



## Full wwPDB EM Validation Report ⓘ

Nov 16, 2023 – 06:53 PM EST

PDB ID : 8THH  
EMDB ID : EMD-41262  
Title : Cryo-EM structure of Nav1.7 with LTG  
Authors : Fan, X.; Huang, J.; Yan, N.  
Deposited on : 2023-07-16  
Resolution : 2.70 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](mailto: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>.

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

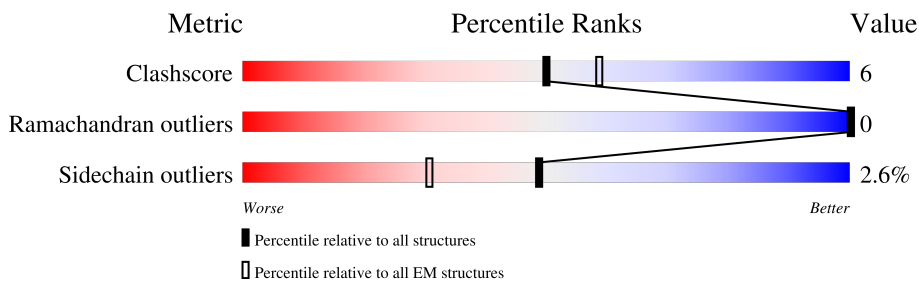
EMDB validation analysis : 0.0.1.dev70  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

# 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 2.70 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	1988	
2	B	218	
3	C	215	
4	D	2	
4	E	2	
4	F	2	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	IYJ	A	2003	-	X	-	-
6	IYJ	A	2004	-	X	-	-

## 2 Entry composition i

There are 11 unique types of molecules in this entry. The entry contains 13319 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 channel protein type 9 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1273	10262	6802	1613	1770	77	0	0

- Molecule 2 is a protein called Sodium channel subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	173	1416	902	232	272	10	0	0

- Molecule 3 is a protein called Sodium channel subunit beta-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	119	971	609	172	180	10	0	0

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



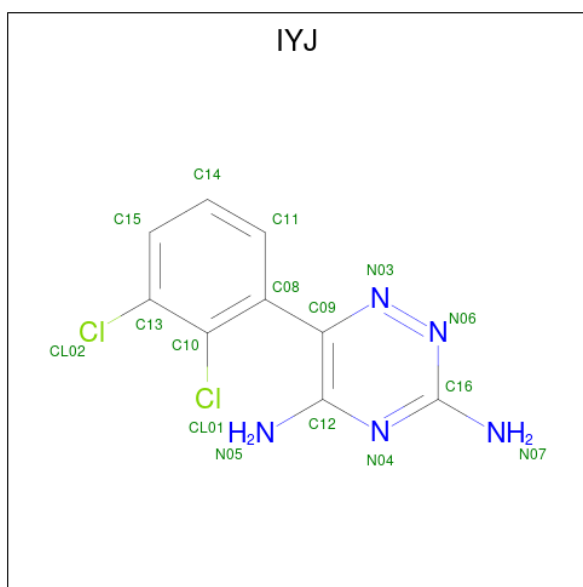
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	2	28	16	2	10	0	0
4	E	2	28	16	2	10	0	0
4	F	2	28	16	2	10	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



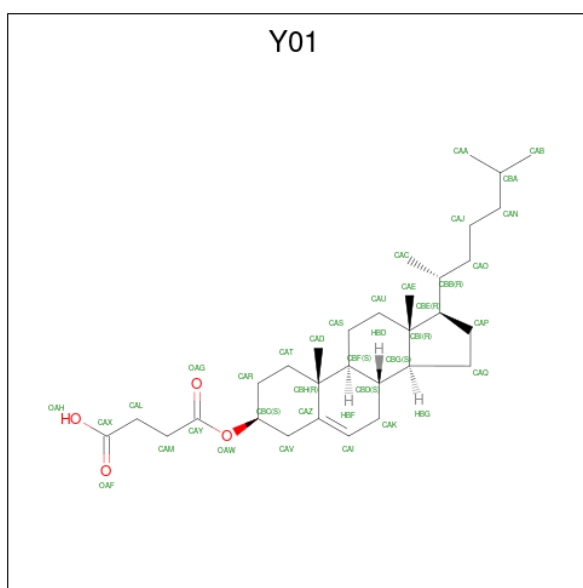
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	A	1	14	8	1	5	0
5	A	1	14	8	1	5	0
5	B	1	14	8	1	5	0
5	B	1	14	8	1	5	0
5	B	1	14	8	1	5	0

- Molecule 6 is (6M)-6-(2,3-dichlorophenyl)-1,2,4-triazine-3,5-diamine (three-letter code: IYJ) (formula:  $C_9H_7Cl_2N_5$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf	
6	A	1	Total	C	Cl	N	0
			16	9	2	5	
6	A	1	Total	C	Cl	N	0
			16	9	2	5	

- Molecule 7 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula:  $C_{31}H_{50}O_4$ ).



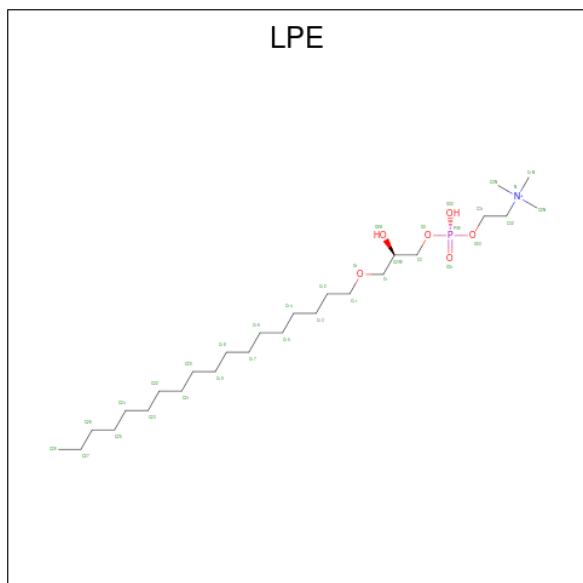
Mol	Chain	Residues	Atoms			AltConf	
7	A	1	Total	C	O		0
			35	31	4		
7	A	1	Total	C	O		0
			35	31	4		

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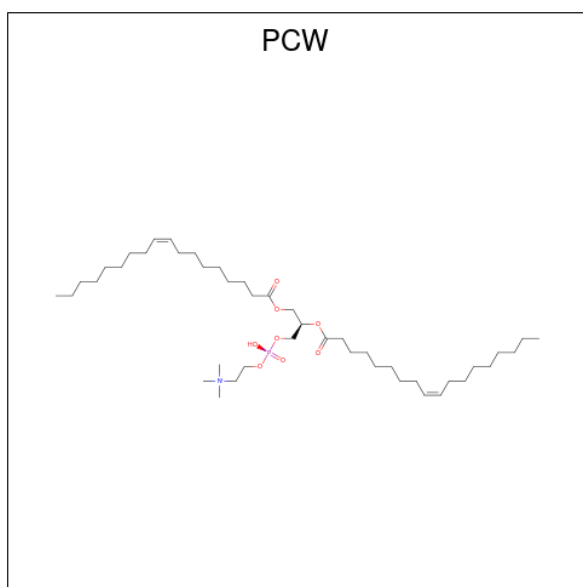
Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			35	31	4	
7	A	1	Total	C	O	0
			35	31	4	

- Molecule 8 is 1-O-OCTADECYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: LPE) (formula:  $C_{26}H_{57}NO_6P$ ).



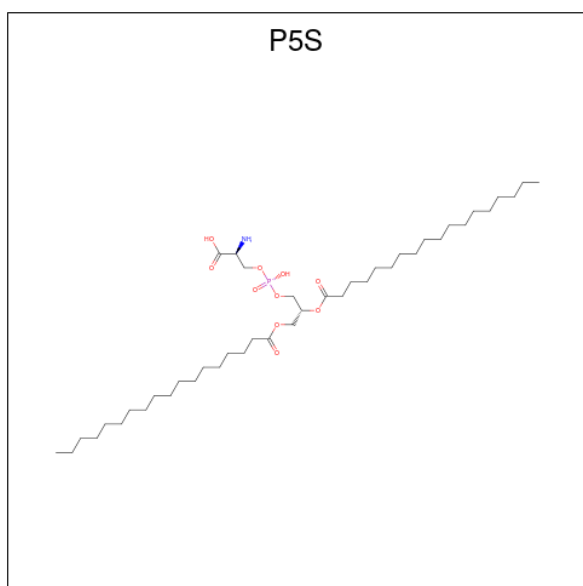
Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
8	A	1	Total	C	N	O	P	0
			28	20	1	6	1	
8	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
8	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
8	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
8	A	1	Total	C	N	O	P	0
			25	17	1	6	1	

- Molecule 9 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula:  $C_{44}H_{85}NO_8P$ ).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
9	A	1	49	39	1	8	1	0
9	A	1	47	37	1	8	1	0
9	A	1	44	34	1	8	1	0

- Molecule 10 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (three-letter code: P5S) (formula: C<sub>42</sub>H<sub>82</sub>NO<sub>10</sub>P).





Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
10	A	1	41	31	1	8	1	0

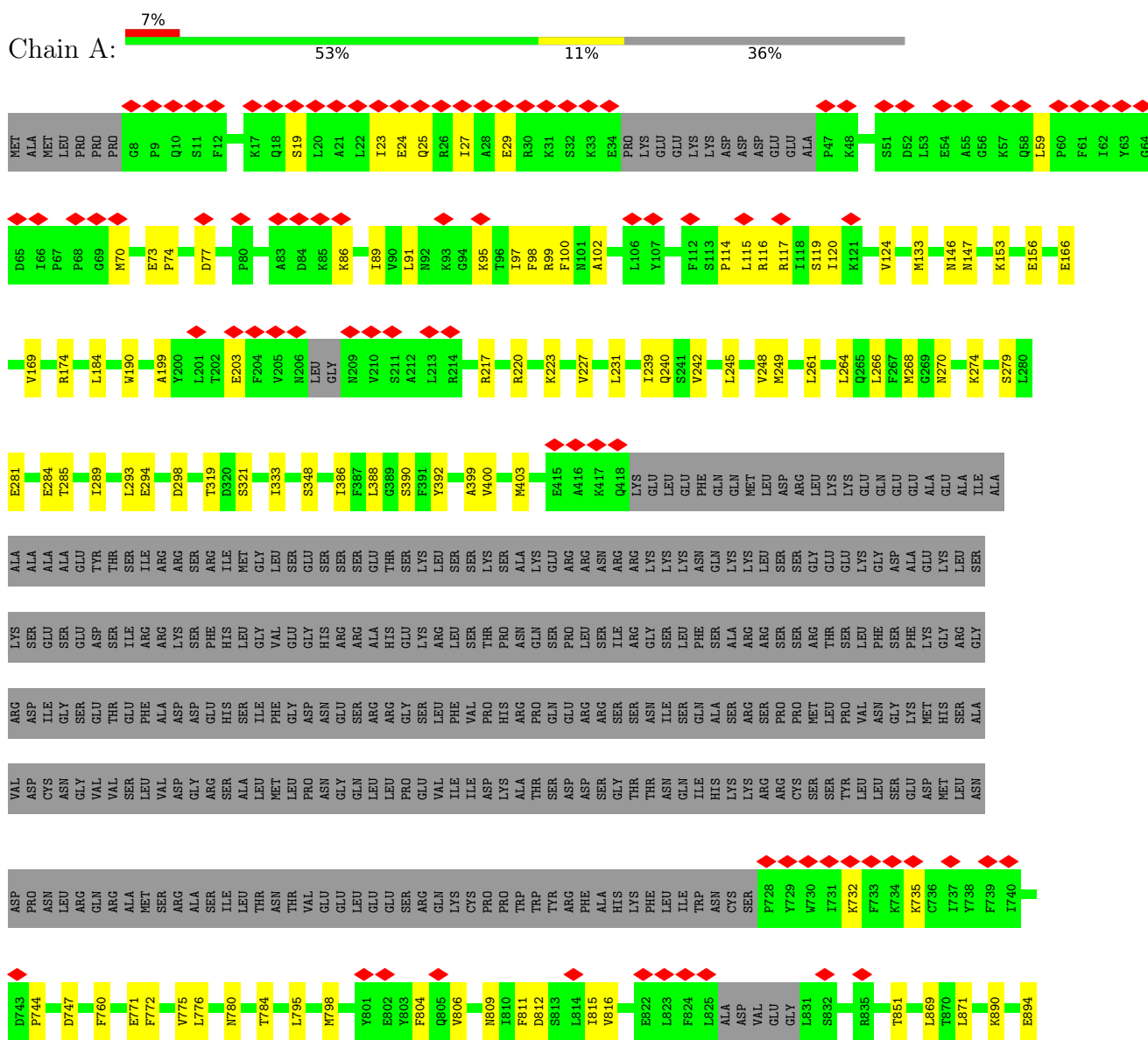
- Molecule 11 is water.

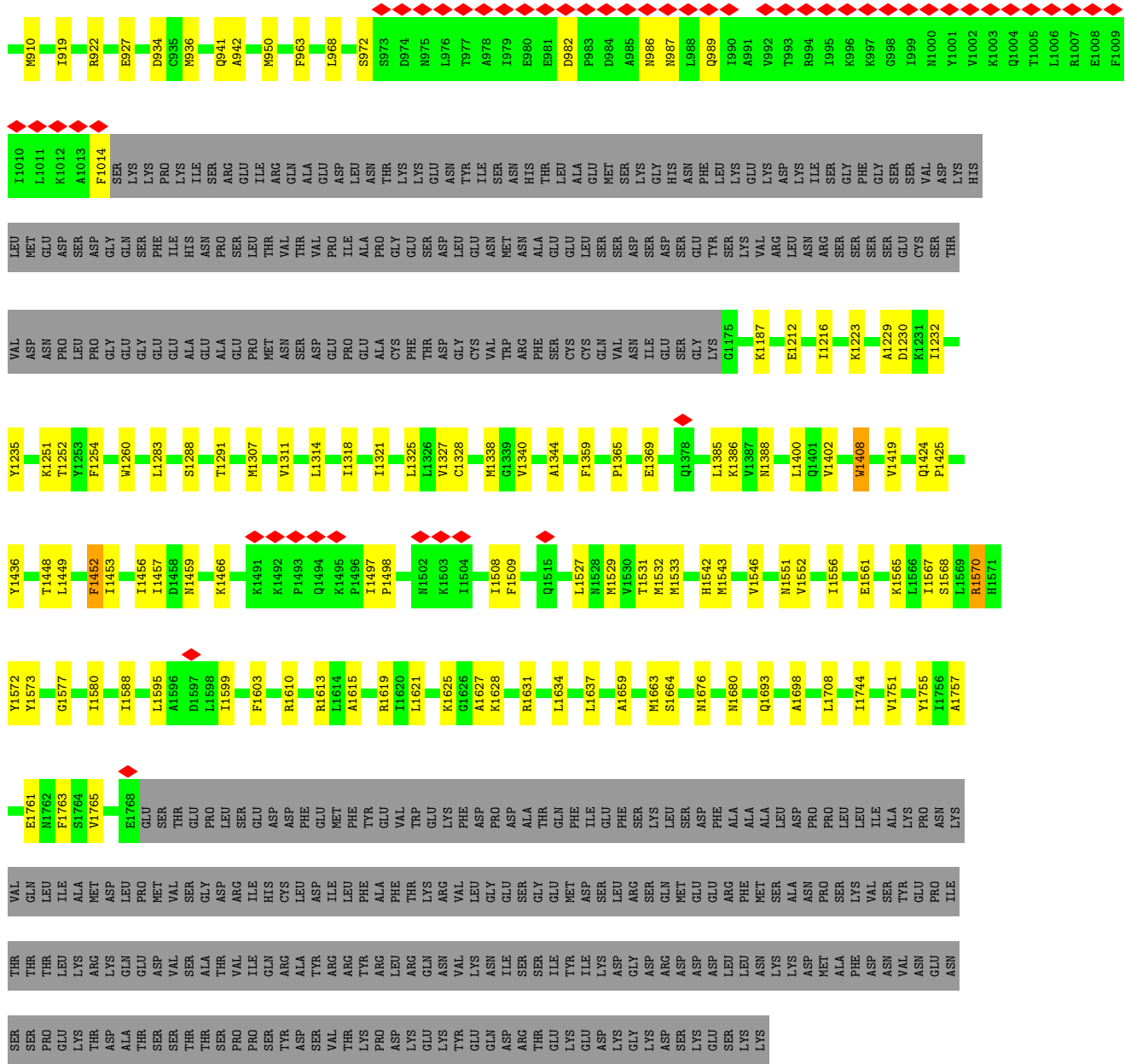
Mol	Chain	Residues	Atoms		AltConf
11	A	9	Total 9	O 9	0
11	B	1	Total 1	O 1	0

### 3 Residue-property plots

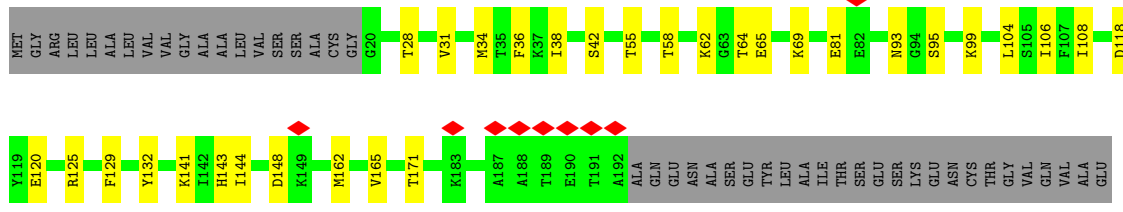
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 channel protein type 9 subunit alpha

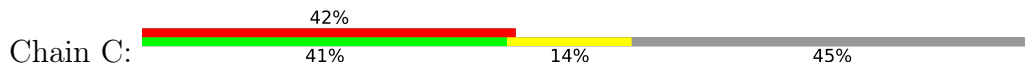


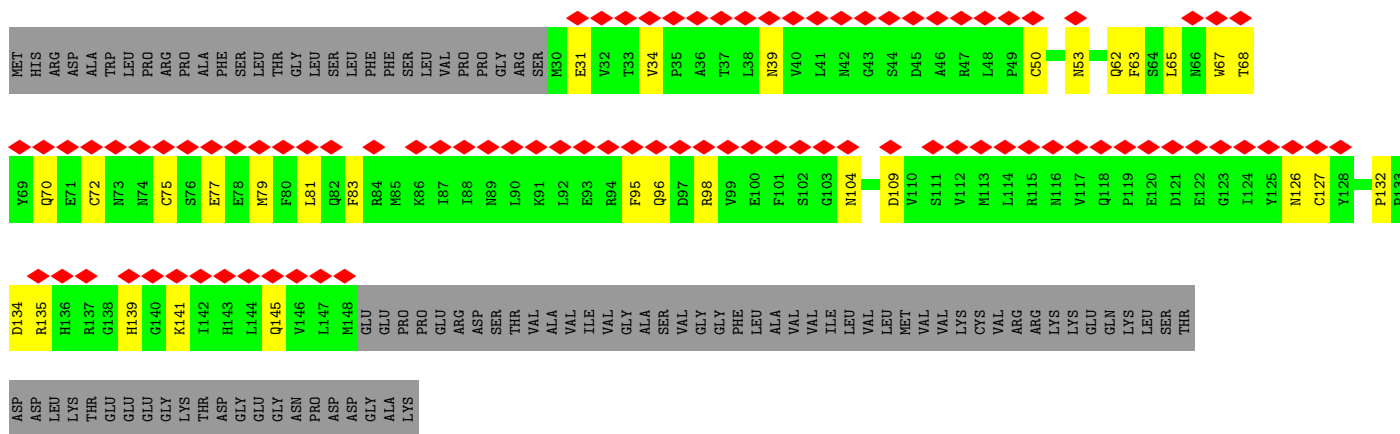


• Molecule 2: Sodium channel subunit beta-1



• Molecule 3: Sodium channel subunit beta-2





● Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



● Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



● Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	294629	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 ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.523	Depositor
Minimum map value	-1.011	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	265.216, 265.216, 265.216	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.036, 1.036, 1.036	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: LPE, IYJ, P5S, Y01, NAG, PCW

