



## Full wwPDB EM Validation Report ⓘ

Feb 20, 2023 – 12:18 PM JST

PDB ID : 7XVE  
EMDB ID : EMD-33484  
Title : Human Nav1.7 mutant class-I  
Authors : Huang, G.; Wu, Q.; Li, Z.; Pan, X.; Yan, N.  
Deposited on : 2022-05-21  
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:

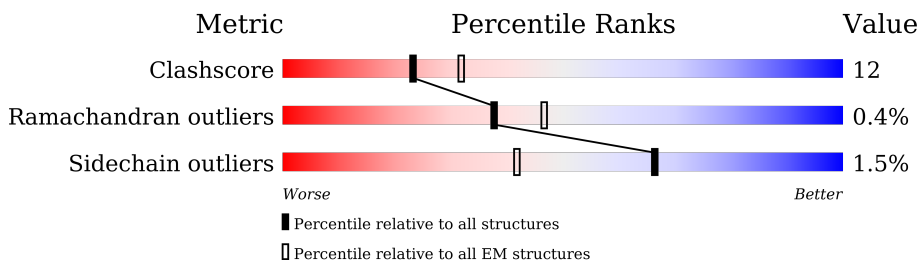
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.32.1

# 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	2022	 6% 50% 13% 37%
2	B	218	 64% 15% 21%
3	C	215	 34% 20% 44%
4	D	2	 100%
4	E	2	 50% 50%

## 2 Entry composition i

There are 11 unique types of molecules in this entry. The entry contains 13659 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	1276	10209	6771	1606	1753	79	1	0

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-33	GLU	-	expression tag	UNP Q15858
A	-32	LYS	-	expression tag	UNP Q15858
A	-31	GLY	-	expression tag	UNP Q15858
A	-30	GLY	-	expression tag	UNP Q15858
A	-29	GLY	-	expression tag	UNP Q15858
A	-28	ALA	-	expression tag	UNP Q15858
A	-27	ARG	-	expression tag	UNP Q15858
A	-26	GLY	-	expression tag	UNP Q15858
A	-25	GLY	-	expression tag	UNP Q15858
A	-24	SER	-	expression tag	UNP Q15858
A	-23	GLY	-	expression tag	UNP Q15858
A	-22	GLY	-	expression tag	UNP Q15858
A	-21	GLY	-	expression tag	UNP Q15858
A	-20	SER	-	expression tag	UNP Q15858
A	-19	TRP	-	expression tag	UNP Q15858
A	-18	SER	-	expression tag	UNP Q15858
A	-17	HIS	-	expression tag	UNP Q15858
A	-16	PRO	-	expression tag	UNP Q15858
A	-15	GLN	-	expression tag	UNP Q15858
A	-14	PHE	-	expression tag	UNP Q15858
A	-13	GLU	-	expression tag	UNP Q15858
A	-12	LYS	-	expression tag	UNP Q15858
A	-11	GLY	-	expression tag	UNP Q15858
A	-10	PHE	-	expression tag	UNP Q15858
A	-9	ASP	-	expression tag	UNP Q15858
A	-8	TYR	-	expression tag	UNP Q15858
A	-7	LYS	-	expression tag	UNP Q15858
A	-6	ASP	-	expression tag	UNP Q15858

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	ASP	-	expression tag	UNP Q15858
A	-4	ASP	-	expression tag	UNP Q15858
A	-3	ASP	-	expression tag	UNP Q15858
A	-2	LYS	-	expression tag	UNP Q15858
A	-1	GLY	-	expression tag	UNP Q15858
A	0	THR	-	expression tag	UNP Q15858
A	156	LYS	GLU	engineered mutation	UNP Q15858
A	779	ARG	GLY	engineered mutation	UNP Q15858
A	866	PHE	LEU	engineered mutation	UNP Q15858
A	870	MET	THR	engineered mutation	UNP Q15858
A	874	PHE	ALA	engineered mutation	UNP Q15858
A	947	PHE	VAL	engineered mutation	UNP Q15858
A	952	PHE	MET	engineered mutation	UNP Q15858
A	953	PHE	VAL	engineered mutation	UNP Q15858
A	1438	ILE	VAL	engineered mutation	UNP Q15858
A	1439	PHE	VAL	engineered mutation	UNP Q15858
A	1454	CYS	GLY	engineered mutation	UNP Q15858

- 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.

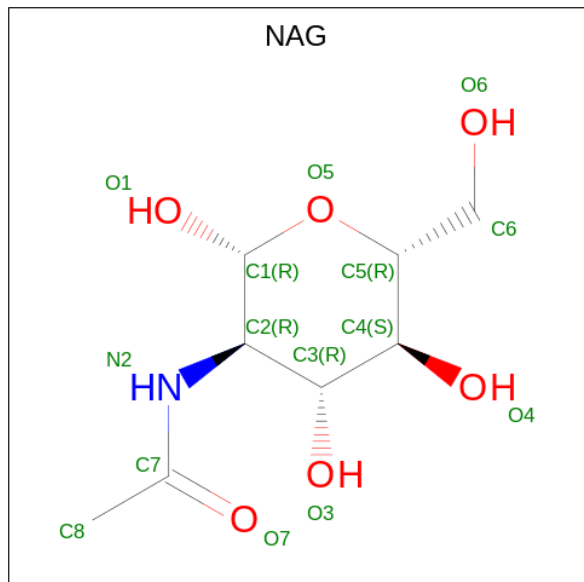
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	120	980	614	173	182	11	0	0

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



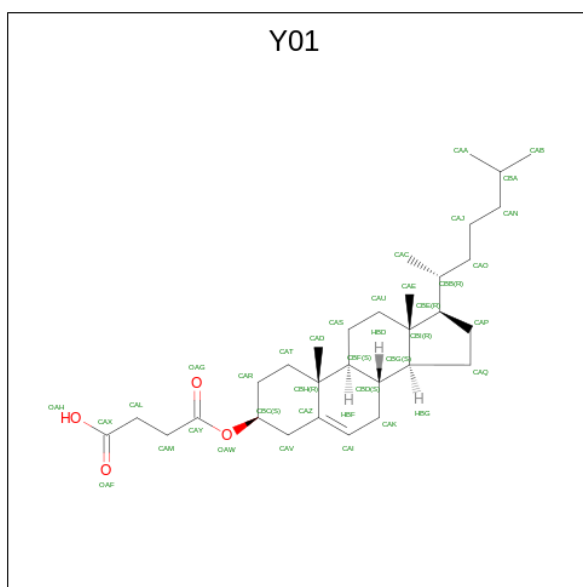
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	2	28	16	2	10	0	0
4	E	2	28	16	2	10	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



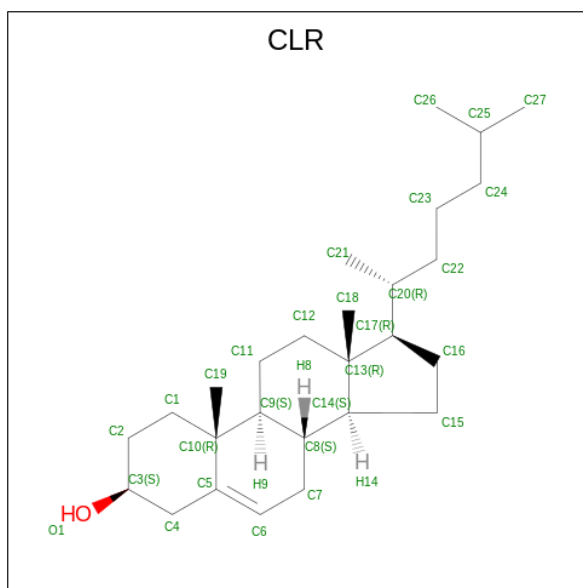
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 6 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula:  $C_{31}H_{50}O_4$ ).



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

- Molecule 7 is CHOLESTEROL (three-letter code: CLR) (formula:  $C_{27}H_{46}O$ ).



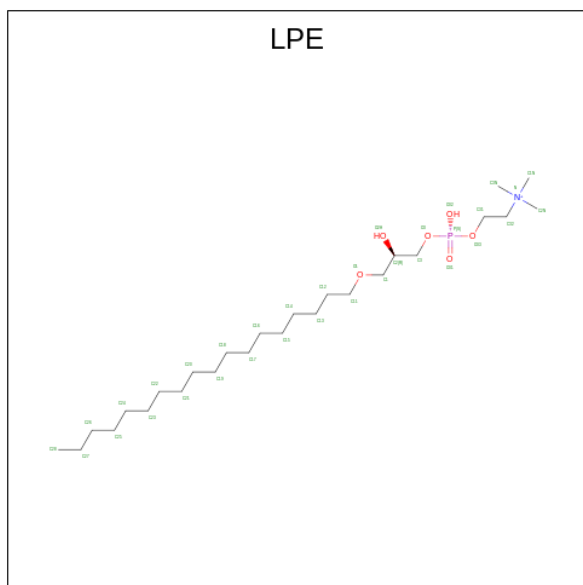
Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			28	27	1	
7	A	1	Total	C	O	0
			28	27	1	
7	A	1	Total	C	O	0
			28	27	1	

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

- Molecule 8 is 1-O-OCTADECYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: LPE) (formula: C<sub>26</sub>H<sub>57</sub>NO<sub>6</sub>P).



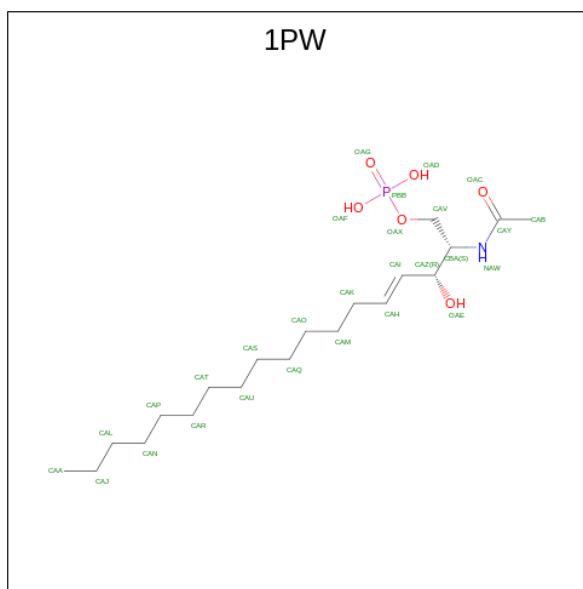
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
8	A	1	25	17	1	6	1	0
8	A	1	25	17	1	6	1	0
8	A	1	20	12	1	6	1	0
8	A	1	28	20	1	6	1	0
8	A	1	28	20	1	6	1	0
8	A	1	25	17	1	6	1	0
8	A	1	25	17	1	6	1	0
8	A	1	25	17	1	6	1	0
8	A	1	25	17	1	6	1	0
8	A	1	25	17	1	6	1	0

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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
			25	17	1	6	1	
8	A	1	Total	C	N	O	P	0
			17	9	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
			17	9	1	6	1	
8	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
8	B	1	Total	C	N	O	P	0
			17	9	1	6	1	

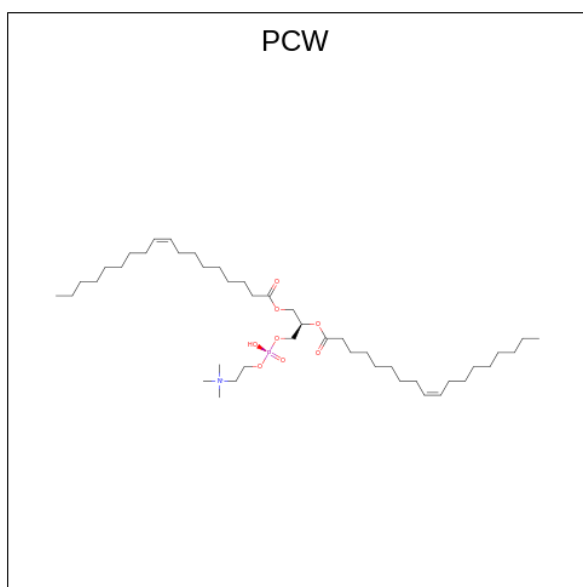
- Molecule 9 is (2S,3R,4E)-2-(acetylamino)-3-hydroxyoctadec-4-en-1-yl dihydrogen phosphate (three-letter code: 1PW) (formula: C<sub>20</sub>H<sub>40</sub>NO<sub>6</sub>P).



