



Full wwPDB EM Validation Report ⓘ

Apr 6, 2026 – 03:33 AM UTC

PDB ID : 21TQ / pdb_000021tq
EMDB ID : EMD-67991
Title : The structure of Nav1.7 with veratridine standing near the IFM motif (site I)
Authors : Fan, X.; Huang, J.; Yan, N.
Deposited on : 2025-12-24
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

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:

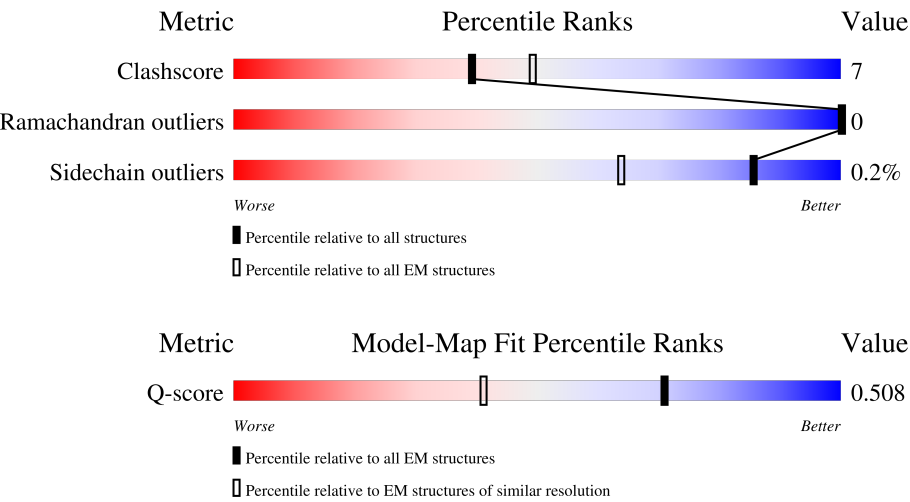
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10327 (2.20 - 3.20)

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	B	173	
2	C	119	
3	A	1988	
4	D	2	

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Mol	Chain	Length	Quality of chain
4	E	2	 100%

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 13098 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 regulatory subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	173	Total	C	N	O	S	0	0
			1417	902	232	273	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	119	Total	C	N	O	S	0	0
			975	611	172	181	11		

- Molecule 3 is a protein called Sodium channel protein type 9 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	1246	Total	C	N	O	S	0	0
			10041	6664	1578	1722	77		

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



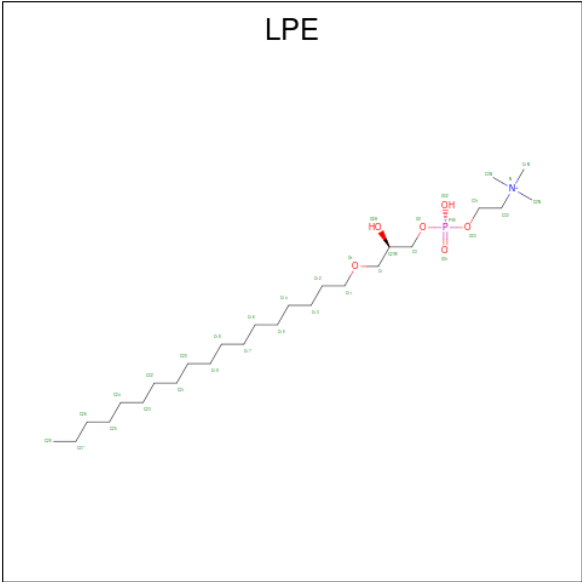
Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



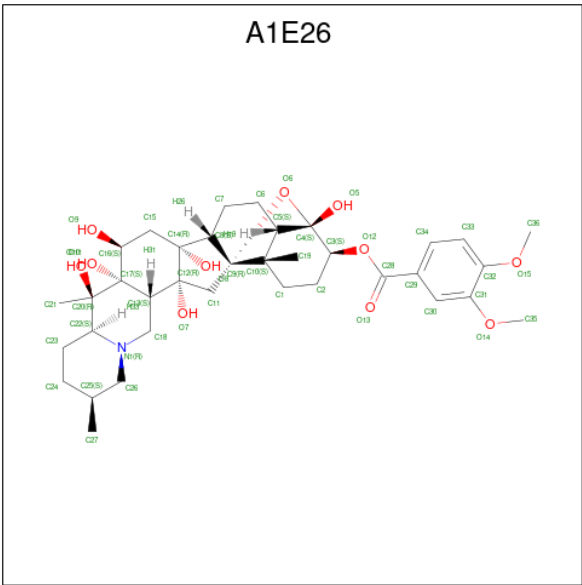
Mol	Chain	Residues	Atoms				AltConf
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 6 is 1-O-OCTADECYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: LPE) (formula: $C_{26}H_{57}NO_6P$).



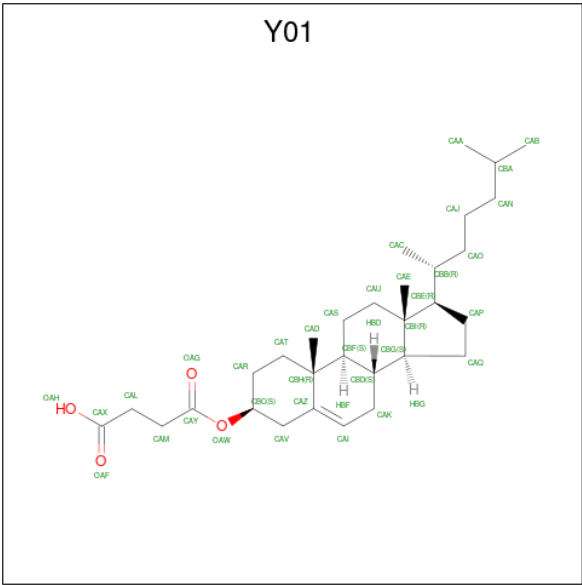
Mol	Chain	Residues	Atoms					AltConf
6	B	1	Total	C	N	O	P	0
			17	9	1	6	1	
6	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
6	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
6	A	1	Total	C	N	O	P	0
			22	14	1	6	1	
6	A	1	Total	C	N	O	P	0
			28	20	1	6	1	
6	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
6	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
6	A	1	Total	C	N	O	P	0
			25	17	1	6	1	

- Molecule 7 is Veratridine (CCD ID: A1E26) (formula: C₃₆H₅₁NO₁₁) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			48	36	1	11	

- Molecule 8 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: C₃₁H₅₀O₄).



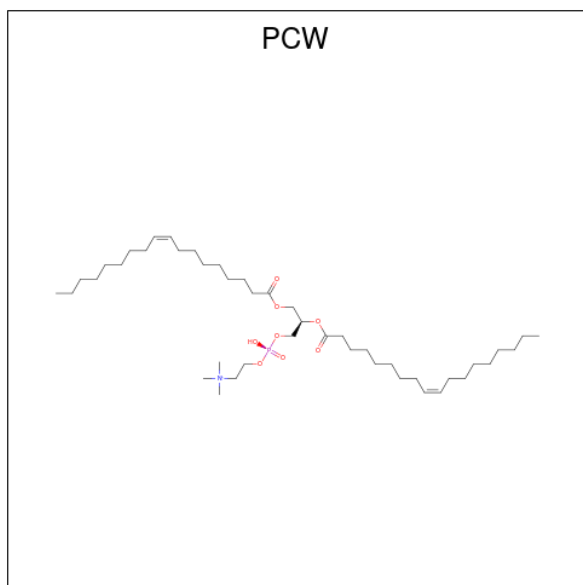
Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total	C	O		0
			35	31	4		
8	A	1	Total	C	O		0
			35	31	4		
8	A	1	Total	C	O		0
			35	31	4		

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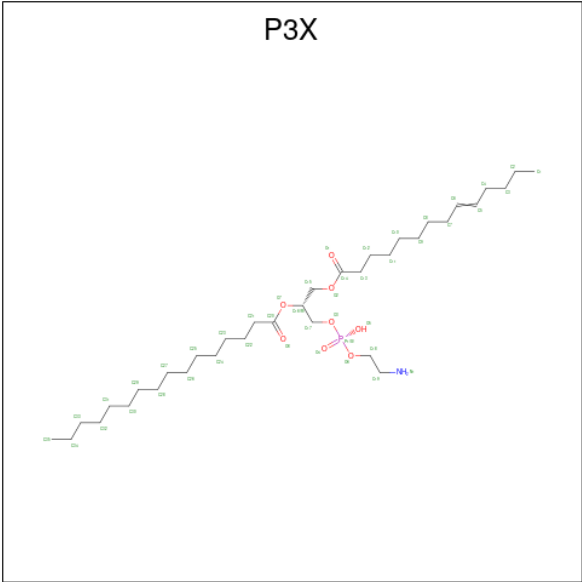
Mol	Chain	Residues	Atoms			AltConf
8	A	1	Total	C	O	0
			35	31	4	

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



Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	N	O	P	0
			53	43	1	8	1	
9	A	1	Total	C	N	O	P	0
			47	37	1	8	1	

- Molecule 10 is (5E,17R,20S)-23-amino-20-hydroxy-14,20-dioxo-15,19,21-trioxa-20lambda 5 -phosphatricos-5-en-17-yl hexadecanoate (CCD ID: P3X) (formula: $C_{35}H_{68}NO_8P$).

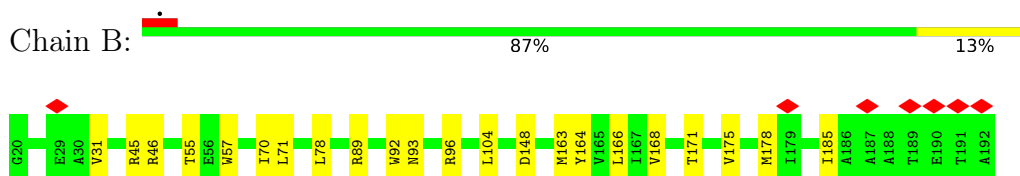


Mol	Chain	Residues	Atoms					AltConf
10	A	1	Total	C	N	O	P	0
			45	35	1	8	1	

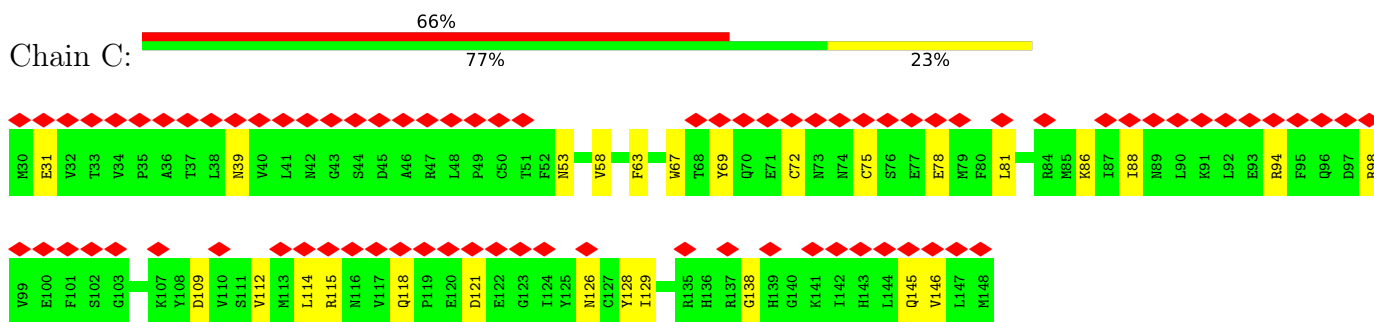
3 Residue-property plots

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.

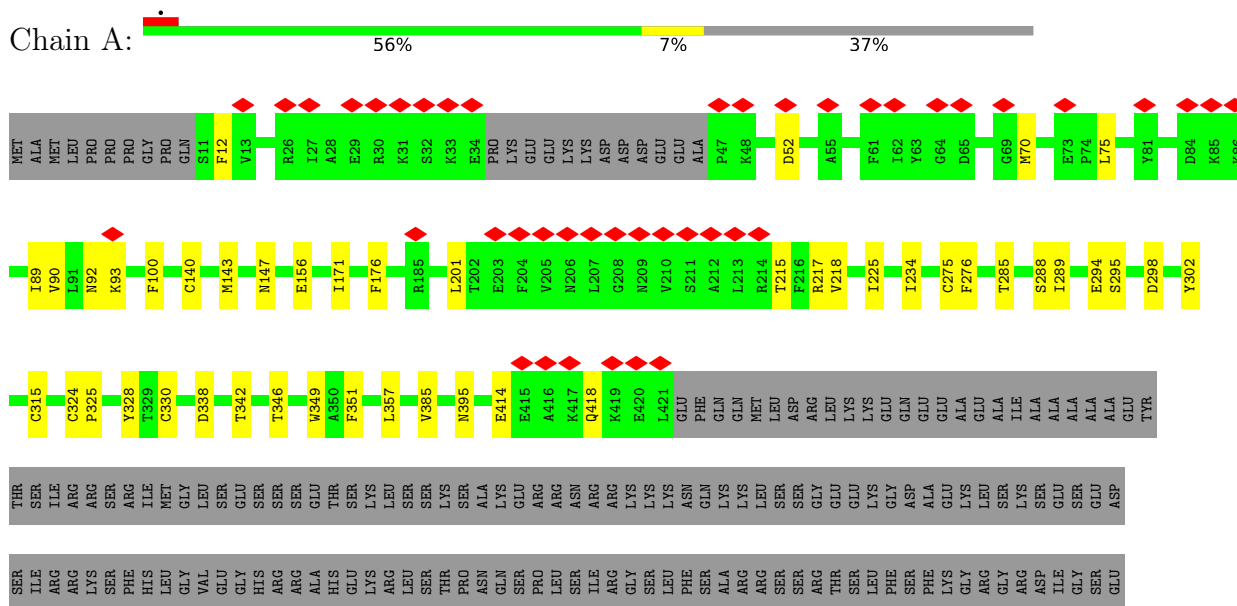
- Molecule 1: Sodium channel regulatory subunit beta-1

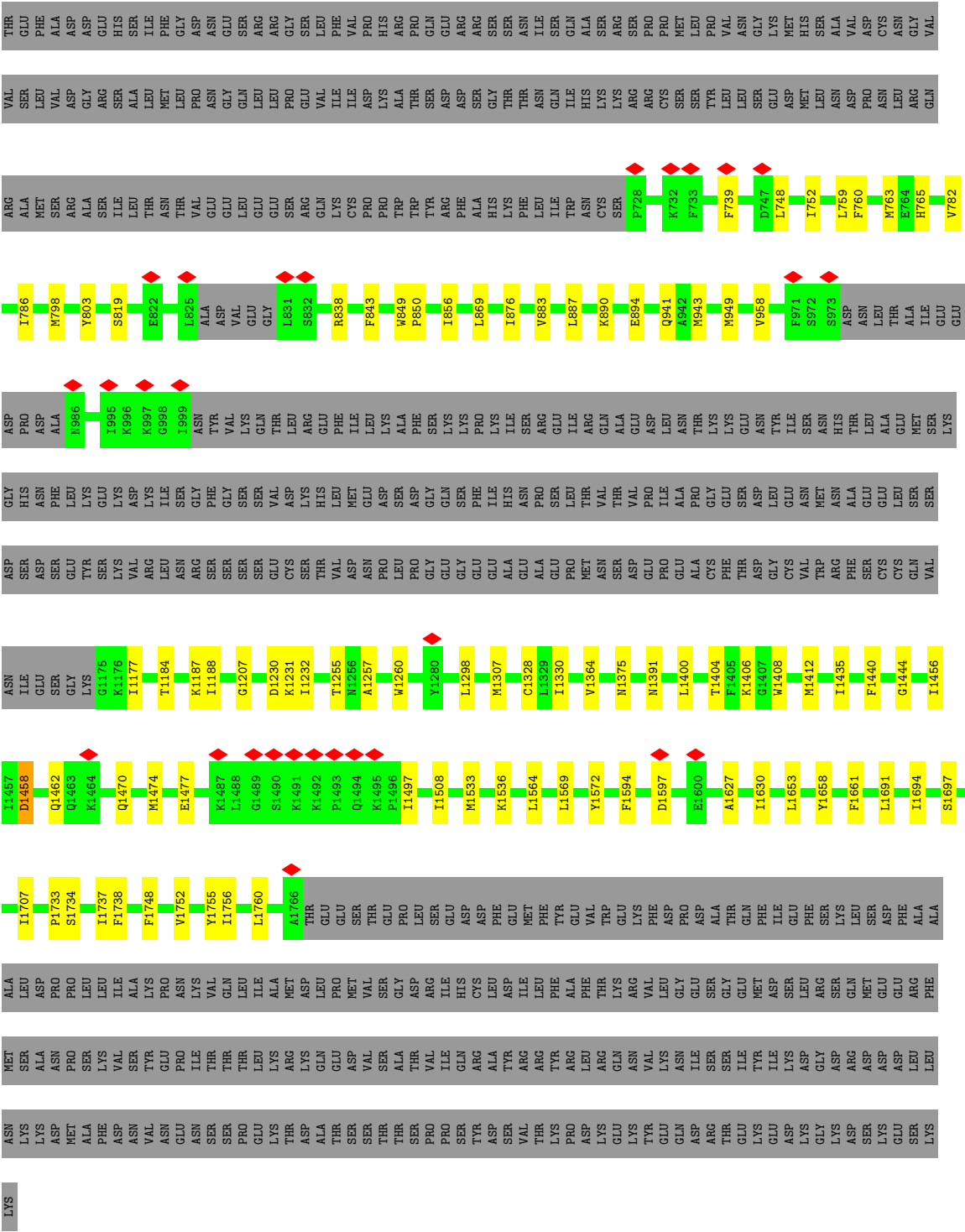


- Molecule 2: Sodium channel regulatory subunit beta-2



- Molecule 3: Sodium channel protein type 9 subunit alpha





● 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

Chain E:

100%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, POINT, POINT, POINT, POINT, POINT, POINT, POINT, POINT, POINT	Depositor
Number of particles used	335177, 335177, 335177, 335177, 335177, 335177, 335177, 335177	Depositor
Resolution determination method	FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION, PHASE FLIPPING AND AMPLITUDE CORRECTION, PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	6.916	Depositor
Minimum map value	-4.583	Depositor
Average map value	-0.006	Depositor
Map value standard deviation	0.135	Depositor
Recommended contour level	0.65	Depositor
Map size (\AA)	356.47998, 356.47998, 356.47998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.114, 1.114, 1.114	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: PCW, LPE, NAG, P3X, Y01, A1E26

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	B	0.14	0/1443	0.28	0/1949
2	C	0.11	0/997	0.27	0/1346
3	A	0.12	0/10285	0.28	0/13930
All	All	0.12	0/12725	0.28	0/17225

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	B	1417	0	1380	25	0
2	C	975	0	937	18	0
3	A	10041	0	10292	145	0
4	D	28	0	25	0	0
4	E	28	0	25	0	0
5	A	42	0	39	0	0
5	B	42	0	39	3	0
6	A	175	0	242	24	0
6	B	17	0	19	4	0
7	A	48	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	140	0	196	30	0
9	A	100	0	143	27	0
10	A	45	0	0	0	0
All	All	13098	0	13337	190	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 7.