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	0.27	0/10511	0.44	0/14239
2	B	0.25	0/1442	0.48	0/1949
3	C	0.25	0/993	0.49	0/1343
All	All	0.26	0/12946	0.45	0/17531

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	10262	0	10498	124	0
2	B	1416	0	1380	14	0
3	C	971	0	930	20	0
4	D	28	0	25	0	0
4	E	28	0	25	0	0
4	F	28	0	25	0	0
5	A	28	0	26	0	0
5	B	42	0	39	0	0
6	A	32	0	0	0	0
7	A	140	0	196	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	153	0	213	2	0
9	A	140	0	195	10	0
10	A	41	0	51	2	0
11	A	9	0	0	0	0
11	B	1	0	0	0	0
All	All	13319	0	13603	161	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 (161) 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:1449:LEU:HD11	1:A:1453:ILE:HD11	1.63	0.78
1:A:1328:CYS:HB3	9:A:2009:PCW:H281	1.68	0.76
1:A:1328:CYS:CB	9:A:2009:PCW:H281	2.19	0.72
1:A:403:MET:HG3	1:A:1763:PHE:HE1	1.58	0.68
1:A:1577:GLY:H	9:A:2013:PCW:H52	1.60	0.66
1:A:100:PHE:HE2	1:A:120:ILE:HG12	1.60	0.66
1:A:294:GLU:N	1:A:294:GLU:OE1	2.27	0.66
1:A:199:ALA:O	1:A:203:GLU:HG2	1.98	0.64
1:A:1659:ALA:O	1:A:1663:MET:HG3	1.97	0.64
1:A:732:LYS:HA	1:A:735:LYS:HE3	1.79	0.64
1:A:77:ASP:OD1	1:A:99:ARG:NH1	2.32	0.63
3:C:65:LEU:HB3	3:C:83:PHE:H	1.63	0.62
2:B:55:THR:HB	2:B:104:LEU:HD22	1.80	0.61
1:A:1625:LYS:O	1:A:1631:ARG:NH1	2.33	0.61
1:A:1402:VAL:HA	1:A:1408:TRP:HB3	1.84	0.60
1:A:910:MET:HG2	1:A:919:ILE:HD12	1.84	0.58
1:A:890:LYS:O	1:A:894:GLU:HG2	2.03	0.58
1:A:285:THR:O	1:A:289:ILE:HD12	2.04	0.57
1:A:1449:LEU:HD11	1:A:1453:ILE:CD1	2.33	0.57
3:C:68:THR:HB	3:C:77:GLU:HB3	1.86	0.57
1:A:98:PHE:HD2	1:A:124:VAL:HG12	1.70	0.57
1:A:184:LEU:O	1:A:190:TRP:NE1	2.36	0.56
1:A:1386:LYS:HD2	1:A:1708:LEU:HB2	1.87	0.56
3:C:72:CYS:SG	3:C:75:CYS:N	2.79	0.56
1:A:936:MET:HG2	1:A:941:GLN:HA	1.88	0.56
1:A:780:ASN:O	1:A:784:THR:HG22	2.07	0.55
1:A:281:GLU:O	1:A:284:GLU:HG3	2.07	0.55
1:A:1229:ALA:HA	1:A:1232:ILE:HG22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:126:ASN:HB3	3:C:139:HIS:HE1	1.72	0.55
1:A:1580:ILE:HD11	9:A:2013:PCW:O11	2.07	0.55
1:A:1508:ILE:HG21	1:A:1567:ILE:HD11	1.90	0.54
1:A:399:ALA:O	1:A:403:MET:HG2	2.08	0.54
1:A:98:PHE:CD2	1:A:124:VAL:HG12	2.43	0.54
1:A:795:LEU:HD21	1:A:804:PHE:HE1	1.72	0.54
1:A:245:LEU:O	1:A:249:MET:HG3	2.07	0.53
1:A:812:ASP:O	1:A:816:VAL:HG23	2.09	0.52
1:A:1328:CYS:SG	1:A:1448:THR:CG2	2.98	0.52
1:A:348:SER:HB3	9:A:2011:PCW:H352	1.91	0.52
1:A:73:GLU:HG3	1:A:74:PRO:HD2	1.90	0.52
1:A:1529:MET:O	1:A:1533:MET:HG3	2.10	0.52
2:B:42:SER:OG	2:B:125:ARG:NH2	2.43	0.51
2:B:120:GLU:OE2	2:B:141:LYS:NZ	2.43	0.51
1:A:1288:SER:O	1:A:1291:THR:HG22	2.10	0.51
3:C:104:ASN:N	3:C:109:ASP:O	2.43	0.51
9:A:2009:PCW:C7	7:A:2018:Y01:CAX	2.89	0.51
1:A:1449:LEU:CD1	1:A:1453:ILE:CD1	2.89	0.50
1:A:1449:LEU:CD1	1:A:1453:ILE:HD11	2.38	0.50
3:C:39:ASN:OD1	3:C:145:GLN:NE2	2.38	0.50
1:A:1693:GLN:NE2	1:A:1698:ALA:O	2.39	0.50
3:C:96:GLN:OE1	3:C:98:ARG:NE	2.44	0.50
1:A:100:PHE:CE2	1:A:120:ILE:HG12	2.44	0.50
1:A:86:LYS:HB3	1:A:102:ALA:HB3	1.94	0.50
1:A:223:LYS:O	1:A:227:VAL:HG13	2.12	0.50
1:A:1340:VAL:O	1:A:1344:ALA:HB2	2.12	0.50
1:A:264:LEU:O	1:A:268:MET:HB2	2.11	0.50
1:A:59:LEU:HD11	1:A:91:LEU:HD11	1.93	0.49
1:A:248:VAL:HG21	1:A:400:VAL:HG21	1.93	0.49
2:B:162:MET:HA	2:B:165:VAL:HG22	1.94	0.49
1:A:1621:LEU:HD22	10:A:2012:P5S:H32A	1.95	0.49
1:A:1365:PRO:HD2	1:A:1369:GLU:HG3	1.95	0.49
1:A:1452:PHE:O	1:A:1456:ILE:HG12	2.12	0.49
2:B:69:LYS:NZ	2:B:81:GLU:OE2	2.46	0.49
3:C:62:GLN:HB3	3:C:132:PRO:HG2	1.94	0.49
1:A:1385:LEU:O	1:A:1388:ASN:ND2	2.46	0.49
1:A:1627:ALA:HA	8:A:2017:LPE:H1N2	1.95	0.49
1:A:1453:ILE:O	1:A:1457:ILE:HG12	2.13	0.48
1:A:1251:LYS:HG3	1:A:1252:THR:N	2.28	0.48
1:A:239:ILE:O	1:A:242:VAL:HG12	2.13	0.48
3:C:70:GLN:NE2	3:C:72:CYS:O	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:MET:HG3	1:A:1763:PHE:CE1	2.43	0.48
1:A:1595:LEU:O	1:A:1599:ILE:HG13	2.14	0.48
1:A:1283:LEU:O	1:A:1283:LEU:HD13	2.14	0.47
7:A:2018:Y01:HAN2	7:A:2018:Y01:HAC2	1.96	0.47
1:A:1761:GLU:O	1:A:1765:VAL:HG23	2.14	0.47
1:A:24:GLU:O	1:A:27:ILE:HG22	2.14	0.47
1:A:744:PRO:HA	1:A:987:ASN:HB3	1.97	0.47
1:A:114:PRO:HA	1:A:117:ARG:HG2	1.97	0.47
1:A:1676:ASN:O	1:A:1680:ASN:ND2	2.48	0.47
1:A:950:MET:HG2	9:A:2011:PCW:H251	1.96	0.47
2:B:129:PHE:HB2	2:B:132:TYR:HB3	1.97	0.47
1:A:1588:ILE:HG22	1:A:1615:ALA:HB1	1.96	0.47
1:A:153:LYS:O	1:A:156:GLU:HG2	2.15	0.46
1:A:231:LEU:HD11	1:A:871:LEU:HD23	1.97	0.46
1:A:274:LYS:HE2	1:A:333:ILE:O	2.14	0.46
1:A:388:LEU:O	1:A:392:TYR:HB3	2.15	0.46
1:A:1338:MET:HE3	1:A:1436:TYR:HE1	1.80	0.46
1:A:1187:LYS:HB2	1:A:1187:LYS:HE2	1.67	0.46
1:A:19:SER:O	1:A:23:ILE:HG12	2.16	0.46
1:A:1235:TYR:HH	2:B:171:THR:HG1	1.60	0.46
1:A:25:GLN:O	1:A:29:GLU:HG2	2.17	0.45
1:A:146:ASN:OD1	1:A:147:ASN:N	2.45	0.45
8:A:2015:LPE:O31	8:A:2015:LPE:O2H	2.30	0.45
1:A:403:MET:CG	1:A:1763:PHE:HE1	2.29	0.45
1:A:1314:LEU:HD12	1:A:1314:LEU:HA	1.81	0.45
1:A:293:LEU:HD22	1:A:298:ASP:HB3	1.98	0.45
1:A:806:VAL:HB	1:A:809:ASN:OD1	2.17	0.45
1:A:851:THR:HG22	1:A:1327:VAL:HG21	1.99	0.45
1:A:1570:ARG:HE	1:A:1570:ARG:HB2	1.63	0.45
1:A:1565:LYS:HE3	1:A:1573:TYR:HE1	1.81	0.44
2:B:38:ILE:HD11	2:B:108:ILE:HD11	1.98	0.44
3:C:34:VAL:HG21	3:C:141:LYS:H	1.82	0.44
3:C:104:ASN:N	3:C:104:ASN:OD1	2.49	0.44
1:A:771:GLU:O	1:A:775:VAL:HG13	2.17	0.44
1:A:1408:TRP:H	1:A:1408:TRP:HD1	1.63	0.44
1:A:1527:LEU:O	1:A:1531:THR:HG23	2.17	0.44
1:A:1757:ALA:O	1:A:1761:GLU:HG2	2.18	0.44
1:A:59:LEU:HG	1:A:97:ILE:HD11	1.99	0.44
1:A:89:ILE:HD13	1:A:89:ILE:HA	1.89	0.44
2:B:28:THR:HG22	2:B:143:HIS:O	2.18	0.44
1:A:968:LEU:O	1:A:972:SER:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1634:LEU:HB3	10:A:2012:P5S:H43A	2.00	0.43
2:B:58:THR:OG1	2:B:120:GLU:HB2	2.17	0.43
1:A:1359:PHE:O	1:A:1424:GLN:NE2	2.47	0.43
3:C:67:TRP:HB2	3:C:81:LEU:HB3	2.01	0.43
1:A:1212:GLU:HA	1:A:1216:ILE:HD12	2.01	0.43
1:A:1254:PHE:O	1:A:1260:TRP:NE1	2.45	0.43
1:A:166:GLU:O	1:A:169:VAL:HG12	2.18	0.43
3:C:34:VAL:HG21	3:C:141:LYS:N	2.33	0.43
1:A:1400:LEU:HD21	1:A:1744:ILE:HD11	2.01	0.43
1:A:1551:ASN:OD1	1:A:1619:ARG:NH2	2.52	0.43
1:A:98:PHE:HE2	1:A:124:VAL:HA	1.84	0.42
1:A:1543:MET:HA	1:A:1546:VAL:HG22	2.01	0.42
3:C:31:GLU:HB3	3:C:53:ASN:OD1	2.19	0.42
3:C:134:ASP:OD1	3:C:135:ARG:N	2.52	0.42
3:C:95:PHE:HA	3:C:98:ARG:HH21	1.84	0.42
1:A:91:LEU:HD12	1:A:91:LEU:HA	1.87	0.42
1:A:942:ALA:HA	9:A:2011:PCW:H131	2.02	0.42
3:C:63:PHE:HE1	3:C:65:LEU:HB2	1.85	0.42
3:C:67:TRP:CZ2	3:C:127:CYS:HB3	2.54	0.42
1:A:922:ARG:HG2	1:A:927:GLU:HB2	2.01	0.42
2:B:64:THR:HG22	2:B:65:GLU:H	1.85	0.42
1:A:59:LEU:HD13	1:A:95:LYS:HG3	2.01	0.42
1:A:1542:HIS:O	1:A:1546:VAL:HG13	2.20	0.42
1:A:986:ASN:HB3	1:A:989:GLN:HG2	2.02	0.41
3:C:126:ASN:HB3	3:C:139:HIS:CE1	2.54	0.41
1:A:261:LEU:HD13	1:A:1532:MET:HE3	2.02	0.41
1:A:963:PHE:HZ	1:A:1453:ILE:HD12	1.85	0.41
9:A:2009:PCW:H72	7:A:2018:Y01:CAX	2.51	0.41
1:A:386:ILE:HA	1:A:390:SER:HB3	2.02	0.41
1:A:1552:VAL:O	1:A:1556:ILE:HG13	2.20	0.41
1:A:1307:MET:O	1:A:1311:VAL:HG23	2.20	0.41
3:C:34:VAL:HG12	3:C:50:CYS:HA	2.02	0.41
1:A:811:PHE:CZ	1:A:815:ILE:HD11	2.55	0.41
1:A:1223:LYS:HB3	1:A:1223:LYS:HE3	1.90	0.41
1:A:1338:MET:HE3	1:A:1436:TYR:CE1	2.56	0.41
1:A:1497:ILE:HG23	1:A:1572:TYR:HD2	1.86	0.41
2:B:36:PHE:CE2	2:B:144:ILE:HD12	2.56	0.41
2:B:38:ILE:HD12	2:B:106:ILE:HD11	2.02	0.41
1:A:1498:PRO:HD2	1:A:1572:TYR:HE2	1.86	0.41
2:B:31:VAL:HG23	2:B:34:MET:HB2	2.02	0.40
1:A:392:TYR:CZ	1:A:1637:LEU:HB2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:LEU:O	1:A:1610:ARG:NH1	2.54	0.40
1:A:1466:LYS:HE2	1:A:1466:LYS:HB2	1.83	0.40
1:A:1509:PHE:HA	1:A:1568:SER:OG	2.21	0.40
1:A:115:LEU:O	1:A:119:SER:OG	2.31	0.40
1:A:760:PHE:CE2	1:A:776:LEU:HA	2.57	0.40
1:A:1318:ILE:HD13	1:A:1318:ILE:HA	1.99	0.40
1:A:1751:VAL:O	1:A:1751:VAL:HG12	2.22	0.40
1:A:1321:ILE:O	1:A:1325:LEU:HB2	2.21	0.40
1:A:1419:VAL:HG23	1:A:1425:PRO:HA	2.03	0.40
1:A:1577:GLY:N	9:A:2013:PCW:H52	2.33	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	1261/1988 (63%)	1228 (97%)	33 (3%)	0	100	100
2	B	171/218 (78%)	170 (99%)	1 (1%)	0	100	100
3	C	117/215 (54%)	113 (97%)	4 (3%)	0	100	100
All	All	1549/2421 (64%)	1511 (98%)	38 (2%)	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	1136/1778 (64%)	1107 (97%)	29 (3%)	46	75
2	B	157/190 (83%)	151 (96%)	6 (4%)	33	62
3	C	111/193 (58%)	110 (99%)	1 (1%)	78	92
All	All	1404/2161 (65%)	1368 (97%)	36 (3%)	49	75

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	MET
1	A	116	ARG
1	A	133	MET
1	A	174	ARG
1	A	217	ARG
1	A	220	ARG
1	A	240	GLN
1	A	270	ASN
1	A	279	SER
1	A	319	THR
1	A	321	SER
1	A	747	ASP
1	A	772	PHE
1	A	798	MET
1	A	869	LEU
1	A	934	ASP
1	A	982	ASP
1	A	1014	PHE
1	A	1230	ASP
1	A	1408	TRP
1	A	1452	PHE
1	A	1459	ASN
1	A	1561	GLU
1	A	1570	ARG
1	A	1603	PHE
1	A	1613	ARG
1	A	1628	LYS
1	A	1664	SER
1	A	1755	TYR
2	B	62	LYS
2	B	93	ASN
2	B	95	SER
2	B	99	LYS
2	B	118	ASP

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Mol	Chain	Res	Type
2	B	148	ASP
3	C	79	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

6 monosaccharides 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	NAG	D	1	1,4	14,14,15	0.42	0	17,19,21	0.95	1 (5%)
4	NAG	D	2	4	14,14,15	0.37	0	17,19,21	0.66	0
4	NAG	E	1	1,4	14,14,15	0.42	0	17,19,21	1.52	3 (17%)
4	NAG	E	2	4	14,14,15	0.33	0	17,19,21	0.85	1 (5%)
4	NAG	F	1	4,2	14,14,15	0.30	0	17,19,21	0.65	0
4	NAG	F	2	4	14,14,15	0.28	0	17,19,21	0.78	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	NAG	D	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	NAG	F	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1	NAG	C4-C3-C2	-3.39	106.05	111.02
4	E	1	NAG	C1-O5-C5	3.38	116.78	112.19
4	E	2	NAG	C1-O5-C5	2.40	115.44	112.19
4	D	1	NAG	C4-C3-C2	2.38	114.50	111.02
4	E	1	NAG	O4-C4-C3	2.23	115.50	110.35

There are no chirality outliers.