Mol	Chain	Residues	Atoms			AltConf	
9	A	1	Total	C	O	P	0
			24	18	5	1	

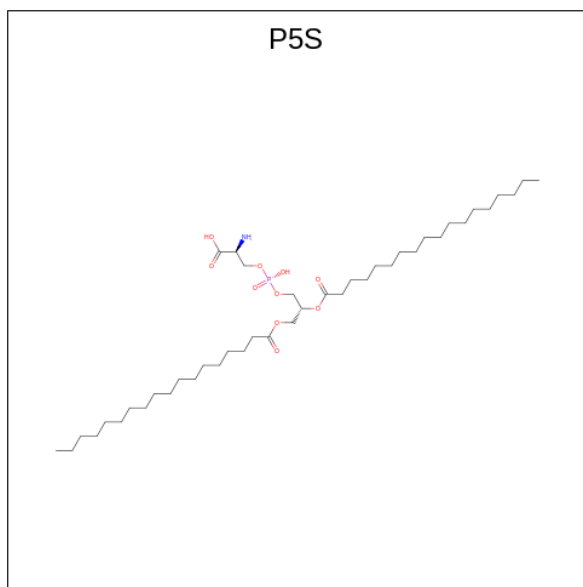
- Molecule 10 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: C<sub>44</sub>H<sub>85</sub>NO<sub>8</sub>P).





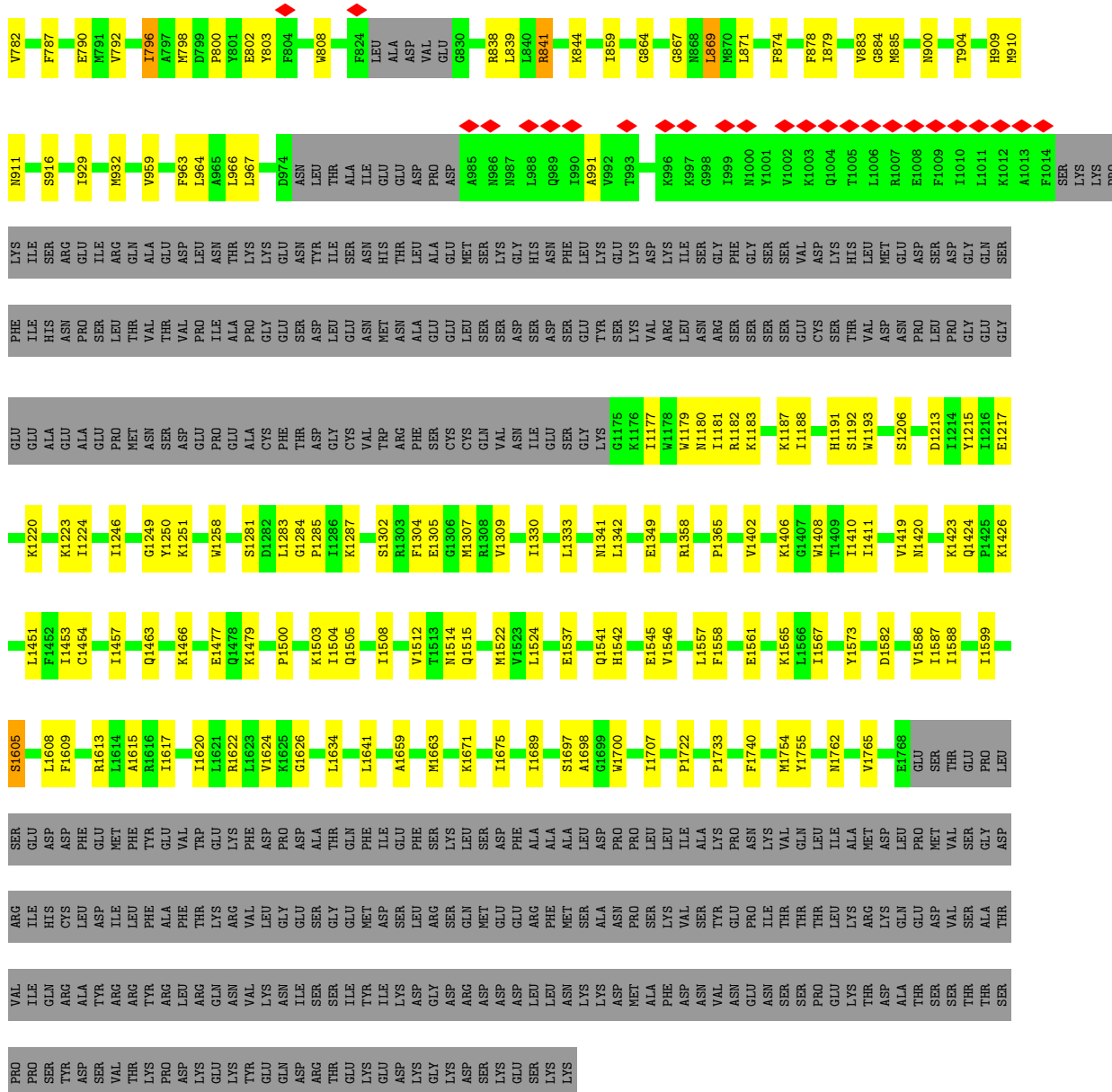
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
10	A	1	53	43	1	8	1	0
10	A	1	47	37	1	8	1	0
10	A	1	44	34	1	8	1	0
10	A	1	44	34	1	8	1	0
10	A	1	44	34	1	8	1	0
10	A	1	44	34	1	8	1	0

- Molecule 11 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).

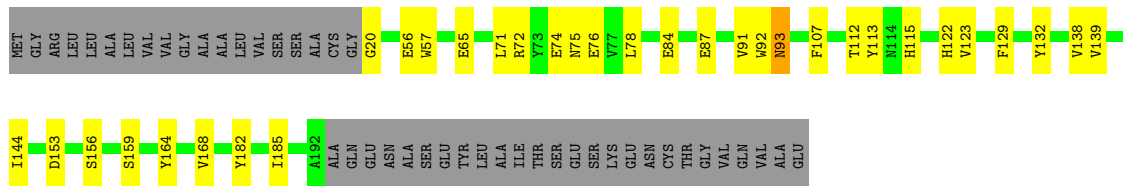


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
11	A	1	34	22	1	10	1	0

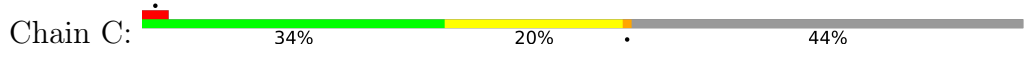


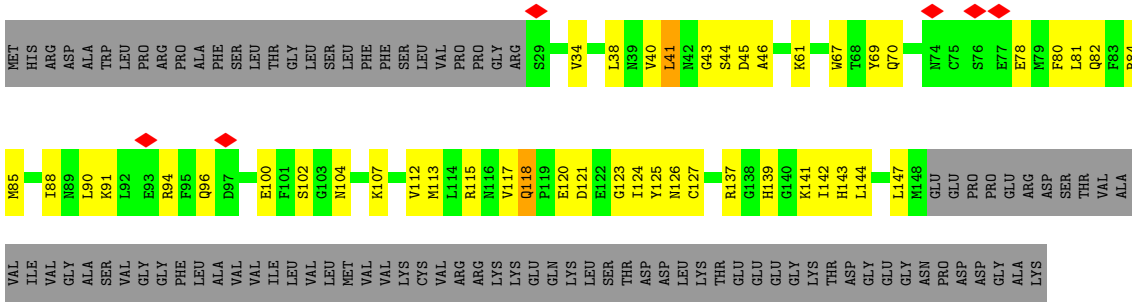


● Molecule 2: Sodium channel subunit beta-1



● 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

Chain D: 100%



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

Chain E: 50%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	249473	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	5.056	Depositor
Minimum map value	-2.043	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.076	Depositor
Recommended contour level	0.36	Depositor
Map size (Å)	346.4, 346.4, 346.4	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0825, 1.0825, 1.0825	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: Y01, 1PW, PCW, CLR, NAG, LPE, P5S

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	0.51	0/10461	0.56	0/14172
2	B	0.54	0/1442	0.53	0/1949
3	C	0.45	0/1002	0.61	0/1354
All	All	0.51	0/12905	0.56	0/17475

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	10209	0	10321	226	0
2	B	1416	0	1380	21	0
3	C	980	0	941	53	0
4	D	28	0	25	0	0
4	E	28	0	25	1	0
5	A	28	0	26	0	0
5	B	56	0	52	1	0
5	C	14	0	13	2	0
6	A	35	0	41	13	0
7	A	112	0	184	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	402	0	546	36	0
8	B	17	0	19	2	0
9	A	24	0	33	0	0
10	A	276	0	383	15	0
11	A	34	0	34	2	0
All	All	13659	0	14023	341	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 12.