All (190) 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)
3:A:349:TRP:CZ2	9:A:2013:PCW:H83	1.78	1.19
3:A:1738:PHE:CE1	6:A:2011:LPE:H3N2	1.85	1.10
3:A:349:TRP:HZ2	9:A:2013:PCW:H83	1.10	1.08
3:A:1738:PHE:HE1	6:A:2011:LPE:H3N2	1.11	1.08
3:A:759:LEU:HD11	8:A:2006:Y01:HAA2	1.29	1.08
3:A:349:TRP:CZ2	9:A:2013:PCW:C8	2.48	0.97
3:A:941:GLN:HE22	9:A:2013:PCW:H52	1.29	0.95
3:A:1330:ILE:HD11	8:A:2006:Y01:HAJ2	1.50	0.93
3:A:1658:TYR:CE1	6:A:2011:LPE:O31	2.25	0.89
3:A:759:LEU:HD11	8:A:2006:Y01:CAA	2.04	0.86
3:A:1328:CYS:SG	9:A:2010:PCW:H283	2.15	0.86
3:A:295:SER:OG	3:A:298:ASP:OD1	1.93	0.86
3:A:849:TRP:HA	8:A:2006:Y01:CAD	2.07	0.84
3:A:1328:CYS:SG	9:A:2010:PCW:C28	2.68	0.82
3:A:941:GLN:NE2	9:A:2013:PCW:H52	1.95	0.79
1:B:89:ARG:HH12	5:B:303:NAG:H81	1.46	0.79
3:A:849:TRP:CD1	8:A:2006:Y01:HAD3	2.20	0.77
3:A:949:MET:HB3	9:A:2013:PCW:H232	1.66	0.76
3:A:414:GLU:O	3:A:418:GLN:NE2	2.21	0.74
3:A:1738:PHE:CE1	6:A:2011:LPE:C3N	2.69	0.73
2:C:78:GLU:OE2	2:C:94:ARG:NH2	2.22	0.73
3:A:1260:TRP:CE3	8:A:2005:Y01:HAE3	2.24	0.73
3:A:1330:ILE:CD1	8:A:2006:Y01:HAJ2	2.18	0.72
3:A:351:PHE:CE2	9:A:2013:PCW:H412	2.24	0.72
1:B:92:TRP:O	1:B:96:ARG:NH2	2.23	0.72
3:A:1391:ASN:HD21	9:A:2010:PCW:H31	1.53	0.72
3:A:1260:TRP:CD2	8:A:2005:Y01:CAE	2.73	0.71
1:B:71:LEU:HD12	1:B:78:LEU:HD11	1.74	0.70
3:A:849:TRP:CE3	8:A:2006:Y01:HAE3	2.27	0.69
3:A:156:GLU:OE2	3:A:217:ARG:NH1	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1260:TRP:CE3	8:A:2005:Y01:CAE	2.76	0.68
3:A:1470:GLN:HA	3:A:1474:MET:HG3	1.74	0.68
3:A:849:TRP:CE3	8:A:2006:Y01:CAE	2.76	0.68
3:A:1404:THR:O	3:A:1406:LYS:NZ	2.25	0.67
3:A:1207:GLY:HA2	6:A:2015:LPE:H112	1.78	0.66
3:A:75:LEU:N	3:A:89:ILE:O	2.28	0.66
3:A:1533:MET:HE1	6:A:2016:LPE:H142	1.78	0.66
3:A:1328:CYS:SG	9:A:2010:PCW:H281	2.38	0.63
2:C:86:LYS:O	2:C:88:ILE:HD12	1.99	0.63
3:A:819:SER:OG	3:A:838:ARG:NH1	2.31	0.62
3:A:1737:ILE:HG21	9:A:2010:PCW:H162	1.82	0.62
3:A:357:LEU:HD23	3:A:385:VAL:HG11	1.81	0.61
3:A:1260:TRP:CD2	8:A:2005:Y01:HAE1	2.35	0.61
3:A:949:MET:CB	9:A:2013:PCW:H20	2.32	0.59
3:A:1658:TYR:CZ	6:A:2011:LPE:O31	2.56	0.59
3:A:351:PHE:CD2	9:A:2013:PCW:H412	2.38	0.58
3:A:1440:PHE:O	3:A:1444:GLY:N	2.34	0.58
2:C:69:TYR:O	2:C:78:GLU:N	2.34	0.58
3:A:887:LEU:HD13	3:A:943:MET:HE2	1.85	0.58
3:A:1477:GLU:N	3:A:1477:GLU:OE1	2.33	0.58
3:A:215:THR:O	3:A:218:VAL:HG12	2.04	0.58
3:A:275:CYS:SG	3:A:315:CYS:SG	3.02	0.58
3:A:798:MET:HE3	3:A:803:TYR:HA	1.85	0.57
3:A:275:CYS:HB3	3:A:328:TYR:HB3	1.85	0.57
1:B:89:ARG:NH1	5:B:303:NAG:H81	2.18	0.57
1:B:178:MET:HG3	6:B:304:LPE:C11	2.34	0.57
2:C:81:LEU:CD2	2:C:112:VAL:HG11	2.35	0.57
2:C:67:TRP:CD1	2:C:81:LEU:HD23	2.40	0.56
3:A:1627:ALA:HB1	3:A:1630:ILE:HD13	1.86	0.56
3:A:1653:LEU:CD1	6:A:2015:LPE:H162	2.36	0.56
3:A:849:TRP:CZ3	8:A:2006:Y01:HAE3	2.41	0.56
3:A:1458:ASP:O	3:A:1462:GLN:HG3	2.07	0.56
3:A:147:ASN:O	3:A:147:ASN:OD1	2.23	0.55
3:A:1400:LEU:HD22	9:A:2010:PCW:H212	1.89	0.55
3:A:1260:TRP:CG	8:A:2005:Y01:HAE1	2.42	0.55
3:A:1207:GLY:CA	6:A:2015:LPE:H112	2.37	0.54
2:C:31:GLU:OE2	2:C:53:ASN:ND2	2.40	0.54
3:A:1230:ASP:OD1	3:A:1231:LYS:N	2.41	0.54
3:A:1298:LEU:HD21	6:A:2011:LPE:H21	1.90	0.54
2:C:72:CYS:SG	2:C:75:CYS:N	2.81	0.53
3:A:1257:ALA:HB1	6:A:2012:LPE:O3	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1406:LYS:HG3	3:A:1700:TRP:HD1	1.73	0.53
3:A:1260:TRP:CD2	8:A:2005:Y01:HAE3	2.42	0.53
3:A:92:ASN:OD1	3:A:93:LYS:N	2.42	0.53
2:C:98:ARG:HH12	2:C:114:LEU:HD11	1.74	0.52
3:A:1364:VAL:O	3:A:1364:VAL:HG23	2.08	0.52
3:A:849:TRP:HA	8:A:2006:Y01:HAD1	1.90	0.52
3:A:748:LEU:O	3:A:752:ILE:HD12	2.09	0.52
3:A:782:VAL:O	3:A:786:ILE:HD12	2.10	0.52
1:B:185:ILE:HD11	3:A:1187:LYS:HD2	1.92	0.51
3:A:276:PHE:CE1	3:A:302:TYR:HB3	2.45	0.51
1:B:70:ILE:HG13	1:B:71:LEU:HD23	1.92	0.51
3:A:1661:PHE:CD2	6:A:2011:LPE:H311	2.46	0.51
3:A:285:THR:O	3:A:289:ILE:HD12	2.11	0.51
3:A:1738:PHE:CD1	6:A:2011:LPE:C3N	2.94	0.51
3:A:1406:LYS:HG3	3:A:1700:TRP:CD1	2.46	0.50
2:C:98:ARG:NH1	2:C:114:LEU:HD11	2.26	0.50
1:B:178:MET:HB3	6:B:304:LPE:C11	2.42	0.50
3:A:275:CYS:HA	3:A:330:CYS:HA	1.94	0.50
3:A:338:ASP:OD2	3:A:342:THR:OG1	2.20	0.50
3:A:876:ILE:CD1	3:A:958:VAL:HG21	2.42	0.50
3:A:218:VAL:HG11	3:A:883:VAL:HG22	1.94	0.49
3:A:849:TRP:CD2	8:A:2006:Y01:CAE	2.95	0.49
3:A:1691:LEU:HD23	3:A:1694:ILE:HD11	1.94	0.49
3:A:1391:ASN:ND2	9:A:2010:PCW:H31	2.26	0.49
3:A:1477:GLU:H	3:A:1477:GLU:CD	2.20	0.49
1:B:55:THR:CG2	1:B:104:LEU:HD12	2.43	0.48
3:A:1738:PHE:CD1	6:A:2011:LPE:H3N2	2.44	0.48
3:A:1257:ALA:CB	6:A:2012:LPE:O3	2.61	0.48
3:A:1435:ILE:HD13	8:A:2007:Y01:HAU1	1.94	0.48
3:A:1756:ILE:O	3:A:1760:LEU:HD13	2.13	0.48
3:A:1257:ALA:HB1	6:A:2012:LPE:C3	2.44	0.48
1:B:55:THR:HG21	1:B:104:LEU:HD12	1.96	0.48
3:A:1497:ILE:HD13	3:A:1569:LEU:HD22	1.96	0.48
8:A:2007:Y01:HAP1	8:A:2007:Y01:HAO2	1.65	0.48
1:B:166:LEU:HD23	3:A:1232:ILE:HD13	1.95	0.48
3:A:276:PHE:HE1	3:A:302:TYR:HB3	1.79	0.48
3:A:1391:ASN:HD21	9:A:2010:PCW:C3	2.24	0.47
3:A:1733:PRO:HG2	6:A:2009:LPE:H311	1.96	0.47
3:A:1307:MET:HE1	3:A:1653:LEU:HD22	1.96	0.47
2:C:129:ILE:HD12	2:C:138:GLY:O	2.15	0.47
3:A:324:CYS:HB2	3:A:325:PRO:CD	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:2010:PCW:H242	9:A:2010:PCW:H272	1.38	0.47
8:A:2017:Y01:HAB3	8:A:2017:Y01:HAJ2	1.75	0.47
3:A:1406:LYS:HE2	3:A:1697:SER:O	2.14	0.47
3:A:351:PHE:CZ	9:A:2013:PCW:H412	2.50	0.46
2:C:58:VAL:HG13	2:C:63:PHE:CD2	2.50	0.46
6:A:2011:LPE:H142	6:A:2011:LPE:H112	1.35	0.46
2:C:109:ASP:OD1	2:C:109:ASP:O	2.34	0.46
3:A:849:TRP:CG	8:A:2006:Y01:HAD3	2.50	0.46
1:B:57:TRP:HB2	1:B:71:LEU:HD23	1.96	0.46
3:A:887:LEU:HD13	3:A:943:MET:CE	2.45	0.46
3:A:843:PHE:CD1	3:A:856:ILE:HD11	2.50	0.46
3:A:234:ILE:HG23	3:A:869:LEU:HD23	1.98	0.46
3:A:1661:PHE:CG	6:A:2011:LPE:H2N3	2.51	0.46
3:A:294:GLU:N	3:A:294:GLU:OE1	2.48	0.45
3:A:1497:ILE:HD11	3:A:1572:TYR:HB2	1.98	0.45
1:B:178:MET:CG	6:B:304:LPE:C11	2.95	0.45
3:A:218:VAL:HG21	3:A:883:VAL:HG23	1.98	0.45
3:A:1594:PHE:O	3:A:1597:ASP:OD1	2.35	0.45
6:A:2009:LPE:H21	9:A:2010:PCW:H131	1.98	0.45
3:A:849:TRP:HA	8:A:2006:Y01:HAD3	1.96	0.44
3:A:949:MET:CB	9:A:2013:PCW:H232	2.40	0.44
1:B:163:MET:HE1	3:A:1231:LYS:CB	2.47	0.44
3:A:1177:ILE:H	3:A:1177:ILE:HD12	1.82	0.44
3:A:1733:PRO:HG2	6:A:2009:LPE:C31	2.48	0.44
2:C:118:GLN:O	2:C:146:VAL:HG21	2.17	0.44
3:A:1456:ILE:HG12	7:A:2004:A1E26:C32	2.48	0.44
3:A:52:ASP:N	3:A:52:ASP:OD1	2.51	0.44
3:A:949:MET:HG3	9:A:2013:PCW:H20	2.00	0.44
3:A:1408:TRP:HE3	3:A:1412:MET:SD	2.41	0.44
3:A:346:THR:HG22	3:A:1536:LYS:HB2	1.99	0.44
3:A:849:TRP:CD2	8:A:2006:Y01:HAE3	2.53	0.44
3:A:890:LYS:O	3:A:894:GLU:OE1	2.36	0.43
3:A:876:ILE:HD13	3:A:958:VAL:HG21	2.00	0.43
1:B:55:THR:HB	1:B:104:LEU:HD12	2.00	0.43
3:A:850:PRO:HD2	8:A:2006:Y01:HAD1	2.00	0.43
2:C:39:ASN:O	2:C:39:ASN:OD1	2.35	0.43
3:A:225:ILE:H	3:A:225:ILE:HD12	1.83	0.43
3:A:752:ILE:HD12	3:A:752:ILE:H	1.83	0.43
3:A:1257:ALA:HB1	6:A:2012:LPE:H31	2.00	0.43
3:A:90:VAL:HG22	3:A:100:PHE:HE1	1.83	0.43
3:A:285:THR:O	3:A:288:SER:N	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:765:HIS:CD2	8:A:2017:Y01:HAL2	2.54	0.43
8:A:2007:Y01:HAB1	8:A:2007:Y01:HAJ2	1.92	0.42
1:B:96:ARG:NH1	5:B:301:NAG:O7	2.47	0.42
1:B:178:MET:CB	6:B:304:LPE:C11	2.98	0.42
3:A:1707:ILE:HG22	3:A:1707:ILE:O	2.18	0.42
1:B:31:VAL:HG13	1:B:148:ASP:O	2.20	0.42
3:A:1508:ILE:HG23	3:A:1564:LEU:HD11	2.01	0.42
1:B:164:TYR:O	1:B:168:VAL:HG23	2.20	0.42
2:C:118:GLN:NE2	2:C:121:ASP:OD2	2.53	0.42
1:B:185:ILE:HD12	3:A:1184:THR:HG22	2.02	0.42
3:A:201:LEU:C	3:A:201:LEU:HD23	2.45	0.42
3:A:949:MET:HB2	9:A:2013:PCW:H20	2.01	0.42
9:A:2013:PCW:H322	9:A:2013:PCW:H122	2.00	0.42
1:B:45:ARG:NH2	3:A:325:PRO:O	2.52	0.41
3:A:140:CYS:HA	3:A:143:MET:HE3	2.01	0.41
3:A:739:PHE:CD1	3:A:739:PHE:C	2.99	0.41
3:A:760:PHE:HA	3:A:763:MET:HE2	2.02	0.41
2:C:126:ASN:HB3	2:C:128:TYR:HE1	1.85	0.41
3:A:1255:THR:HB	8:A:2005:Y01:HAL2	2.02	0.41
1:B:46:ARG:HD2	3:A:324:CYS:HA	2.03	0.41
3:A:349:TRP:HZ2	9:A:2013:PCW:C8	1.96	0.41
2:C:98:ARG:NH2	2:C:115:ARG:O	2.52	0.41
3:A:12:PHE:HB3	3:A:70:MET:SD	2.61	0.41
3:A:171:ILE:CD1	3:A:176:PHE:CE1	3.03	0.41
3:A:1748:PHE:O	3:A:1752:VAL:HG23	2.21	0.41
9:A:2010:PCW:H122	9:A:2010:PCW:H152	1.84	0.41
1:B:163:MET:HE1	3:A:1231:LYS:HB3	2.03	0.40
1:B:178:MET:HE1	3:A:1188:ILE:CD1	2.51	0.40
2:C:145:GLN:OE1	2:C:145:GLN:N	2.55	0.40
3:A:849:TRP:CD2	8:A:2006:Y01:HAE1	2.56	0.40
8:A:2017:Y01:HAP1	8:A:2017:Y01:HAO2	1.54	0.40
3:A:1734:SER:OG	6:A:2009:LPE:H32	2.22	0.40
9:A:2013:PCW:C43	6:A:2016:LPE:H141	2.52	0.40
1:B:171:THR:O	1:B:175:VAL:HG23	2.21	0.40
3:A:289:ILE:HD12	3:A:289:ILE:H	1.86	0.40
3:A:395:ASN:OD1	3:A:1755:TYR:CD1	2.75	0.40
3:A:1260:TRP:CZ3	8:A:2005:Y01:HAE3	2.56	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	B	171/173 (99%)	171 (100%)	0	0	100	100
2	C	117/119 (98%)	115 (98%)	2 (2%)	0	100	100
3	A	1234/1988 (62%)	1216 (98%)	18 (2%)	0	100	100
All	All	1522/2280 (67%)	1502 (99%)	20 (1%)	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	B	157/157 (100%)	156 (99%)	1 (1%)	78	91
2	C	112/112 (100%)	112 (100%)	0	100	100
3	A	1111/1778 (62%)	1109 (100%)	2 (0%)	87	95
All	All	1380/2047 (67%)	1377 (100%)	3 (0%)	85	95

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

Mol	Chain	Res	Type
1	B	93	ASN
3	A	1375	ASN
3	A	1458	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13)

such sidechains are listed below:

Mol	Chain	Res	Type
2	C	53	ASN
2	C	96	GLN
2	C	131	ASN
3	A	240	GLN
3	A	336	ASN
3	A	941	GLN
3	A	1379	ASN
3	A	1463	GLN
3	A	1502	ASN
3	A	1505	GLN
3	A	1551	ASN
3	A	1753	ASN
3	A	1762	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

4 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	0.24	0	17,19,21	0.55	0
4	NAG	D	2	4	14,14,15	0.24	0	17,19,21	0.39	0
4	NAG	E	1	3,4	14,14,15	0.36	0	17,19,21	0.47	0
4	NAG	E	2	4	14,14,15	0.50	0	17,19,21	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
4	NAG	D	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	NAG	E	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

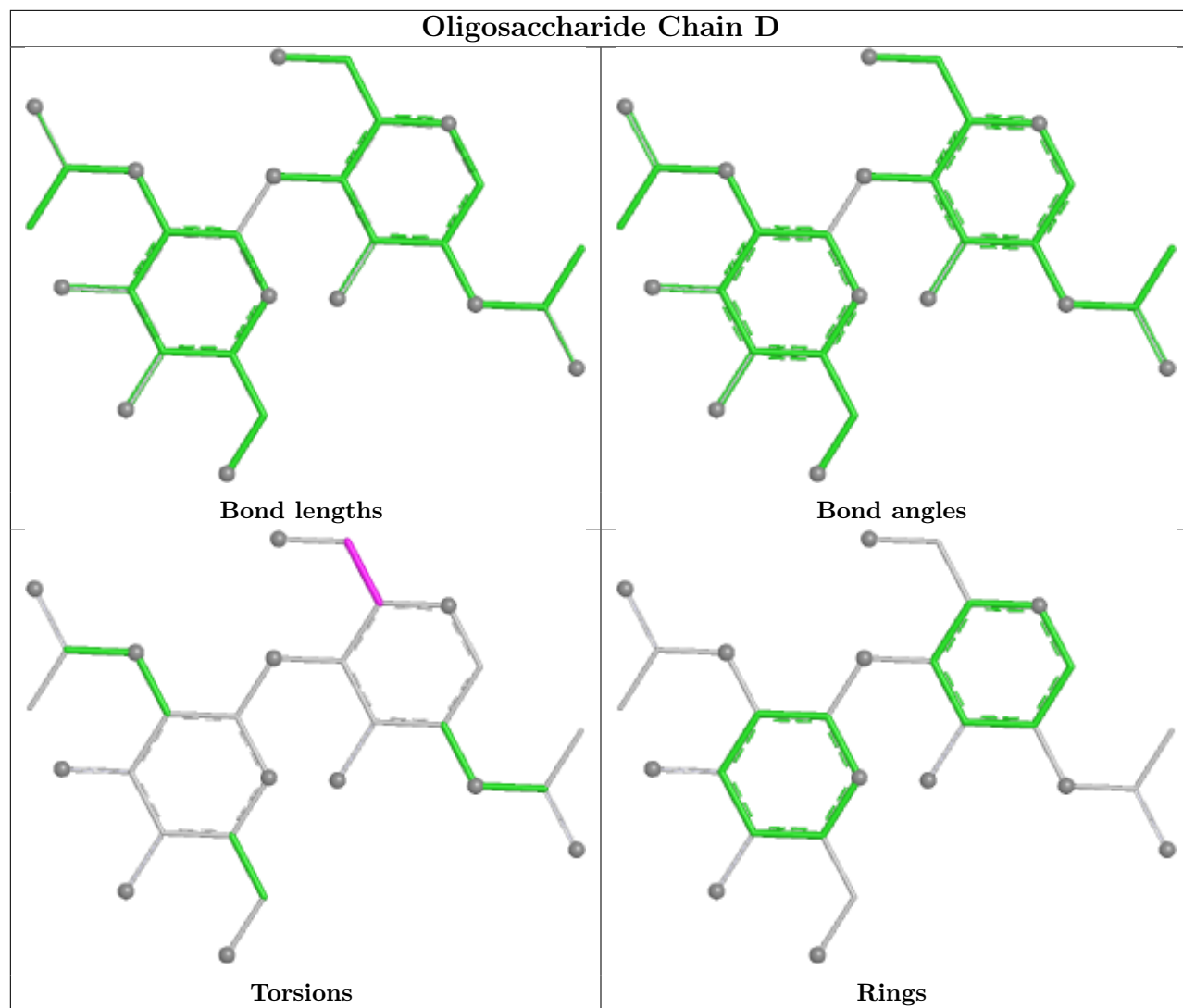
All (4) torsion outliers are listed below:

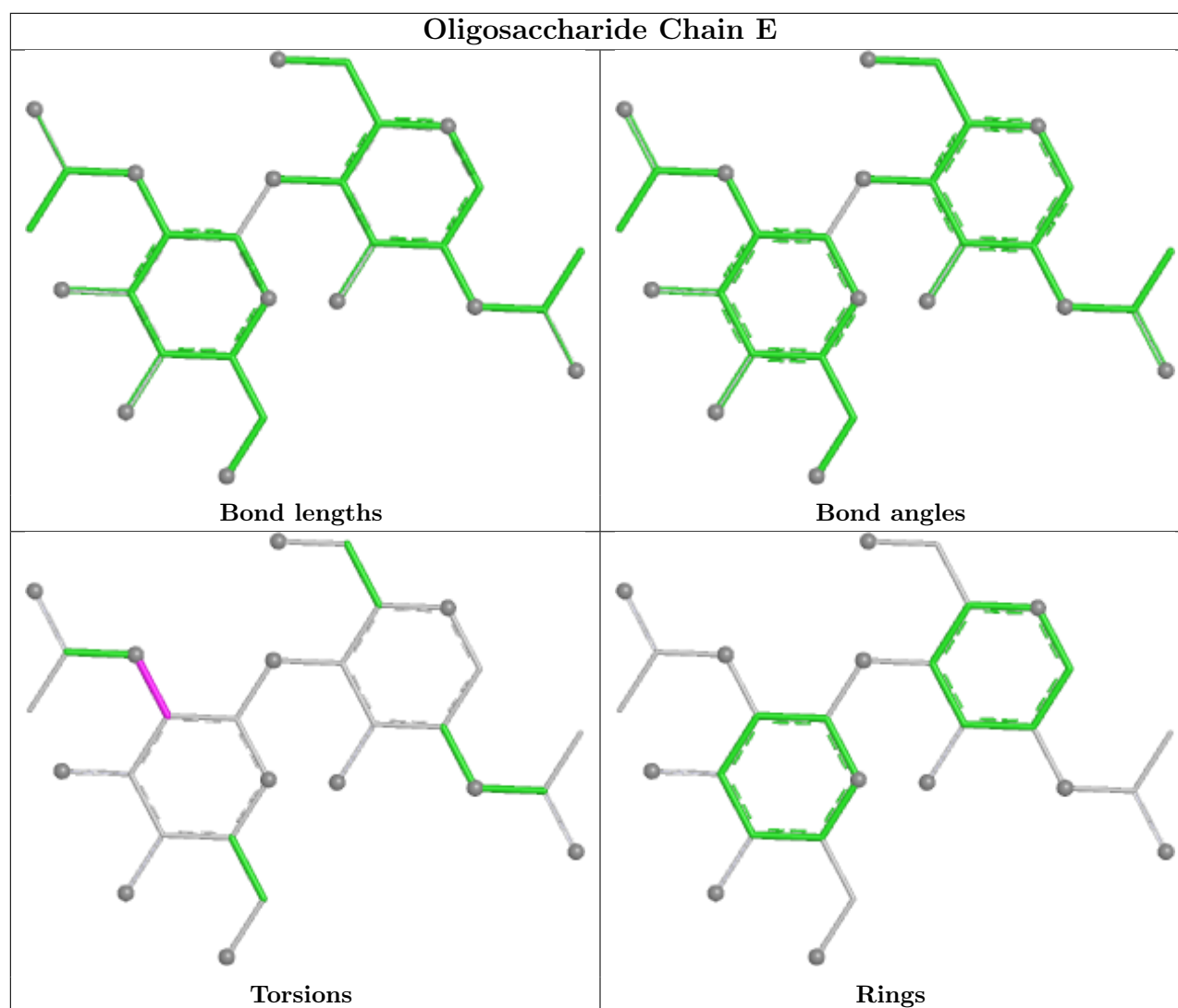
Mol	Chain	Res	Type	Atoms
4	D	1	NAG	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
4	E	2	NAG	C1-C2-N2-C7
4	E	2	NAG	C3-C2-N2-C7

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](#)

22 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	$\# Z > 2$
9	PCW	A	2010	-	52,52,53	0.38	0	58,60,61	0.40	0
6	LPE	A	2015	-	24,24,33	0.30	0	28,30,39	0.40	0
6	LPE	A	2009	-	24,24,33	0.32	0	25,27,39	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	LPE	A	2012	-	27,27,33	0.27	0	31,33,39	0.36	0
5	NAG	A	2003	3	14,14,15	0.21	0	17,19,21	0.41	0
8	Y01	A	2007	-	38,38,38	0.48	0	57,57,57	0.50	0
6	LPE	B	304	-	16,16,33	0.35	0	20,22,39	0.41	0
5	NAG	B	301	1	14,14,15	0.15	0	17,19,21	0.46	0
5	NAG	A	2001	3	14,14,15	0.26	0	17,19,21	0.57	0
6	LPE	A	2008	-	24,24,33	0.31	0	28,30,39	0.35	0
5	NAG	A	2002	3	14,14,15	0.22	0	17,19,21	0.49	0
9	PCW	A	2013	-	46,46,53	0.35	0	52,54,61	0.36	0
7	A1E26	A	2004	-	51,55,55	0.90	3 (5%)	63,95,95	0.80	3 (4%)
5	NAG	B	303	1	14,14,15	0.33	0	17,19,21	0.45	0
8	Y01	A	2006	-	38,38,38	0.50	0	57,57,57	0.73	0
6	LPE	A	2014	-	24,24,33	0.30	0	28,30,39	0.40	0
8	Y01	A	2017	-	38,38,38	0.48	0	57,57,57	0.52	0
6	LPE	A	2011	-	21,21,33	0.34	0	25,27,39	0.39	0
8	Y01	A	2005	-	38,38,38	0.47	0	57,57,57	0.62	0
10	P3X	A	2018	-	44,44,44	1.08	5 (11%)	47,49,49	1.31	4 (8%)
5	NAG	B	302	1	14,14,15	0.24	0	17,19,21	0.44	0
6	LPE	A	2016	-	24,24,33	0.29	0	28,30,39	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
9	PCW	A	2010	-	-	26/56/56/57	-
6	LPE	A	2015	-	-	16/25/25/34	-
6	LPE	A	2009	-	-	4/25/25/34	-
6	LPE	A	2012	-	-	4/28/28/34	-
5	NAG	A	2003	3	-	0/6/23/26	0/1/1/1
8	Y01	A	2007	-	-	15/19/77/77	0/4/4/4
6	LPE	B	304	-	-	10/17/17/34	-
5	NAG	B	301	1	-	2/6/23/26	0/1/1/1
5	NAG	A	2001	3	-	0/6/23/26	0/1/1/1
6	LPE	A	2008	-	-	17/25/25/34	-
5	NAG	A	2002	3	-	0/6/23/26	0/1/1/1
9	PCW	A	2013	-	-	35/50/50/57	-
7	A1E26	A	2004	-	-	1/12/138/138	0/1/8/8
5	NAG	B	303	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	Y01	A	2006	-	-	8/19/77/77	0/4/4/4
6	LPE	A	2014	-	-	12/25/25/34	-
8	Y01	A	2017	-	-	11/19/77/77	0/4/4/4
6	LPE	A	2011	-	-	16/22/22/34	-
8	Y01	A	2005	-	-	15/19/77/77	0/4/4/4
10	P3X	A	2018	-	-	24/48/48/48	-
5	NAG	B	302	1	-	0/6/23/26	0/1/1/1
6	LPE	A	2016	-	-	15/25/25/34	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2004	A1E26	C22-N1	4.06	1.52	1.48
10	A	2018	P3X	C6-C5	3.67	1.52	1.31
7	A	2004	A1E26	C17-C20	-3.50	1.52	1.57
7	A	2004	A1E26	C26-N1	2.54	1.51	1.47
10	A	2018	P3X	O7-C16	-2.52	1.40	1.46
10	A	2018	P3X	O2-C15	-2.46	1.39	1.45
10	A	2018	P3X	O2-C14	2.10	1.39	1.33
10	A	2018	P3X	O7-C20	2.08	1.40	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	2018	P3X	O7-C20-C21	5.27	122.89	111.48
10	A	2018	P3X	O2-C14-C13	3.53	122.60	111.83
10	A	2018	P3X	C17-C16-C15	-2.83	105.18	111.78
7	A	2004	A1E26	C26-N1-C18	2.69	112.44	108.69
7	A	2004	A1E26	C20-C22-N1	2.64	107.89	105.41
7	A	2004	A1E26	O8-C14-C12	-2.45	104.29	110.47
10	A	2018	P3X	O2-C14-O1	-2.17	118.19	123.63

There are no chirality outliers.

All (232) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	304	LPE	O1-C1-C2-O2H
6	B	304	LPE	O2H-C2-C3-O3
6	B	304	LPE	C3-O3-P-O32
6	B	304	LPE	C3-O3-P-O33

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Mol	Chain	Res	Type	Atoms
6	A	2008	LPE	C3-O3-P-O31
6	A	2008	LPE	C31-O33-P-O3
6	A	2008	LPE	C31-O33-P-O31
6	A	2008	LPE	C31-O33-P-O32
6	A	2008	LPE	O33-C31-C32-N
6	A	2009	LPE	C31-O33-P-O31
6	A	2009	LPE	C32-C31-O33-P
6	A	2011	LPE	O1-C1-C2-O2H
6	A	2011	LPE	O1-C1-C2-C3
6	A	2011	LPE	C1-C2-C3-O3
6	A	2011	LPE	C3-O3-P-O31
6	A	2011	LPE	C3-O3-P-O32
6	A	2011	LPE	C3-O3-P-O33
6	A	2011	LPE	C31-O33-P-O3
6	A	2011	LPE	C31-O33-P-O32
6	A	2014	LPE	O1-C1-C2-O2H
6	A	2014	LPE	C3-O3-P-O33
6	A	2014	LPE	C31-O33-P-O3
6	A	2014	LPE	C31-O33-P-O32
6	A	2015	LPE	C1-C2-C3-O3
6	A	2015	LPE	C31-O33-P-O31
6	A	2015	LPE	C32-C31-O33-P
6	A	2015	LPE	O33-C31-C32-N
6	A	2016	LPE	C1-C2-C3-O3
6	A	2016	LPE	O2H-C2-C3-O3
6	A	2016	LPE	C3-O3-P-O31
6	A	2016	LPE	C31-O33-P-O3
6	A	2016	LPE	C31-O33-P-O31
6	A	2016	LPE	O33-C31-C32-N
8	A	2005	Y01	CAV-CBC-OAW-CAY
8	A	2005	Y01	CAM-CAY-OAW-CBC
8	A	2007	Y01	CAX-CAL-CAM-CAY
8	A	2017	Y01	CAC-CBB-CBE-CBI
9	A	2010	PCW	O3P-C1-C2-O2
9	A	2010	PCW	C32-C31-O2-C2
9	A	2010	PCW	O31-C31-O2-C2
9	A	2010	PCW	C4-O4P-P-O2P
9	A	2013	PCW	C40-C41-C42-C43
9	A	2013	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

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Mol	Chain	Res	Type	Atoms
10	A	2018	P3X	C21-C20-O7-C16
10	A	2018	P3X	C17-O3-P1-O5
10	A	2018	P3X	O1-C14-O2-C15
8	A	2007	Y01	CAV-CBC-OAW-CAY
8	A	2005	Y01	OAG-CAY-OAW-CBC
10	A	2018	P3X	C13-C14-O2-C15
6	A	2011	LPE	C11-C12-C13-C14
8	A	2017	Y01	CAC-CBB-CBE-CAP
8	A	2017	Y01	CAO-CBB-CBE-CAP
8	A	2017	Y01	CAO-CBB-CBE-CBI
9	A	2010	PCW	C18-C19-C20-C21
10	A	2018	P3X	O8-C20-O7-C16
6	A	2016	LPE	C31-C32-N-C2N
6	A	2011	LPE	O2H-C2-C3-O3
9	A	2013	PCW	C12-C11-O3-C3
10	A	2018	P3X	C26-C27-C28-C29
8	A	2005	Y01	CAJ-CAO-CBB-CBE
9	A	2013	PCW	O11-C11-O3-C3
8	A	2007	Y01	CAJ-CAO-CBB-CAC
8	A	2007	Y01	CAJ-CAO-CBB-CBE
6	B	304	LPE	C1-C2-C3-O3
9	A	2010	PCW	C12-C13-C14-C15
10	A	2018	P3X	C24-C25-C26-C27
6	A	2008	LPE	C31-C32-N-C2N
6	A	2014	LPE	C31-C32-N-C3N
8	A	2007	Y01	CAO-CBB-CBE-CBI
8	A	2017	Y01	CAJ-CAO-CBB-CBE
9	A	2010	PCW	C24-C25-C26-C27
6	A	2015	LPE	O2H-C2-C3-O3
6	A	2008	LPE	O1-C1-C2-O2H
10	A	2018	P3X	C28-C29-C30-C31
8	A	2005	Y01	CAJ-CAO-CBB-CAC
9	A	2010	PCW	C14-C15-C16-C17
8	A	2006	Y01	CAJ-CAO-CBB-CBE
6	A	2016	LPE	O1-C11-C12-C13
6	A	2015	LPE	C31-C32-N-C3N
8	A	2006	Y01	CAJ-CAO-CBB-CAC
8	A	2005	Y01	CAO-CAJ-CAN-CBA
8	A	2017	Y01	CAO-CAJ-CAN-CBA
9	A	2010	PCW	C31-C32-C33-C34
8	A	2007	Y01	CAC-CBB-CBE-CBI
6	A	2008	LPE	O1-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
9	A	2010	PCW	C12-C11-O3-C3
8	A	2007	Y01	CAO-CAJ-CAN-CBA
6	B	304	LPE	C31-C32-N-C1N
6	B	304	LPE	C31-C32-N-C2N
6	B	304	LPE	C31-C32-N-C3N
6	A	2008	LPE	C31-C32-N-C3N
6	A	2014	LPE	C31-C32-N-C1N
6	A	2016	LPE	C31-C32-N-C3N
6	A	2011	LPE	O1-C11-C12-C13
6	A	2014	LPE	O1-C1-C2-C3
9	A	2013	PCW	C38-C39-C40-C41
8	A	2006	Y01	CAJ-CAN-CBA-CAA
9	A	2010	PCW	O11-C11-O3-C3
9	A	2013	PCW	C32-C31-O2-C2
6	A	2008	LPE	C31-C32-N-C1N
6	A	2016	LPE	C31-C32-N-C1N
8	A	2006	Y01	CAJ-CAN-CBA-CAB
6	A	2015	LPE	C13-C14-C15-C16
6	A	2015	LPE	C11-C12-C13-C14
6	A	2014	LPE	C14-C15-C16-C17
9	A	2010	PCW	C15-C16-C17-C18
9	A	2013	PCW	O31-C31-O2-C2
8	A	2007	Y01	CAC-CBB-CBE-CAP
10	A	2018	P3X	C21-C22-C23-C24
6	A	2008	LPE	C13-C14-C15-C16
6	A	2016	LPE	C15-C16-C17-C18
6	A	2014	LPE	C31-C32-N-C2N
6	A	2015	LPE	C31-C32-N-C2N
10	A	2018	P3X	C10-C11-C12-C13
6	A	2008	LPE	C15-C16-C17-C18
9	A	2010	PCW	C23-C24-C25-C26
6	A	2016	LPE	C11-C12-C13-C14
6	A	2008	LPE	C14-C15-C16-C17
9	A	2010	PCW	C42-C43-C44-C45
9	A	2013	PCW	C35-C36-C37-C38
10	A	2018	P3X	C9-C10-C11-C12
8	A	2006	Y01	CAM-CAY-OAW-CBC
8	A	2006	Y01	OAG-CAY-OAW-CBC
6	A	2011	LPE	C12-C13-C14-C15
9	A	2013	PCW	C34-C35-C36-C37
6	A	2015	LPE	C31-C32-N-C1N
9	A	2013	PCW	C4-C5-N-C7