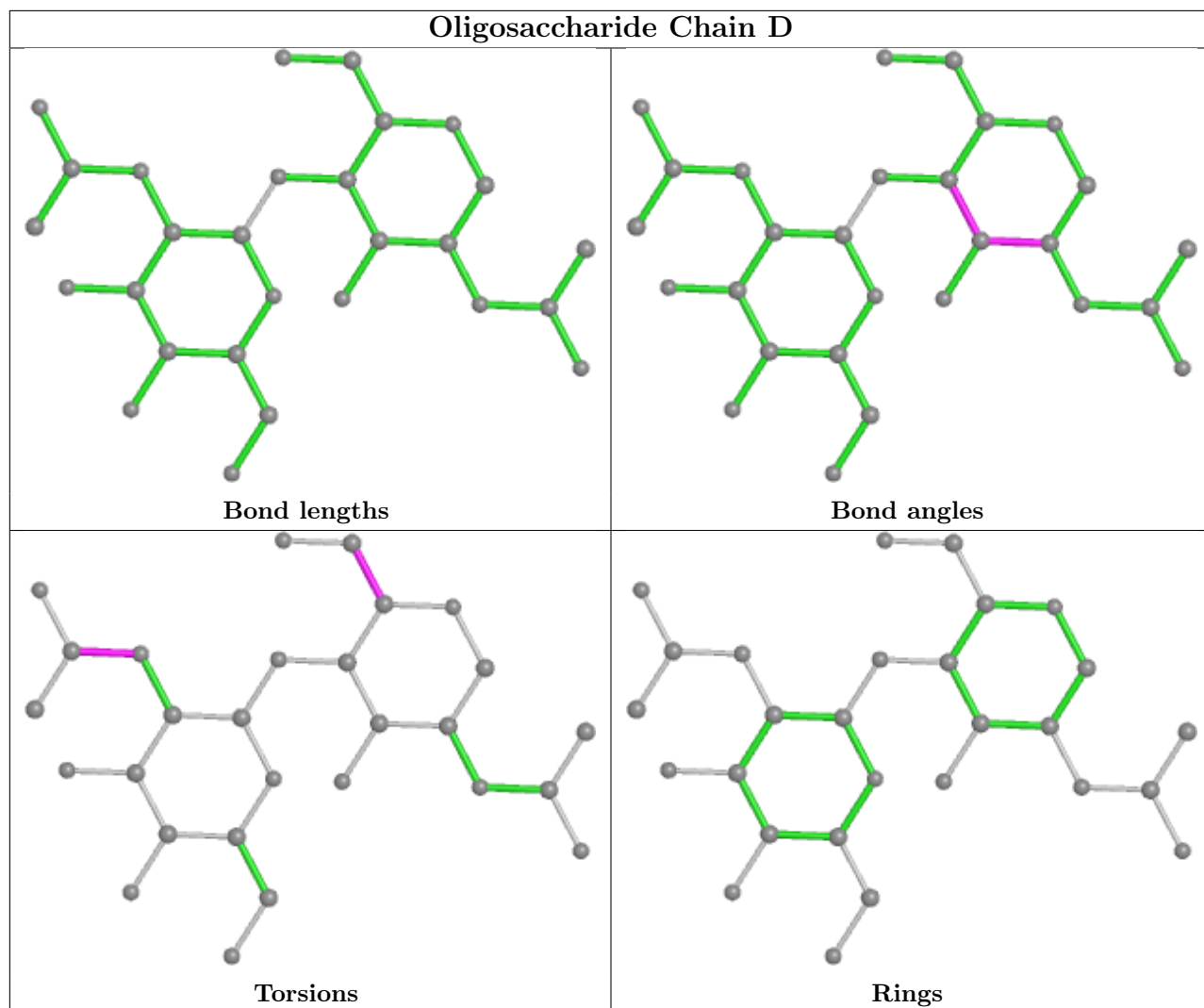
All (4) torsion outliers are listed below:

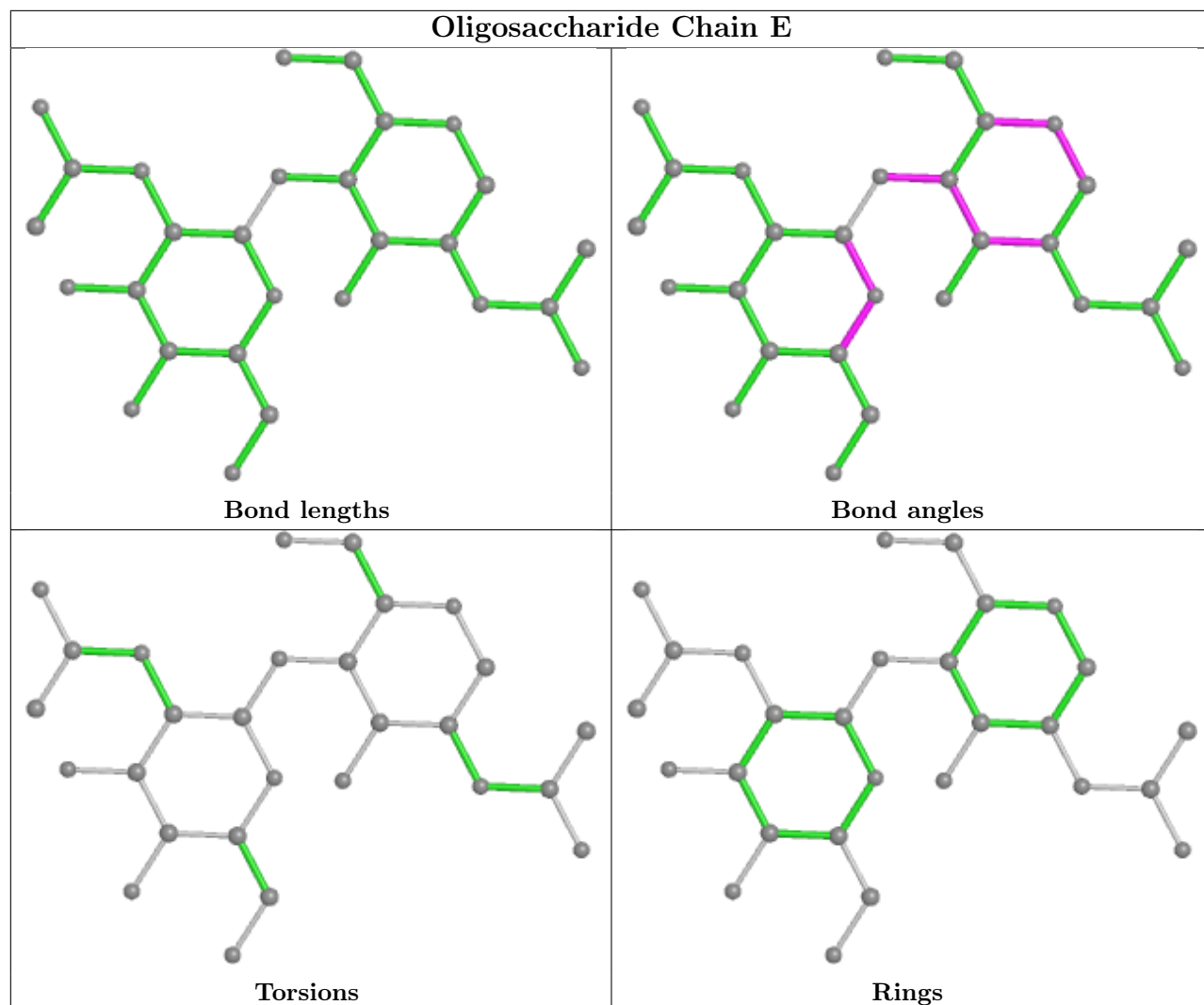
Mol	Chain	Res	Type	Atoms
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
4	D	1	NAG	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6

There are no ring outliers.

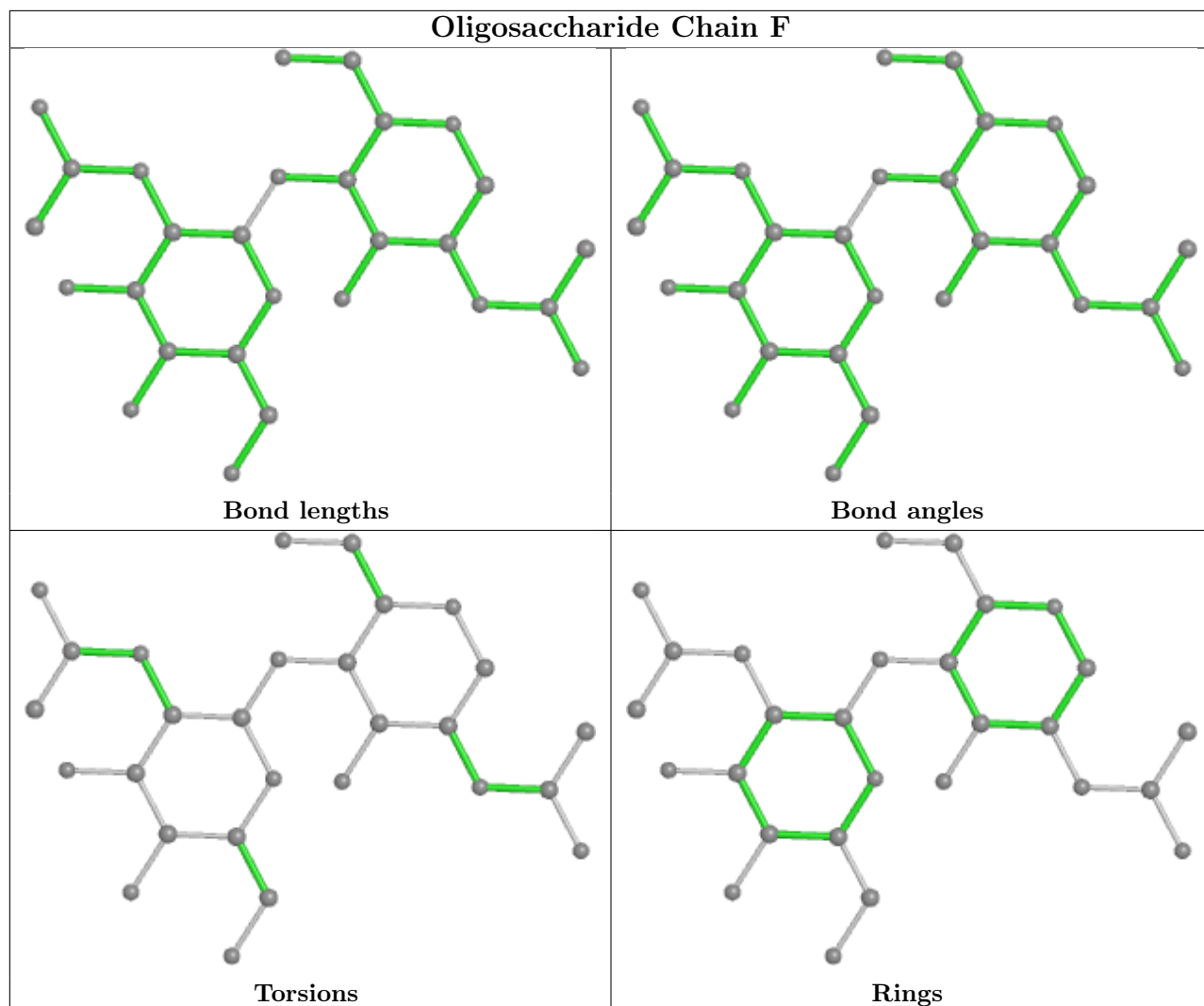
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.









## 5.6 Ligand geometry [i](#)

21 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$
8	LPE	A	2017	-	24,24,33	0.28	0	28,30,39	0.36	0
5	NAG	B	301	2	14,14,15	0.29	0	17,19,21	0.60	0
7	Y01	A	2018	-	38,38,38	0.49	0	57,57,57	0.64	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	P5S	A	2012	-	40,40,53	0.30	0	43,45,60	0.40	0
5	NAG	A	2001	1	14,14,15	0.29	0	17,19,21	0.57	0
9	PCW	A	2011	-	46,46,53	0.32	0	52,54,61	0.38	0
5	NAG	A	2002	1	14,14,15	0.37	0	17,19,21	0.81	1 (5%)
7	Y01	A	2006	-	38,38,38	0.45	0	57,57,57	0.66	0
5	NAG	B	303	2	14,14,15	0.32	0	17,19,21	0.76	0
8	LPE	A	2014	-	24,24,33	0.28	0	28,30,39	0.42	0
7	Y01	A	2007	-	38,38,38	0.47	0	57,57,57	0.66	0
8	LPE	A	2016	-	24,24,33	0.28	0	28,30,39	0.36	0
8	LPE	A	2010	-	27,27,33	0.26	0	31,33,39	0.33	0
9	PCW	A	2013	-	43,43,53	0.32	0	49,51,61	0.41	0
5	NAG	B	302	2	14,14,15	0.27	0	17,19,21	0.65	0
6	IYJ	A	2003	-	17,17,17	2.76	9 (52%)	24,24,24	4.59	10 (41%)
7	Y01	A	2005	-	38,38,38	0.44	0	57,57,57	0.49	0
9	PCW	A	2009	-	48,48,53	0.41	0	54,56,61	0.30	0
8	LPE	A	2015	-	24,24,33	0.28	0	28,30,39	0.32	0
6	IYJ	A	2004	-	17,17,17	2.83	9 (52%)	24,24,24	4.74	11 (45%)
8	LPE	A	2008	-	24,24,33	0.32	0	25,27,39	0.40	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
8	LPE	A	2017	-	-	4/25/25/34	-
5	NAG	B	301	2	-	1/6/23/26	0/1/1/1
7	Y01	A	2018	-	-	9/19/77/77	0/4/4/4
10	P5S	A	2012	-	-	12/44/44/59	-
5	NAG	A	2001	1	-	4/6/23/26	0/1/1/1
9	PCW	A	2011	-	-	14/50/50/57	-
5	NAG	A	2002	1	-	0/6/23/26	0/1/1/1
7	Y01	A	2006	-	-	9/19/77/77	0/4/4/4
5	NAG	B	303	2	-	2/6/23/26	0/1/1/1
8	LPE	A	2014	-	-	13/25/25/34	-
7	Y01	A	2007	-	-	2/19/77/77	0/4/4/4
8	LPE	A	2016	-	-	5/25/25/34	-
8	LPE	A	2010	-	-	9/28/28/34	-
9	PCW	A	2013	-	-	9/47/47/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	302	2	-	0/6/23/26	0/1/1/1
6	IYJ	A	2003	-	-	0/4/4/4	0/2/2/2
7	Y01	A	2005	-	-	4/19/77/77	0/4/4/4
9	PCW	A	2009	-	-	25/52/52/57	-
8	LPE	A	2015	-	-	4/25/25/34	-
6	IYJ	A	2004	-	-	0/4/4/4	0/2/2/2
8	LPE	A	2008	-	-	14/25/25/34	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2004	IYJ	C09-C12	-5.75	1.38	1.45
6	A	2003	IYJ	C16-N07	5.74	1.45	1.33
6	A	2004	IYJ	C16-N07	5.73	1.45	1.33
6	A	2003	IYJ	C09-C12	-5.18	1.39	1.45
6	A	2003	IYJ	C12-N05	4.55	1.45	1.34
6	A	2004	IYJ	C12-N05	4.46	1.45	1.34
6	A	2003	IYJ	C08-C09	3.74	1.53	1.49
6	A	2004	IYJ	C08-C09	3.43	1.53	1.49
6	A	2003	IYJ	C16-N04	-2.96	1.30	1.35
6	A	2004	IYJ	C16-N04	-2.94	1.30	1.35
6	A	2003	IYJ	C10-CL01	2.73	1.78	1.72
6	A	2004	IYJ	C10-CL01	2.72	1.78	1.72
6	A	2003	IYJ	C16-N06	-2.72	1.32	1.35
6	A	2004	IYJ	C16-N06	-2.65	1.32	1.35
6	A	2004	IYJ	C13-CL02	2.33	1.79	1.73
6	A	2004	IYJ	C12-N04	-2.33	1.31	1.35
6	A	2003	IYJ	C13-CL02	2.15	1.78	1.73
6	A	2003	IYJ	C12-N04	-2.03	1.32	1.35

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	2003	IYJ	N07-C16-N06	-14.70	103.34	117.26
6	A	2004	IYJ	N07-C16-N06	-14.49	103.53	117.26
6	A	2004	IYJ	N04-C16-N06	12.81	134.31	125.57
6	A	2003	IYJ	N04-C16-N06	12.50	134.10	125.57
6	A	2004	IYJ	C16-N04-C12	-6.22	110.13	116.99
6	A	2004	IYJ	C12-C09-N03	6.08	123.52	119.98
6	A	2003	IYJ	C16-N04-C12	-6.03	110.34	116.99
6	A	2003	IYJ	C12-C09-N03	5.53	123.20	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	2004	IYJ	C16-N06-N03	-4.57	114.07	117.38
6	A	2003	IYJ	C16-N06-N03	-4.17	114.37	117.38
6	A	2004	IYJ	C09-N03-N06	-3.95	116.11	120.43
6	A	2003	IYJ	C09-N03-N06	-3.84	116.23	120.43
6	A	2004	IYJ	C08-C09-C12	-3.46	118.06	122.34
6	A	2003	IYJ	N07-C16-N04	3.41	122.56	117.25
6	A	2004	IYJ	N07-C16-N04	3.15	122.15	117.25
6	A	2004	IYJ	C09-C12-N05	-3.08	118.55	121.11
6	A	2004	IYJ	C09-C12-N04	2.70	121.85	120.09
6	A	2003	IYJ	C09-C12-N04	2.57	121.77	120.09
6	A	2003	IYJ	C08-C09-C12	-2.51	119.23	122.34
6	A	2003	IYJ	C09-C12-N05	-2.25	119.24	121.11
5	A	2002	NAG	C1-O5-C5	2.23	115.22	112.19
7	A	2018	Y01	CAP-CBE-CBB	2.11	115.42	112.15
6	A	2004	IYJ	C09-C08-C10	-2.06	117.95	120.97

There are no chirality outliers.

