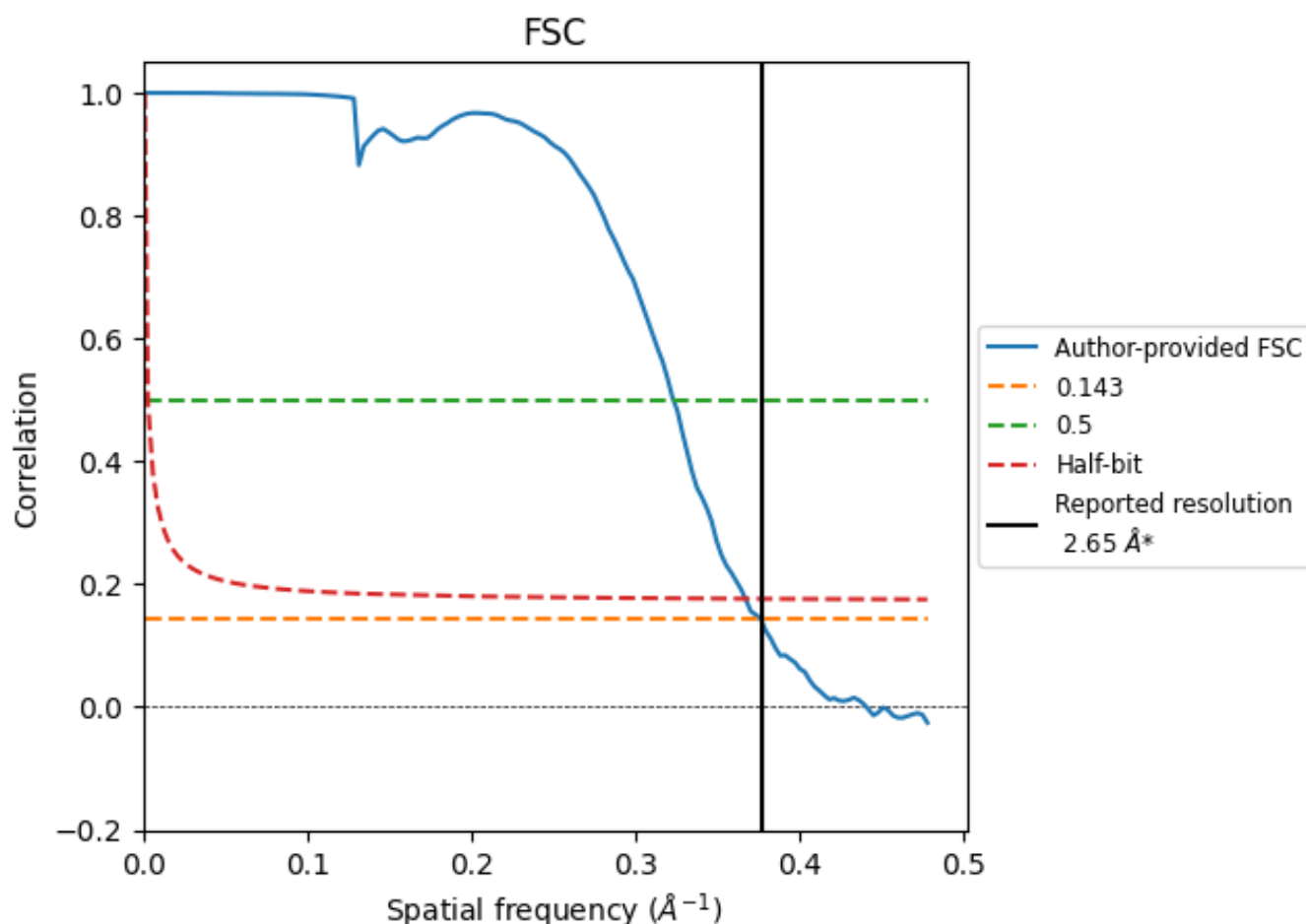


*Reported resolution corresponds to spatial frequency of 0.377 Å⁻¹

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 0.377 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.65	-	-
Author-provided FSC curve	2.65	3.09	2.72
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