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Mol	Chain	Res	Type	Atoms
9	A	2010	PCW	C22-C23-C24-C25
6	A	2015	LPE	C14-C15-C16-C17
10	A	2018	P3X	C7-C8-C9-C10
8	A	2007	Y01	CAR-CBC-OAW-CAY
9	A	2013	PCW	C39-C40-C41-C42
6	A	2016	LPE	C2-C3-O3-P
6	A	2008	LPE	C1-C2-C3-O3
8	A	2007	Y01	CAO-CBB-CBE-CAP
10	A	2018	P3X	C4-C5-C6-C7
9	A	2013	PCW	C36-C37-C38-C39
9	A	2010	PCW	C21-C22-C23-C24
9	A	2010	PCW	O3P-C1-C2-C3
9	A	2013	PCW	C1-C2-C3-O3
9	A	2013	PCW	C12-C13-C14-C15
9	A	2013	PCW	C4-C5-N-C6
10	A	2018	P3X	C11-C10-C9-C8
9	A	2013	PCW	C18-C19-C20-C21
9	A	2013	PCW	C22-C23-C24-C25
8	A	2005	Y01	CAN-CAJ-CAO-CBB
6	A	2014	LPE	C13-C14-C15-C16
9	A	2013	PCW	O2-C2-C3-O3
7	A	2004	A1E26	C2-C3-O12-C28
9	A	2010	PCW	C34-C35-C36-C37
6	A	2008	LPE	C12-C13-C14-C15
8	A	2017	Y01	CAJ-CAN-CBA-CAA
9	A	2010	PCW	C25-C26-C27-C28
10	A	2018	P3X	C3-C4-C5-C6
6	A	2015	LPE	C16-C17-C18-C19
9	A	2010	PCW	C1-C2-C3-O3
10	A	2018	P3X	C22-C23-C24-C25
9	A	2010	PCW	O2-C2-C3-O3
8	A	2017	Y01	CAJ-CAO-CBB-CAC
6	A	2015	LPE	C15-C16-C17-C18
8	A	2017	Y01	CAJ-CAN-CBA-CAB
9	A	2013	PCW	C33-C34-C35-C36
9	A	2013	PCW	C20-C21-C22-C23
8	A	2007	Y01	CAM-CAY-OAW-CBC
6	B	304	LPE	O33-C31-C32-N
6	A	2011	LPE	O33-C31-C32-N
6	A	2014	LPE	O33-C31-C32-N
9	A	2010	PCW	O4P-C4-C5-N
6	A	2008	LPE	O2H-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
6	A	2008	LPE	C2-C1-O1-C11
9	A	2013	PCW	C4-C5-N-C8
8	A	2007	Y01	OAG-CAY-OAW-CBC
6	A	2016	LPE	C16-C17-C18-C19
9	A	2013	PCW	O3P-C1-C2-O2
6	A	2015	LPE	C12-C11-O1-C1
10	A	2018	P3X	O2-C15-C16-O7
10	A	2018	P3X	O2-C15-C16-C17
9	A	2010	PCW	C32-C33-C34-C35
6	A	2012	LPE	C3-O3-P-O31
6	A	2012	LPE	C31-O33-P-O31
6	A	2014	LPE	C3-O3-P-O31
10	A	2018	P3X	C17-O3-P1-O4
10	A	2018	P3X	C17-O3-P1-O6
10	A	2018	P3X	C16-C17-O3-P1
6	A	2016	LPE	C12-C11-O1-C1
8	A	2005	Y01	CAX-CAL-CAM-CAY
9	A	2013	PCW	C23-C24-C25-C26
10	A	2018	P3X	C20-C21-C22-C23
5	B	301	NAG	C4-C5-C6-O6
9	A	2010	PCW	C19-C20-C21-C22
6	A	2011	LPE	C2-C1-O1-C11
6	A	2015	LPE	C2-C1-O1-C11
9	A	2010	PCW	C16-C17-C18-C19
5	B	303	NAG	O5-C5-C6-O6
6	B	304	LPE	O1-C1-C2-C3
8	A	2005	Y01	CAJ-CAN-CBA-CAA
8	A	2006	Y01	CAM-CAL-CAX-OAH
9	A	2013	PCW	C37-C38-C39-C40
6	A	2009	LPE	C14-C15-C16-C17
8	A	2007	Y01	CAM-CAL-CAX-OAH
9	A	2013	PCW	C32-C33-C34-C35
8	A	2007	Y01	CAM-CAL-CAX-OAF
8	A	2005	Y01	CAO-CBB-CBE-CAP
8	A	2005	Y01	CAC-CBB-CBE-CBI
8	A	2006	Y01	CAM-CAL-CAX-OAF
10	A	2018	P3X	C12-C13-C14-O2
8	A	2005	Y01	CAM-CAL-CAX-OAH
8	A	2005	Y01	CAJ-CAN-CBA-CAB
6	A	2012	LPE	C2-C3-O3-P
8	A	2017	Y01	CAM-CAL-CAX-OAH
6	A	2012	LPE	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
6	A	2011	LPE	C12-C11-O1-C1
9	A	2013	PCW	C17-C18-C19-C20
10	A	2018	P3X	C5-C6-C7-C8
8	A	2005	Y01	CAM-CAL-CAX-OAF
5	B	301	NAG	O5-C5-C6-O6
8	A	2017	Y01	CAM-CAL-CAX-OAF
8	A	2005	Y01	CAO-CBB-CBE-CBI
6	A	2009	LPE	C13-C14-C15-C16
9	A	2013	PCW	C19-C20-C21-C22
9	A	2013	PCW	O3P-C1-C2-C3
6	A	2015	LPE	C12-C13-C14-C15
9	A	2013	PCW	O3-C11-C12-C13
9	A	2013	PCW	O11-C11-C12-C13
8	A	2007	Y01	CAL-CAM-CAY-OAW
9	A	2013	PCW	C14-C15-C16-C17
9	A	2010	PCW	O3-C11-C12-C13
6	A	2011	LPE	C13-C14-C15-C16
9	A	2013	PCW	C11-C12-C13-C14

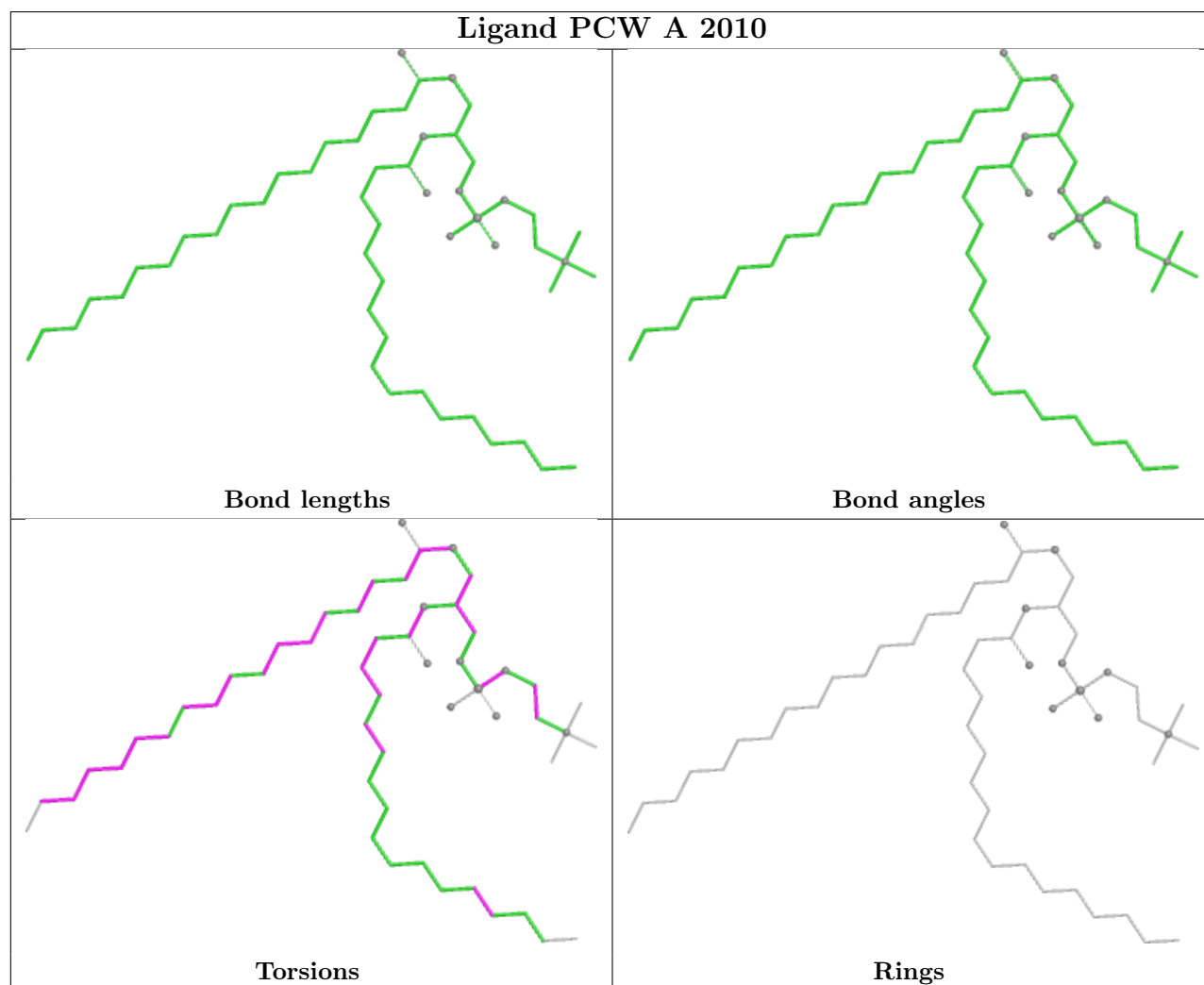
There are no ring outliers.

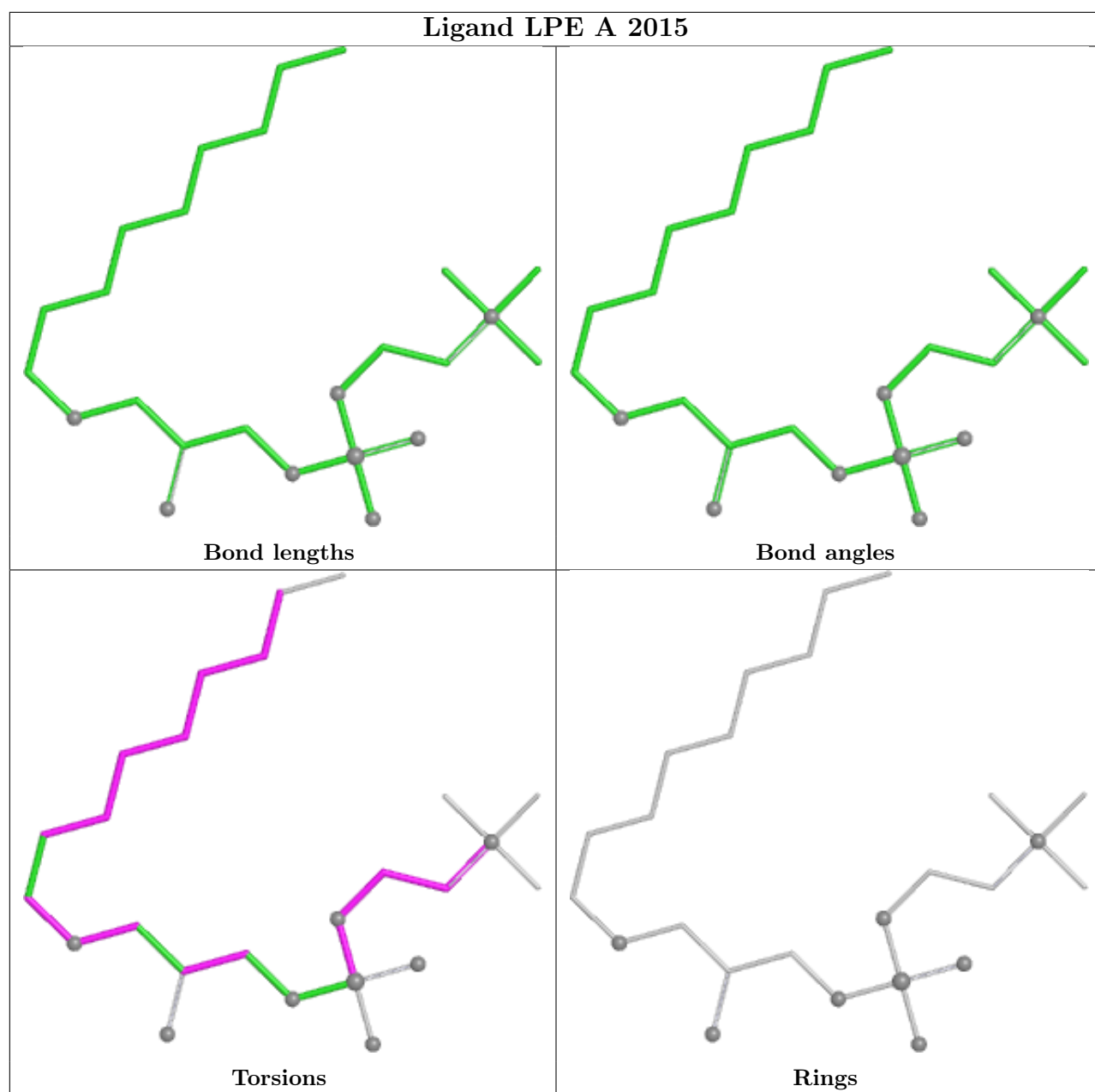
15 monomers are involved in 87 short contacts:

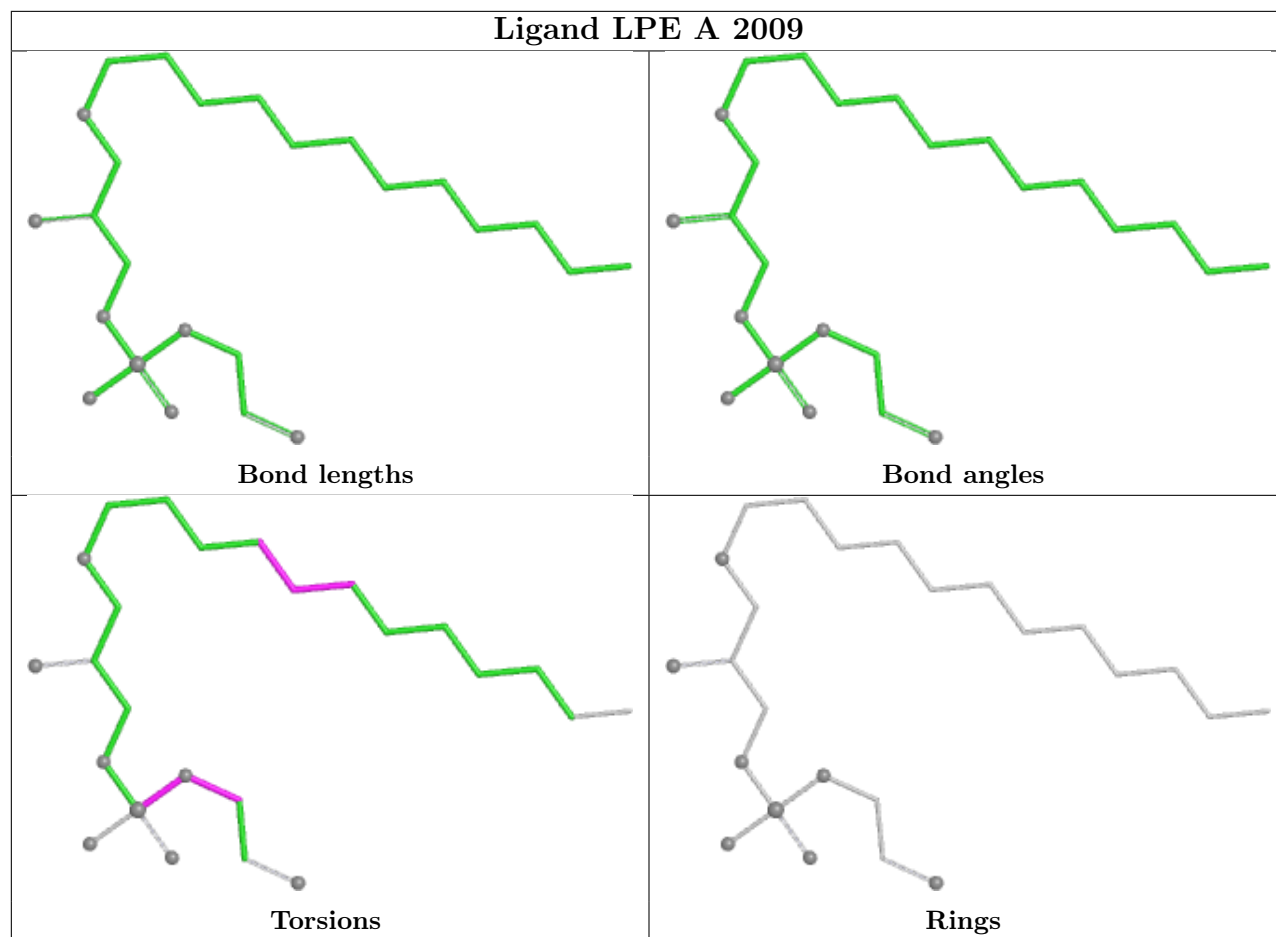
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	2010	PCW	11	0
6	A	2015	LPE	3	0
6	A	2009	LPE	4	0
6	A	2012	LPE	4	0
8	A	2007	Y01	3	0
6	B	304	LPE	4	0
5	B	301	NAG	1	0
9	A	2013	PCW	16	0
7	A	2004	A1E26	1	0
5	B	303	NAG	2	0
8	A	2006	Y01	16	0
8	A	2017	Y01	3	0
6	A	2011	LPE	11	0
8	A	2005	Y01	8	0
6	A	2016	LPE	2	0

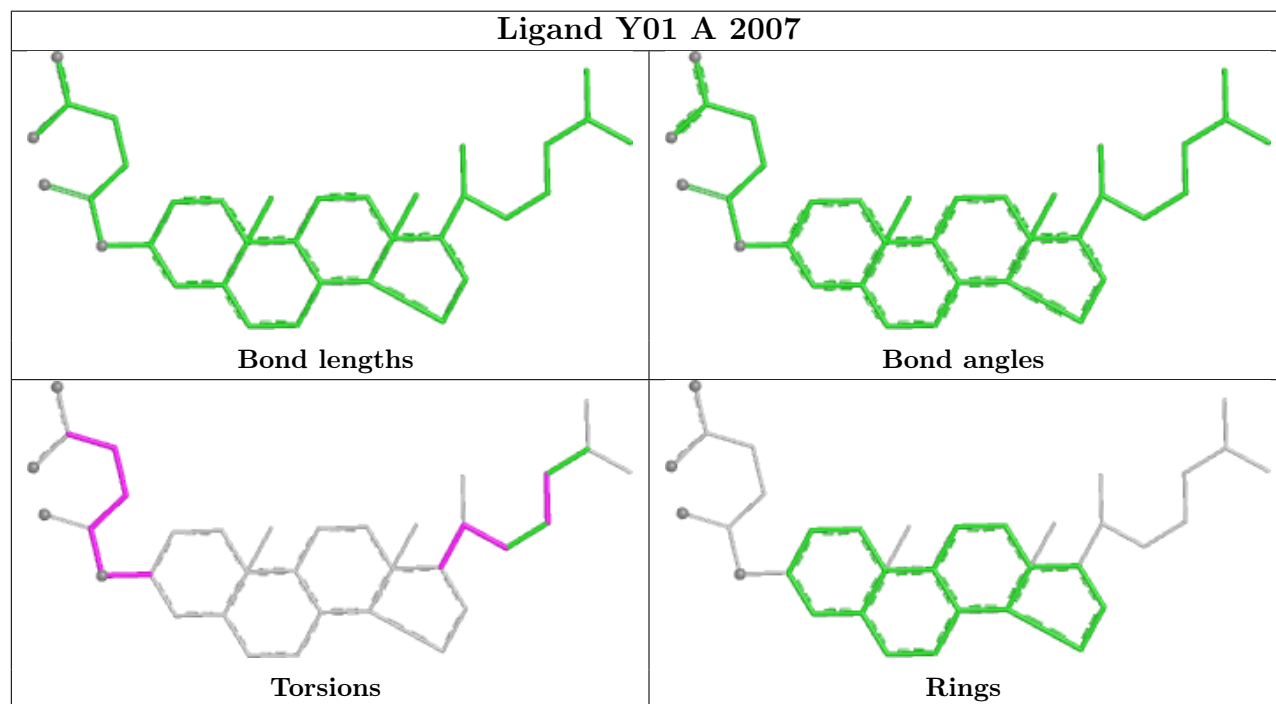
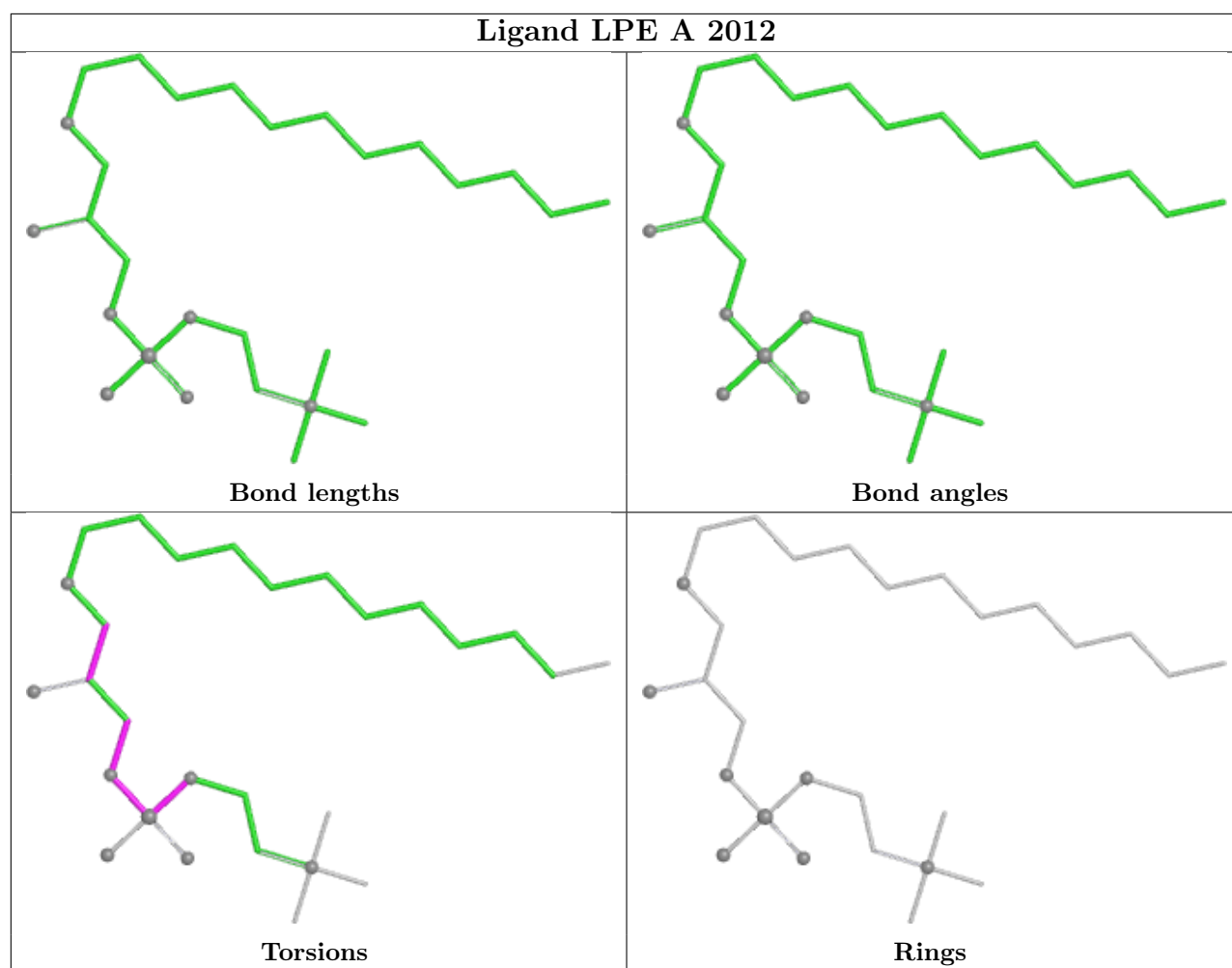
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