All (140) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	2008	LPE	C31-O33-P-O32
8	A	2008	LPE	O33-C31-C32-N
8	A	2010	LPE	C2-C3-O3-P
8	A	2014	LPE	C3-O3-P-O31
8	A	2014	LPE	O33-C31-C32-N
8	A	2015	LPE	C31-O33-P-O31
8	A	2016	LPE	C31-O33-P-O31
8	A	2016	LPE	C32-C31-O33-P
9	A	2009	PCW	O4P-C4-C5-N
9	A	2009	PCW	C1-O3P-P-O2P
9	A	2013	PCW	C4-O4P-P-O1P
9	A	2013	PCW	C4-O4P-P-O2P
9	A	2013	PCW	C4-O4P-P-O3P
10	A	2012	P5S	N-CA-CB-OG
9	A	2009	PCW	O11-C11-O3-C3
7	A	2006	Y01	CAC-CBB-CBE-CAP
7	A	2006	Y01	CAC-CBB-CBE-CBI
7	A	2006	Y01	CAO-CBB-CBE-CBI
7	A	2006	Y01	CAV-CBC-OAW-CAY
9	A	2009	PCW	C12-C11-O3-C3
7	A	2018	Y01	CAJ-CAO-CBB-CAC
7	A	2006	Y01	CAO-CBB-CBE-CAP

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Mol	Chain	Res	Type	Atoms
8	A	2014	LPE	C31-C32-N-C2N
5	B	303	NAG	C8-C7-N2-C2
5	B	303	NAG	O7-C7-N2-C2
8	A	2008	LPE	O2H-C2-C3-O3
8	A	2014	LPE	O2H-C2-C3-O3
10	A	2012	P5S	C39-C38-O37-C2
9	A	2009	PCW	C24-C25-C26-C27
5	A	2001	NAG	C8-C7-N2-C2
7	A	2018	Y01	CAM-CAY-OAW-CBC
8	A	2014	LPE	C1-C2-C3-O3
7	A	2018	Y01	CAO-CBB-CBE-CBI
7	A	2018	Y01	CAJ-CAO-CBB-CBE
5	A	2001	NAG	O7-C7-N2-C2
7	A	2018	Y01	CAC-CBB-CBE-CAP
7	A	2018	Y01	CAC-CBB-CBE-CBI
7	A	2006	Y01	CAR-CBC-OAW-CAY
7	A	2018	Y01	OAG-CAY-OAW-CBC
8	A	2008	LPE	C31-O33-P-O3
8	A	2014	LPE	C3-O3-P-O33
10	A	2012	P5S	O47-C38-O37-C2
8	A	2014	LPE	C31-C32-N-C1N
9	A	2009	PCW	C35-C36-C37-C38
7	A	2006	Y01	CAJ-CAN-CBA-CAA
8	A	2014	LPE	C31-C32-N-C3N
8	A	2008	LPE	C14-C15-C16-C17
9	A	2009	PCW	C33-C34-C35-C36
8	A	2008	LPE	C11-C12-C13-C14
5	A	2001	NAG	C1-C2-N2-C7
9	A	2009	PCW	C22-C23-C24-C25
9	A	2013	PCW	O31-C31-O2-C2
9	A	2013	PCW	C32-C31-O2-C2
8	A	2008	LPE	C12-C13-C14-C15
9	A	2009	PCW	C1-O3P-P-O4P
9	A	2009	PCW	C18-C19-C20-C21
8	A	2008	LPE	O1-C1-C2-O2H
7	A	2006	Y01	CAJ-CAN-CBA-CAB
8	A	2008	LPE	O1-C11-C12-C13
7	A	2006	Y01	CAN-CAJ-CAO-CBB
9	A	2011	PCW	O2-C31-C32-C33
8	A	2015	LPE	C2-C3-O3-P
8	A	2008	LPE	C13-C14-C15-C16
8	A	2014	LPE	C31-O33-P-O3

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms
9	A	2009	PCW	C4-O4P-P-O3P
9	A	2011	PCW	O2-C2-C3-O3
9	A	2009	PCW	C31-C32-C33-C34
8	A	2014	LPE	C2-C3-O3-P
8	A	2016	LPE	C2-C1-O1-C11
8	A	2016	LPE	C31-O33-P-O3
10	A	2012	P5S	C41-C42-C43-C44
9	A	2009	PCW	C2-C1-O3P-P
8	A	2008	LPE	C31-O33-P-O31
9	A	2009	PCW	C1-O3P-P-O1P
9	A	2009	PCW	C4-O4P-P-O1P
8	A	2010	LPE	C32-C31-O33-P
8	A	2014	LPE	C32-C31-O33-P
9	A	2011	PCW	C5-C4-O4P-P
9	A	2013	PCW	C5-C4-O4P-P
10	A	2012	P5S	CA-CB-OG-P12
8	A	2008	LPE	C1-C2-C3-O3
8	A	2010	LPE	O33-C31-C32-N
8	A	2015	LPE	O33-C31-C32-N
8	A	2016	LPE	O33-C31-C32-N
8	A	2017	LPE	O33-C31-C32-N
9	A	2011	PCW	O4P-C4-C5-N
7	A	2005	Y01	CAJ-CAO-CBB-CBE
8	A	2008	LPE	C16-C17-C18-C19
9	A	2011	PCW	C19-C20-C21-C22
9	A	2011	PCW	C37-C38-C39-C40
8	A	2010	LPE	C3-O3-P-O33
8	A	2010	LPE	C31-O33-P-O3
8	A	2015	LPE	C31-O33-P-O3
8	A	2017	LPE	C3-O3-P-O33
8	A	2017	LPE	C31-O33-P-O3
9	A	2011	PCW	C4-O4P-P-O3P
9	A	2013	PCW	C1-O3P-P-O4P
10	A	2012	P5S	CB-OG-P12-O16
9	A	2011	PCW	C34-C35-C36-C37
9	A	2009	PCW	C37-C38-C39-C40
9	A	2013	PCW	C19-C20-C21-C22
10	A	2012	P5S	C20-C21-C22-C23
10	A	2012	P5S	C1-C2-C3-O16
9	A	2009	PCW	C13-C14-C15-C16
9	A	2009	PCW	C17-C18-C19-C20
8	A	2010	LPE	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
9	A	2009	PCW	O31-C31-O2-C2
9	A	2011	PCW	C14-C15-C16-C17
10	A	2012	P5S	C40-C41-C42-C43
7	A	2005	Y01	CAJ-CAO-CBB-CAC
8	A	2010	LPE	O1-C11-C12-C13
9	A	2009	PCW	C38-C39-C40-C41
9	A	2009	PCW	C16-C17-C18-C19
9	A	2011	PCW	C17-C18-C19-C20
7	A	2007	Y01	CAM-CAL-CAX-OAH
10	A	2012	P5S	O19-C17-C20-C21
9	A	2011	PCW	C1-C2-C3-O3
9	A	2009	PCW	C19-C20-C21-C22
7	A	2007	Y01	CAM-CAL-CAX-OAF
7	A	2018	Y01	CAO-CBB-CBE-CAP
9	A	2011	PCW	O31-C31-C32-C33
5	A	2001	NAG	C3-C2-N2-C7
9	A	2009	PCW	O2-C31-C32-C33
8	A	2017	LPE	C12-C13-C14-C15
8	A	2010	LPE	C2-C1-O1-C11
9	A	2009	PCW	O31-C31-C32-C33
10	A	2012	P5S	O18-C17-C20-C21
9	A	2009	PCW	C12-C13-C14-C15
8	A	2008	LPE	C3-O3-P-O31
8	A	2010	LPE	C31-O33-P-O31
8	A	2014	LPE	C3-O3-P-O32
8	A	2014	LPE	C31-O33-P-O32
9	A	2011	PCW	C4-O4P-P-O2P
9	A	2013	PCW	C1-O3P-P-O2P
7	A	2018	Y01	CAJ-CAN-CBA-CAB
10	A	2012	P5S	O18-C17-O19-C1
9	A	2011	PCW	C15-C16-C17-C18
7	A	2005	Y01	CAL-CAM-CAY-OAW
7	A	2005	Y01	CAL-CAM-CAY-OAG
5	B	301	NAG	C4-C5-C6-O6

There are no ring outliers.

7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	2017	LPE	1	0
7	A	2018	Y01	3	0
10	A	2012	P5S	2	0

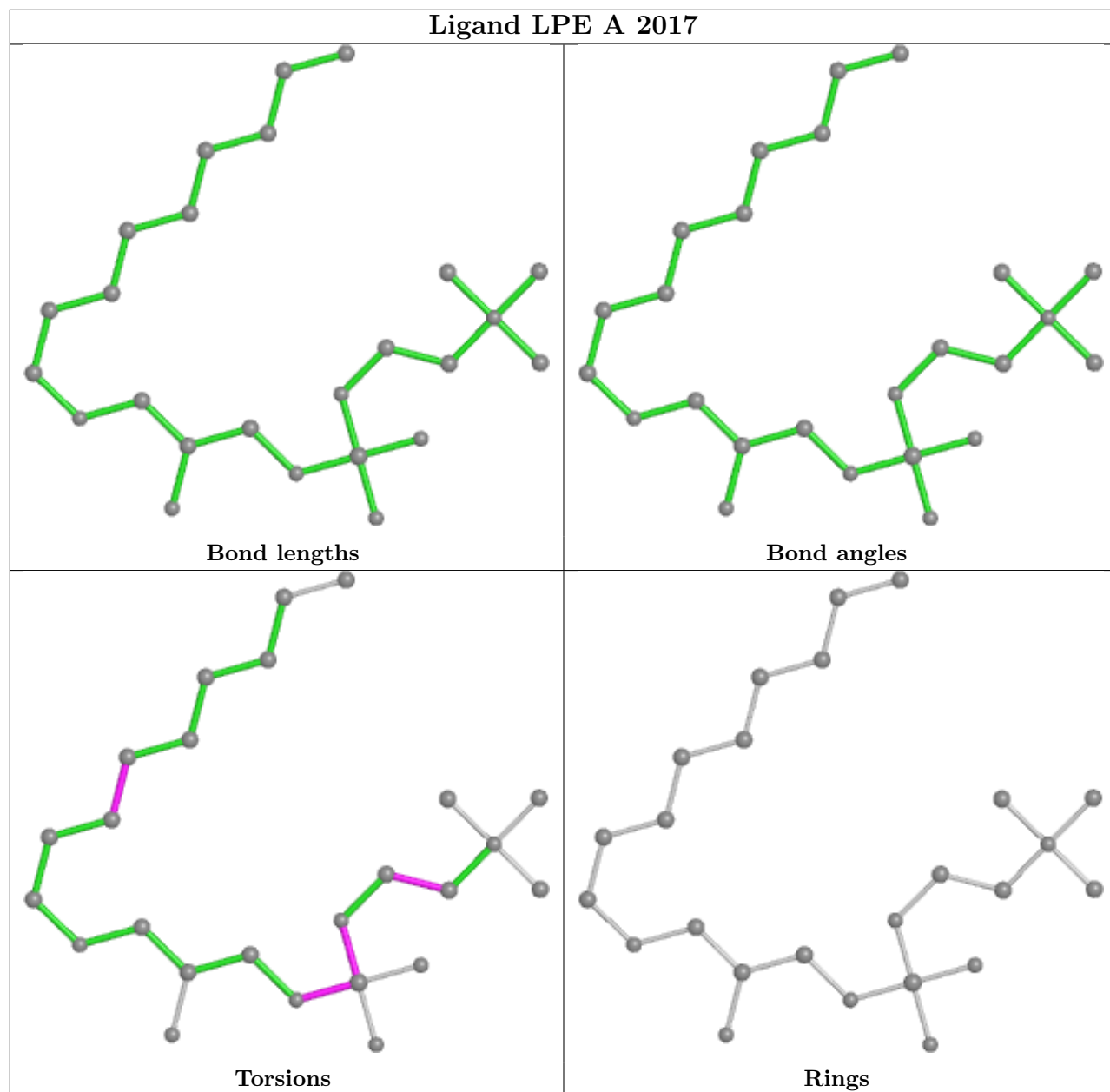
*Continued on next page...*

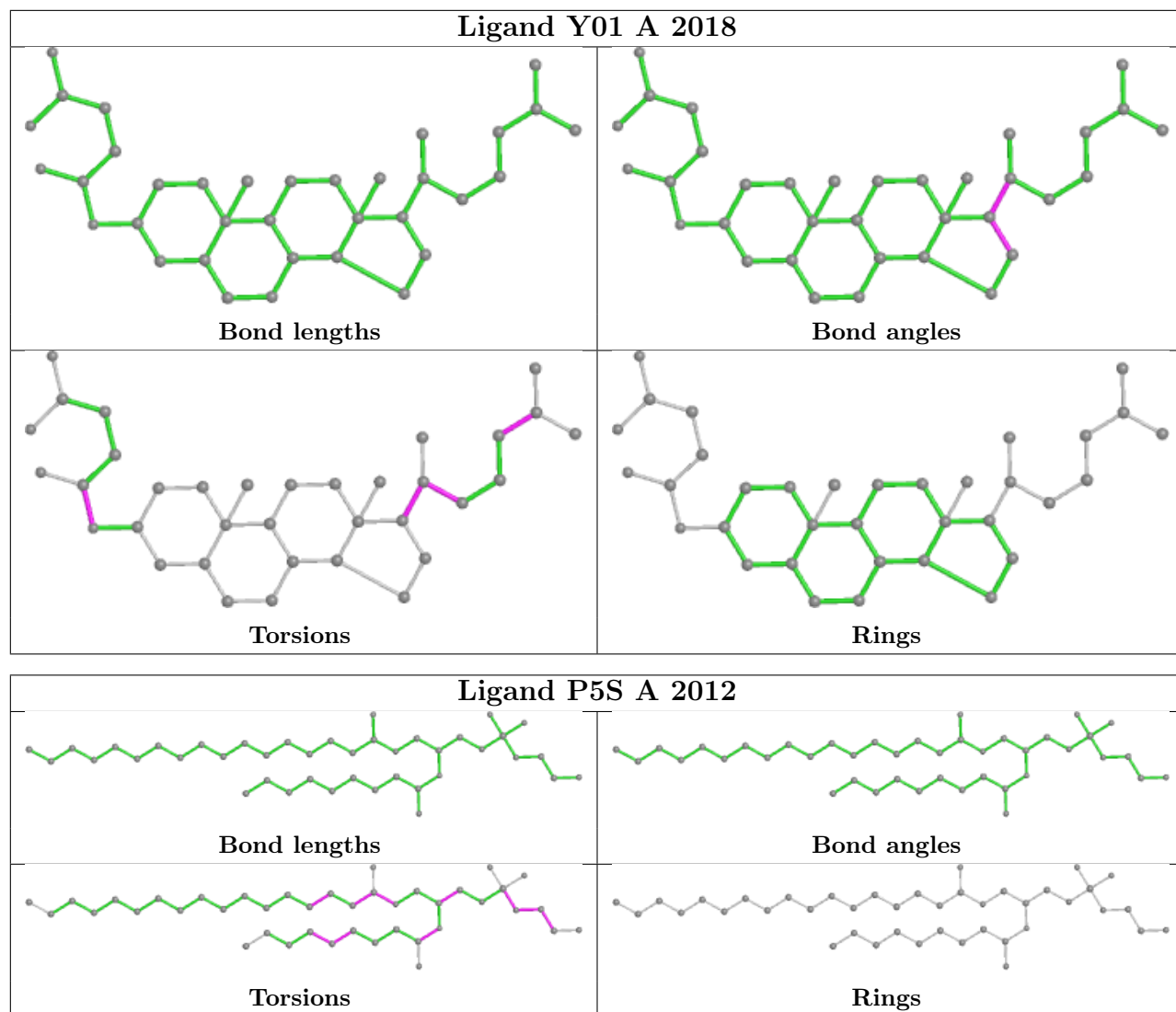
*Continued from previous page...*

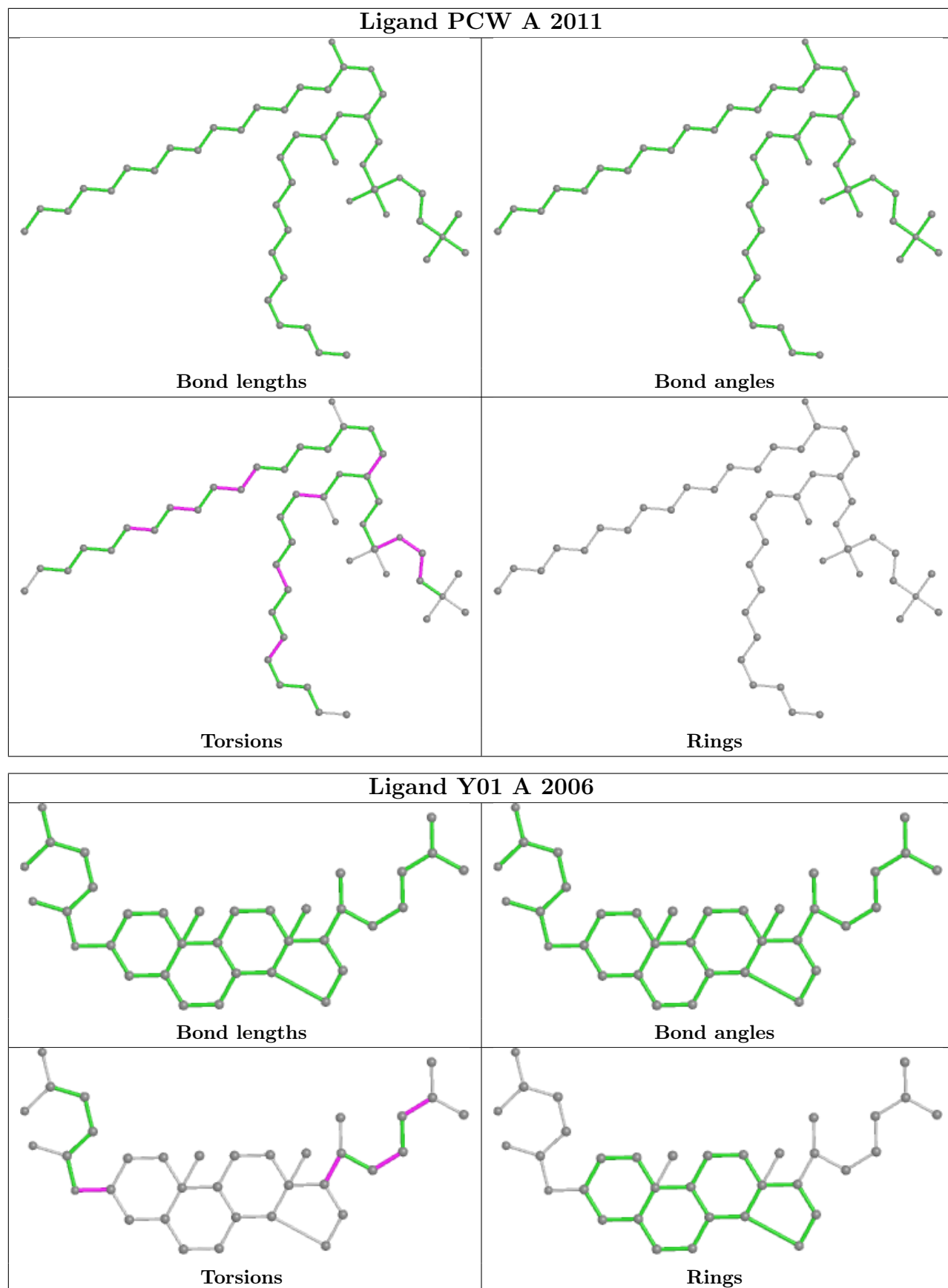
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	2011	PCW	3	0
9	A	2013	PCW	3	0
9	A	2009	PCW	4	0
8	A	2015	LPE	1	0