All (341) 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)
6:A:2003:Y01:CAK	6:A:2003:Y01:CAI	1.74	1.65
6:A:2003:Y01:CAZ	6:A:2003:Y01:CAV	1.78	1.60
1:A:89:ILE:HD11	1:A:99:ARG:NH1	1.60	1.15
3:C:104:ASN:ND2	3:C:107:LYS:HG3	1.64	1.12
1:A:874[A]:PHE:CD1	7:A:2004:CLR:H272	1.86	1.11
1:A:140:CYS:SG	1:A:878:PHE:HE2	1.78	1.06
3:C:104:ASN:HD22	3:C:107:LYS:CD	1.74	1.00
1:A:162:ILE:HG12	8:A:2030:LPE:H151	1.46	0.96
1:A:874[A]:PHE:CD1	7:A:2004:CLR:C27	2.51	0.92
6:A:2003:Y01:CAI	6:A:2003:Y01:CBF	2.37	0.92
1:A:808:TRP:CZ2	1:A:841:ARG:HG3	2.06	0.90
1:A:800:PRO:HA	1:A:803:TYR:HD2	1.36	0.89
3:C:104:ASN:HD22	3:C:107:LYS:CG	1.84	0.89
1:A:750:ILE:HD12	1:A:790:GLU:OE2	1.71	0.89
1:A:140:CYS:HG	1:A:878:PHE:HE2	0.91	0.89
3:C:104:ASN:ND2	3:C:107:LYS:CG	2.36	0.88
1:A:808:TRP:CH2	1:A:841:ARG:HA	2.08	0.87
1:A:808:TRP:CZ2	1:A:841:ARG:HA	2.10	0.86
1:A:140:CYS:SG	1:A:878:PHE:CE2	2.69	0.85
1:A:874[A]:PHE:HD1	7:A:2004:CLR:H272	1.41	0.84
1:A:162:ILE:CG1	8:A:2030:LPE:H151	2.08	0.83
1:A:808:TRP:CZ2	1:A:841:ARG:CG	2.63	0.81
6:A:2003:Y01:CAI	6:A:2003:Y01:CAV	2.55	0.81
6:A:2003:Y01:CAV	6:A:2003:Y01:CBH	2.55	0.81
1:A:808:TRP:HZ2	1:A:841:ARG:CG	1.93	0.80
3:C:40:VAL:CG1	3:C:117:VAL:HG11	2.12	0.80
1:A:874[B]:PHE:CD2	7:A:2004:CLR:H273	2.17	0.80
1:A:1762:ASN:HA	1:A:1765:VAL:HG12	1.61	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:800:PRO:HA	1:A:803:TYR:CD2	2.17	0.79
1:A:750:ILE:CD1	1:A:790:GLU:OE2	2.33	0.77
1:A:219:LEU:HA	1:A:222:LEU:HD12	1.68	0.76
1:A:874[B]:PHE:CG	7:A:2004:CLR:C27	2.70	0.75
1:A:874[A]:PHE:CG	7:A:2004:CLR:C27	2.70	0.75
3:C:104:ASN:HD22	3:C:107:LYS:HD2	1.49	0.74
1:A:874[A]:PHE:CG	7:A:2004:CLR:H272	2.21	0.74
1:A:162:ILE:HG12	8:A:2030:LPE:C15	2.18	0.74
1:A:874[B]:PHE:CB	7:A:2004:CLR:C27	2.67	0.73
1:A:60:PRO:HB2	1:A:62:ILE:HG12	1.70	0.73
3:C:40:VAL:HG11	3:C:117:VAL:HG11	1.71	0.72
1:A:307:GLU:OE1	1:A:307:GLU:HA	1.88	0.71
1:A:1191:HIS:HD2	1:A:1193:TRP:H	1.38	0.71
3:C:38:LEU:HG	3:C:144:LEU:HG	1.72	0.71
1:A:388:LEU:O	1:A:392:TYR:HB3	1.90	0.70
1:A:101:ASN:ND2	1:A:103:THR:HB	2.06	0.70
6:A:2003:Y01:CAK	6:A:2003:Y01:CAZ	2.53	0.69
1:A:47:PRO:HB2	1:A:81:TYR:CE2	2.27	0.69
1:A:162:ILE:HG13	8:A:2030:LPE:H141	1.75	0.69
1:A:874[A]:PHE:CB	7:A:2004:CLR:C27	2.71	0.69
1:A:163:TYR:O	1:A:166:GLU:HB3	1.92	0.69
1:A:67:PRO:HB2	1:A:70:MET:HG3	1.75	0.69
1:A:874[B]:PHE:CB	7:A:2004:CLR:H272	2.22	0.69
1:A:869:LEU:HD12	1:A:869:LEU:O	1.94	0.68
1:A:874[A]:PHE:HB2	7:A:2004:CLR:H272	1.75	0.68
1:A:91:LEU:HD23	1:A:97:ILE:HA	1.74	0.68
3:C:100:GLU:O	3:C:112:VAL:HG13	1.93	0.68
3:C:102:SER:OG	3:C:113:MET:HB2	1.94	0.67
1:A:120:ILE:HD13	1:A:173:ALA:HB1	1.76	0.66
1:A:874[A]:PHE:CB	7:A:2004:CLR:H272	2.25	0.66
1:A:59:LEU:HD22	1:A:91:LEU:HD13	1.76	0.66
1:A:787:PHE:O	1:A:790:GLU:HG2	1.95	0.66
1:A:1508:ILE:O	1:A:1512:VAL:HG22	1.96	0.66
1:A:196:ILE:HG12	1:A:200:TYR:CE2	2.30	0.66
10:A:2009:PCW:H412	10:A:2009:PCW:H20	1.78	0.65
1:A:89:ILE:HD11	1:A:99:ARG:HH11	1.59	0.65
1:A:89:ILE:CD1	1:A:99:ARG:NH1	2.51	0.65
1:A:348:SER:HB2	10:A:2012:PCW:H321	1.78	0.65
1:A:30:ARG:NH2	1:A:84:ASP:OD2	2.29	0.65
2:B:123:VAL:HB	2:B:138:VAL:HG13	1.77	0.65
3:C:70:GLN:HB2	3:C:124:ILE:HB	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ILE:HG13	8:A:2030:LPE:C14	2.26	0.65
1:A:874[B]:PHE:CG	7:A:2004:CLR:H273	2.32	0.65
1:A:808:TRP:HH2	1:A:841:ARG:HA	1.63	0.64
2:B:74:GLU:HG3	2:B:75:ASN:H	1.61	0.64
1:A:808:TRP:NE1	1:A:844:LYS:HD2	2.14	0.63
1:A:1305:GLU:O	1:A:1309:VAL:HG13	1.97	0.63
1:A:778:ILE:O	1:A:782:VAL:HG23	1.98	0.63
3:C:38:LEU:HB3	3:C:144:LEU:HA	1.80	0.63
1:A:158:THR:HA	8:A:2030:LPE:H12	1.80	0.62
1:A:196:ILE:HG12	1:A:200:TYR:HE2	1.62	0.62
1:A:751:THR:HG23	1:A:841:ARG:HH21	1.63	0.62
1:A:1707:ILE:HD12	1:A:1740:PHE:HE2	1.64	0.62
1:A:900:ASN:ND2	1:A:904:THR:O	2.33	0.62
1:A:1504:ILE:HD12	1:A:1504:ILE:H	1.65	0.62
1:A:1565:LYS:HE3	1:A:1573:TYR:HE2	1.65	0.62
1:A:808:TRP:HZ2	1:A:841:ARG:HG2	1.65	0.61
2:B:65:GLU:N	2:B:65:GLU:OE1	2.34	0.61
3:C:147:LEU:HD12	3:C:147:LEU:O	1.99	0.61
2:B:91:VAL:HG12	2:B:92:TRP:N	2.15	0.61
1:A:874[B]:PHE:HB3	7:A:2004:CLR:H272	1.81	0.60
2:B:164:TYR:O	2:B:168:VAL:HG12	2.01	0.60
1:A:9:PRO:HB3	1:A:63:TYR:O	2.01	0.60
2:B:57:TRP:HB2	2:B:71:LEU:HG	1.81	0.60
1:A:50:SER:HB2	1:A:53:LEU:HB2	1.84	0.59
1:A:750:ILE:HG21	1:A:790:GLU:OE1	2.02	0.59
1:A:1365:PRO:HG3	4:E:1:NAG:H61	1.83	0.59
1:A:1641:LEU:HD22	8:A:2015:LPE:H162	1.83	0.59
1:A:1762:ASN:HA	1:A:1765:VAL:CG1	2.31	0.59
1:A:758:THR:HA	1:A:761:MET:HE2	1.84	0.58
8:A:2005:LPE:H122	8:A:2008:LPE:H322	1.85	0.58
8:A:2006:LPE:H21	10:A:2009:PCW:H152	1.84	0.58
1:A:967:LEU:HB3	1:A:1454:CYS:SG	2.43	0.58
1:A:47:PRO:HB2	1:A:81:TYR:CD2	2.39	0.58
1:A:410:GLN:O	1:A:413:ILE:HG13	2.02	0.58
1:A:89:ILE:HG12	1:A:99:ARG:HG3	1.86	0.58
3:C:91:LYS:O	3:C:91:LYS:HG3	2.05	0.57
1:A:196:ILE:CG1	1:A:200:TYR:HE2	2.17	0.57
3:C:40:VAL:HG12	3:C:117:VAL:HG11	1.86	0.57
3:C:38:LEU:CD2	3:C:144:LEU:HD12	2.35	0.57
3:C:81:LEU:HD22	3:C:112:VAL:HG21	1.87	0.56
3:C:34:VAL:HB	3:C:142:ILE:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:ILE:O	1:A:390:SER:HB3	2.05	0.56
1:A:1477:GLU:HB2	8:A:2015:LPE:H3N3	1.88	0.56
1:A:874[A]:PHE:HB2	7:A:2004:CLR:C27	2.34	0.56
1:A:157:TYR:O	1:A:160:THR:OG1	2.21	0.56
1:A:808:TRP:HZ2	1:A:841:ARG:HA	1.68	0.56
1:A:1605:SER:OG	1:A:1608:LEU:HB2	2.05	0.55
1:A:867:GLY:HA3	7:A:2004:CLR:H122	1.88	0.55
1:A:909:HIS:HD2	1:A:911:ASN:H	1.55	0.55
2:B:129:PHE:HB2	2:B:132:TYR:HB3	1.88	0.55
3:C:123:GLY:O	3:C:143:HIS:ND1	2.39	0.55
1:A:162:ILE:CG1	8:A:2030:LPE:C15	2.79	0.55
8:A:2017:LPE:H3N2	8:A:2018:LPE:H121	1.88	0.55
3:C:82:GLN:HG3	3:C:90:LEU:HD21	1.88	0.55
1:A:196:ILE:O	1:A:200:TYR:HD2	1.90	0.55
3:C:91:LYS:NZ	3:C:96:GLN:O	2.37	0.54
1:A:91:LEU:CD2	1:A:97:ILE:HA	2.37	0.54
1:A:216:PHE:O	1:A:219:LEU:HB2	2.08	0.54
1:A:874[A]:PHE:CG	7:A:2004:CLR:H271	2.41	0.53
1:A:874[A]:PHE:CD1	7:A:2004:CLR:H271	2.41	0.53
3:C:137:ARG:HE	5:C:301:NAG:H62	1.73	0.53
1:A:808:TRP:HE1	1:A:844:LYS:HD2	1.72	0.53
3:C:124:ILE:C	3:C:125:TYR:HD2	2.12	0.53
1:A:143:MET:O	1:A:885:MET:HE1	2.08	0.53
2:B:75:ASN:OD1	2:B:76:GLU:N	2.42	0.53
1:A:839:LEU:HD13	1:A:1330:ILE:HG23	1.91	0.53
1:A:1213:ASP:OD2	1:A:1215:TYR:HB2	2.09	0.53
1:A:798:MET:HG2	1:A:802:GLU:HB2	1.91	0.53
1:A:1182:ARG:NH1	8:A:2026:LPE:H122	2.22	0.53
1:A:1188:ILE:HA	8:A:2032:LPE:H2N2	1.92	0.52
1:A:1177:ILE:O	1:A:1181:ILE:HG12	2.09	0.52
3:C:40:VAL:HG11	3:C:46:ALA:HB2	1.90	0.52
1:A:351:PHE:HE1	10:A:2012:PCW:H412	1.74	0.52
1:A:1567:ILE:HG22	11:A:2031:P5S:H20A	1.91	0.52
3:C:61:LYS:HA	3:C:85:MET:SD	2.50	0.52
1:A:99:ARG:HD2	1:A:181:PHE:CZ	2.45	0.52
2:B:153:ASP:OD1	2:B:153:ASP:N	2.38	0.51
3:C:38:LEU:HD23	3:C:144:LEU:HD12	1.92	0.51
1:A:874[B]:PHE:HB3	7:A:2004:CLR:C27	2.38	0.51
1:A:1333:LEU:HD22	6:A:2003:Y01:HAB2	1.93	0.51
1:A:1181:ILE:HD12	8:B:301:LPE:H32	1.91	0.51
1:A:222:LEU:C	1:A:224:THR:H	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1514:ASN:OD1	1:A:1515:GLN:N	2.43	0.51
1:A:859:ILE:HD11	1:A:1451:LEU:HD21	1.93	0.50
1:A:792:VAL:O	1:A:796:ILE:HG22	2.11	0.50
1:A:231:LEU:HD11	1:A:871:LEU:HD23	1.93	0.50
1:A:1180:ASN:HB3	2:B:182:TYR:HE1	1.77	0.50
1:A:59:LEU:HD22	1:A:91:LEU:CD1	2.40	0.50
1:A:161:GLY:HA3	8:A:2030:LPE:H122	1.94	0.50
1:A:869:LEU:HD11	1:A:959:VAL:HG13	1.94	0.50
1:A:1249:GLY:HA2	8:A:2026:LPE:H141	1.94	0.49
3:C:67:TRP:CE2	3:C:127:CYS:HB3	2.47	0.49
1:A:356:ARG:HD2	1:A:929:ILE:HD13	1.93	0.49
1:A:154:ASN:O	1:A:158:THR:OG1	2.27	0.49
1:A:100:PHE:HD1	1:A:174:ARG:HB3	1.76	0.49
1:A:92:ASN:C	1:A:94:GLY:H	2.15	0.49
1:A:1500:PRO:HG3	1:A:1505:GLN:HG2	1.95	0.49
3:C:137:ARG:NE	5:C:301:NAG:H62	2.28	0.49
1:A:217:ARG:NH2	1:A:220:ARG:HH12	2.11	0.49
2:B:112:THR:HG22	2:B:113:TYR:H	1.78	0.49
2:B:115:HIS:O	2:B:144:ILE:HD11	2.13	0.49
1:A:1659:ALA:O	1:A:1663:MET:HG3	2.13	0.49
1:A:89:ILE:HD11	1:A:99:ARG:HH12	1.67	0.48
1:A:1588:ILE:HG22	1:A:1615:ALA:HB1	1.95	0.48