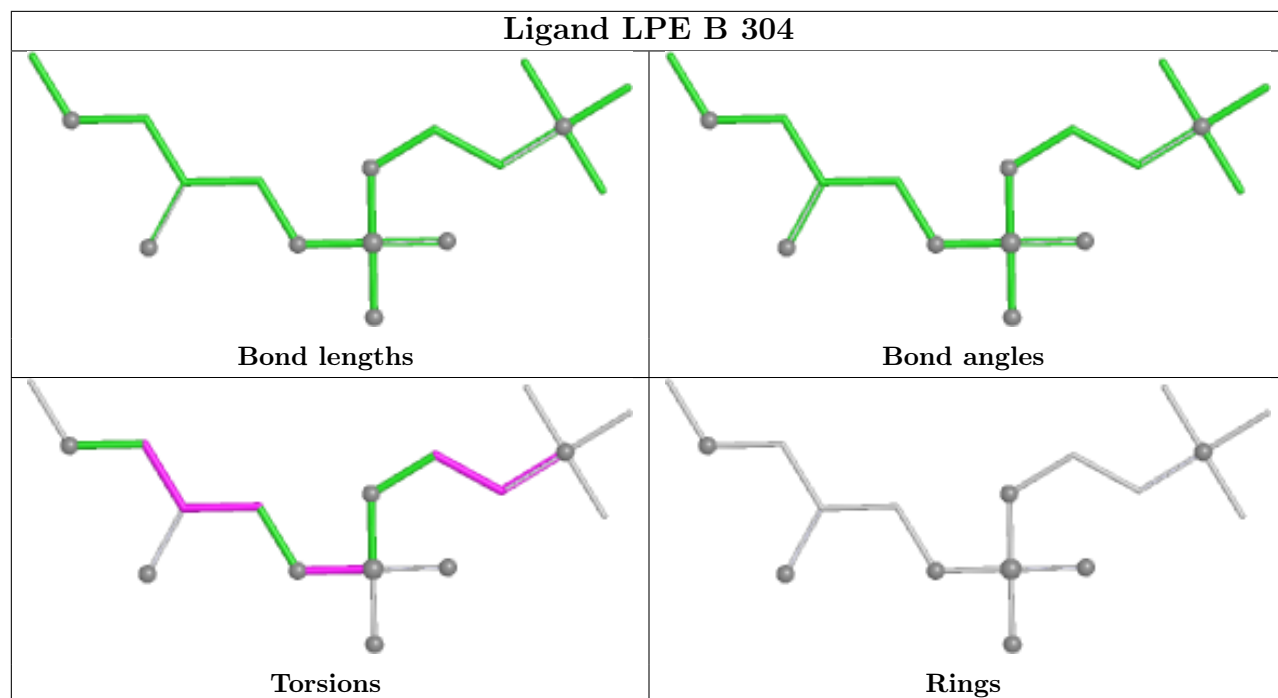
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

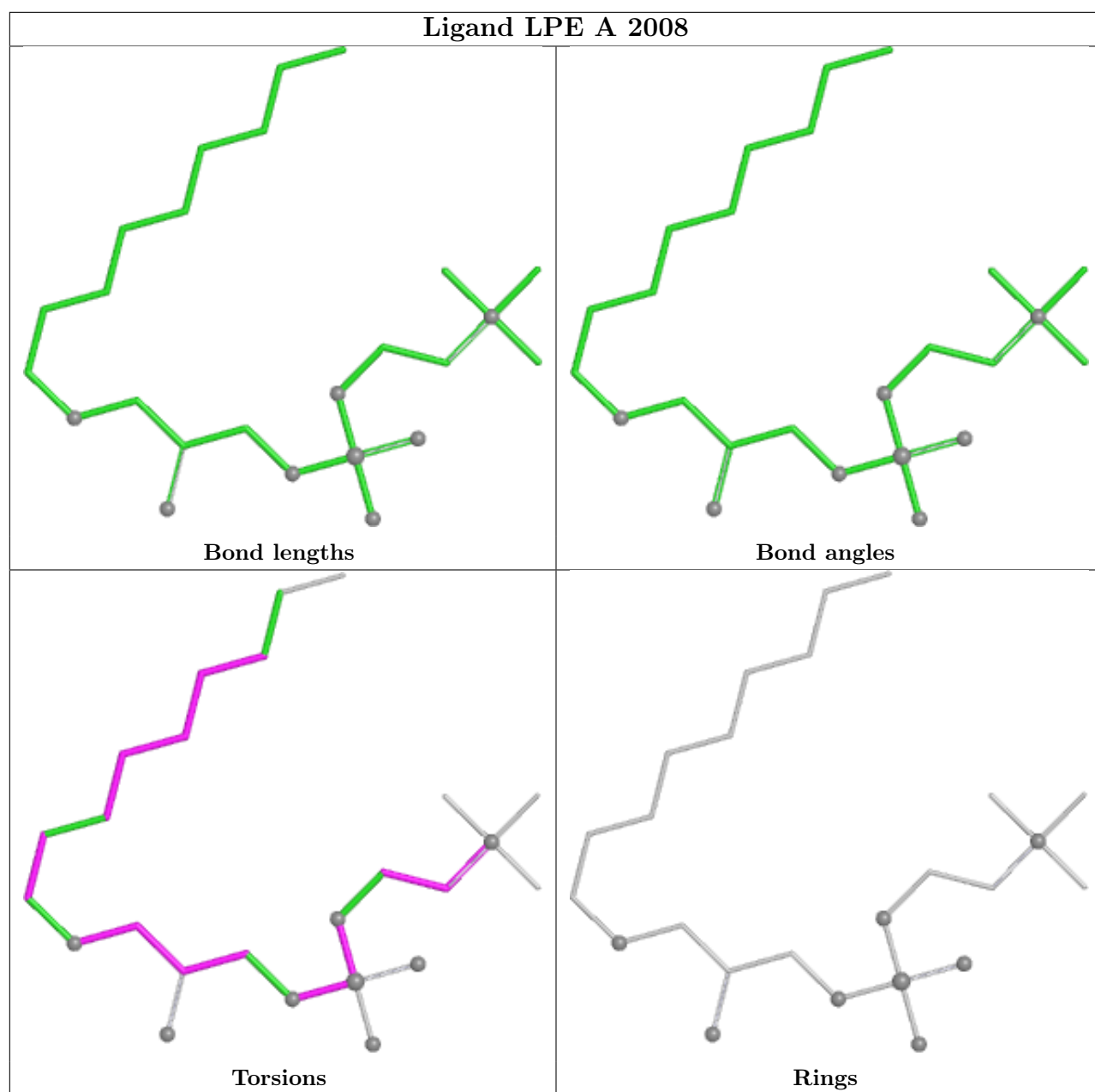


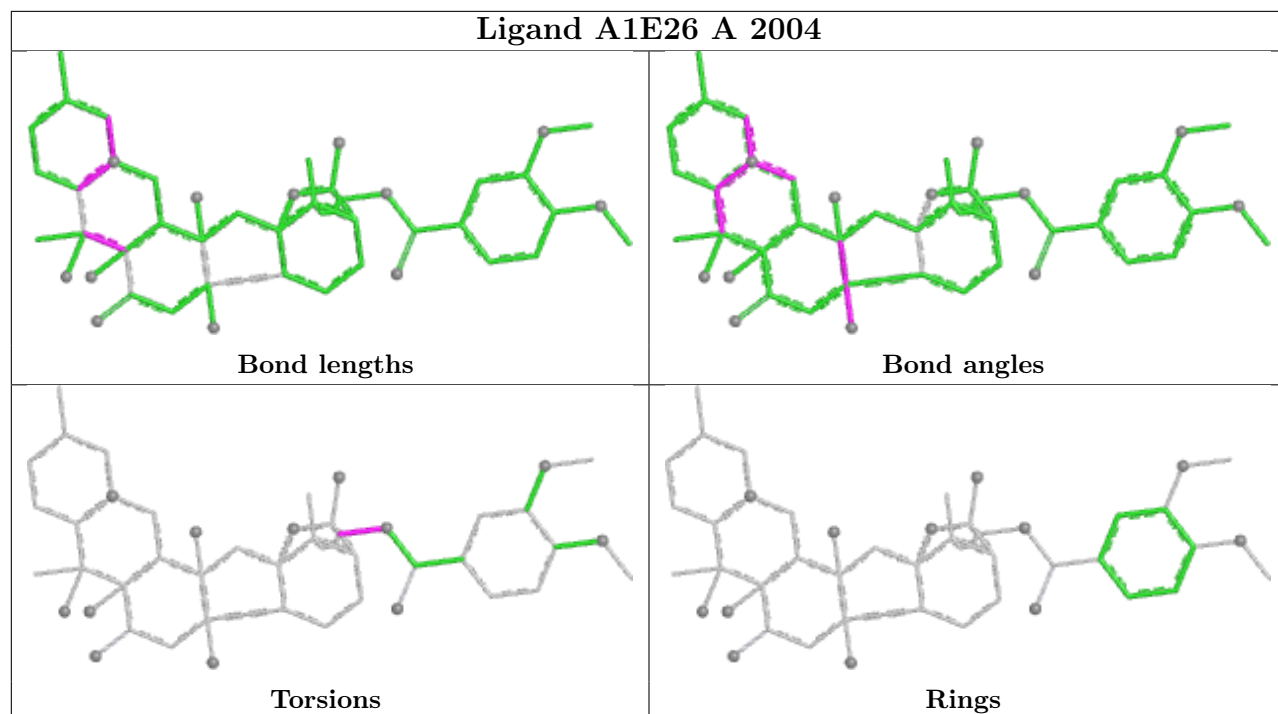
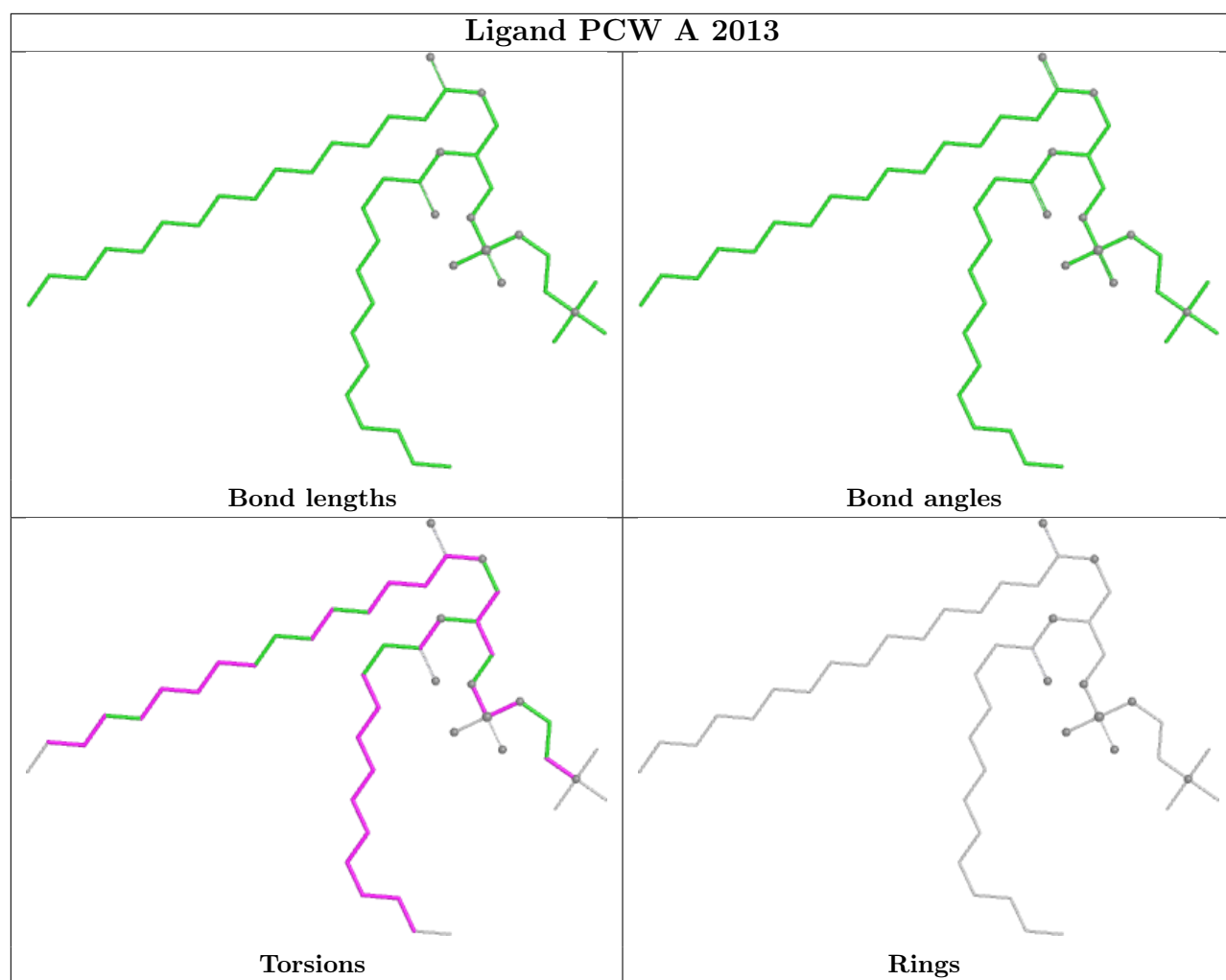