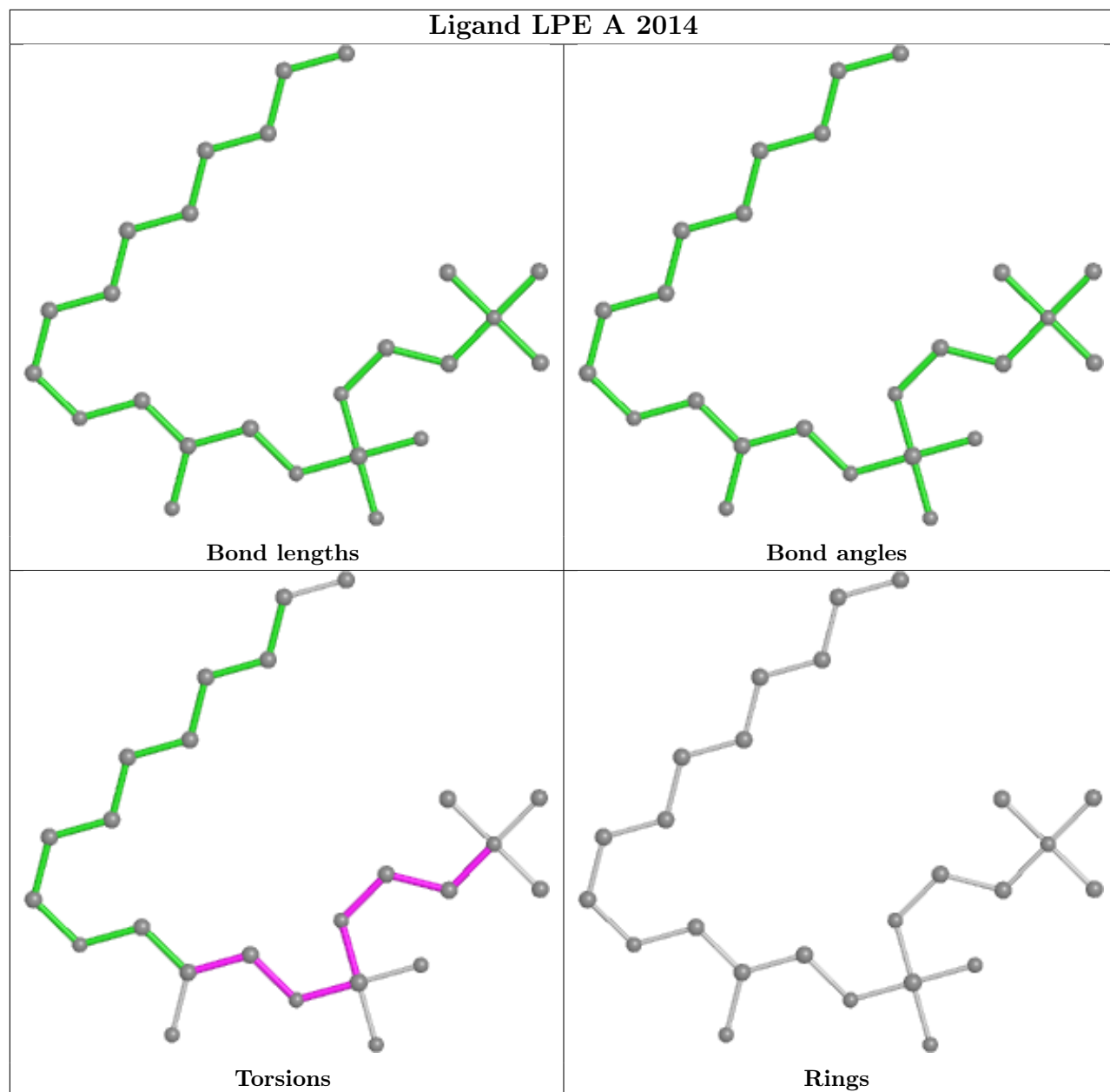
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

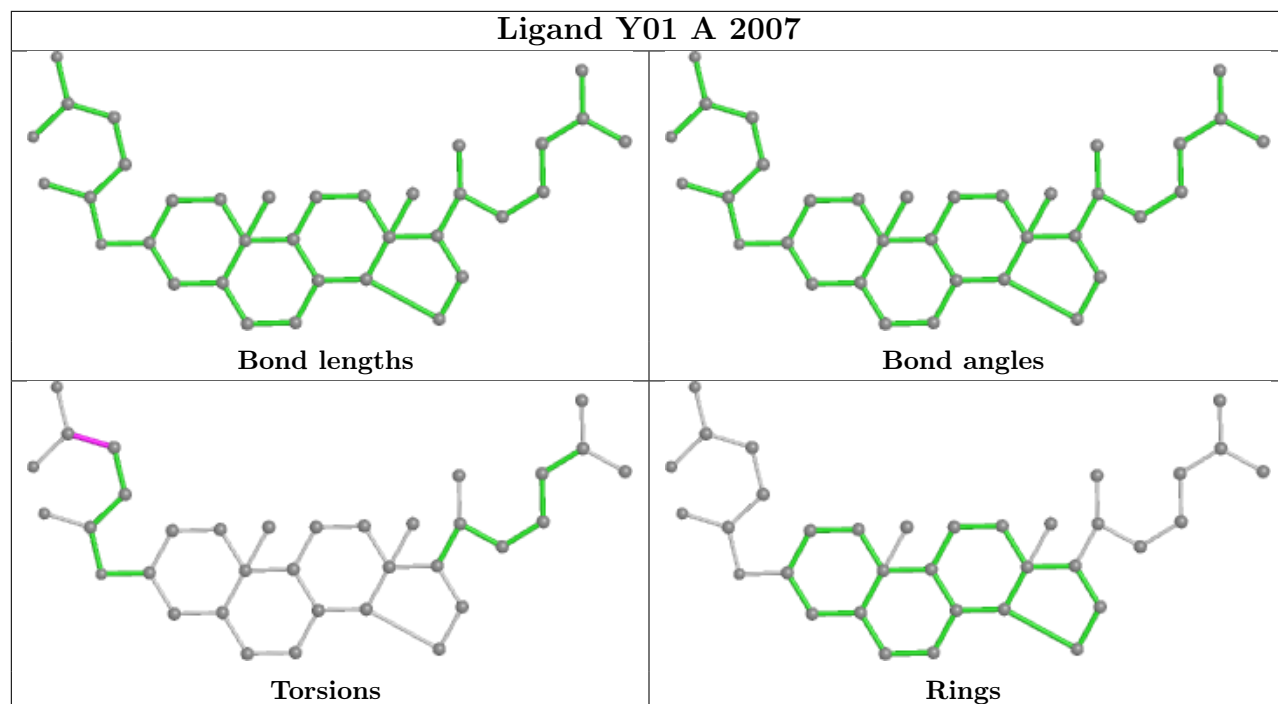


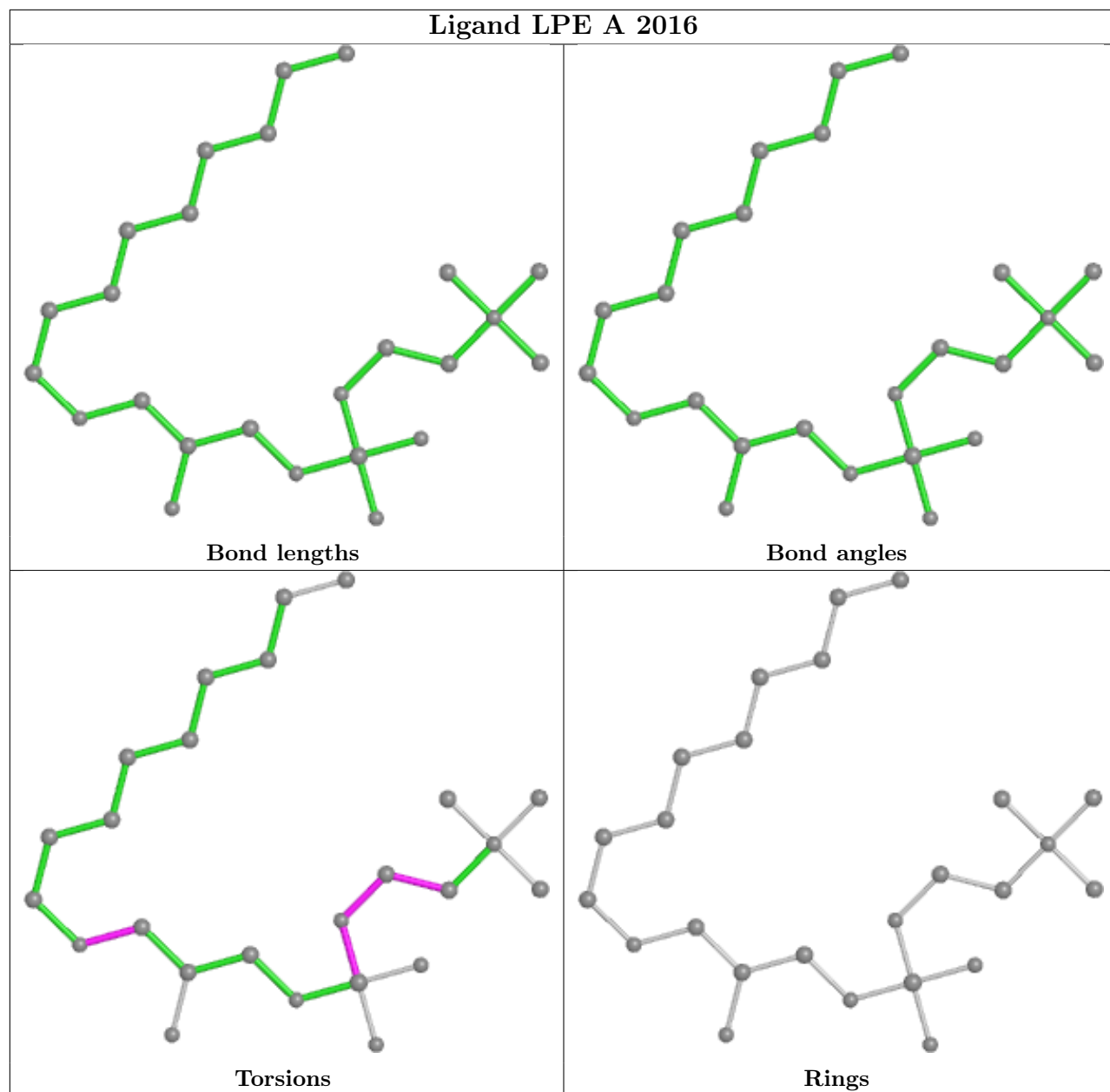


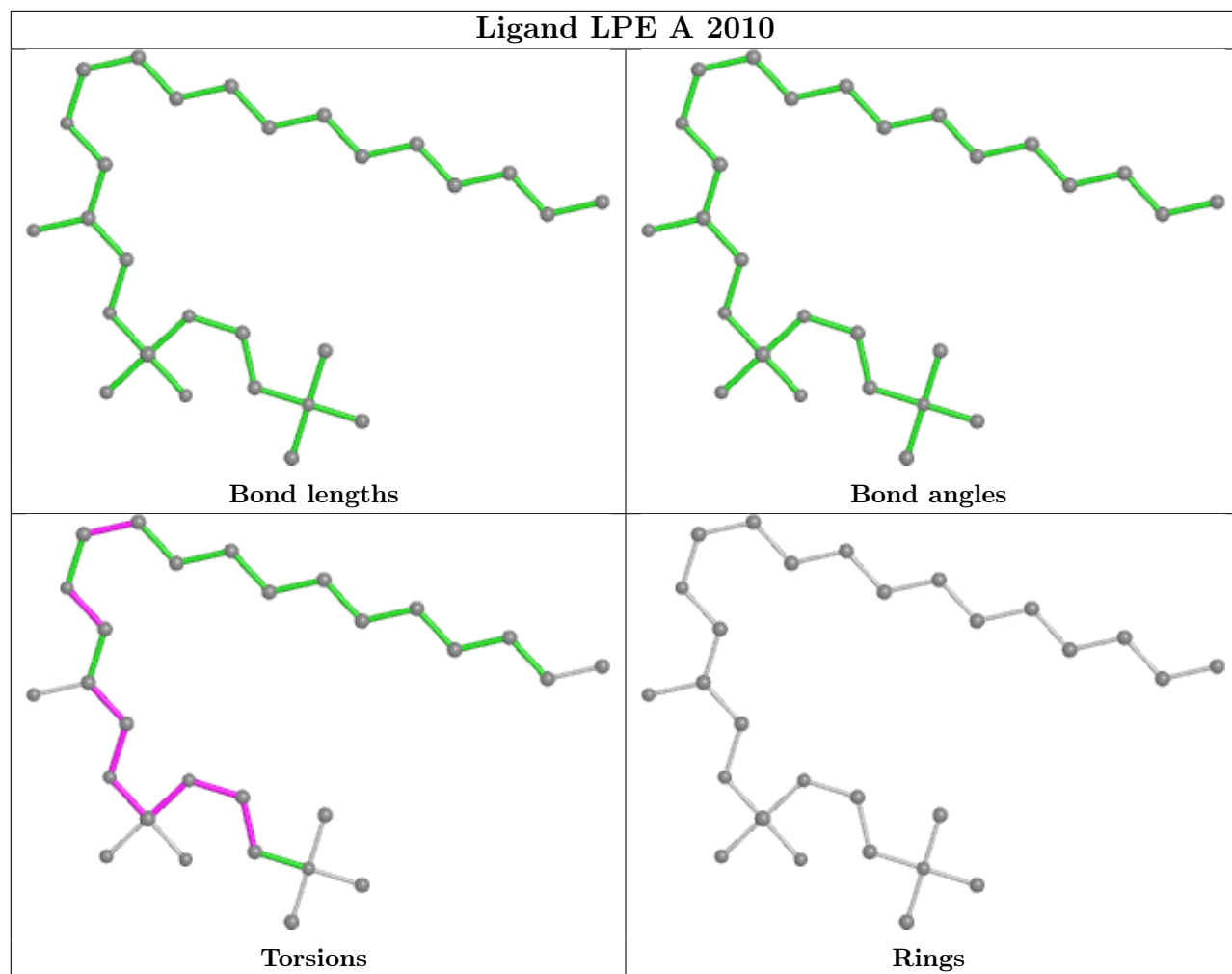


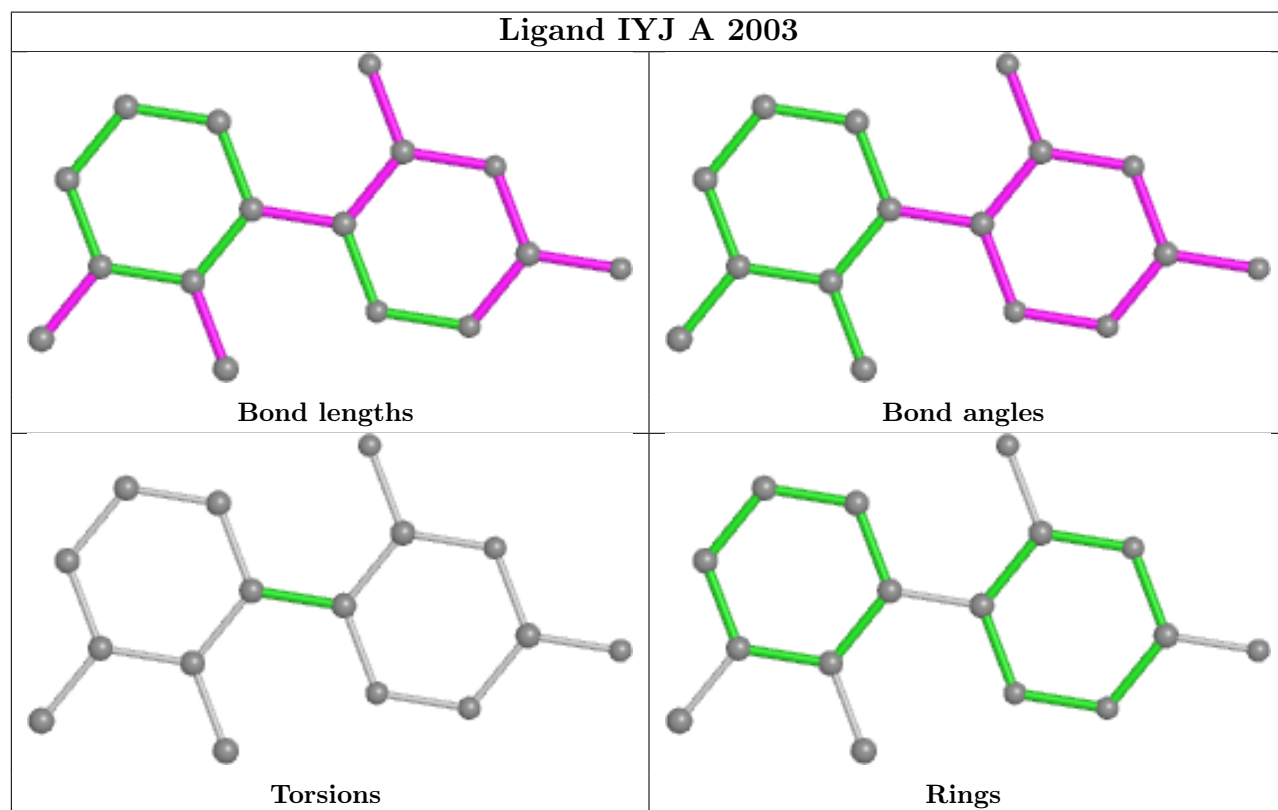
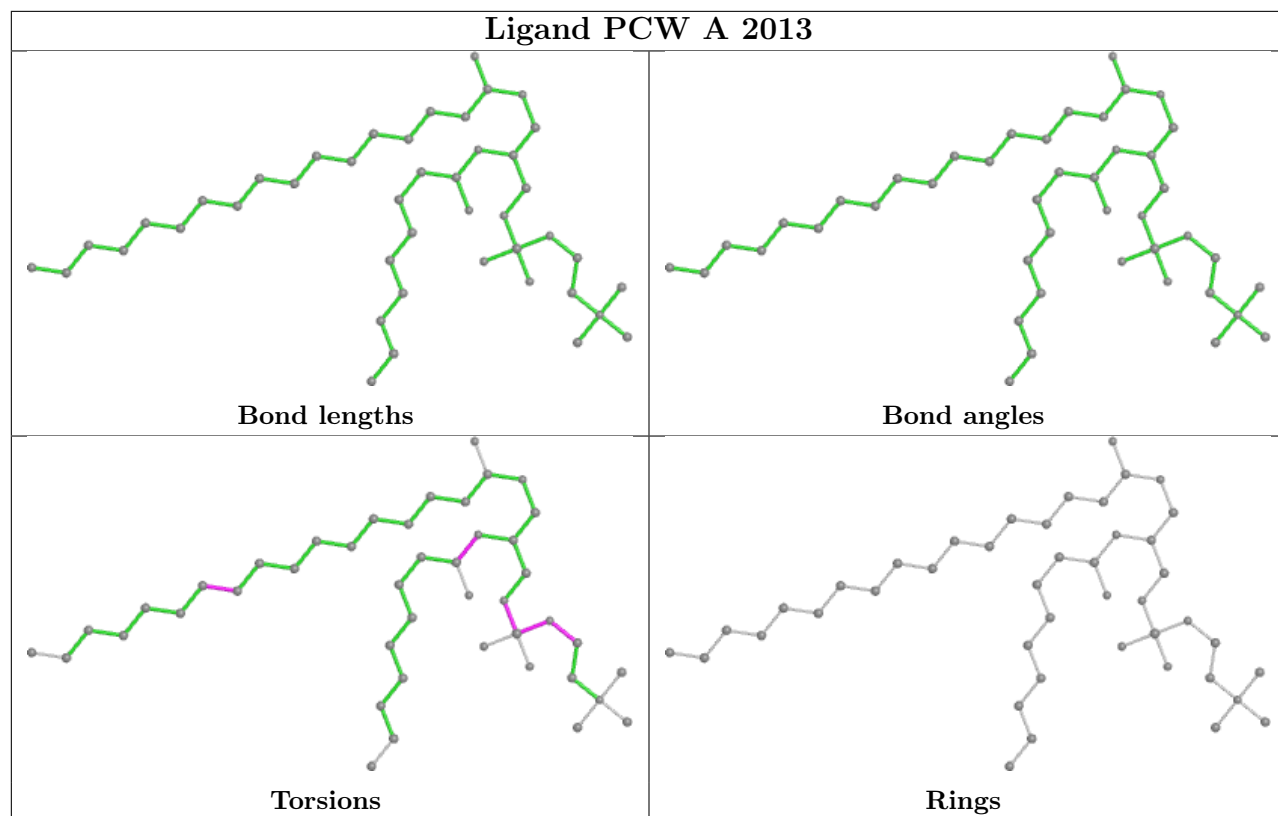