8:B:301:LPE:H312	8:B:301:LPE:H3N2	1.57	0.48
3:C:44:SER:O	3:C:117:VAL:HG12	2.14	0.48
3:C:104:ASN:HB3	3:C:107:LYS:HB2	1.95	0.48
1:A:1402:VAL:HA	1:A:1408:TRP:HB3	1.95	0.48
1:A:1410:ILE:HD12	1:A:1411:ILE:HG13	1.95	0.48
3:C:45:ASP:HB3	3:C:113:MET:CE	2.44	0.48
1:A:320:ASP:HB3	8:A:2017:LPE:H2N3	1.95	0.48
1:A:879:ILE:O	1:A:883:VAL:HG23	2.13	0.48
1:A:1609:PHE:CE2	1:A:1613:ARG:HD2	2.49	0.48
1:A:1733:PRO:HD2	8:A:2006:LPE:N	2.28	0.48
1:A:1542:HIS:O	1:A:1546:VAL:HG12	2.14	0.47
1:A:1419:VAL:HG21	1:A:1426:LYS:HD3	1.96	0.47
2:B:78:LEU:CD1	2:B:92:TRP:HB2	2.45	0.47
1:A:1284:GLY:HA2	1:A:1287:LYS:NZ	2.29	0.47
1:A:215:THR:O	1:A:218:VAL:HG22	2.14	0.47
1:A:1220:LYS:O	1:A:1224:ILE:HG12	2.15	0.47
1:A:203:GLU:HG2	1:A:204:PHE:CE1	2.50	0.47
1:A:1179:TRP:HD1	1:A:1183:LYS:HZ3	1.61	0.47
1:A:1410:ILE:HD12	1:A:1411:ILE:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:91:VAL:CG1	2:B:92:TRP:N	2.77	0.47
2:B:84:GLU:HA	2:B:87:GLU:HG2	1.97	0.47
3:C:61:LYS:O	3:C:84:ARG:NH1	2.47	0.47
1:A:387:PHE:HA	1:A:391:PHE:HD2	1.80	0.47
10:A:2013:PCW:H122	10:A:2013:PCW:H151	1.73	0.47
5:B:305:NAG:O7	5:B:305:NAG:O3	2.32	0.47
1:A:884:GLY:HA3	1:A:910:MET:HE1	1.97	0.46
1:A:1182:ARG:HG3	1:A:1246:ILE:O	2.15	0.46
1:A:1304:PHE:HB2	1:A:1307:MET:HG3	1.97	0.46
3:C:126:ASN:OD1	3:C:139:HIS:NE2	2.46	0.46
10:A:2014:PCW:H121	10:A:2028:PCW:H32	1.96	0.46
1:A:104:PRO:HB2	1:A:107:TYR:HA	1.98	0.46
1:A:222:LEU:HD22	1:A:231:LEU:HD13	1.97	0.46
1:A:1246:ILE:HG12	8:A:2026:LPE:H182	1.97	0.46
7:A:2021:CLR:H222	7:A:2021:CLR:H162	1.77	0.46
3:C:70:GLN:CB	3:C:124:ILE:HB	2.45	0.46
1:A:311:ASP:OD2	1:A:335:ARG:NH2	2.48	0.45
1:A:1671:LYS:HG2	1:A:1675:ILE:HG22	1.98	0.45
1:A:1424:GLN:HE21	1:A:1424:GLN:HB2	1.59	0.45
3:C:104:ASN:HD22	3:C:107:LYS:CE	2.29	0.45
1:A:1524:LEU:HD13	1:A:1557:LEU:HD13	1.99	0.45
1:A:213:LEU:HD22	1:A:216:PHE:CE2	2.52	0.45
1:A:1217:GLU:OE2	1:A:1217:GLU:HA	2.17	0.45
3:C:84:ARG:HD2	3:C:84:ARG:HA	1.79	0.45
1:A:298:ASP:OD2	1:A:298:ASP:N	2.47	0.45
8:A:2026:LPE:H2N2	8:A:2026:LPE:H312	1.60	0.45
2:B:93:ASN:OD1	2:B:107:PHE:HB2	2.17	0.45
3:C:41:LEU:CD1	3:C:147:LEU:HD11	2.47	0.45
3:C:41:LEU:HD13	3:C:147:LEU:HD11	1.98	0.45
1:A:1187:LYS:HE2	2:B:185:ILE:HD12	1.98	0.45
1:A:1251:LYS:HB3	1:A:1251:LYS:HE2	1.87	0.44
2:B:56:GLU:HG2	2:B:72:ARG:HG3	1.99	0.44
3:C:41:LEU:HD13	3:C:147:LEU:CD1	2.48	0.44
3:C:43:GLY:HA2	3:C:118:GLN:HE22	1.81	0.44
1:A:367:TYR:OH	1:A:1689:ILE:HG23	2.17	0.44
1:A:1406:LYS:HE2	1:A:1698:ALA:HA	1.99	0.44
8:A:2008:LPE:H1N2	8:A:2008:LPE:H311	1.64	0.44
8:A:2032:LPE:H3N2	8:A:2032:LPE:H312	1.71	0.44
6:A:2003:Y01:CAV	6:A:2003:Y01:CAD	2.95	0.44
2:B:122:HIS:ND1	2:B:139:VAL:HG22	2.32	0.44
3:C:45:ASP:OD2	3:C:115:ARG:NH1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:2018:LPE:H1N2	8:A:2018:LPE:H312	1.71	0.44
1:A:272:LYS:HG3	1:A:336:ASN:ND2	2.33	0.44
1:A:1558:PHE:O	1:A:1561:GLU:HG3	2.17	0.44
1:A:1634:LEU:HB3	10:A:2013:PCW:H351	2.00	0.44
1:A:775:VAL:O	1:A:778:ILE:HG13	2.17	0.44
1:A:808:TRP:CE2	1:A:841:ARG:HG3	2.50	0.44
1:A:60:PRO:CB	1:A:62:ILE:HG12	2.42	0.43
1:A:1609:PHE:CZ	1:A:1613:ARG:HD2	2.53	0.43
1:A:89:ILE:CG1	1:A:99:ARG:HG3	2.48	0.43
3:C:61:LYS:HE2	3:C:61:LYS:HB2	1.90	0.43
6:A:2003:Y01:CAZ	6:A:2003:Y01:CBC	2.79	0.43
1:A:271:LEU:HD12	1:A:343:SER:HA	2.00	0.43
8:A:2010:LPE:H151	8:A:2011:LPE:H192	2.00	0.43
1:A:787:PHE:HA	1:A:790:GLU:CD	2.39	0.43
1:A:1182:ARG:HH12	8:A:2026:LPE:H141	1.84	0.43
1:A:1622:ARG:C	1:A:1624:VAL:H	2.21	0.43
10:A:2014:PCW:H211	10:A:2014:PCW:H182	1.66	0.43
1:A:1582:ASP:O	1:A:1586:VAL:HG23	2.18	0.43
6:A:2003:Y01:HAD1	6:A:2003:Y01:HAV1	2.01	0.43
8:A:2019:LPE:H3N3	8:A:2019:LPE:H311	1.78	0.43
1:A:268:MET:HG2	1:A:1537:GLU:HG2	2.00	0.43
1:A:398:LEU:HD11	1:A:964:LEU:HD23	2.00	0.43
1:A:1522:MET:CE	1:A:1626:GLY:H	2.32	0.43
1:A:1697:SER:O	1:A:1700:TRP:HD1	2.02	0.43
1:A:405:TYR:CE2	1:A:966:LEU:HA	2.54	0.43
1:A:754:ILE:HD13	1:A:838:ARG:HB2	1.99	0.43
1:A:1754:MET:HE3	1:A:1754:MET:HB3	1.89	0.43
2:B:112:THR:HG22	2:B:113:TYR:N	2.33	0.43
1:A:295:SER:O	1:A:299:PHE:HD2	2.00	0.42
1:A:1349:GLU:OE1	1:A:1358:ARG:HD3	2.19	0.42
1:A:396:LEU:HD23	1:A:396:LEU:HA	1.85	0.42
1:A:1191:HIS:CD2	1:A:1193:TRP:H	2.26	0.42
10:A:2014:PCW:H82	10:A:2014:PCW:H41	1.85	0.42
1:A:213:LEU:HD23	1:A:213:LEU:HA	1.84	0.42
1:A:285:THR:H	1:A:288:SER:HB3	1.84	0.42
1:A:1722:PRO:HD2	2:B:20:GLY:O	2.19	0.42
1:A:17:LYS:H	1:A:17:LYS:HG3	1.67	0.42
1:A:187:PRO:HA	1:A:190:TRP:HD1	1.83	0.42
1:A:839:LEU:HD11	1:A:1333:LEU:HD23	2.02	0.42
1:A:1479:LYS:HE3	1:A:1479:LYS:HB2	1.92	0.42
3:C:70:GLN:N	3:C:124:ILE:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:LEU:HD21	1:A:97:ILE:HG12	2.01	0.42
1:A:1258:TRP:HE1	8:A:2011:LPE:H1N3	1.85	0.42
1:A:1599:ILE:HG22	1:A:1599:ILE:O	2.20	0.42
7:A:2021:CLR:H183	7:A:2021:CLR:H20	1.84	0.42
3:C:141:LYS:HB2	3:C:141:LYS:HE2	1.87	0.42
1:A:1206:SER:HB2	8:A:2019:LPE:H112	2.02	0.42
1:A:1342:LEU:HD11	7:A:2021:CLR:H72	2.01	0.42
3:C:112:VAL:HG12	3:C:113:MET:N	2.34	0.42
1:A:101:ASN:HD21	1:A:103:THR:HB	1.80	0.42
1:A:764:GLU:OE1	1:A:1341:ASN:ND2	2.52	0.42
1:A:1220:LYS:O	1:A:1223:LYS:HG2	2.20	0.42
1:A:1617:ILE:O	1:A:1620:ILE:HG12	2.19	0.42
1:A:198:PHE:CZ	1:A:207:LEU:HD23	2.55	0.41
10:A:2029:PCW:H132	10:A:2029:PCW:H32	2.02	0.41
3:C:104:ASN:ND2	3:C:107:LYS:CD	2.59	0.41
3:C:112:VAL:CG1	3:C:113:MET:N	2.83	0.41
1:A:16:THR:O	1:A:17:LYS:C	2.57	0.41
1:A:85:LYS:HB2	1:A:85:LYS:HE2	1.87	0.41
1:A:1420:ASN:HB2	1:A:1423:LYS:HG3	2.01	0.41
3:C:82:GLN:HB2	3:C:88:ILE:HB	2.01	0.41
1:A:23:ILE:HG23	1:A:84:ASP:O	2.20	0.41
1:A:808:TRP:CZ2	1:A:841:ARG:CA	2.93	0.41
1:A:1283:LEU:O	1:A:1285:PRO:HD2	2.21	0.41
8:A:2018:LPE:H141	8:A:2019:LPE:H2N2	2.02	0.41
1:A:120:ILE:CD1	1:A:173:ALA:HB1	2.46	0.41
7:A:2023:CLR:H273	8:A:2025:LPE:H1N2	2.02	0.41
1:A:1250:TYR:HB3	7:A:2023:CLR:H151	2.01	0.41
1:A:222:LEU:C	1:A:224:THR:N	2.74	0.41
1:A:1217:GLU:OE1	1:A:1223:LYS:HE3	2.20	0.41
8:A:2016:LPE:H112	8:A:2016:LPE:H142	1.98	0.41
3:C:38:LEU:HD21	3:C:144:LEU:HD12	2.03	0.41
1:A:744:PRO:HB3	1:A:991:ALA:HB2	2.03	0.41
1:A:864:GLY:HA2	7:A:2004:CLR:H12	2.03	0.41
1:A:1182:ARG:HD3	8:A:2026:LPE:H1N2	2.02	0.41
6:A:2003:Y01:HAO2	6:A:2003:Y01:HAP1	1.32	0.41
7:A:2023:CLR:H222	7:A:2023:CLR:H162	1.84	0.41
3:C:61:LYS:NZ	3:C:61:LYS:H	2.19	0.41
1:A:1463:GLN:O	1:A:1466:LYS:HG2	2.21	0.41
1:A:1541:GLN:O	1:A:1545:GLU:OE2	2.39	0.41
10:A:2009:PCW:H41	10:A:2009:PCW:H63	1.68	0.41
8:A:2024:LPE:H32	8:A:2026:LPE:H121	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:2030:LPE:H1N2	8:A:2030:LPE:H312	1.80	0.41
1:A:743:ASP:HB3	1:A:744:PRO:HD3	2.03	0.41
1:A:808:TRP:HZ2	1:A:841:ARG:CA	2.32	0.41
1:A:1213:ASP:OD2	1:A:1215:TYR:N	2.48	0.41
6:A:2003:Y01:HAC2	6:A:2003:Y01:HAJ1	1.83	0.41
10:A:2012:PCW:H182	10:A:2012:PCW:H211	1.80	0.41
7:A:2021:CLR:H8	7:A:2021:CLR:H182	1.80	0.41
10:A:2029:PCW:H341	11:A:2031:P5S:H44	2.03	0.41
1:A:185:ARG:HD2	1:A:185:ARG:HA	1.94	0.40
1:A:59:LEU:HD12	1:A:60:PRO:HD2	2.03	0.40
1:A:224:THR:HA	1:A:232:LYS:NZ	2.36	0.40
1:A:231:LEU:HD23	1:A:231:LEU:HA	1.90	0.40
1:A:1504:ILE:O	1:A:1508:ILE:HG13	2.21	0.40
10:A:2012:PCW:H83	10:A:2012:PCW:H42	1.60	0.40
8:A:2024:LPE:H2N2	8:A:2024:LPE:H312	1.92	0.40
1:A:1453:ILE:O	1:A:1457:ILE:HG12	2.21	0.40
1:A:1587:ILE:HG21	10:A:2029:PCW:H20	2.03	0.40
8:A:2015:LPE:H1N2	8:A:2015:LPE:H312	1.85	0.40
3:C:67:TRP:HB3	3:C:80:PHE:CE1	2.55	0.40
3:C:69:TYR:HB3	3:C:78:GLU:HG2	2.03	0.40
1:A:761:MET:O	1:A:764:GLU:HG2	2.22	0.40
1:A:1283:LEU:HD12	1:A:1283:LEU:HA	1.95	0.40
1:A:1503:LYS:H	1:A:1503:LYS:HG3	1.68	0.40
3:C:94:ARG:HH22	3:C:121:ASP:HA	1.86	0.40
1:A:345:ASP:HB3	1:A:1537:GLU:HB2	2.04	0.40
6:A:2003:Y01:HAE2	6:A:2003:Y01:HBB	1.66	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	1265/2022 (63%)	1200 (95%)	60 (5%)	5 (0%)	34	60
2	B	171/218 (78%)	163 (95%)	8 (5%)	0	100	100
3	C	118/215 (55%)	106 (90%)	11 (9%)	1 (1%)	19	43
All	All	1554/2455 (63%)	1469 (94%)	79 (5%)	6 (0%)	38	60