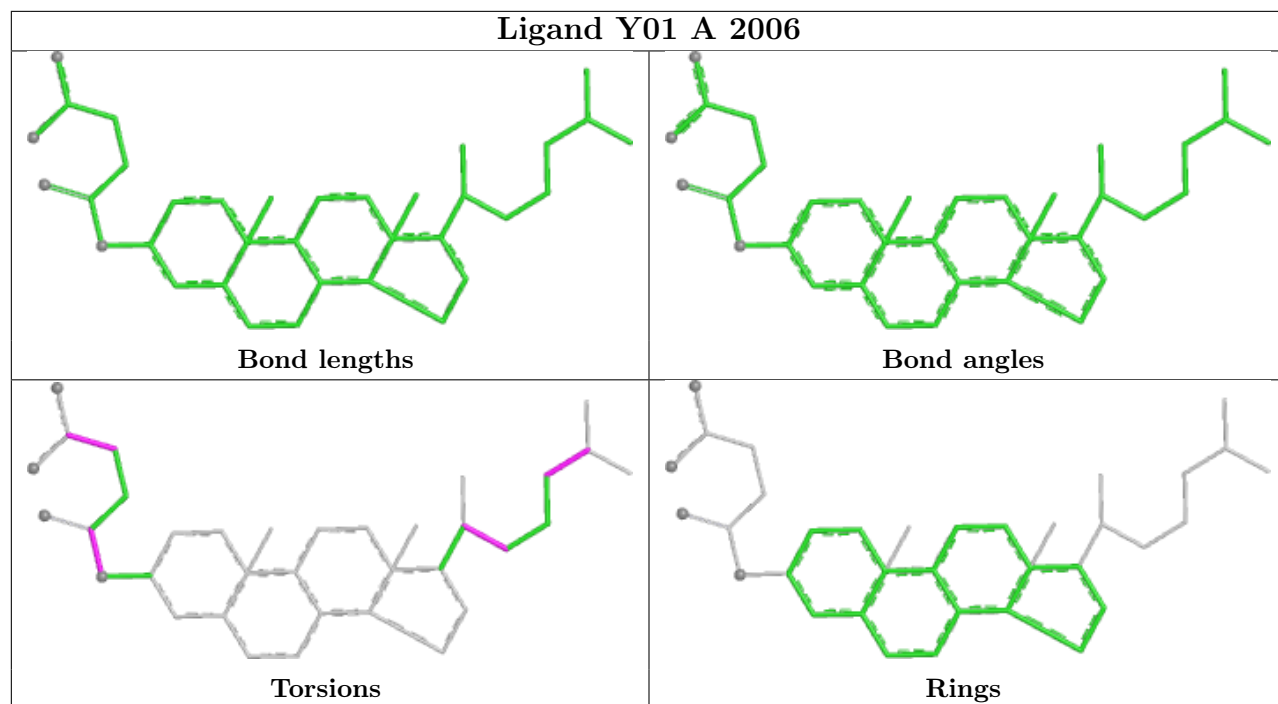


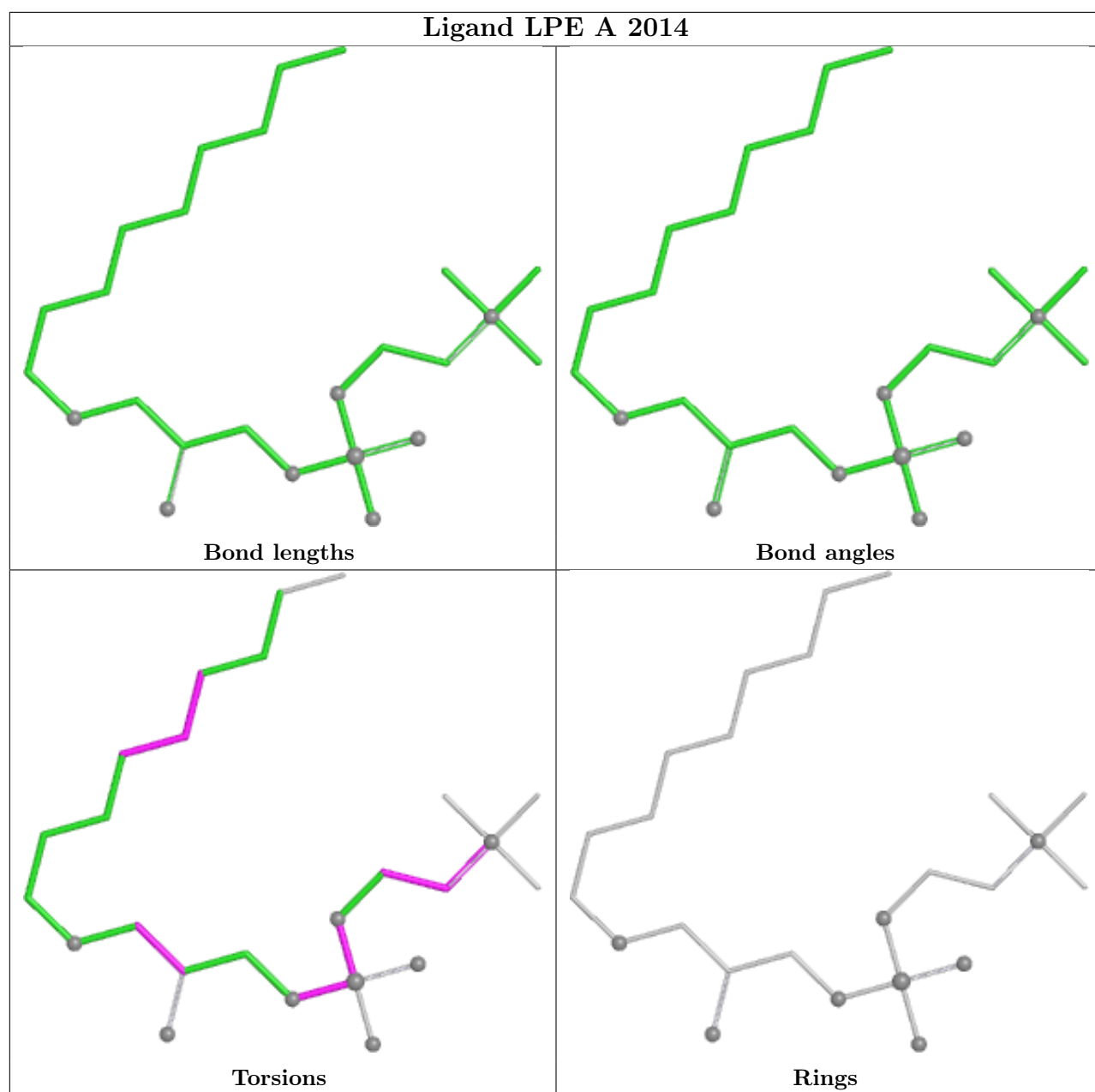


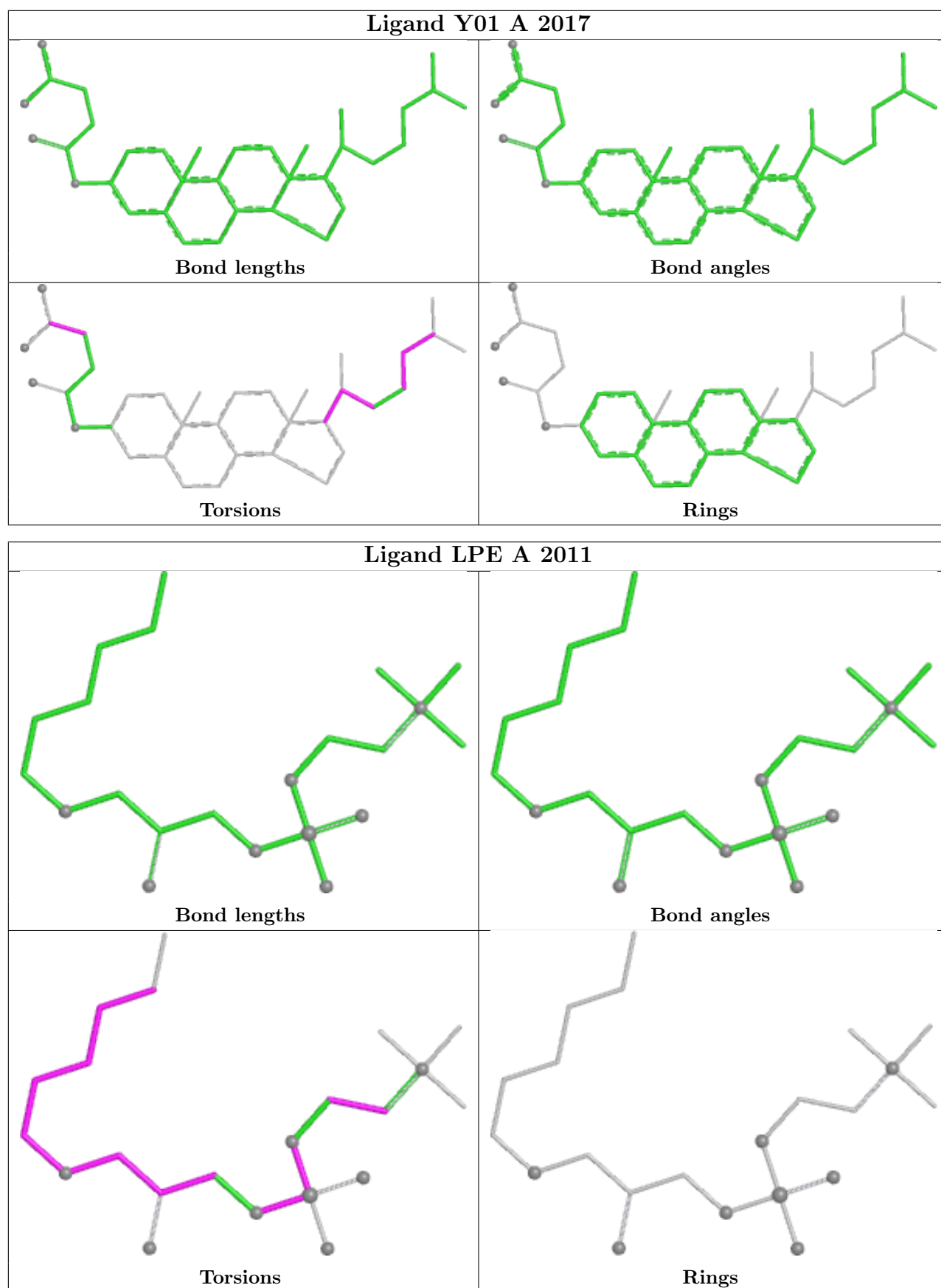


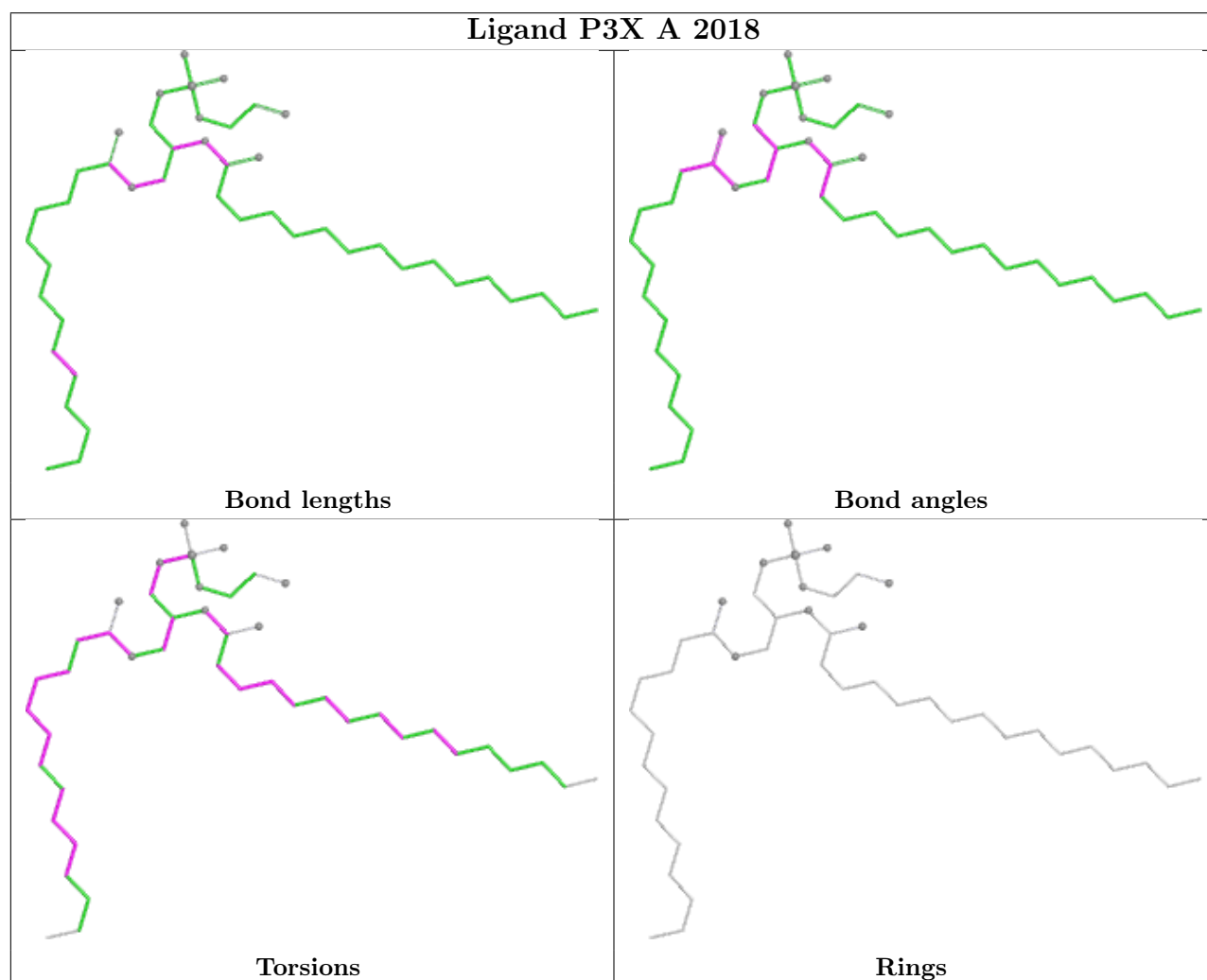
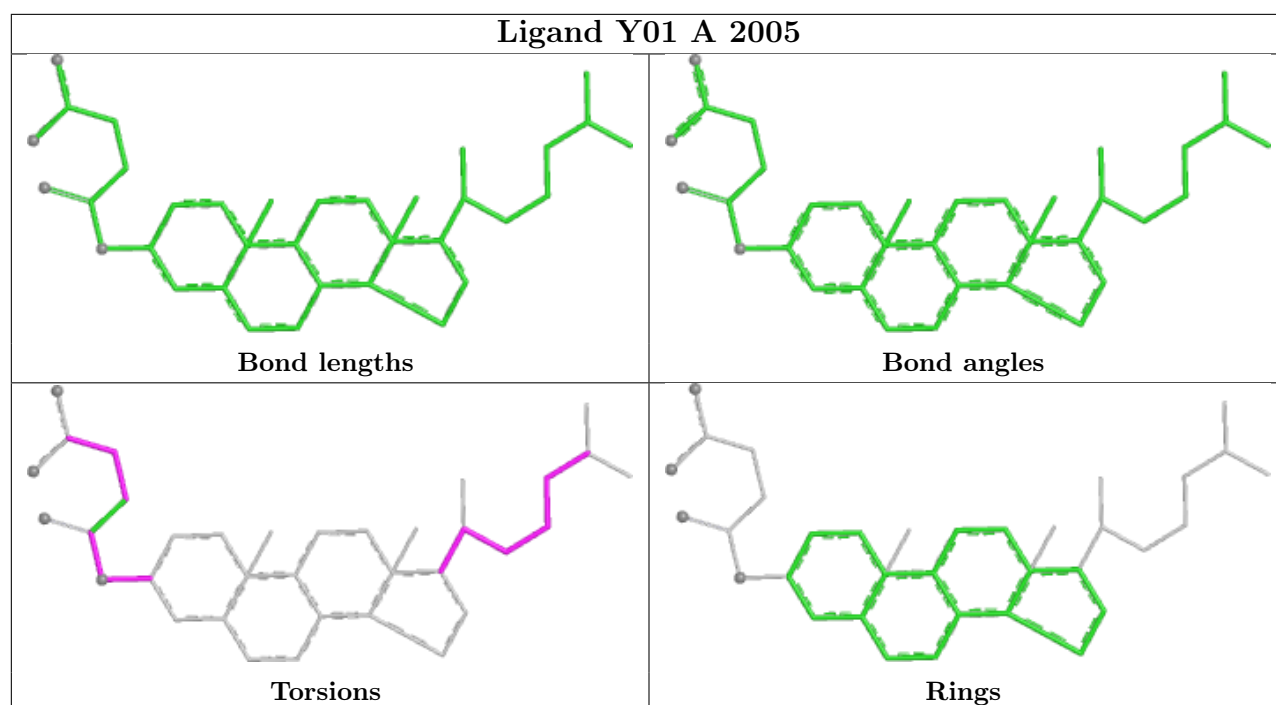


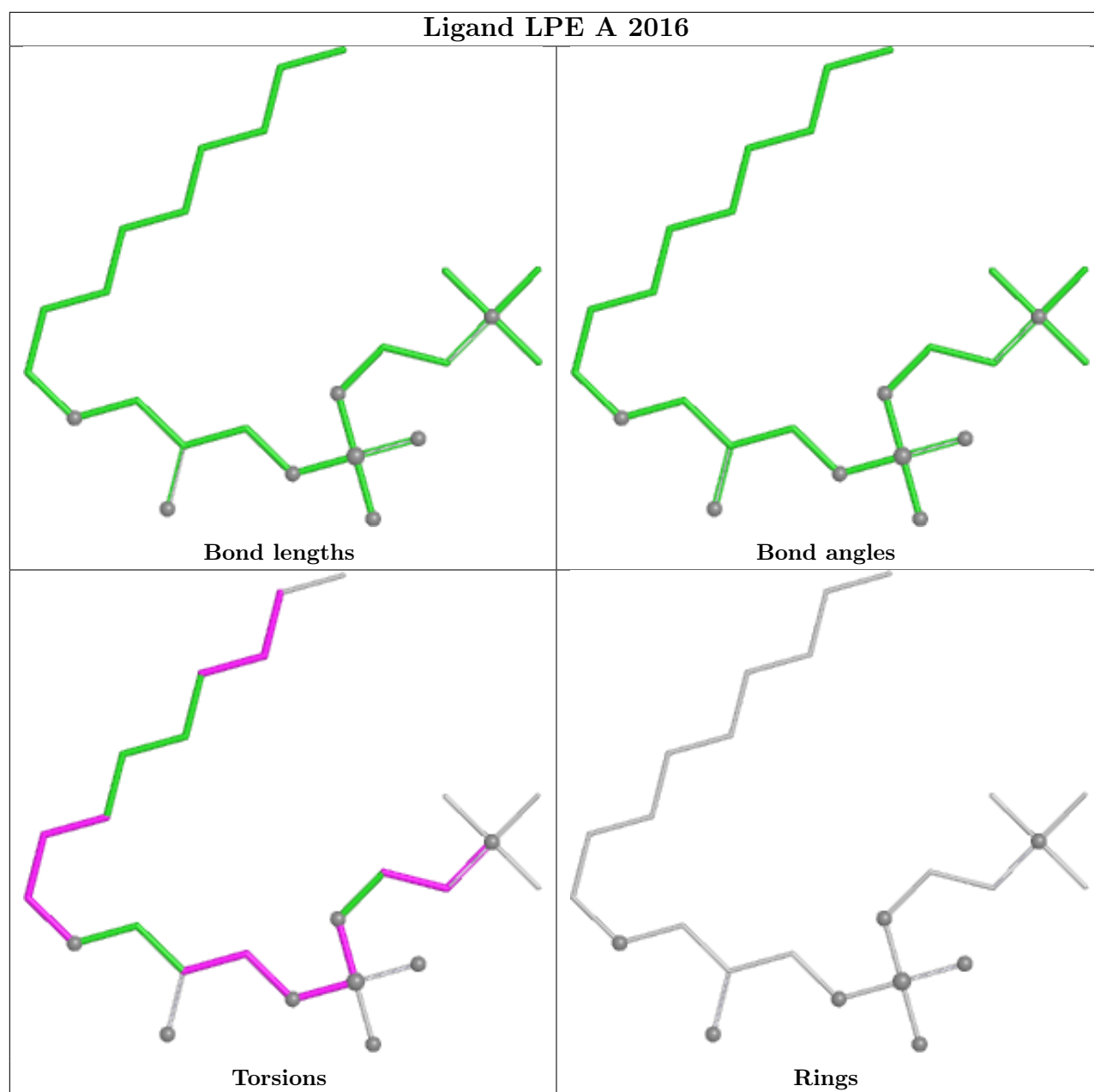












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

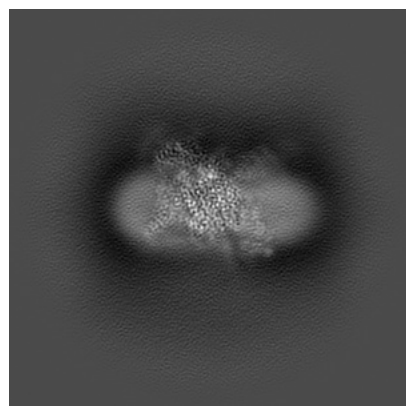
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-67991. These allow visual inspection of the internal detail of the map and identification of artifacts.