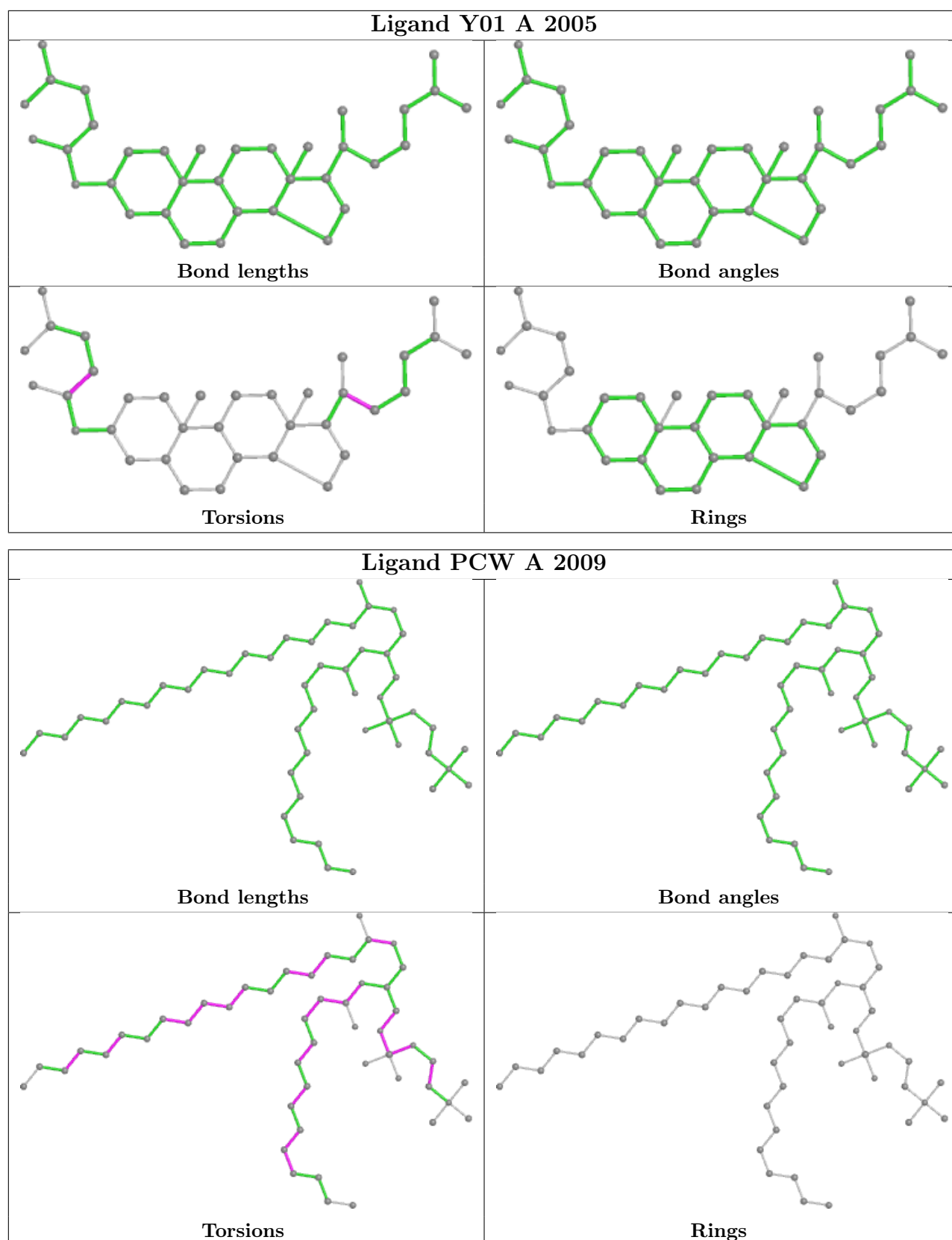


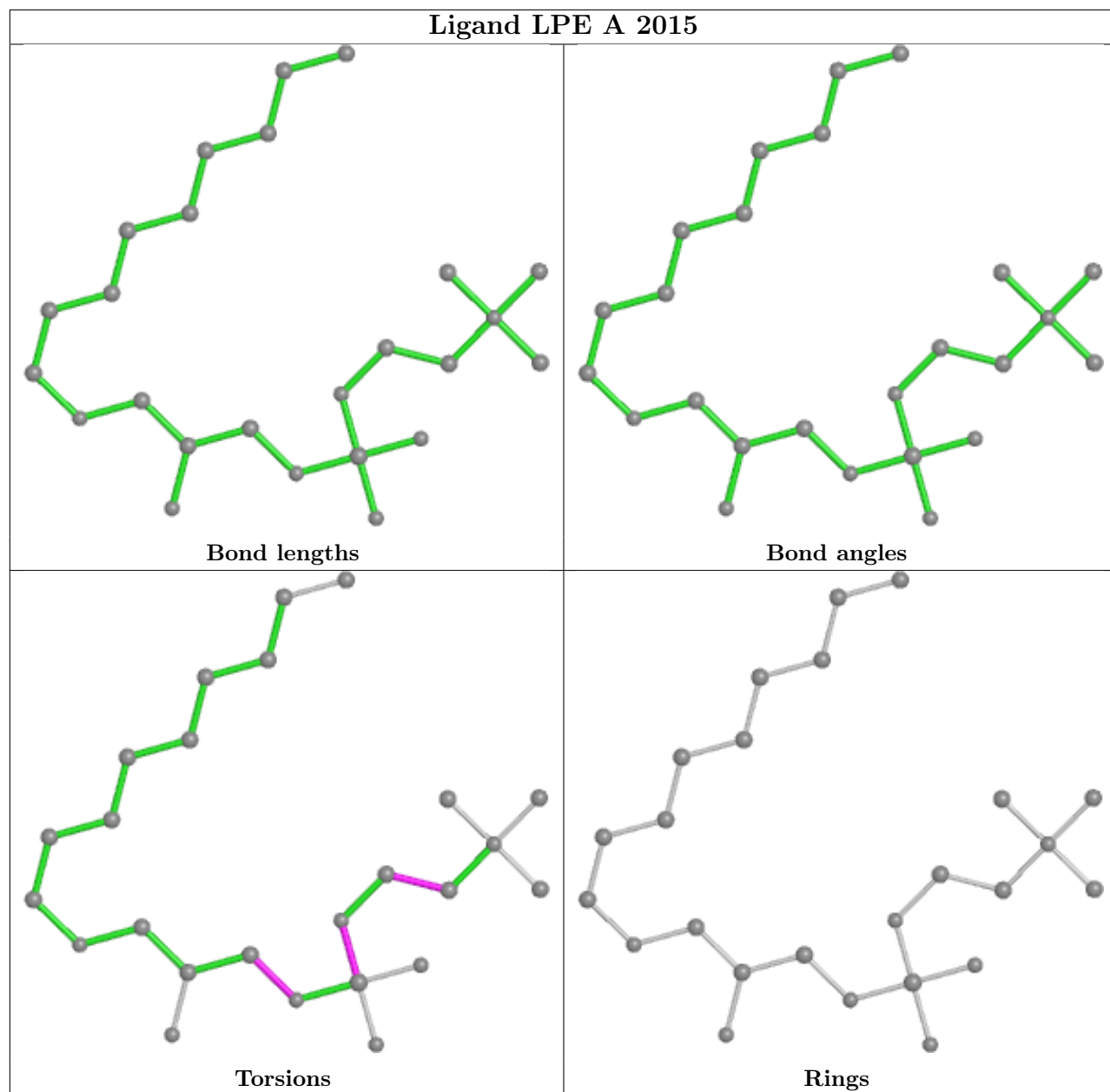


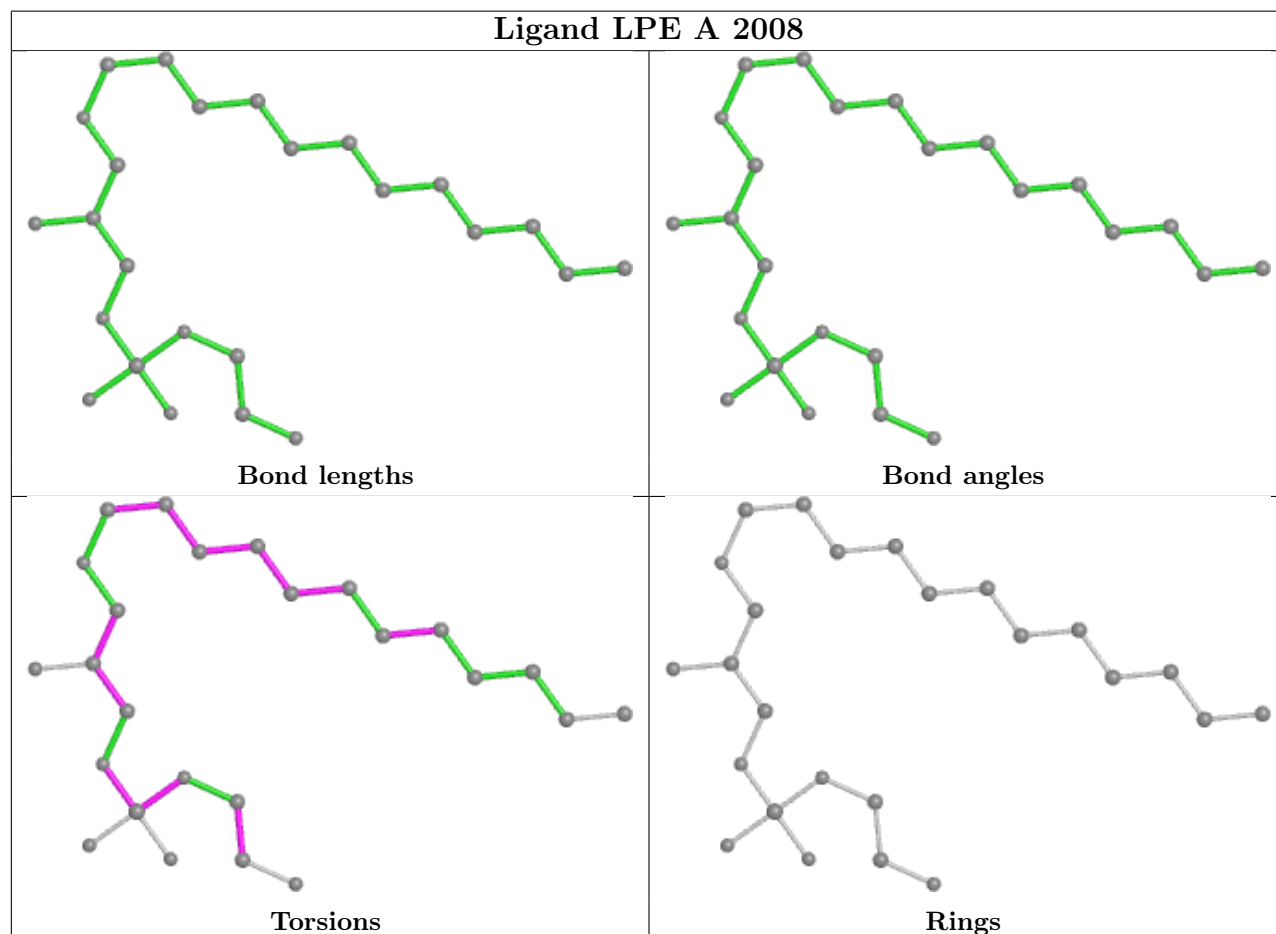
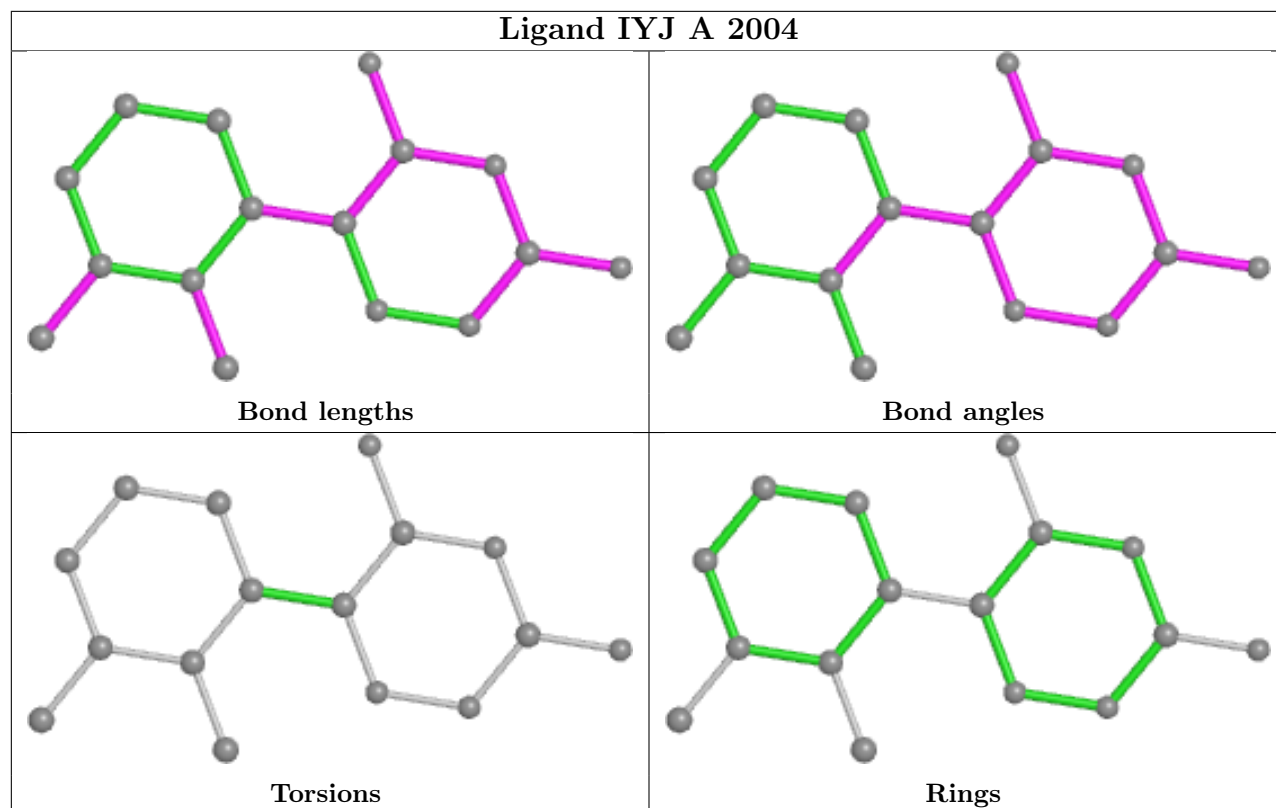












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

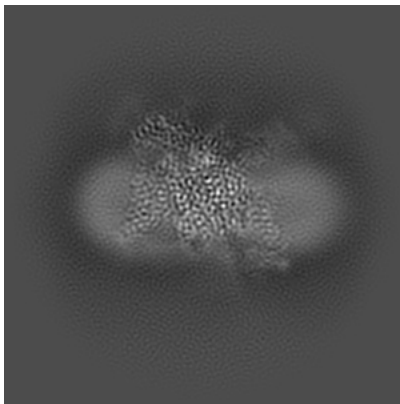
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41262. These allow visual inspection of the internal detail of the map and identification of artifacts.

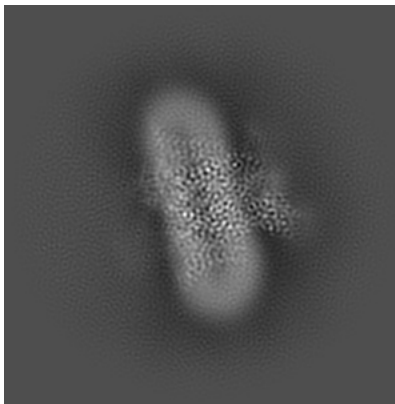
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

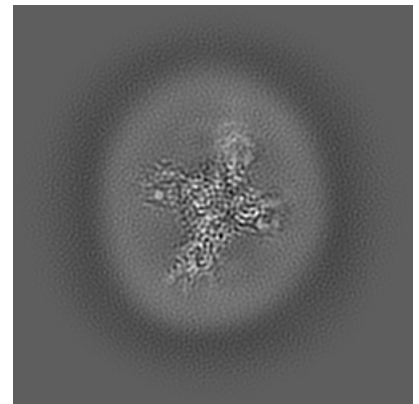
#### 6.1.1 Primary map



X

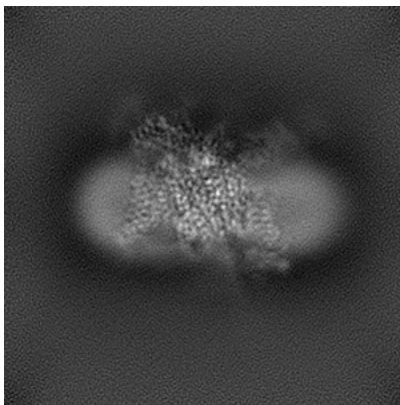


Y

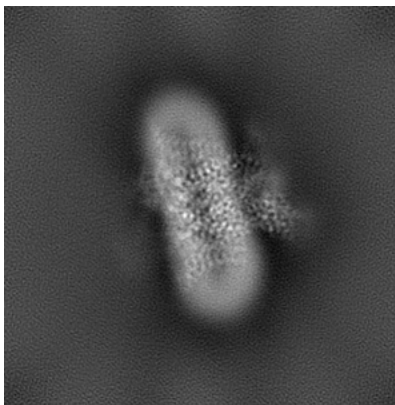


Z

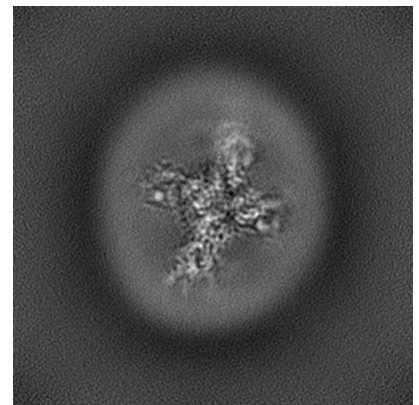
#### 6.1.2 Raw map



X



Y

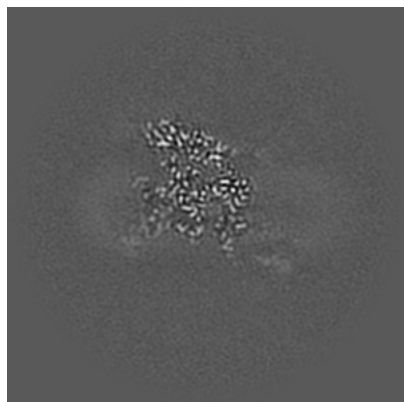


Z

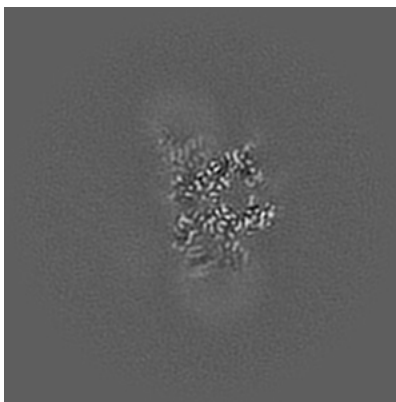
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