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	PHE
1	A	93	LYS
1	A	10	GLN
1	A	52	ASP
1	A	223	LYS
3	C	120	GLU

### 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	1110/1804 (62%)	1095 (99%)	15 (1%)	67	86
2	B	157/190 (83%)	154 (98%)	3 (2%)	57	82
3	C	113/193 (58%)	111 (98%)	2 (2%)	59	83
All	All	1380/2187 (63%)	1360 (99%)	20 (1%)	66	86

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	ASN
1	A	146	ASN
1	A	166	GLU
1	A	780	ASN
1	A	796	ILE
1	A	841	ARG
1	A	869	LEU

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Mol	Chain	Res	Type
1	A	916	SER
1	A	932	MET
1	A	963	PHE
1	A	1192	SER
1	A	1281	SER
1	A	1302	SER
1	A	1605	SER
1	A	1755	TYR
2	B	93	ASN
2	B	156	SER
2	B	159	SER
3	C	41	LEU
3	C	118	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	139	ASN
1	A	147	ASN
1	A	270	ASN
1	A	336	ASN
1	A	395	ASN
1	A	409	ASN
1	A	412	ASN
1	A	765	HIS
1	A	780	ASN
1	A	805	GLN
1	A	861	ASN
1	A	956	ASN
1	A	961	ASN
1	A	1191	HIS
1	A	1276	ASN
1	A	1341	ASN
1	A	1363	GLN
1	A	1424	GLN
1	A	1470	GLN
1	A	1515	GLN
1	A	1541	GLN
1	A	1676	ASN
2	B	134	HIS
3	C	104	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	4,1	14,14,15	0.36	0	17,19,21	0.51	0
4	NAG	D	2	4	14,14,15	0.29	0	17,19,21	0.58	0
4	NAG	E	1	4,1	14,14,15	0.44	0	17,19,21	0.93	1 (5%)
4	NAG	E	2	4	14,14,15	0.30	0	17,19,21	0.79	1 (5%)

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	4,1	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	NAG	E	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1	NAG	C1-O5-C5	2.26	115.25	112.19
4	E	2	NAG	O5-C1-C2	-2.26	107.73	111.29

There are no chirality outliers.

All (6) torsion outliers are listed below:

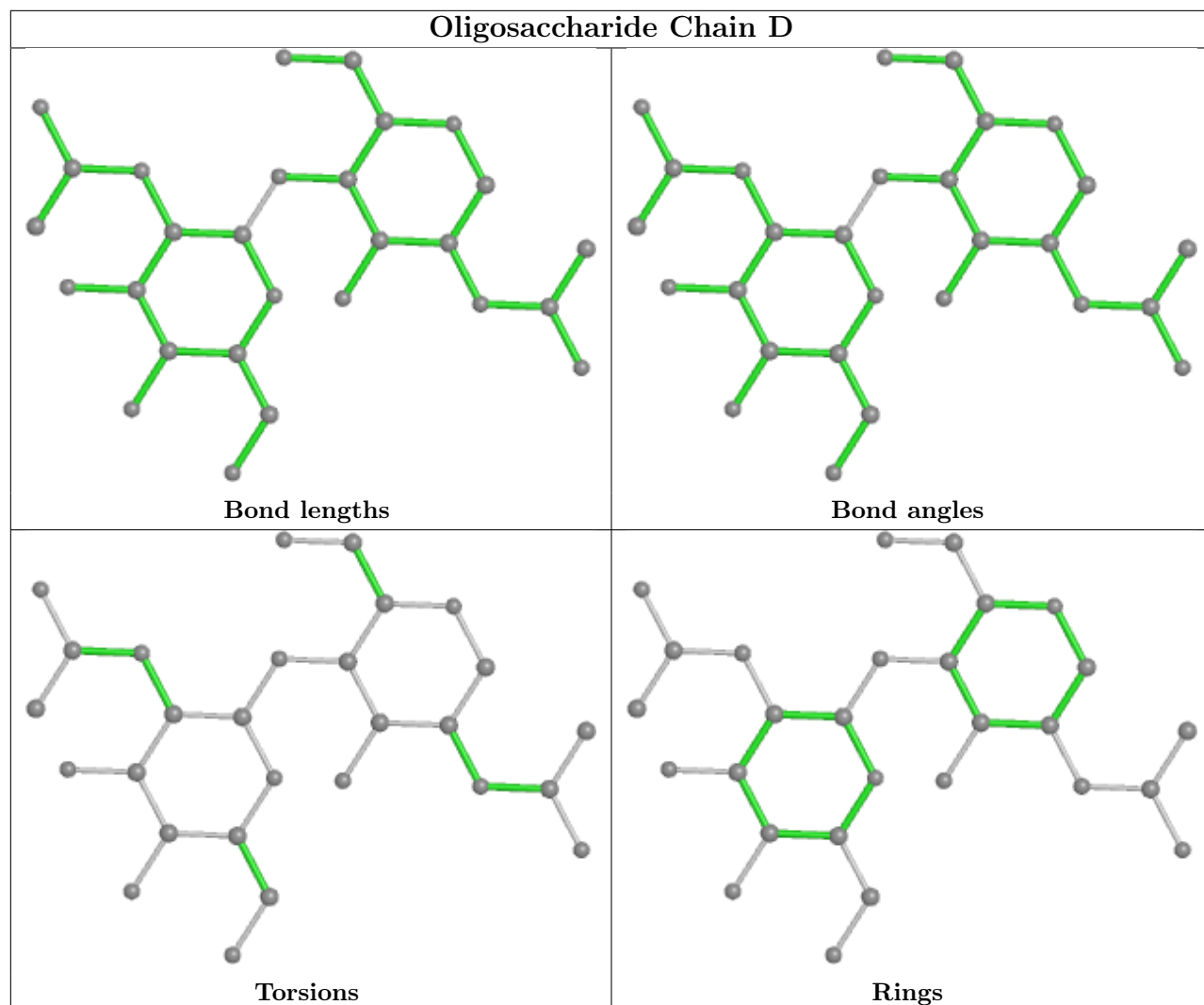
Mol	Chain	Res	Type	Atoms
4	E	1	NAG	C8-C7-N2-C2
4	E	1	NAG	O7-C7-N2-C2
4	E	2	NAG	C8-C7-N2-C2
4	E	2	NAG	O7-C7-N2-C2
4	E	1	NAG	O5-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6

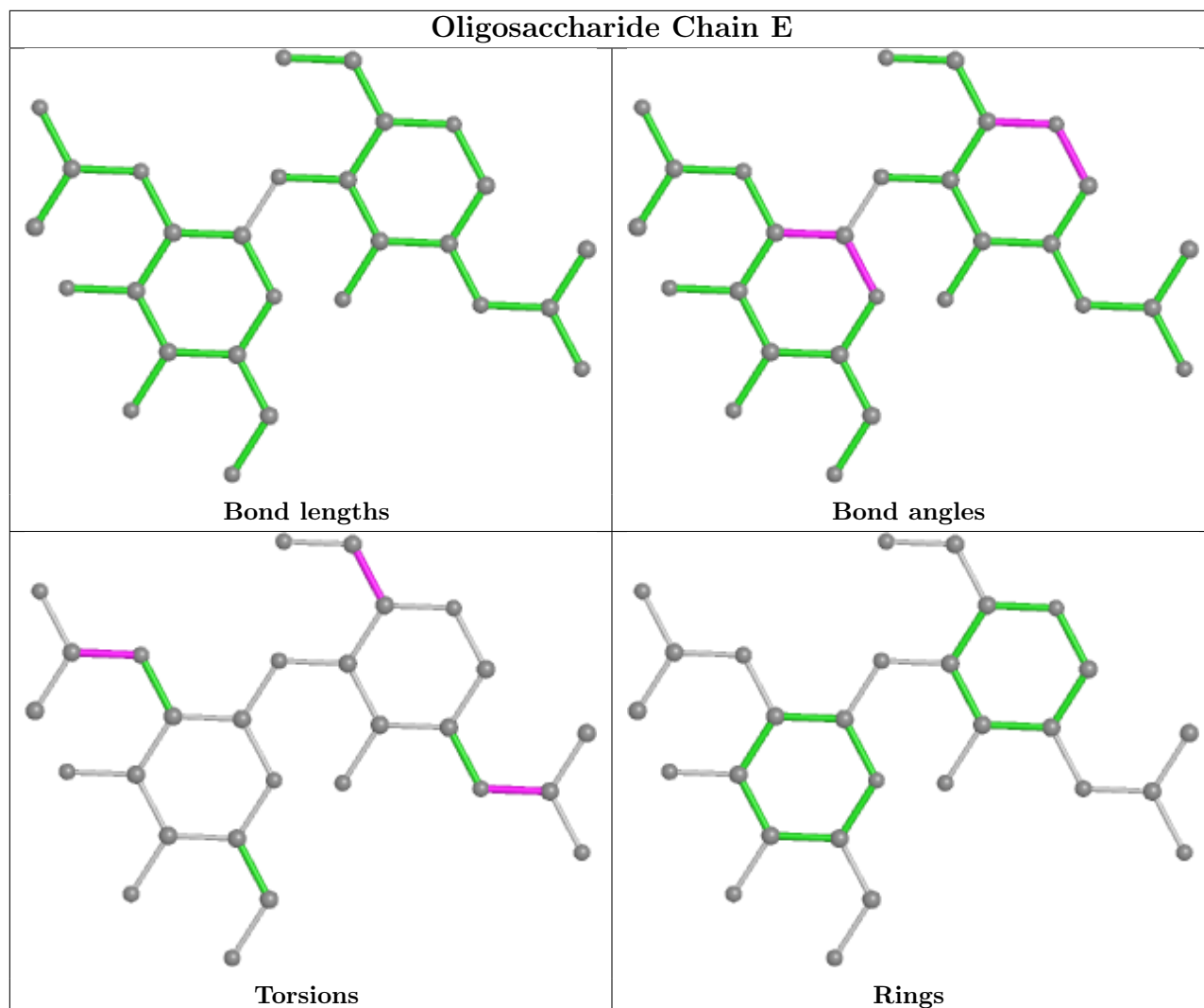
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1	NAG	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 oligosaccharide.