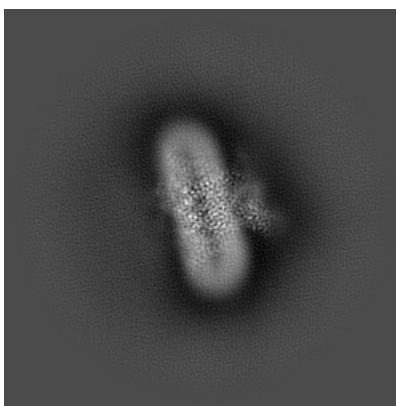
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

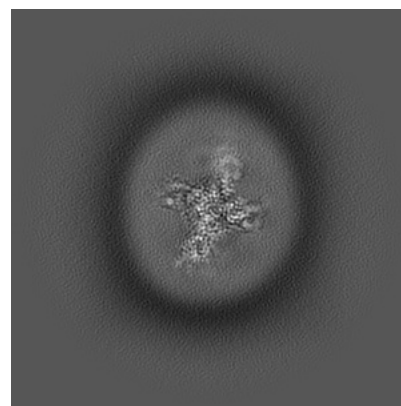
6.1.1 Primary map



X

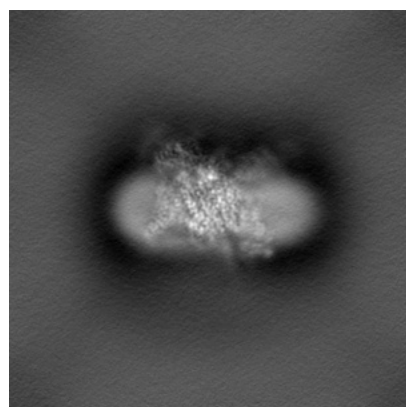


Y

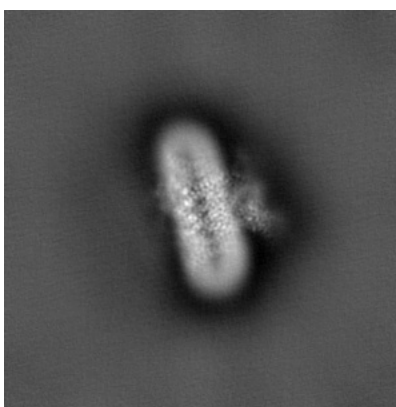


Z

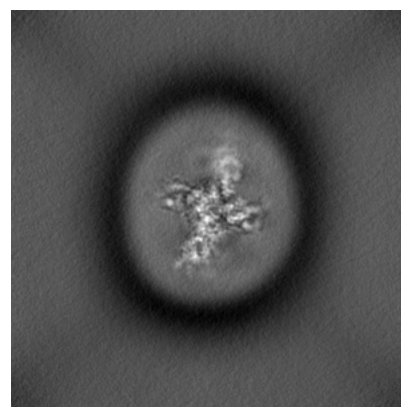
6.1.2 Raw map



X



Y

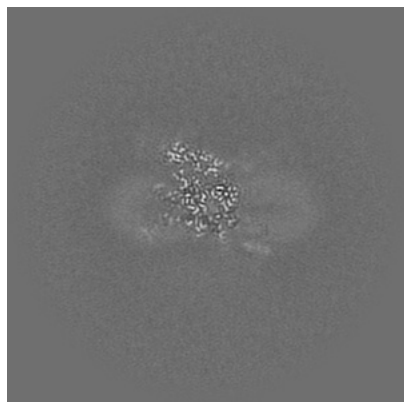


Z

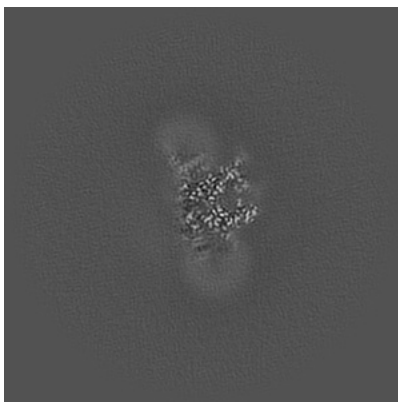
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

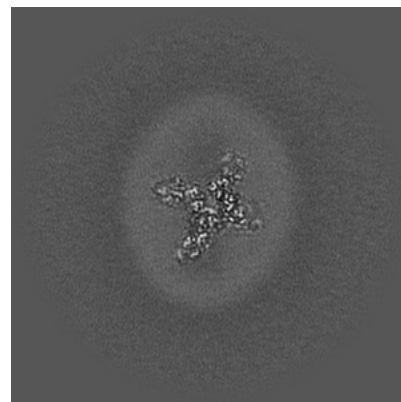
6.2.1 Primary map



X Index: 160

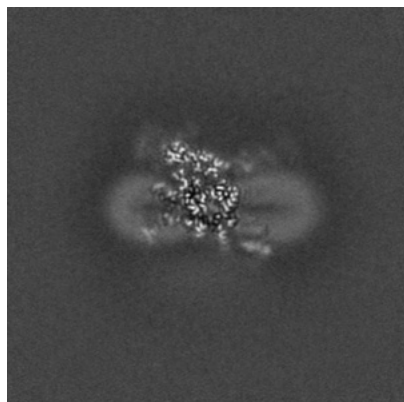


Y Index: 160

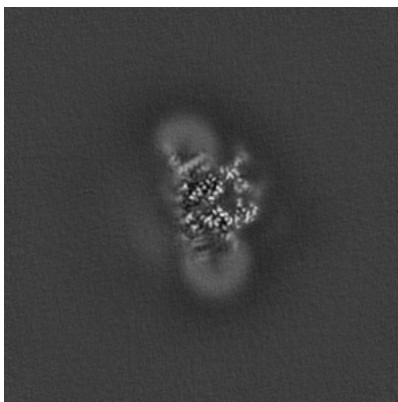


Z Index: 160

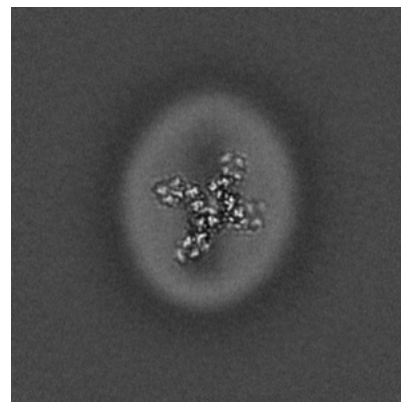
6.2.2 Raw map



X Index: 160



Y Index: 160

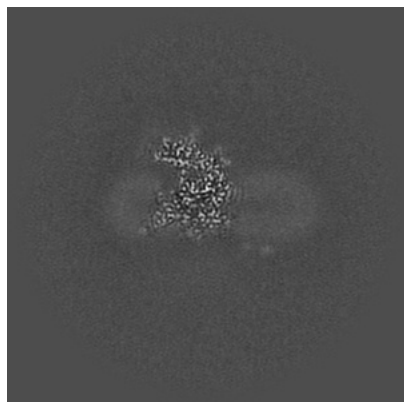


Z Index: 160

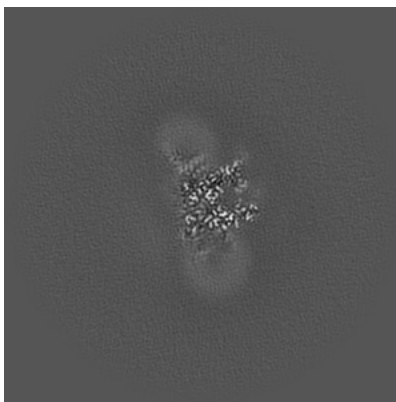
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

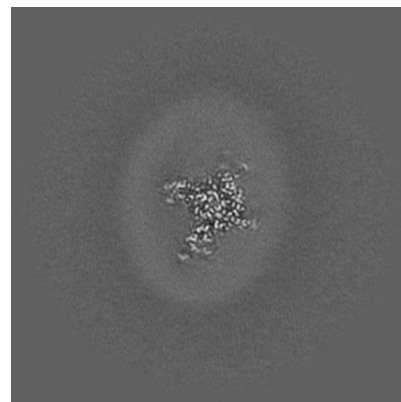
6.3.1 Primary map



X Index: 153

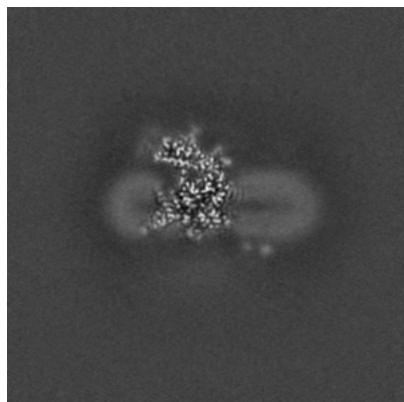


Y Index: 159

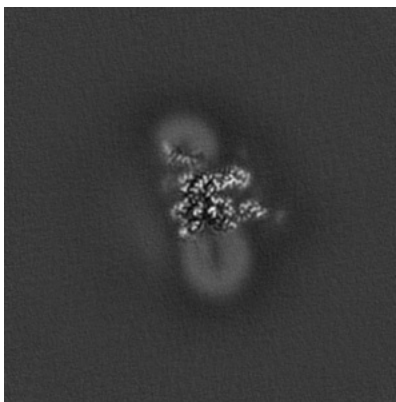


Z Index: 167

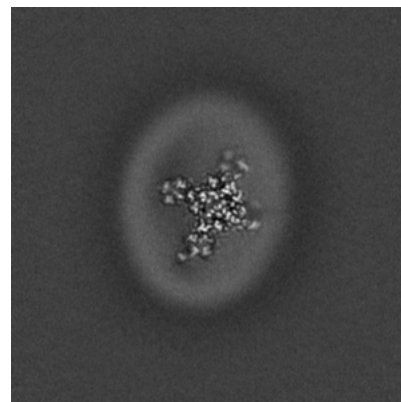
6.3.2 Raw map



X Index: 153



Y Index: 153

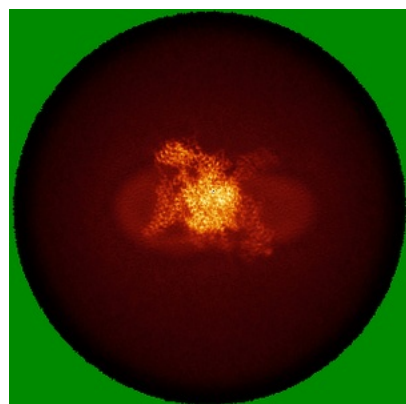


Z Index: 166

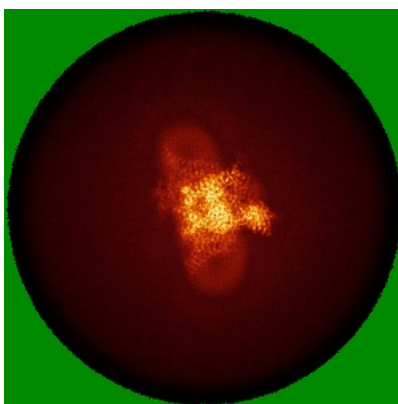
The images above show the largest variance slices of the map in three orthogonal directions.

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

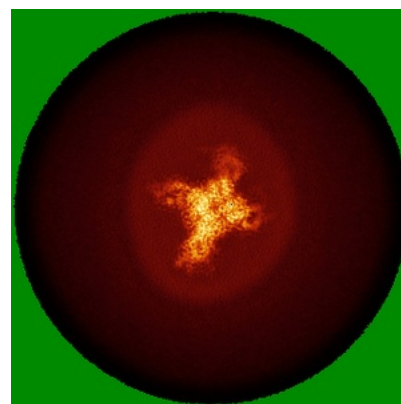
6.4.1 Primary map



X

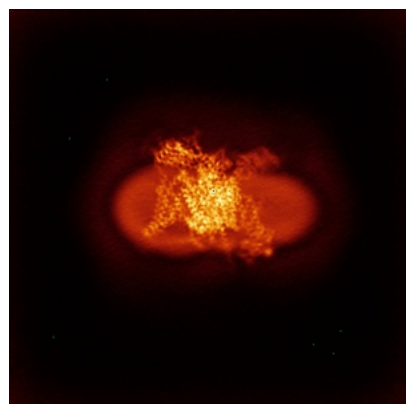


Y

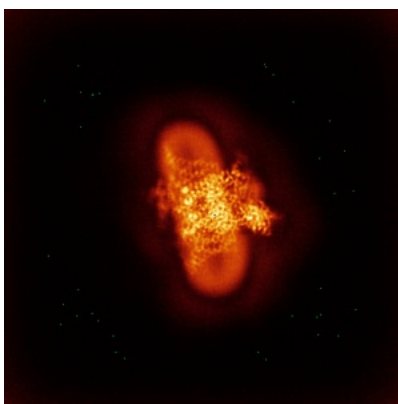


Z

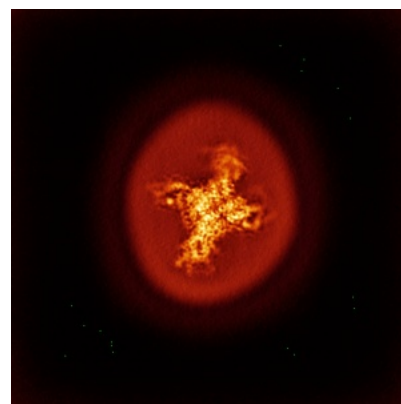
6.4.2 Raw map



X



Y

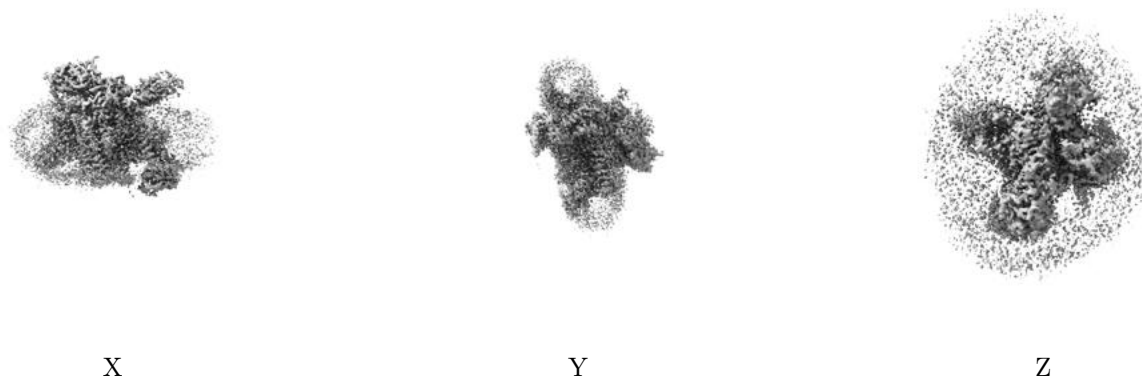


Z

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.

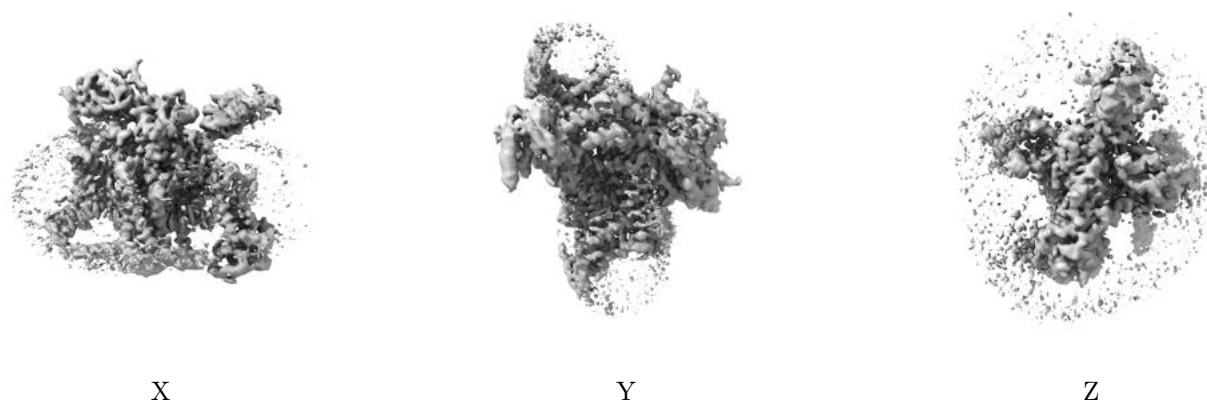
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.65. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

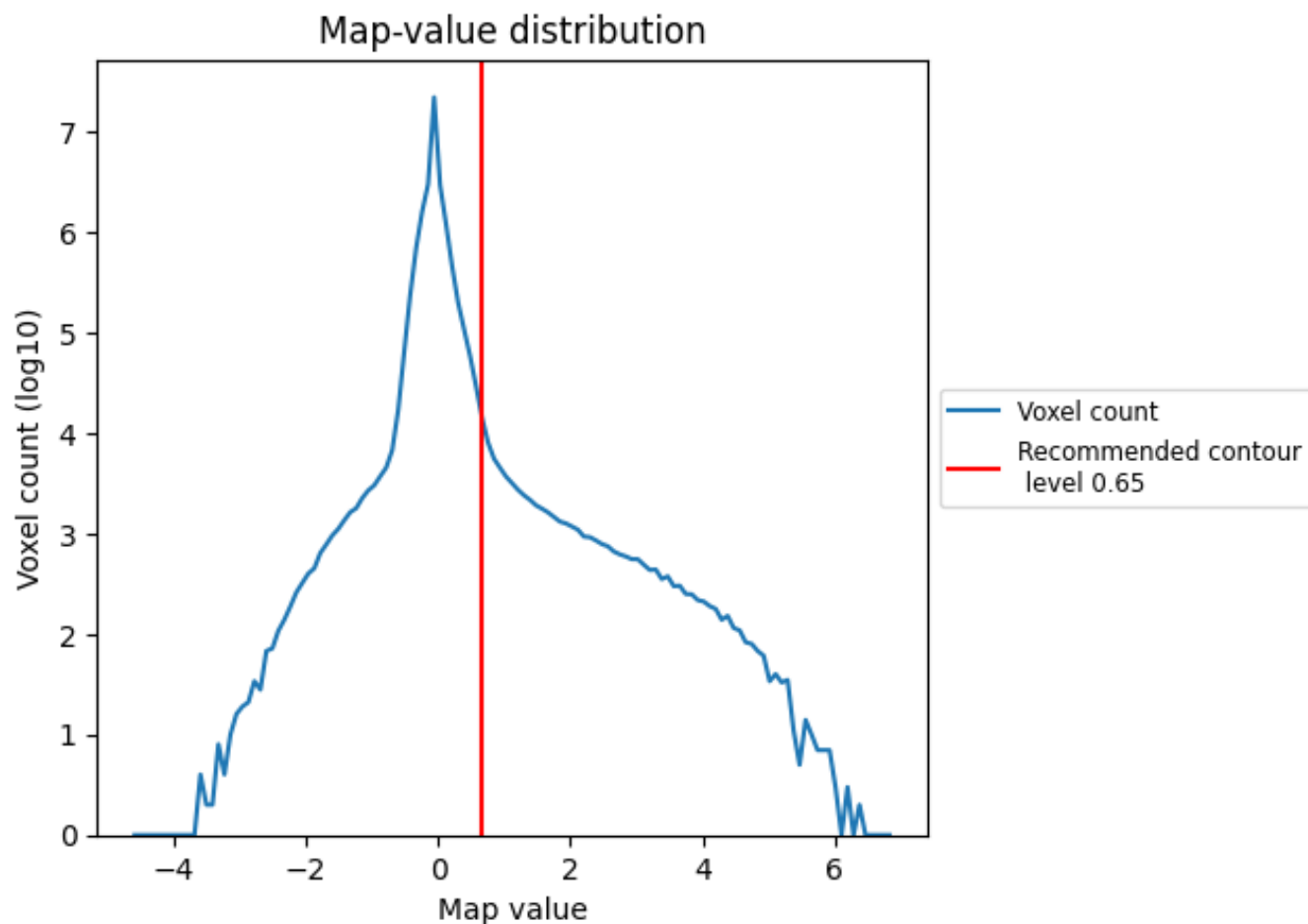
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