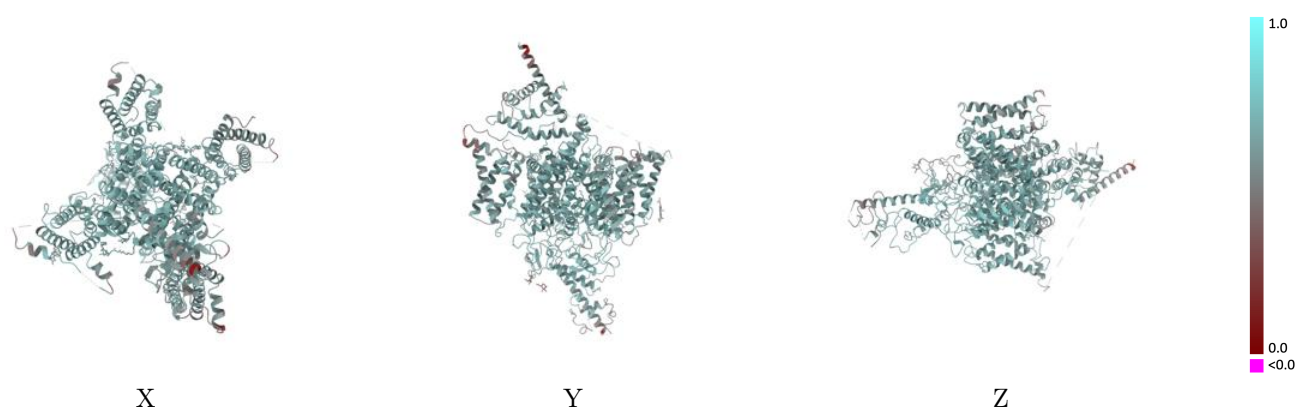
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-30470 and PDB model 7CU3. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

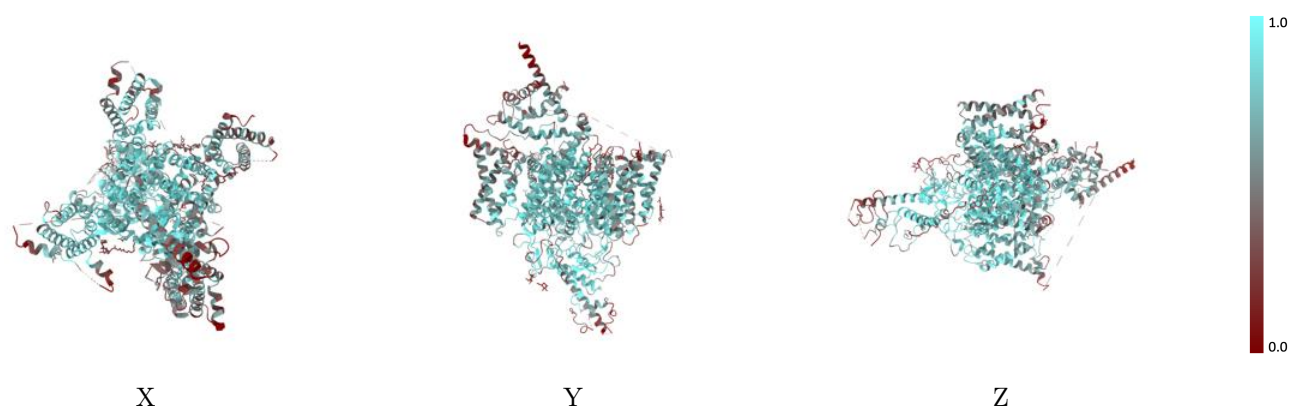
This section was not generated.