## 5.6 Ligand geometry [i](#)

38 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	2011	-	27,27,33	0.51	0	31,33,39	0.56	0
9	1PW	A	2007	-	23,23,27	0.41	0	24,26,32	0.47	0
10	PCW	A	2029	-	43,43,53	1.05	2 (4%)	49,51,61	1.06	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	CLR	A	2022	-	31,31,31	0.73	0	48,48,48	1.14	4 (8%)
8	LPE	A	2005	-	24,24,33	0.52	0	28,30,39	0.69	0
8	LPE	A	2030	-	24,24,33	0.53	0	28,30,39	0.63	0
7	CLR	A	2023	-	31,31,31	0.70	0	48,48,48	1.12	3 (6%)
5	NAG	B	303	2	14,14,15	0.35	0	17,19,21	0.62	0
8	LPE	A	2015	-	24,24,33	0.53	0	28,30,39	0.60	0
11	P5S	A	2031	-	32,33,53	1.15	2 (6%)	36,40,60	1.87	4 (11%)
10	PCW	A	2014	-	43,43,53	1.06	2 (4%)	49,51,61	1.20	4 (8%)
8	LPE	A	2010	-	27,27,33	0.50	0	31,33,39	0.58	0
5	NAG	A	2001	1	14,14,15	0.28	0	17,19,21	0.56	0
5	NAG	B	302	2	14,14,15	0.28	0	17,19,21	0.60	0
8	LPE	A	2008	-	19,19,33	0.62	0	23,25,39	0.56	0
8	LPE	A	2032	-	16,16,33	0.66	0	20,22,39	0.68	0
8	LPE	A	2026	-	24,24,33	0.87	0	28,30,39	0.91	1 (3%)
5	NAG	B	305	2	14,14,15	0.66	1 (7%)	17,19,21	0.48	0
8	LPE	A	2025	-	16,16,33	0.92	0	20,22,39	1.16	1 (5%)
7	CLR	A	2021	-	31,31,31	0.80	1 (3%)	48,48,48	1.30	7 (14%)
5	NAG	B	304	2	14,14,15	0.29	0	17,19,21	0.63	0
8	LPE	A	2016	-	24,24,33	0.85	0	28,30,39	0.92	1 (3%)
8	LPE	A	2018	-	24,24,33	0.56	0	28,30,39	0.61	1 (3%)
10	PCW	A	2013	-	43,43,53	1.03	2 (4%)	49,51,61	1.03	3 (6%)
8	LPE	A	2006	-	24,24,33	0.33	0	25,27,39	0.61	0
8	LPE	B	301	-	16,16,33	0.94	0	20,22,39	1.05	1 (5%)
8	LPE	A	2020	-	24,24,33	0.54	0	28,30,39	0.59	0
10	PCW	A	2028	-	43,43,53	1.04	2 (4%)	49,51,61	1.07	4 (8%)
10	PCW	A	2009	-	52,52,53	0.92	2 (3%)	58,60,61	0.97	4 (6%)
7	CLR	A	2004	-	31,31,31	0.70	0	48,48,48	0.99	2 (4%)
8	LPE	A	2017	-	24,24,33	0.53	0	28,30,39	0.59	0
8	LPE	A	2027	-	16,16,33	0.62	0	20,22,39	0.62	0
5	NAG	A	2002	1	14,14,15	0.30	0	17,19,21	0.46	0
6	Y01	A	2003	-	38,38,38	7.55	22 (57%)	57,57,57	2.33	13 (22%)
8	LPE	A	2024	-	24,24,33	0.54	0	28,30,39	0.60	0
5	NAG	C	301	3	14,14,15	0.42	0	17,19,21	0.35	0
8	LPE	A	2019	-	24,24,33	0.88	0	28,30,39	0.98	1 (3%)
10	PCW	A	2012	-	46,46,53	0.99	2 (4%)	52,54,61	1.03	3 (5%)

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	2011	-	-	10/28/28/34	-
9	1PW	A	2007	-	-	3/22/22/29	-
10	PCW	A	2029	-	-	11/47/47/57	-
7	CLR	A	2022	-	-	3/10/68/68	0/4/4/4
8	LPE	A	2005	-	-	9/25/25/34	-
8	LPE	A	2030	-	-	6/25/25/34	-
7	CLR	A	2023	-	-	4/10/68/68	0/4/4/4
5	NAG	B	303	2	-	0/6/23/26	0/1/1/1
8	LPE	A	2015	-	-	7/25/25/34	-
11	P5S	A	2031	-	-	14/39/39/59	-
10	PCW	A	2014	-	-	9/47/47/57	-
8	LPE	A	2010	-	-	8/28/28/34	-
5	NAG	A	2001	1	-	2/6/23/26	0/1/1/1
5	NAG	B	302	2	-	3/6/23/26	0/1/1/1
8	LPE	A	2008	-	-	5/20/20/34	-
8	LPE	A	2032	-	-	8/17/17/34	-
8	LPE	A	2026	-	-	16/25/25/34	-
5	NAG	B	305	2	-	4/6/23/26	0/1/1/1
8	LPE	A	2025	-	-	11/17/17/34	-
7	CLR	A	2021	-	-	6/10/68/68	0/4/4/4
5	NAG	B	304	2	-	2/6/23/26	0/1/1/1
8	LPE	A	2016	-	-	12/25/25/34	-
8	LPE	A	2018	-	-	7/25/25/34	-
10	PCW	A	2013	-	-	13/47/47/57	-
8	LPE	A	2006	-	-	13/25/25/34	-
8	LPE	B	301	-	-	9/17/17/34	-
8	LPE	A	2020	-	-	7/25/25/34	-
10	PCW	A	2028	-	-	11/47/47/57	-
10	PCW	A	2009	-	-	9/56/56/57	-
7	CLR	A	2004	-	-	1/10/68/68	0/4/4/4
8	LPE	A	2017	-	-	10/25/25/34	-
8	LPE	A	2027	-	-	7/17/17/34	-
5	NAG	A	2002	1	-	3/6/23/26	0/1/1/1
6	Y01	A	2003	-	-	12/19/77/77	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	LPE	A	2024	-	-	6/25/25/34	-
5	NAG	C	301	3	-	2/6/23/26	0/1/1/1
8	LPE	A	2019	-	-	14/25/25/34	-
10	PCW	A	2012	-	-	13/50/50/57	-

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2003	Y01	CAK-CBD	-25.12	1.10	1.53
6	A	2003	Y01	CBD-CBG	-19.73	1.15	1.53
6	A	2003	Y01	CAU-CAS	-17.98	1.15	1.53
6	A	2003	Y01	CBH-CAZ	-12.96	1.27	1.52
6	A	2003	Y01	CAV-CAZ	12.17	1.78	1.51
6	A	2003	Y01	CAK-CAI	11.32	1.74	1.50
6	A	2003	Y01	CAT-CBH	7.33	1.68	1.54
6	A	2003	Y01	CAT-CAR	7.17	1.68	1.53
6	A	2003	Y01	CAQ-CAP	6.24	1.71	1.54
6	A	2003	Y01	CBI-CBE	6.17	1.66	1.55
6	A	2003	Y01	CBD-CBF	-5.70	1.42	1.53
6	A	2003	Y01	CAQ-CBG	5.01	1.64	1.54
6	A	2003	Y01	CBB-CBE	-4.62	1.46	1.54
6	A	2003	Y01	CAR-CBC	-4.49	1.39	1.51
6	A	2003	Y01	CAU-CBI	-4.46	1.46	1.54
10	A	2014	PCW	O2-C31	4.40	1.46	1.34
10	A	2029	PCW	O3-C11	4.37	1.46	1.33
10	A	2028	PCW	O3-C11	4.36	1.46	1.33
11	A	2031	P5S	O19-C17	4.32	1.46	1.33
10	A	2013	PCW	O3-C11	4.25	1.45	1.33
10	A	2012	PCW	O3-C11	4.24	1.45	1.33
10	A	2009	PCW	O3-C11	4.16	1.45	1.33
10	A	2013	PCW	O2-C31	4.08	1.45	1.34
10	A	2029	PCW	O2-C31	4.07	1.45	1.34
11	A	2031	P5S	O37-C38	4.05	1.45	1.34
10	A	2028	PCW	O2-C31	4.05	1.45	1.34
10	A	2012	PCW	O2-C31	4.01	1.45	1.34
10	A	2009	PCW	O2-C31	3.98	1.45	1.34
10	A	2014	PCW	O3-C11	3.62	1.43	1.33
6	A	2003	Y01	OAW-CAY	3.56	1.44	1.34
6	A	2003	Y01	CBH-CBF	3.55	1.62	1.56
6	A	2003	Y01	CAD-CBH	2.97	1.59	1.54
6	A	2003	Y01	CAV-CBC	2.51	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2003	Y01	CAM-CAY	2.26	1.57	1.50
5	B	305	NAG	O5-C1	-2.11	1.40	1.43
6	A	2003	Y01	CAS-CBF	2.07	1.57	1.53
6	A	2003	Y01	CAL-CAX	2.06	1.55	1.50
7	A	2021	CLR	C13-C14	-2.06	1.51	1.55

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	2031	P5S	OG-CB-CA	8.60	115.56	108.06
6	A	2003	Y01	CAK-CAI-CAZ	-7.08	112.00	125.06
6	A	2003	Y01	CAV-CAZ-CAI	-6.47	111.28	120.61
6	A	2003	Y01	CBH-CAZ-CAI	-6.04	113.66	122.90
6	A	2003	Y01	CAQ-CBG-CBD	-5.30	110.35	119.08
6	A	2003	Y01	CBI-CBE-CBB	-5.18	111.37	119.49
10	A	2014	PCW	O2-C31-C32	4.99	122.26	111.50
10	A	2012	PCW	O2-C31-C32	4.20	120.56	111.50
6	A	2003	Y01	OAW-CAY-CAM	4.17	120.49	111.50
10	A	2013	PCW	O2-C31-C32	4.07	120.27	111.50
8	A	2025	LPE	C3N-N-C2N	4.00	119.26	108.97
8	A	2026	LPE	C3N-N-C2N	3.93	119.08	108.97
8	A	2016	LPE	C3N-N-C2N	3.92	119.05	108.97
8	A	2019	LPE	C3N-N-C2N	3.87	118.92	108.97
8	B	301	LPE	C3N-N-C2N	3.83	118.82	108.97
10	A	2009	PCW	O2-C31-C32	3.81	119.72	111.50
10	A	2028	PCW	O2-C31-C32	3.75	119.59	111.50
10	A	2029	PCW	O2-C31-C32	3.74	119.56	111.50
11	A	2031	P5S	O37-C38-C39	3.55	119.16	111.50
6	A	2003	Y01	CAD-CBH-CBF	-3.46	107.56	111.68
6	A	2003	Y01	CAE-CBI-CBE	-3.36	105.45	111.71
7	A	2021	CLR	C8-C7-C6	-3.25	108.07	112.73
6	A	2003	Y01	CAU-CBI-CBE	3.20	121.36	116.57
10	A	2014	PCW	O3-C11-C12	3.15	121.80	111.91
7	A	2021	CLR	C17-C13-C14	3.11	103.76	100.07
10	A	2028	PCW	O3-C11-C12	2.96	121.19	111.91
6	A	2003	Y01	CAP-CAQ-CBG	-2.92	99.35	105.13
7	A	2021	CLR	C13-C14-C8	-2.90	110.09	114.38
10	A	2029	PCW	O3-C11-C12	2.84	120.82	111.91
6	A	2003	Y01	CAV-CAZ-CBH	-2.81	112.69	116.42
7	A	2023	CLR	C4-C5-C10	2.78	120.11	116.42
10	A	2009	PCW	C2-O2-C31	-2.77	110.98	117.79
7	A	2022	CLR	C8-C7-C6	-2.71	108.83	112.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	2003	Y01	CAQ-CBG-CBI	-2.67	100.63	103.84
7	A	2021	CLR	C13-C17-C20	-2.67	115.31	119.49
10	A	2028	PCW	C2-O2-C31	-2.66	111.23	117.79
11	A	2031	P5S	O19-C17-C20	2.65	120.22	111.91
11	A	2031	P5S	OXT-C-O	-2.59	118.21	124.09
10	A	2012	PCW	O3-C11-C12	2.45	119.58	111.91
10	A	2009	PCW	O3-C11-C12	2.39	119.41	111.91
6	A	2003	Y01	CAC-CBB-CBE	-2.36	109.31	112.92
10	A	2012	PCW	C2-O2-C31	-2.35	112.01	117.79
7	A	2004	CLR	C4-C5-C10	2.33	119.52	116.42
7	A	2004	CLR	C11-C9-C10	-2.31	110.04	113.08
7	A	2021	CLR	C9-C10-C5	2.30	113.26	109.65
7	A	2021	CLR	C19-C10-C9	-2.25	109.00	111.68
10	A	2013	PCW	O3-C11-C12	2.20	118.82	111.91
10	A	2014	PCW	O3-C11-O11	-2.20	118.05	123.59
7	A	2022	CLR	C17-C13-C14	2.14	102.61	100.07
7	A	2021	CLR	C11-C9-C10	-2.12	110.28	113.08
8	A	2018	LPE	C31-C32-N	-2.11	108.75	115.78
7	A	2023	CLR	C13-C17-C20	-2.09	116.21	119.49
10	A	2028	PCW	O2-C31-O31	-2.09	118.65	123.70
10	A	2013	PCW	C2-O2-C31	-2.08	112.66	117.79
7	A	2022	CLR	C13-C14-C8	-2.07	111.32	114.38
10	A	2009	PCW	O2-C31-O31	-2.06	118.72	123.70
7	A	2023	CLR	C4-C5-C6	-2.06	117.64	120.61
10	A	2014	PCW	C3-C2-C1	-2.06	106.93	111.79
7	A	2022	CLR	C19-C10-C9	-2.04	109.25	111.68

There are no chirality outliers.