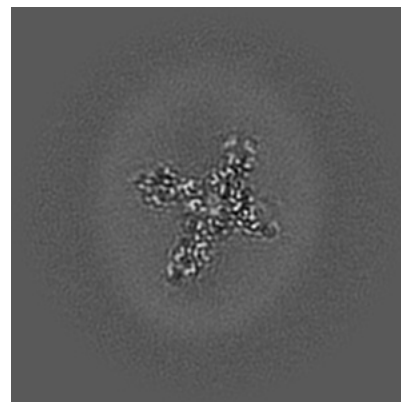
### 6.2.1 Primary map



X Index: 128

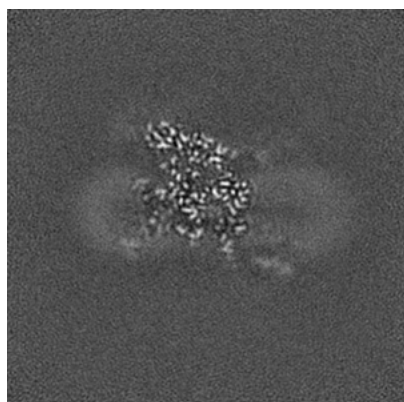


Y Index: 128

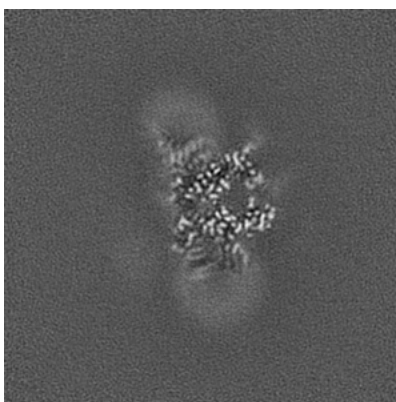


Z Index: 128

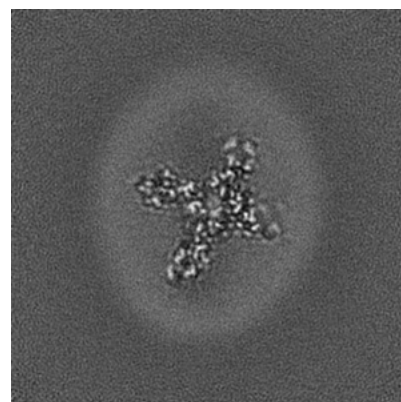
### 6.2.2 Raw map



X Index: 128



Y Index: 128

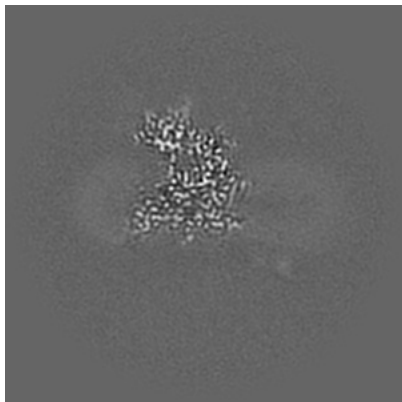


Z Index: 128

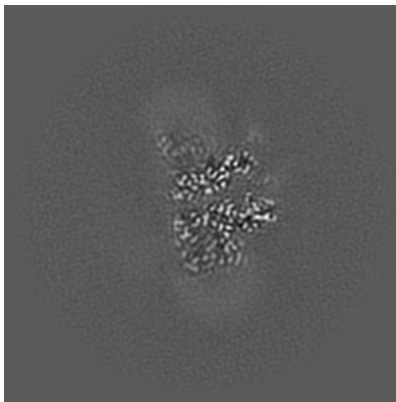
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

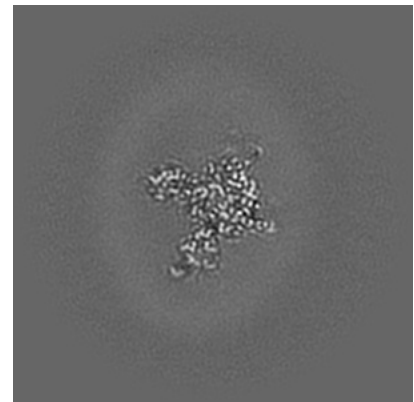
### 6.3.1 Primary map



X Index: 121

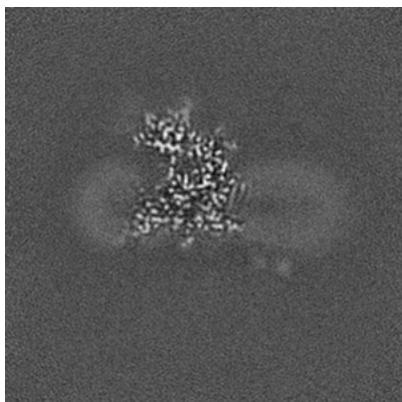


Y Index: 131

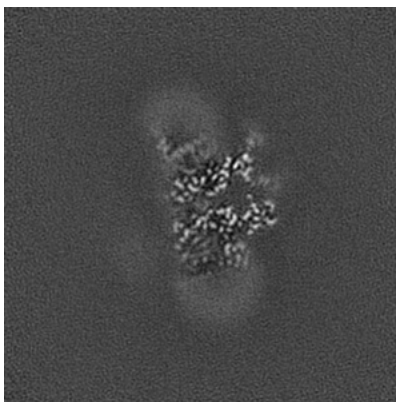


Z Index: 135

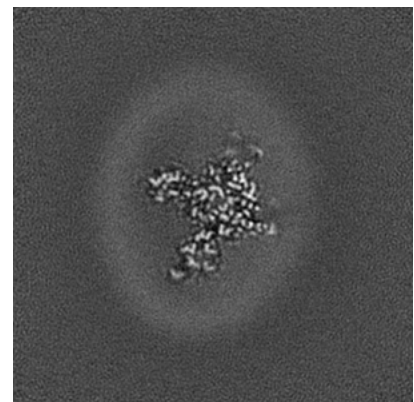
### 6.3.2 Raw map



X Index: 121



Y Index: 130

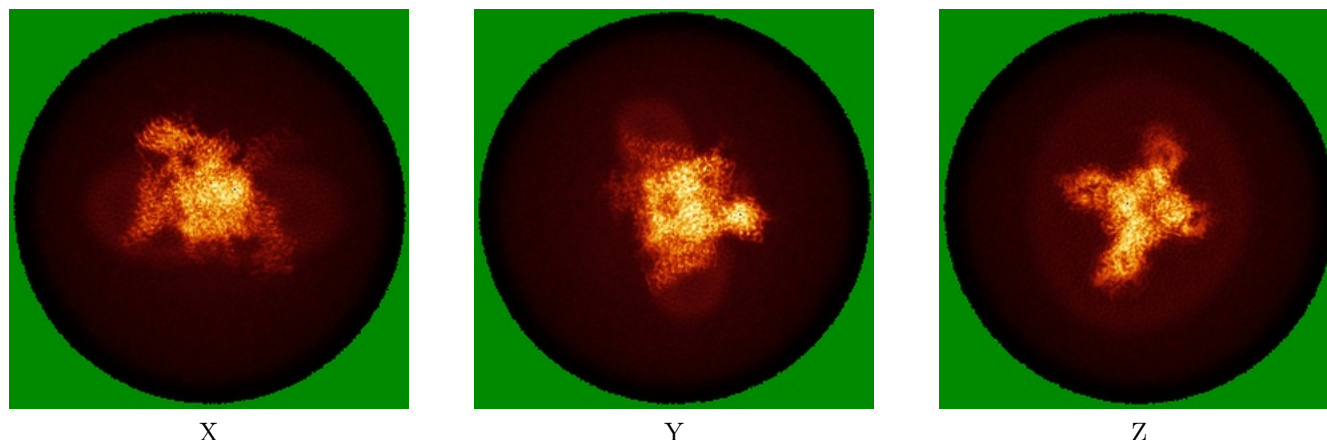


Z Index: 135

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

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

### 6.4.1 Primary map

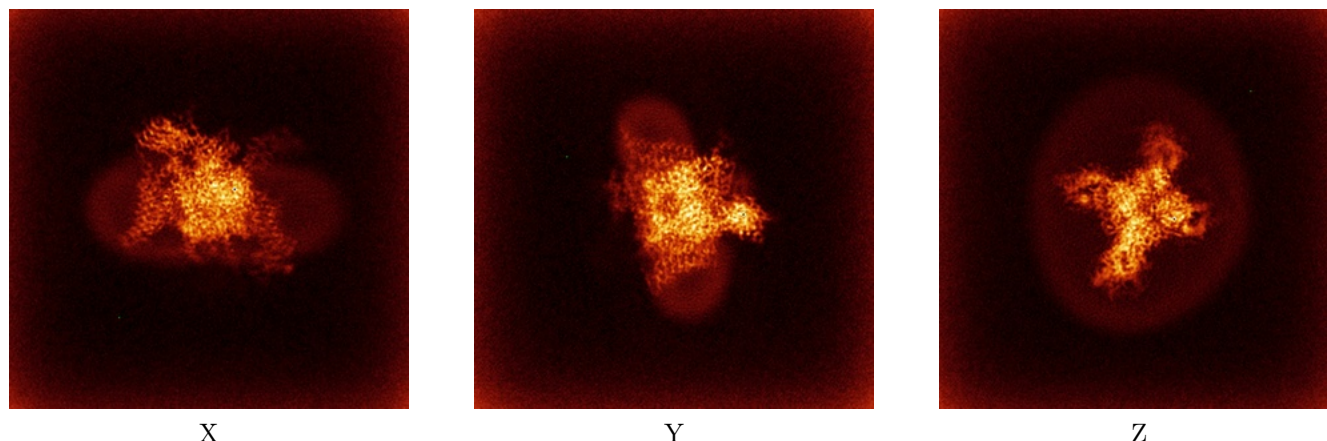


X

Y

Z

### 6.4.2 Raw map



X

Y

Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



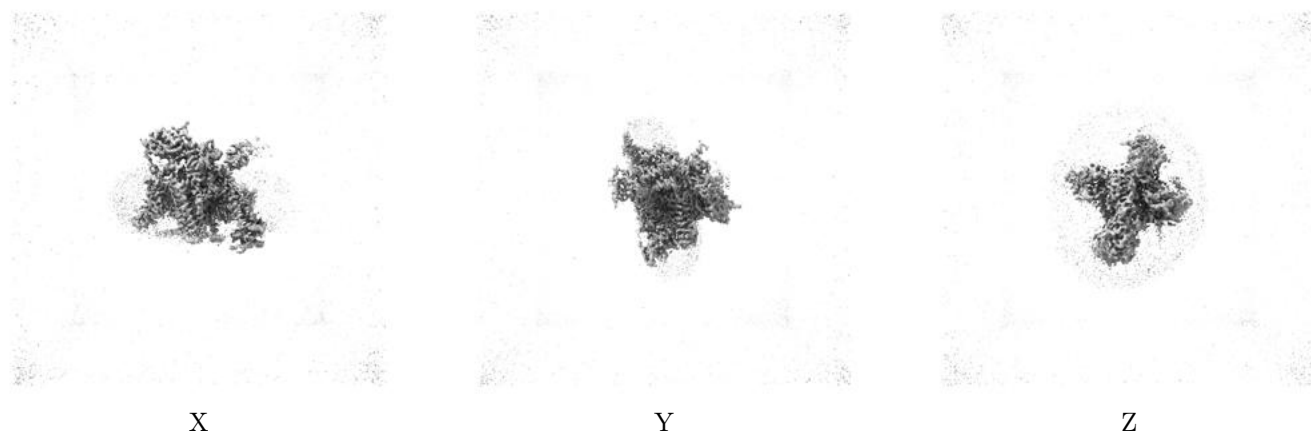
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. 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.

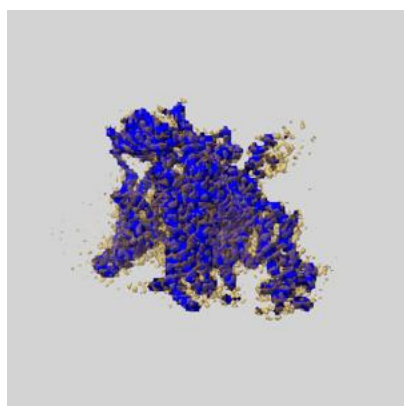
## 6.6 Mask visualisation [i](#)

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

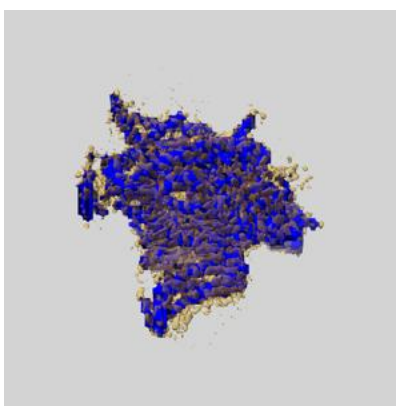
A mask typically either:

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

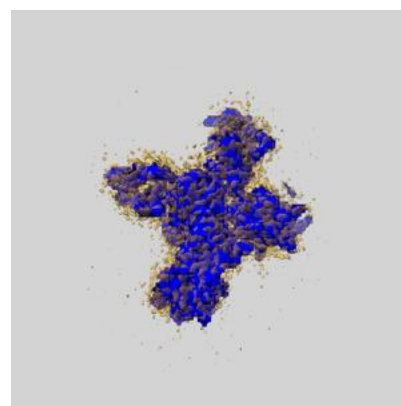
### 6.6.1 emd\_41262\_msk\_1.map [i](#)



X



Y

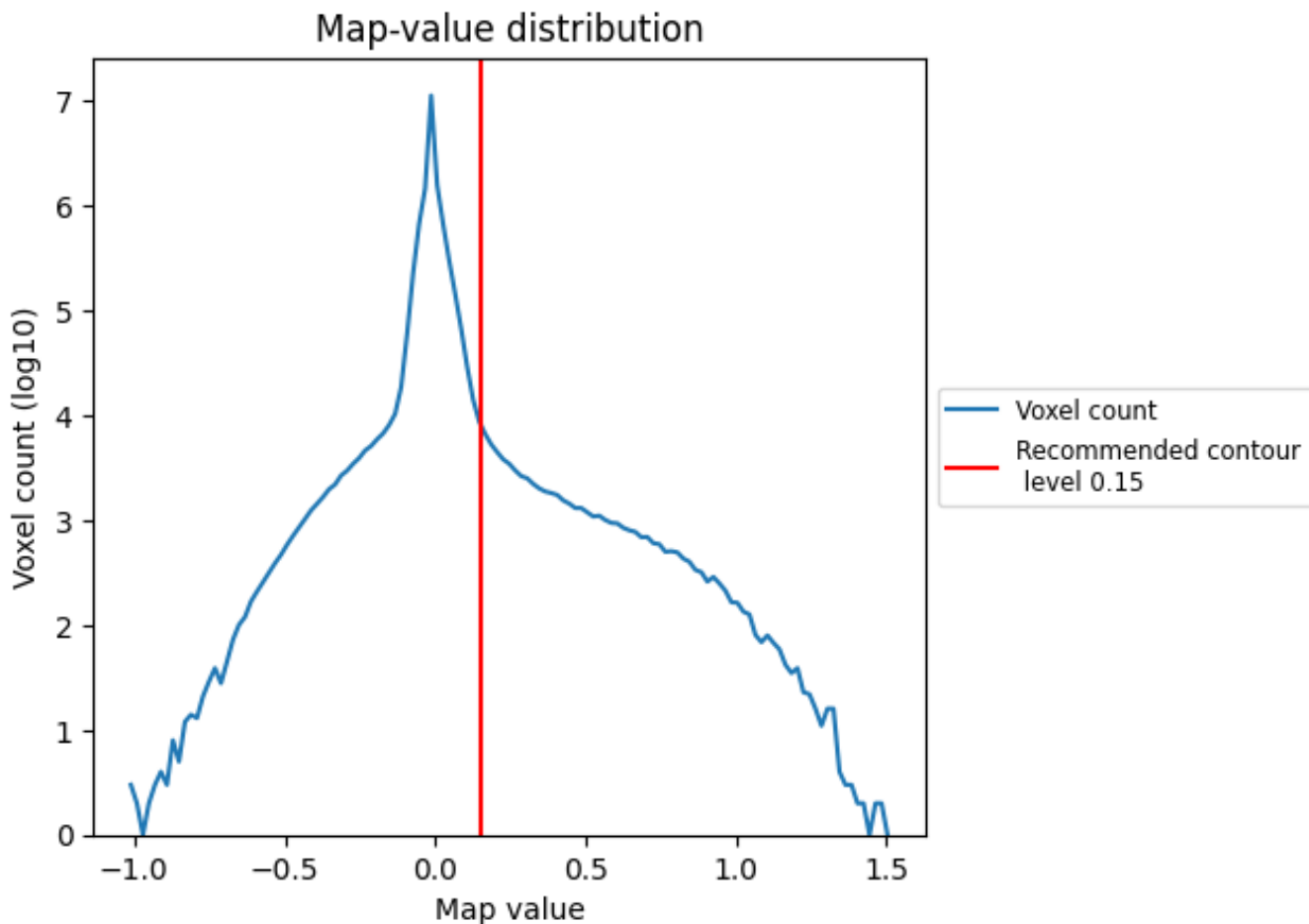


Z

## 7 Map analysis [i](#)

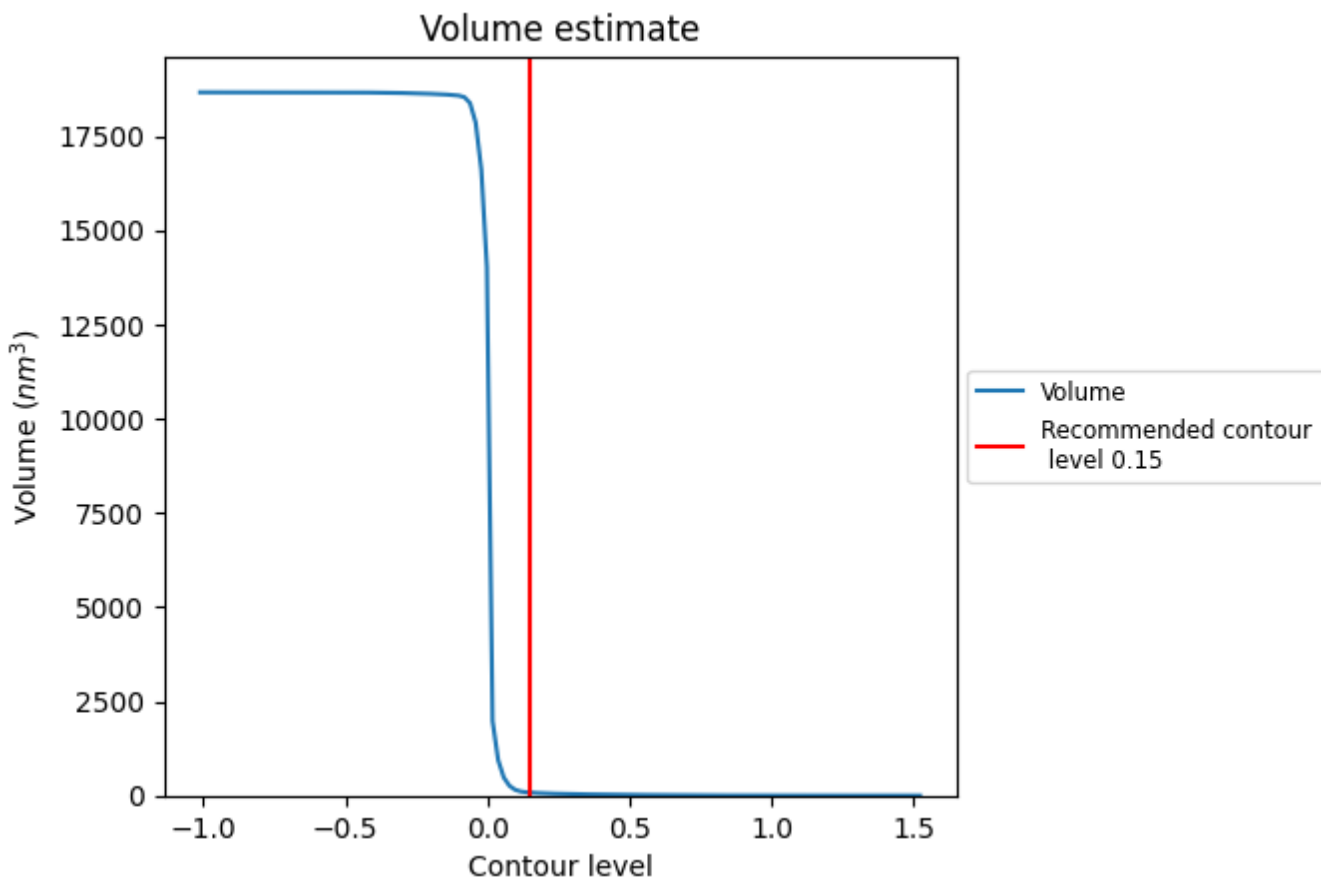
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