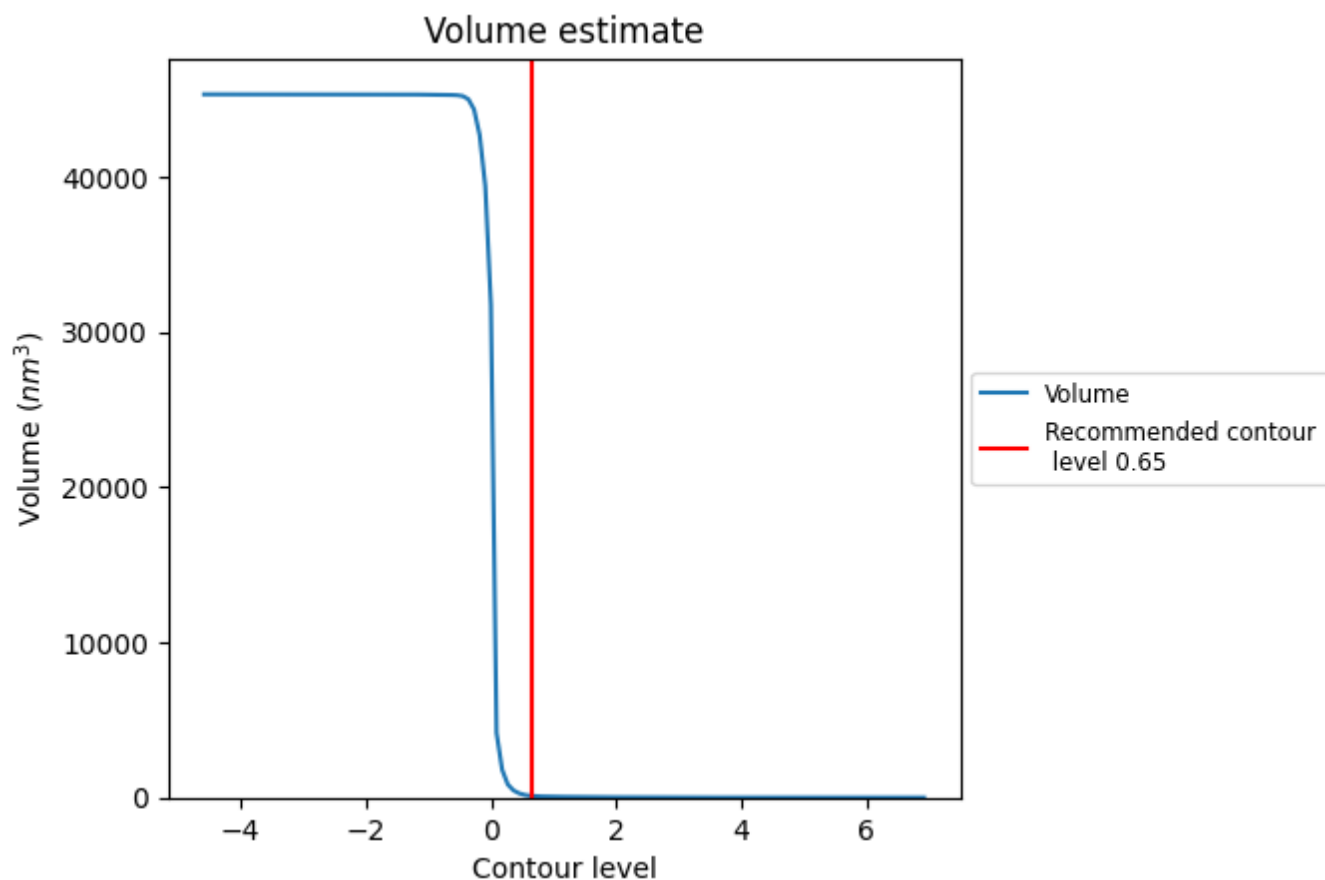
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

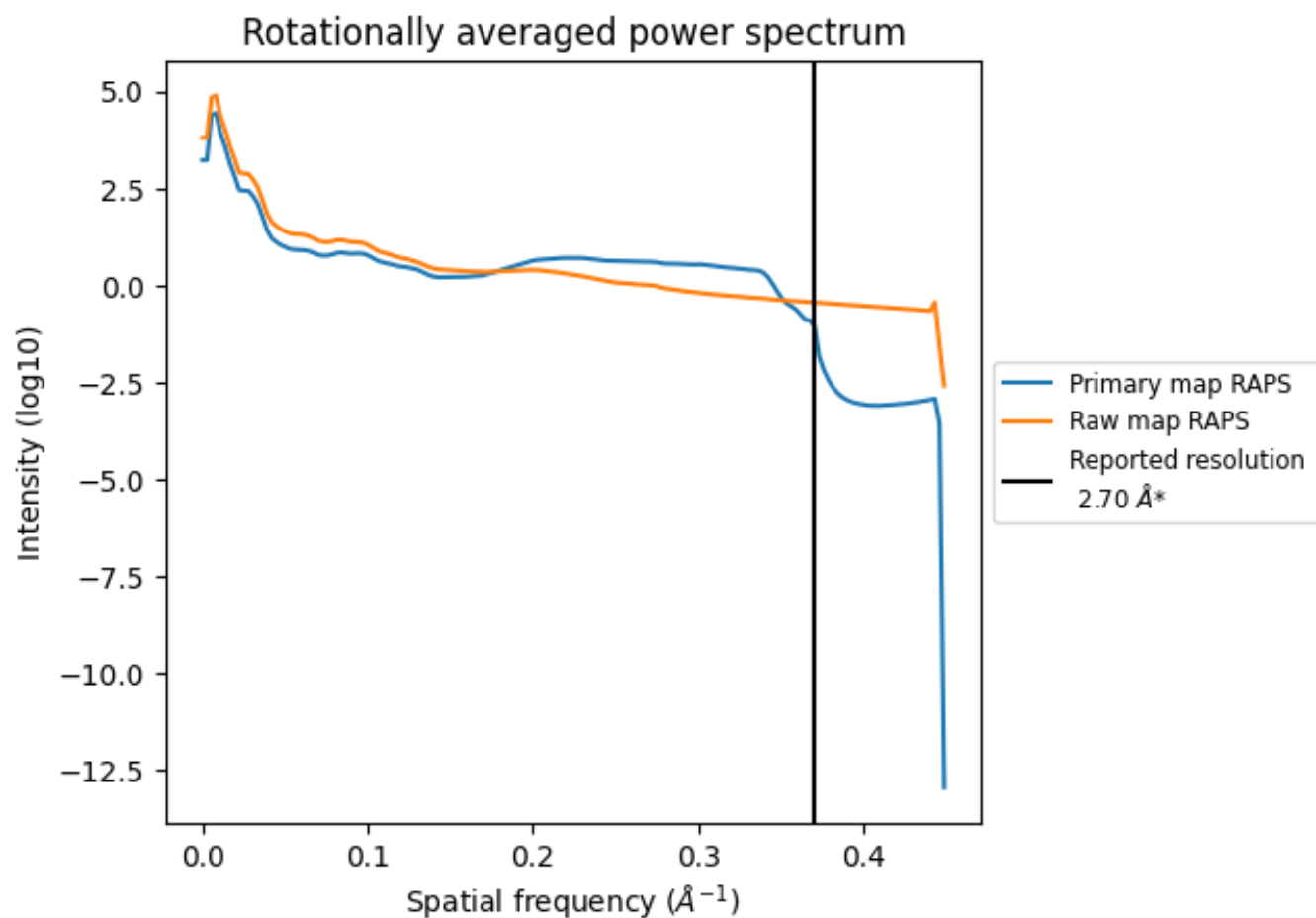
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 105 nm³; this corresponds to an approximate mass of 95 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 ⓘ

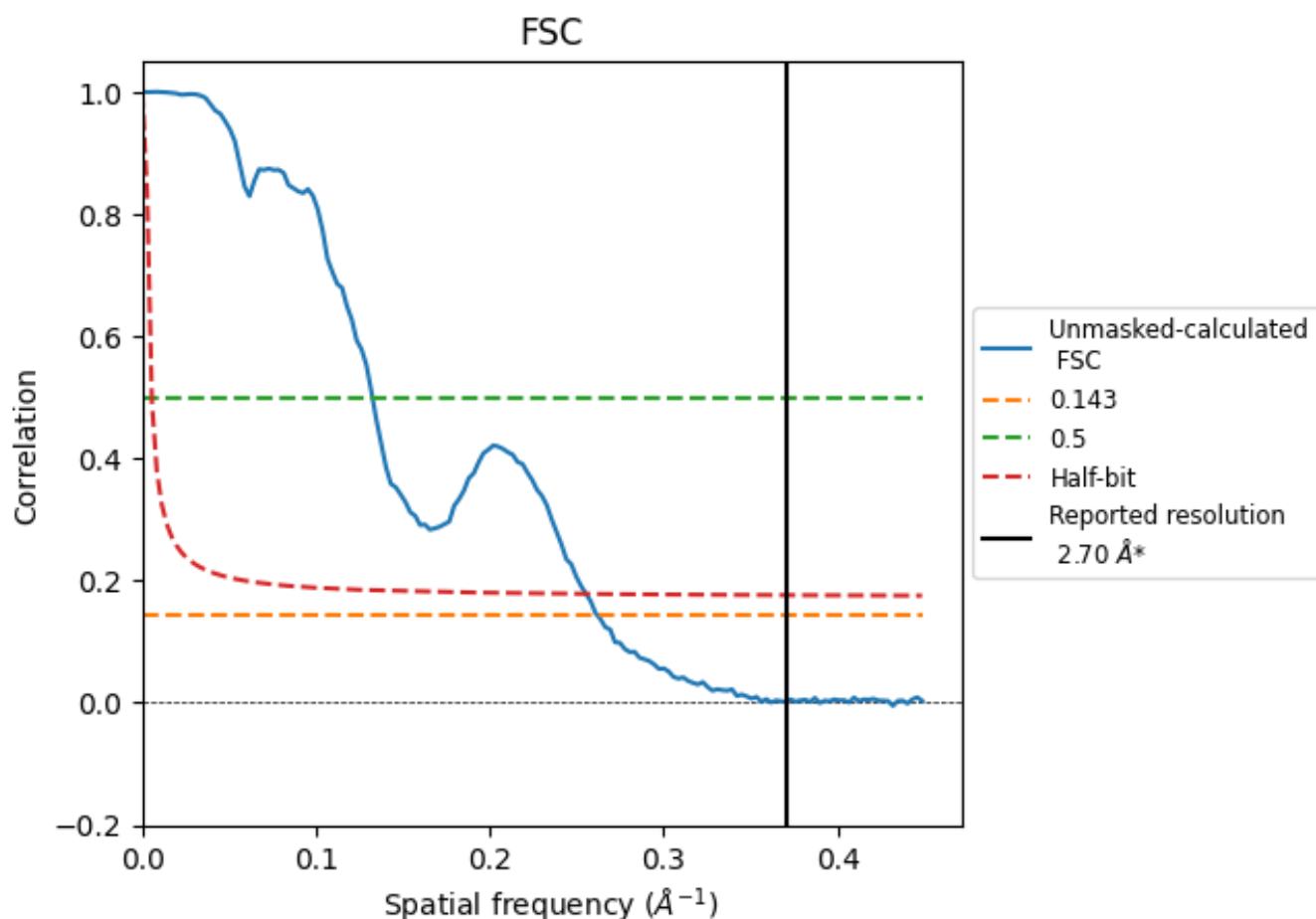


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

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 0.370 \AA^{-1}

8.2 Resolution estimates [i](#)

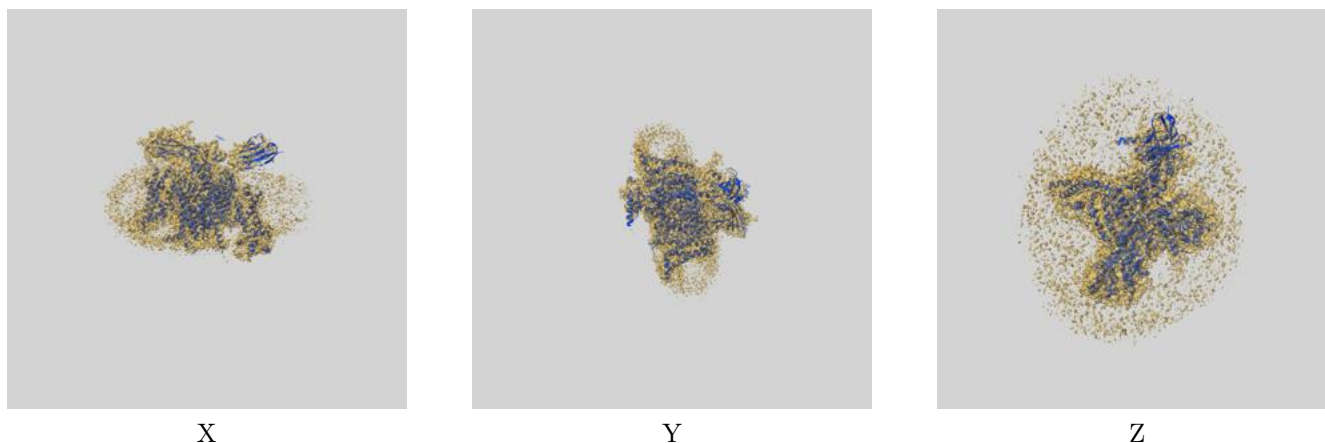
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.82	7.55	3.92

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

9 Map-model fit [i](#)

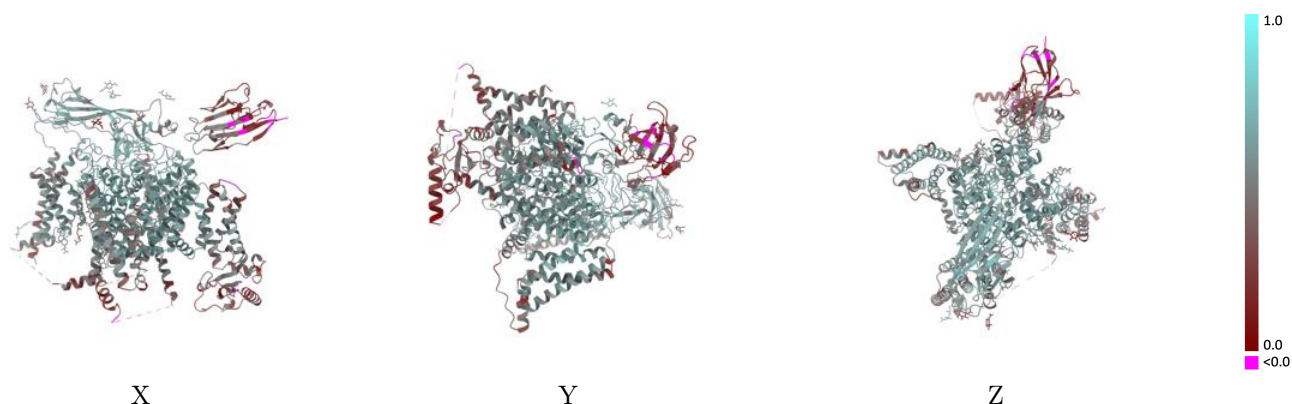
This section contains information regarding the fit between EMDB map EMD-67991 and PDB model 21TQ. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



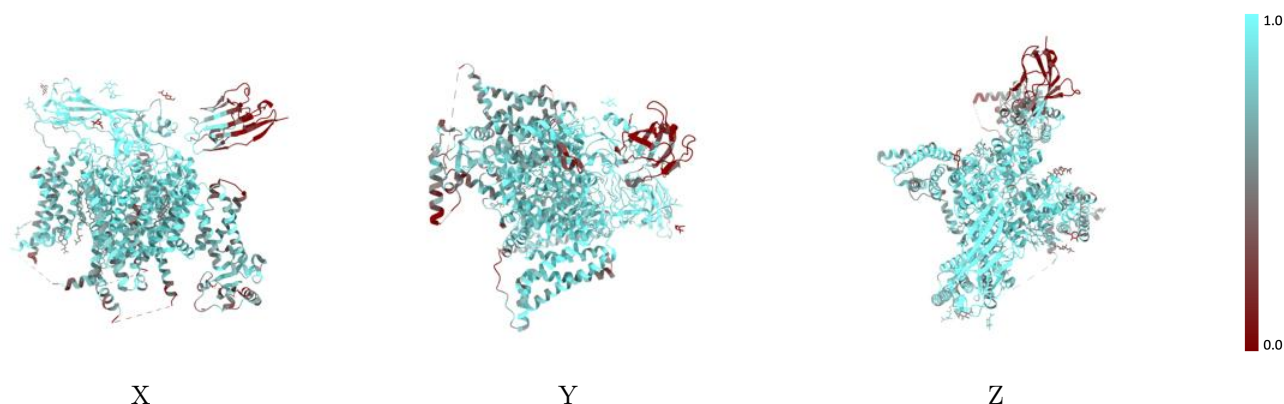
The images above show the 3D surface view of the map at the recommended contour level 0.65 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



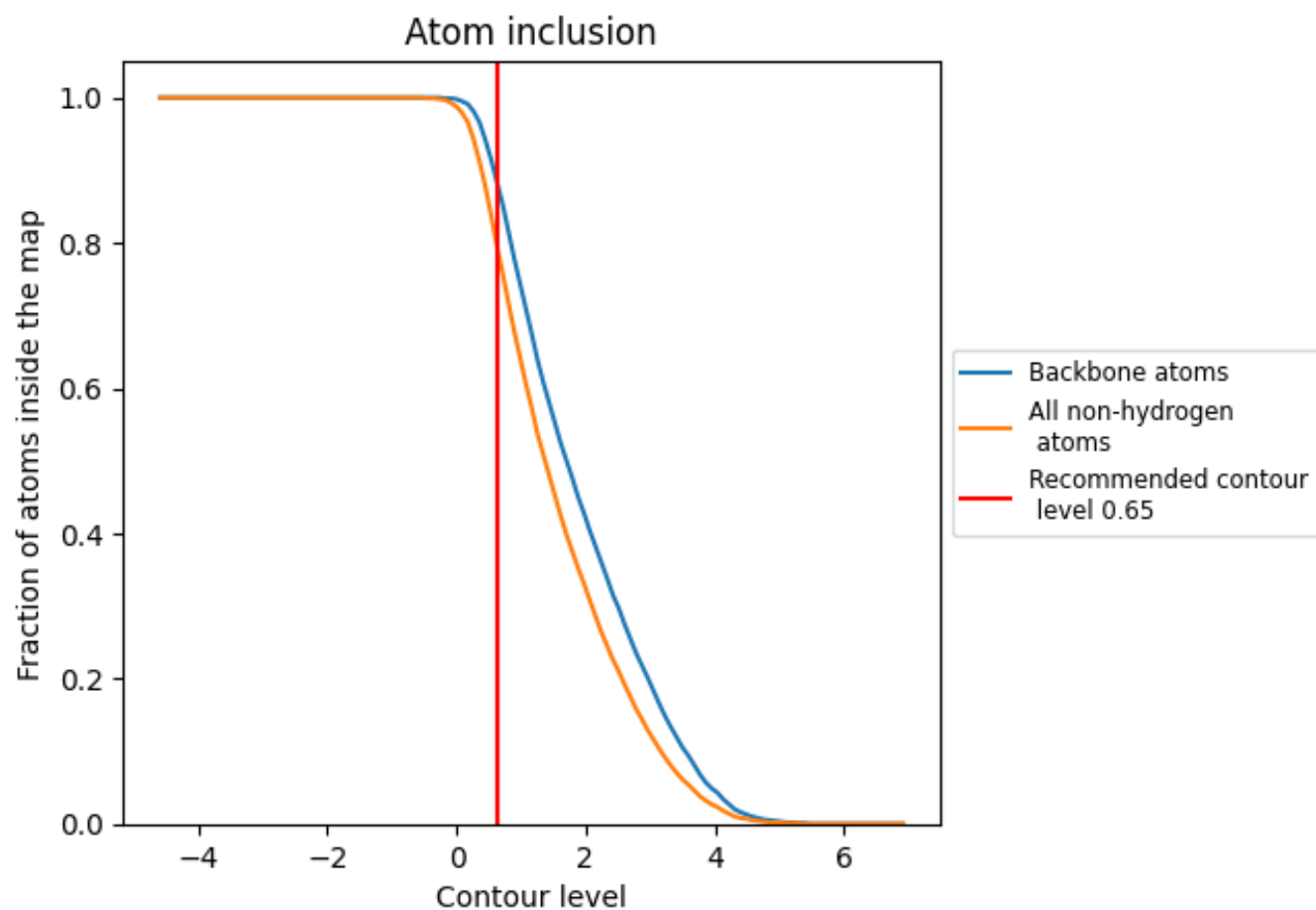
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.65).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 79% 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 (0.65) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7860	<div></div> 0.5080
A	<div></div> 0.8200	<div></div> 0.5280
B	<div></div> 0.8390	<div></div> 0.5260
C	<div></div> 0.3340	<div></div> 0.2690
D	<div></div> 0.8930	<div></div> 0.5330
E	<div></div> 0.6790	<div></div> 0.4150