All (290) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2001	NAG	C8-C7-N2-C2
5	A	2001	NAG	O7-C7-N2-C2
5	B	304	NAG	C8-C7-N2-C2
5	B	304	NAG	O7-C7-N2-C2
6	A	2003	Y01	CAC-CBB-CBE-CBI
6	A	2003	Y01	OAG-CAY-OAW-CBC
8	A	2005	LPE	O33-C31-C32-N
8	A	2006	LPE	O1-C1-C2-C3
8	A	2006	LPE	C31-O33-P-O32
8	A	2006	LPE	O33-C31-C32-N
8	A	2008	LPE	C3-O3-P-O31

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Mol	Chain	Res	Type	Atoms
8	A	2008	LPE	C3-O3-P-O32
8	A	2008	LPE	O33-C31-C32-N
8	A	2010	LPE	C31-O33-P-O31
8	A	2010	LPE	C31-O33-P-O32
8	A	2011	LPE	C3-O3-P-O31
8	A	2011	LPE	C3-O3-P-O32
8	A	2011	LPE	C3-O3-P-O33
8	A	2011	LPE	C31-O33-P-O32
8	A	2015	LPE	C3-O3-P-O33
8	A	2016	LPE	C31-O33-P-O31
8	A	2017	LPE	C3-O3-P-O31
8	A	2017	LPE	C3-O3-P-O32
8	A	2017	LPE	C3-O3-P-O33
8	A	2017	LPE	C31-O33-P-O3
8	A	2018	LPE	C31-O33-P-O3
8	A	2019	LPE	C31-O33-P-O3
8	A	2019	LPE	C31-O33-P-O31
8	A	2019	LPE	C31-O33-P-O32
8	A	2024	LPE	O33-C31-C32-N
8	A	2025	LPE	C31-O33-P-O31
8	A	2025	LPE	C31-O33-P-O32
8	A	2025	LPE	O33-C31-C32-N
8	A	2026	LPE	O1-C1-C2-O2H
8	A	2026	LPE	C1-C2-C3-O3
8	A	2026	LPE	C3-O3-P-O31
8	A	2026	LPE	C3-O3-P-O32
8	A	2026	LPE	O33-C31-C32-N
8	A	2027	LPE	C3-O3-P-O32
8	A	2027	LPE	C31-O33-P-O3
8	A	2030	LPE	C3-O3-P-O32
8	A	2030	LPE	C31-O33-P-O31
8	A	2030	LPE	C31-O33-P-O32
8	A	2032	LPE	C3-O3-P-O31
8	A	2032	LPE	C3-O3-P-O32
8	A	2032	LPE	C3-O3-P-O33
8	A	2032	LPE	C31-O33-P-O3
8	A	2032	LPE	C31-O33-P-O31
8	A	2032	LPE	O33-C31-C32-N
8	B	301	LPE	O1-C1-C2-C3
8	B	301	LPE	C31-O33-P-O31
8	B	301	LPE	C31-O33-P-O32
8	B	301	LPE	O33-C31-C32-N

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Mol	Chain	Res	Type	Atoms
10	A	2009	PCW	C32-C31-O2-C2
10	A	2012	PCW	O4P-C4-C5-N
10	A	2012	PCW	C1-O3P-P-O2P
10	A	2012	PCW	C4-O4P-P-O1P
10	A	2012	PCW	C4-O4P-P-O2P
10	A	2012	PCW	C4-O4P-P-O3P
10	A	2013	PCW	O4P-C4-C5-N
10	A	2014	PCW	C32-C31-O2-C2
10	A	2014	PCW	O31-C31-O2-C2
10	A	2014	PCW	C1-O3P-P-O1P
10	A	2028	PCW	C32-C31-O2-C2
10	A	2028	PCW	C1-O3P-P-O2P
10	A	2028	PCW	C1-O3P-P-O4P
10	A	2028	PCW	C4-O4P-P-O3P
10	A	2029	PCW	C32-C31-O2-C2
10	A	2029	PCW	C1-O3P-P-O2P
10	A	2009	PCW	O11-C11-O3-C3
10	A	2009	PCW	C12-C11-O3-C3
10	A	2029	PCW	O11-C11-O3-C3
11	A	2031	P5S	O18-C17-O19-C1
10	A	2009	PCW	O31-C31-O2-C2
10	A	2028	PCW	O31-C31-O2-C2
10	A	2029	PCW	O31-C31-O2-C2
11	A	2031	P5S	C20-C17-O19-C1
6	A	2003	Y01	CAM-CAY-OAW-CBC
6	A	2003	Y01	CAJ-CAO-CBB-CAC
6	A	2003	Y01	CAC-CBB-CBE-CAP
6	A	2003	Y01	CAO-CBB-CBE-CBI
7	A	2021	CLR	C13-C17-C20-C22
10	A	2029	PCW	C12-C11-O3-C3
6	A	2003	Y01	CAO-CBB-CBE-CAP
5	A	2002	NAG	C8-C7-N2-C2
5	A	2002	NAG	O7-C7-N2-C2
8	A	2026	LPE	O2H-C2-C3-O3
8	A	2006	LPE	O1-C1-C2-O2H
8	B	301	LPE	O1-C1-C2-O2H
7	A	2021	CLR	C13-C17-C20-C21
5	C	301	NAG	O5-C5-C6-O6
5	B	305	NAG	C1-C2-N2-C7
10	A	2013	PCW	C12-C11-O3-C3
6	A	2003	Y01	CAJ-CAO-CBB-CBE
8	A	2025	LPE	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
8	A	2025	LPE	C2-C1-O1-C11
10	A	2013	PCW	O11-C11-O3-C3
7	A	2021	CLR	C16-C17-C20-C21
5	B	302	NAG	C8-C7-N2-C2
5	B	305	NAG	C4-C5-C6-O6
10	A	2012	PCW	C31-C32-C33-C34
6	A	2003	Y01	CAX-CAL-CAM-CAY
8	A	2026	LPE	C31-C32-N-C3N
7	A	2021	CLR	C16-C17-C20-C22
8	A	2019	LPE	O1-C11-C12-C13
8	A	2025	LPE	O2H-C2-C3-O3
8	A	2016	LPE	O1-C1-C2-O2H
8	A	2024	LPE	O1-C1-C2-O2H
8	A	2005	LPE	C3-O3-P-O33
8	A	2006	LPE	C31-O33-P-O3
8	A	2008	LPE	C3-O3-P-O33
8	A	2010	LPE	C31-O33-P-O3
8	A	2015	LPE	C31-O33-P-O3
8	A	2019	LPE	C3-O3-P-O33
8	A	2024	LPE	C31-O33-P-O3
8	A	2025	LPE	C31-O33-P-O3
8	A	2026	LPE	C3-O3-P-O33
8	A	2027	LPE	C3-O3-P-O33
8	A	2030	LPE	C3-O3-P-O33
8	A	2030	LPE	C31-O33-P-O3
8	B	301	LPE	C31-O33-P-O3
10	A	2029	PCW	C1-O3P-P-O4P
11	A	2031	P5S	C3-O16-P12-OG
5	B	302	NAG	O7-C7-N2-C2
8	A	2006	LPE	C12-C13-C14-C15
8	A	2016	LPE	O1-C1-C2-C3
8	A	2024	LPE	O1-C1-C2-C3
8	A	2026	LPE	O1-C1-C2-C3
8	A	2005	LPE	C12-C13-C14-C15
5	C	301	NAG	C4-C5-C6-O6
8	A	2006	LPE	O1-C11-C12-C13
8	A	2019	LPE	C14-C15-C16-C17
8	A	2019	LPE	O1-C1-C2-O2H
8	A	2026	LPE	C12-C13-C14-C15
7	A	2004	CLR	C21-C20-C22-C23
8	A	2006	LPE	C14-C15-C16-C17
8	A	2026	LPE	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
8	A	2016	LPE	C12-C13-C14-C15
8	A	2026	LPE	C15-C16-C17-C18
5	B	305	NAG	O5-C5-C6-O6
8	A	2026	LPE	C31-C32-N-C1N
8	A	2026	LPE	C31-C32-N-C2N
8	A	2016	LPE	C14-C15-C16-C17
8	A	2006	LPE	C16-C17-C18-C19
8	A	2006	LPE	C13-C14-C15-C16
10	A	2012	PCW	O31-C31-O2-C2
10	A	2028	PCW	C12-C11-O3-C3
8	A	2005	LPE	C13-C14-C15-C16
8	A	2006	LPE	C11-C12-C13-C14
10	A	2012	PCW	C32-C31-O2-C2
10	A	2013	PCW	C32-C31-O2-C2
11	A	2031	P5S	C39-C38-O37-C2
10	A	2013	PCW	C13-C14-C15-C16
10	A	2013	PCW	O31-C31-O2-C2
11	A	2031	P5S	O47-C38-O37-C2
7	A	2023	CLR	C13-C17-C20-C22
10	A	2028	PCW	C32-C33-C34-C35
6	A	2003	Y01	CAN-CAJ-CAO-CBB
10	A	2013	PCW	C1-O3P-P-O4P
10	A	2014	PCW	C1-O3P-P-O4P
8	A	2008	LPE	C11-C12-C13-C14
11	A	2031	P5S	C1-C2-C3-O16
8	A	2017	LPE	O1-C11-C12-C13
10	A	2028	PCW	O11-C11-O3-C3
8	A	2019	LPE	C2-C1-O1-C11
5	A	2002	NAG	O5-C5-C6-O6
5	B	302	NAG	O5-C5-C6-O6
8	A	2005	LPE	C14-C15-C16-C17
7	A	2023	CLR	C16-C17-C20-C21
7	A	2023	CLR	C13-C17-C20-C21
8	A	2010	LPE	C2-C1-O1-C11
11	A	2031	P5S	C2-C3-O16-P12
7	A	2023	CLR	C16-C17-C20-C22
8	A	2019	LPE	C13-C14-C15-C16
8	A	2025	LPE	O1-C1-C2-C3
10	A	2014	PCW	C16-C17-C18-C19
8	A	2016	LPE	C16-C17-C18-C19
8	A	2016	LPE	C11-C12-C13-C14
8	A	2019	LPE	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
8	A	2019	LPE	C12-C13-C14-C15
8	A	2017	LPE	C2-C3-O3-P
11	A	2031	P5S	O37-C2-C3-O16
8	A	2016	LPE	C12-C11-O1-C1
8	A	2020	LPE	C12-C11-O1-C1
8	A	2011	LPE	C15-C16-C17-C18
8	A	2019	LPE	C16-C17-C18-C19
8	A	2025	LPE	O1-C1-C2-O2H
11	A	2031	P5S	N-CA-CB-OG
8	A	2011	LPE	C31-O33-P-O3
8	A	2016	LPE	C31-O33-P-O3
8	A	2026	LPE	C31-O33-P-O3
10	A	2009	PCW	C4-O4P-P-O3P
8	A	2005	LPE	C3-O3-P-O31
8	A	2011	LPE	C31-O33-P-O31
8	A	2015	LPE	C3-O3-P-O32
8	A	2015	LPE	C31-O33-P-O31
8	A	2016	LPE	C3-O3-P-O32
8	A	2017	LPE	C31-O33-P-O31
8	A	2018	LPE	C31-O33-P-O32
8	A	2019	LPE	C3-O3-P-O32
8	A	2024	LPE	C31-O33-P-O32
8	A	2027	LPE	C3-O3-P-O31
8	A	2027	LPE	C31-O33-P-O32
8	B	301	LPE	C3-O3-P-O31
10	A	2013	PCW	C1-O3P-P-O1P
10	A	2013	PCW	C1-O3P-P-O2P
10	A	2014	PCW	C1-O3P-P-O2P
10	A	2028	PCW	C4-O4P-P-O1P
10	A	2029	PCW	C1-O3P-P-O1P
11	A	2031	P5S	C3-O16-P12-O15
8	A	2032	LPE	C2-C1-O1-C11
8	A	2032	LPE	C32-C31-O33-P
8	A	2005	LPE	C15-C16-C17-C18
8	A	2005	LPE	C2-C1-O1-C11
8	A	2011	LPE	C2-C1-O1-C11
8	A	2024	LPE	C2-C1-O1-C11
8	A	2010	LPE	O33-C31-C32-N
8	A	2011	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