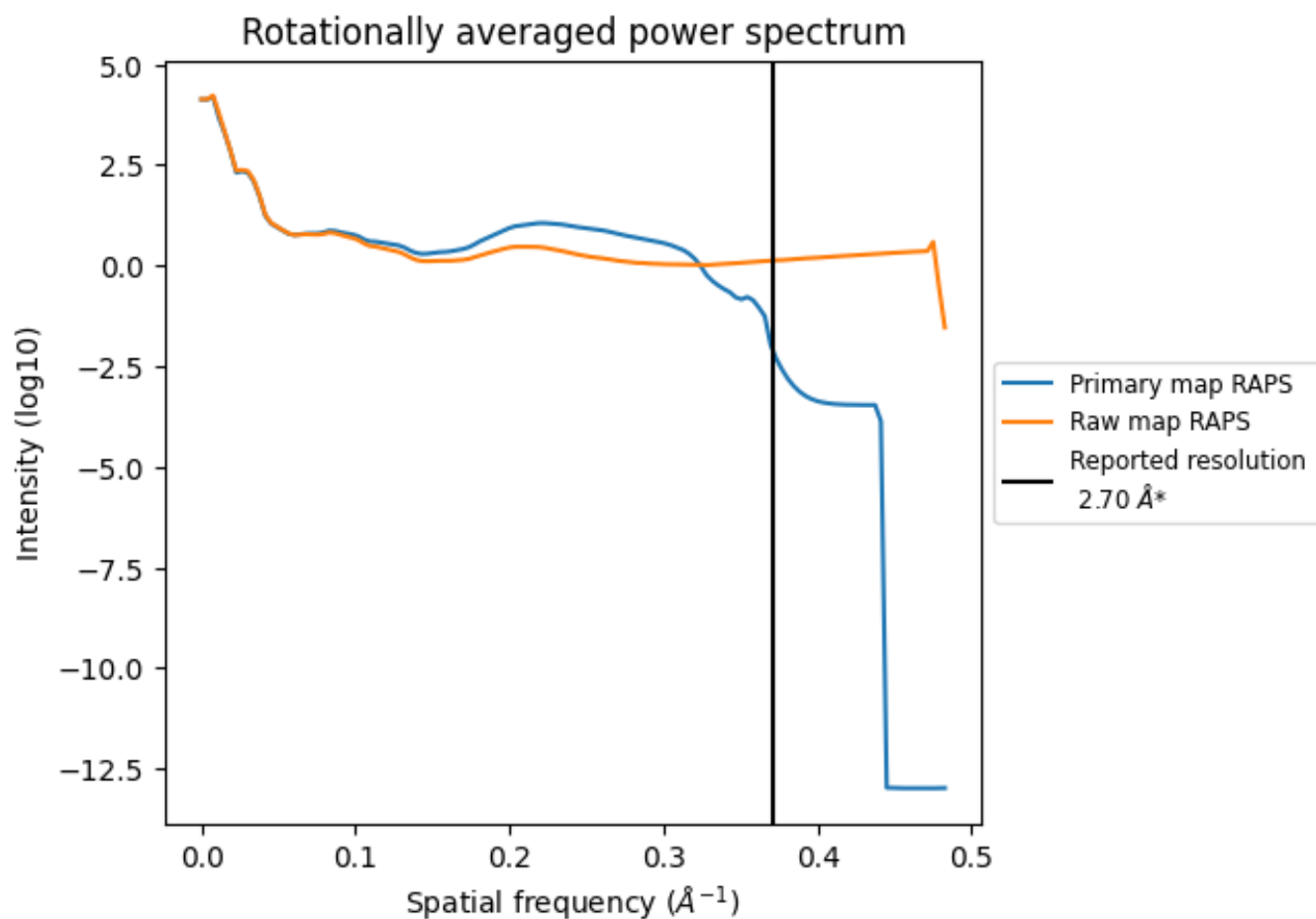
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 79 nm<sup>3</sup>; this corresponds to an approximate mass of 71 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](#)

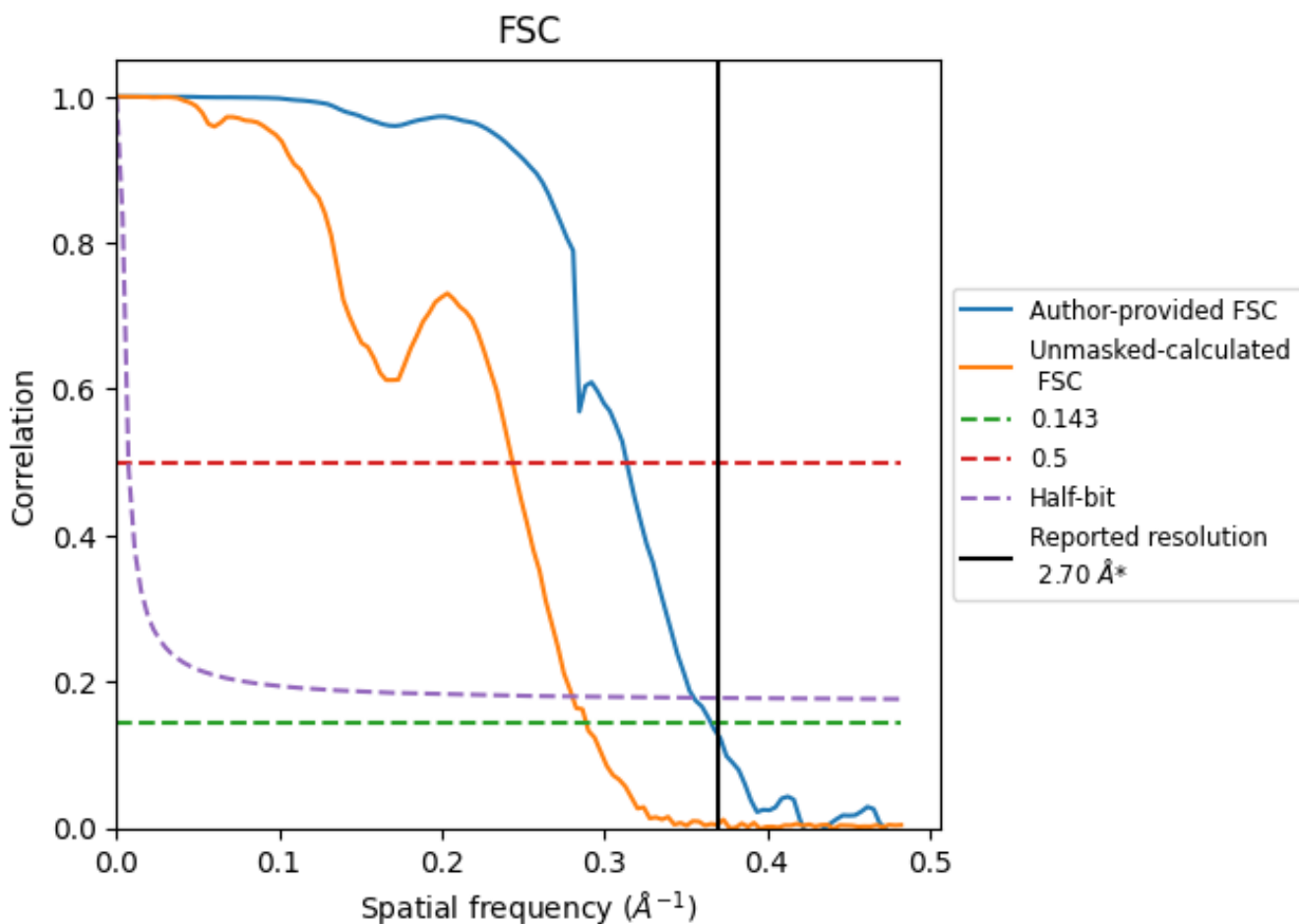


\*Reported resolution corresponds to spatial frequency of 0.370 Å<sup>-1</sup>

## 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 0.370 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

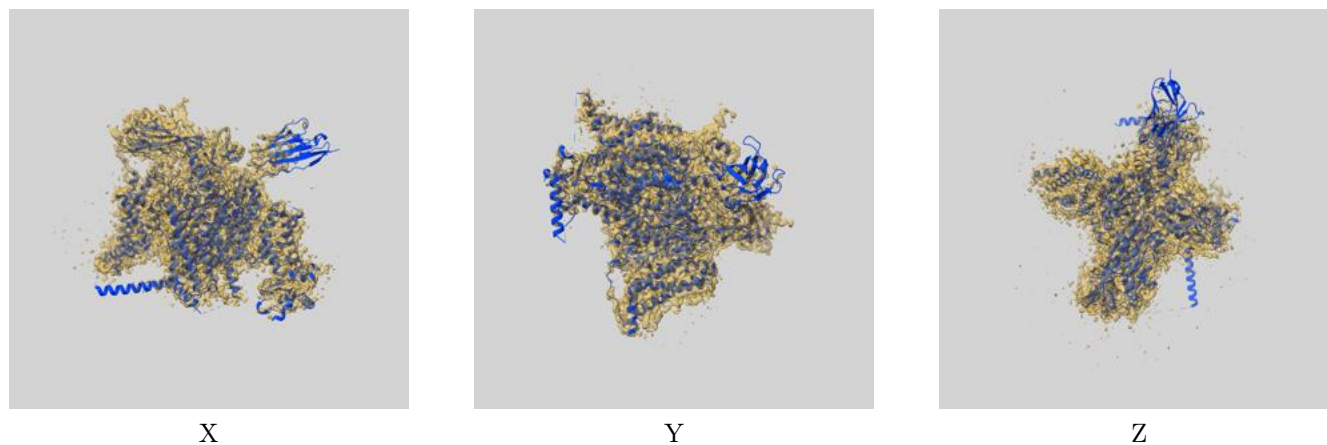
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.73	3.19	2.82
Unmasked-calculated*	3.46	4.11	3.57

\*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 3.46 differs from the reported value 2.7 by more than 10 %

## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-41262 and PDB model 8THH. Per-residue inclusion information can be found in section 3 on page 10.

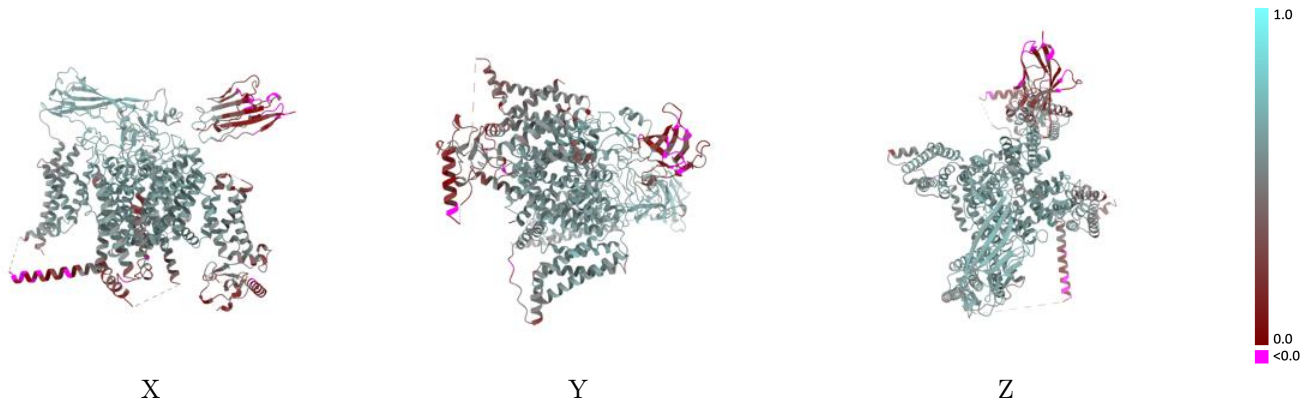
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.15 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.

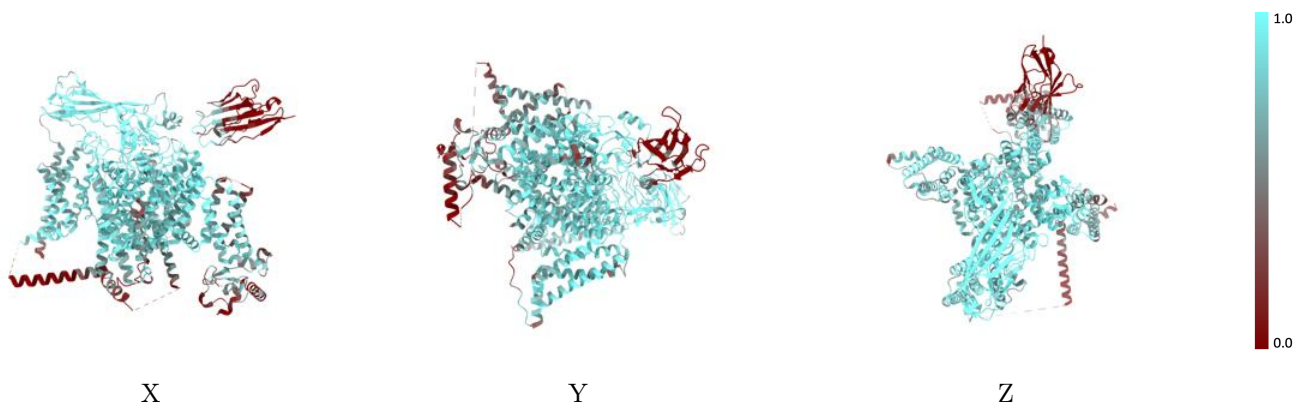


## 9.2 Q-score mapped to coordinate model [\(i\)](#)



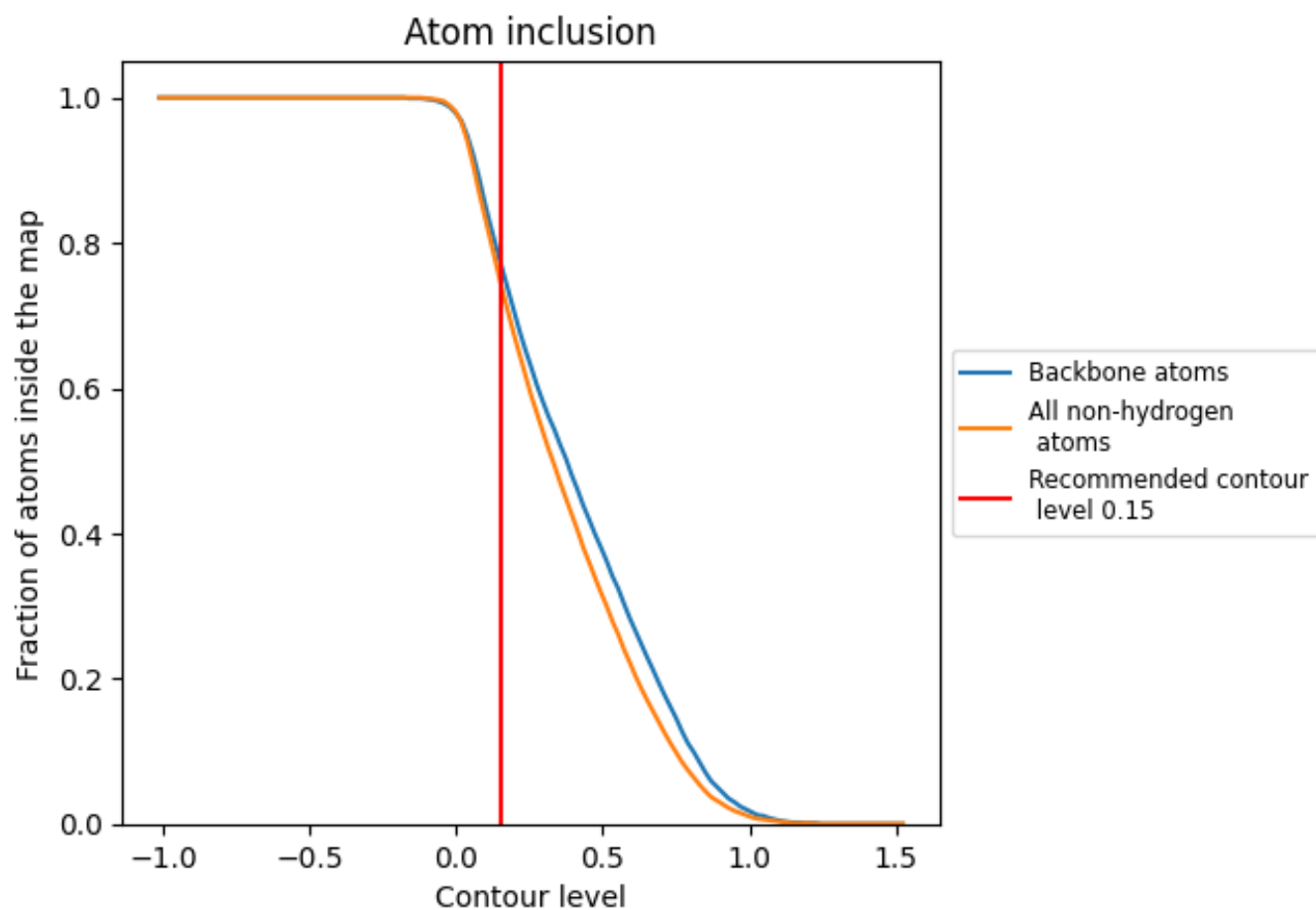
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).















## 9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 75% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7470	 0.5110
A	 0.7800	 0.5260
B	 0.8480	 0.5730
C	 0.2210	 0.2510
D	 0.6430	 0.4500
E	 0.8210	 0.5450
F	 0.9640	 0.5650