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



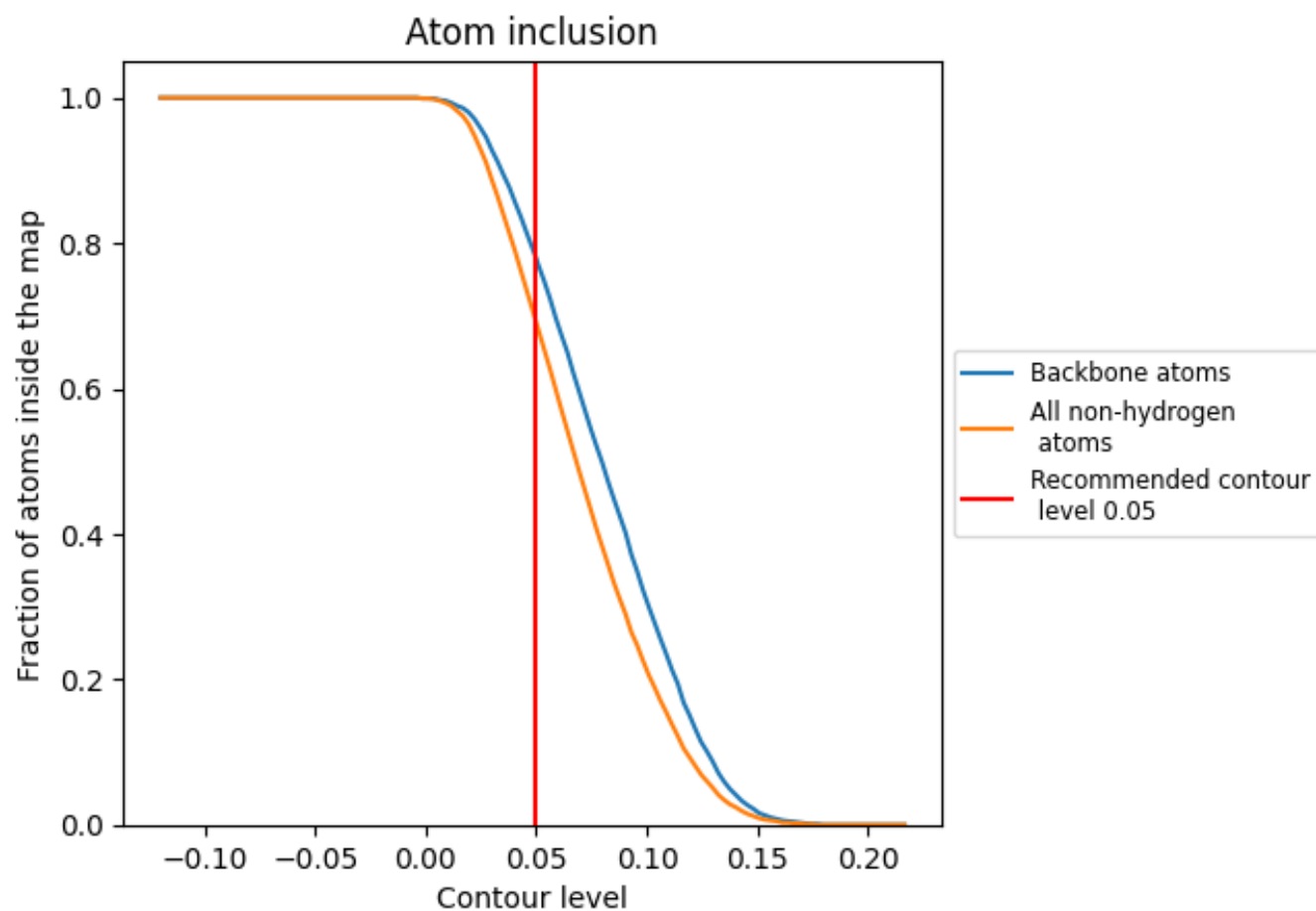
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 69% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6900	0.6180
A	0.6990	0.6210
B	0.6260	0.5980