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Mol	Chain	Res	Type	Atoms
8	A	2018	LPE	O33-C31-C32-N
8	A	2019	LPE	O33-C31-C32-N
8	A	2020	LPE	O33-C31-C32-N
8	A	2027	LPE	O33-C31-C32-N
8	A	2030	LPE	O33-C31-C32-N
10	A	2014	PCW	O4P-C4-C5-N
10	A	2028	PCW	O4P-C4-C5-N
10	A	2029	PCW	O4P-C4-C5-N
8	A	2005	LPE	C16-C17-C18-C19
8	A	2015	LPE	C12-C11-O1-C1
8	A	2020	LPE	C14-C15-C16-C17
8	A	2020	LPE	C31-O33-P-O3
8	A	2025	LPE	C3-O3-P-O33
10	A	2012	PCW	C1-O3P-P-O4P
10	A	2013	PCW	C4-O4P-P-O3P
11	A	2031	P5S	CB-OG-P12-O16
8	A	2018	LPE	C12-C11-O1-C1
8	A	2026	LPE	C11-C12-C13-C14
8	A	2020	LPE	C12-C13-C14-C15
10	A	2013	PCW	C12-C13-C14-C15
10	A	2009	PCW	C19-C20-C21-C22
5	B	305	NAG	C3-C2-N2-C7
7	A	2021	CLR	C22-C23-C24-C25
8	A	2010	LPE	C2-C3-O3-P
10	A	2028	PCW	C31-C32-C33-C34
11	A	2031	P5S	C-CA-CB-OG
7	A	2022	CLR	C13-C17-C20-C21
8	A	2017	LPE	C12-C13-C14-C15
6	A	2003	Y01	CAM-CAL-CAX-OAF
8	A	2017	LPE	C13-C14-C15-C16
8	B	301	LPE	C2-C1-O1-C11
10	A	2014	PCW	C23-C24-C25-C26
10	A	2029	PCW	C33-C34-C35-C36
10	A	2029	PCW	C31-C32-C33-C34
10	A	2009	PCW	O2-C2-C3-O3
10	A	2029	PCW	O2-C2-C3-O3
6	A	2003	Y01	CAM-CAL-CAX-OAH
8	B	301	LPE	C1-C2-C3-O3
10	A	2012	PCW	C39-C40-C41-C42
11	A	2031	P5S	C39-C40-C41-C42
7	A	2022	CLR	C13-C17-C20-C22
8	A	2018	LPE	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
8	A	2010	LPE	C12-C11-O1-C1
8	A	2018	LPE	C3-O3-P-O33
10	A	2009	PCW	C37-C38-C39-C40
10	A	2013	PCW	C17-C18-C19-C20
10	A	2009	PCW	C1-C2-C3-O3
10	A	2012	PCW	C37-C38-C39-C40
7	A	2022	CLR	C16-C17-C20-C22
8	A	2006	LPE	C18-C19-C20-C21
10	A	2012	PCW	O2-C31-C32-C33
8	A	2020	LPE	C2-C3-O3-P
8	A	2016	LPE	C13-C14-C15-C16
7	A	2021	CLR	C21-C20-C22-C23
8	A	2015	LPE	C31-O33-P-O32
8	A	2020	LPE	C31-O33-P-O31
10	A	2014	PCW	C4-O4P-P-O2P
11	A	2031	P5S	CB-OG-P12-O13
9	A	2007	1PW	CAL-CAN-CAP-CAR
8	A	2011	LPE	C12-C13-C14-C15
8	A	2010	LPE	C32-C31-O33-P
8	A	2018	LPE	C32-C31-O33-P
8	A	2025	LPE	C32-C31-O33-P
8	A	2027	LPE	C32-C31-O33-P
10	A	2013	PCW	C5-C4-O4P-P
9	A	2007	1PW	CAP-CAR-CAT-CAU
10	A	2012	PCW	O31-C31-C32-C33
9	A	2007	1PW	CAN-CAP-CAR-CAT
8	A	2006	LPE	C2-C1-O1-C11

There are no ring outliers.

29 monomers are involved in 95 short contacts:

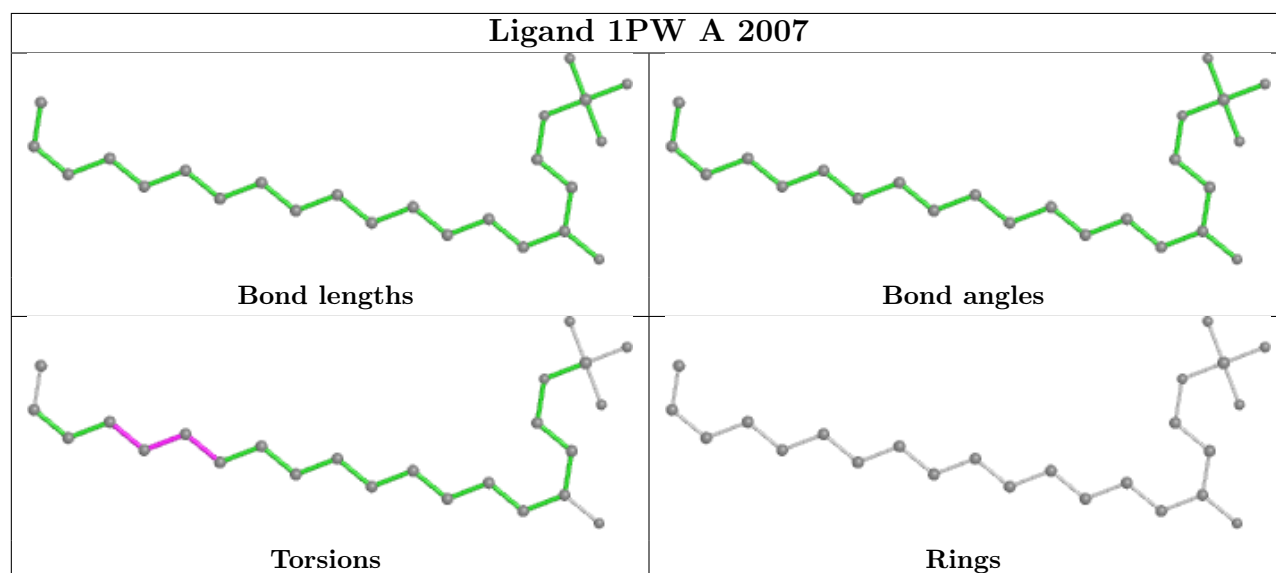
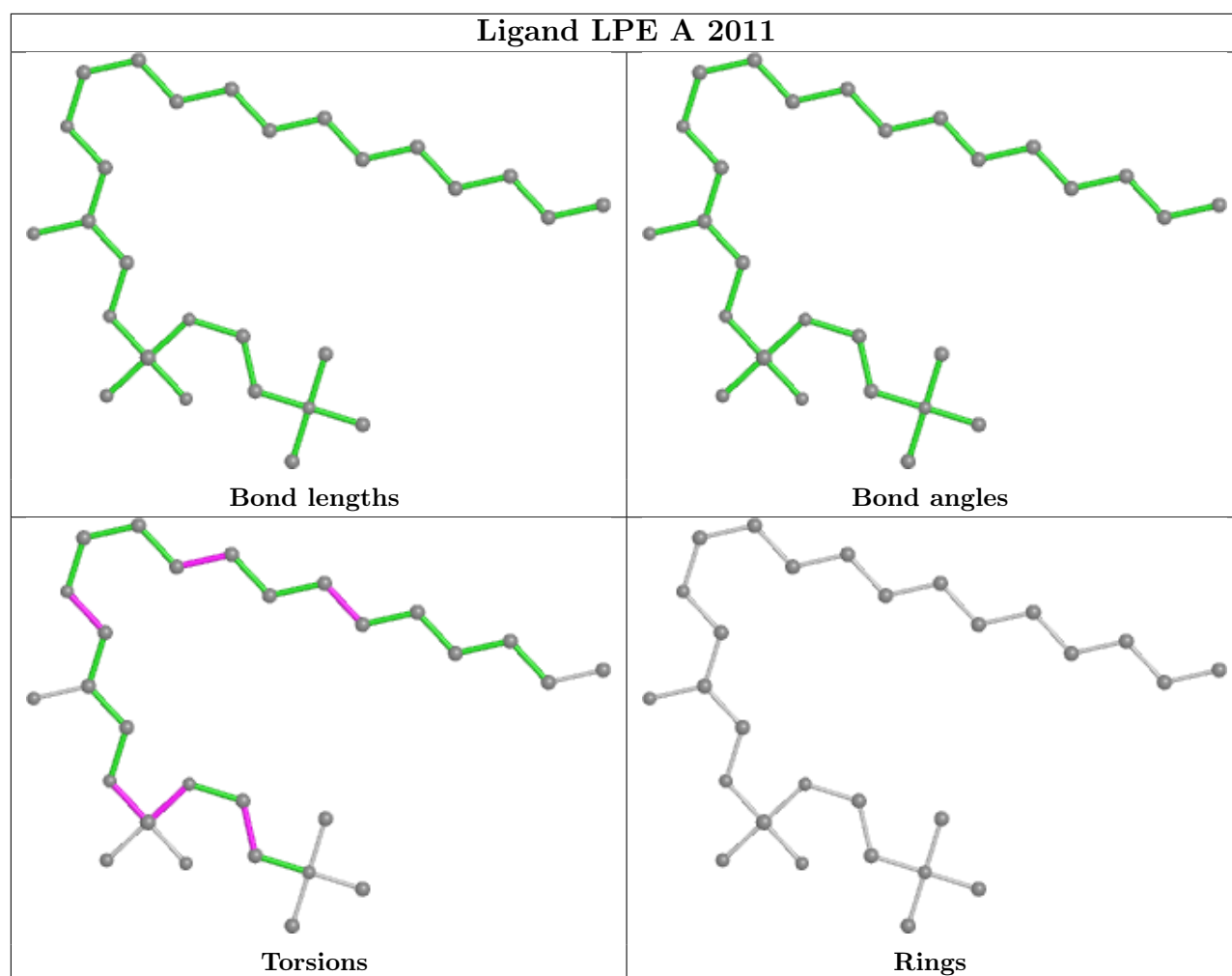
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	2011	LPE	2	0
10	A	2029	PCW	3	0
8	A	2005	LPE	1	0
8	A	2030	LPE	9	0
7	A	2023	CLR	3	0
8	A	2015	LPE	3	0
11	A	2031	P5S	2	0
10	A	2014	PCW	3	0
8	A	2010	LPE	1	0
8	A	2008	LPE	2	0

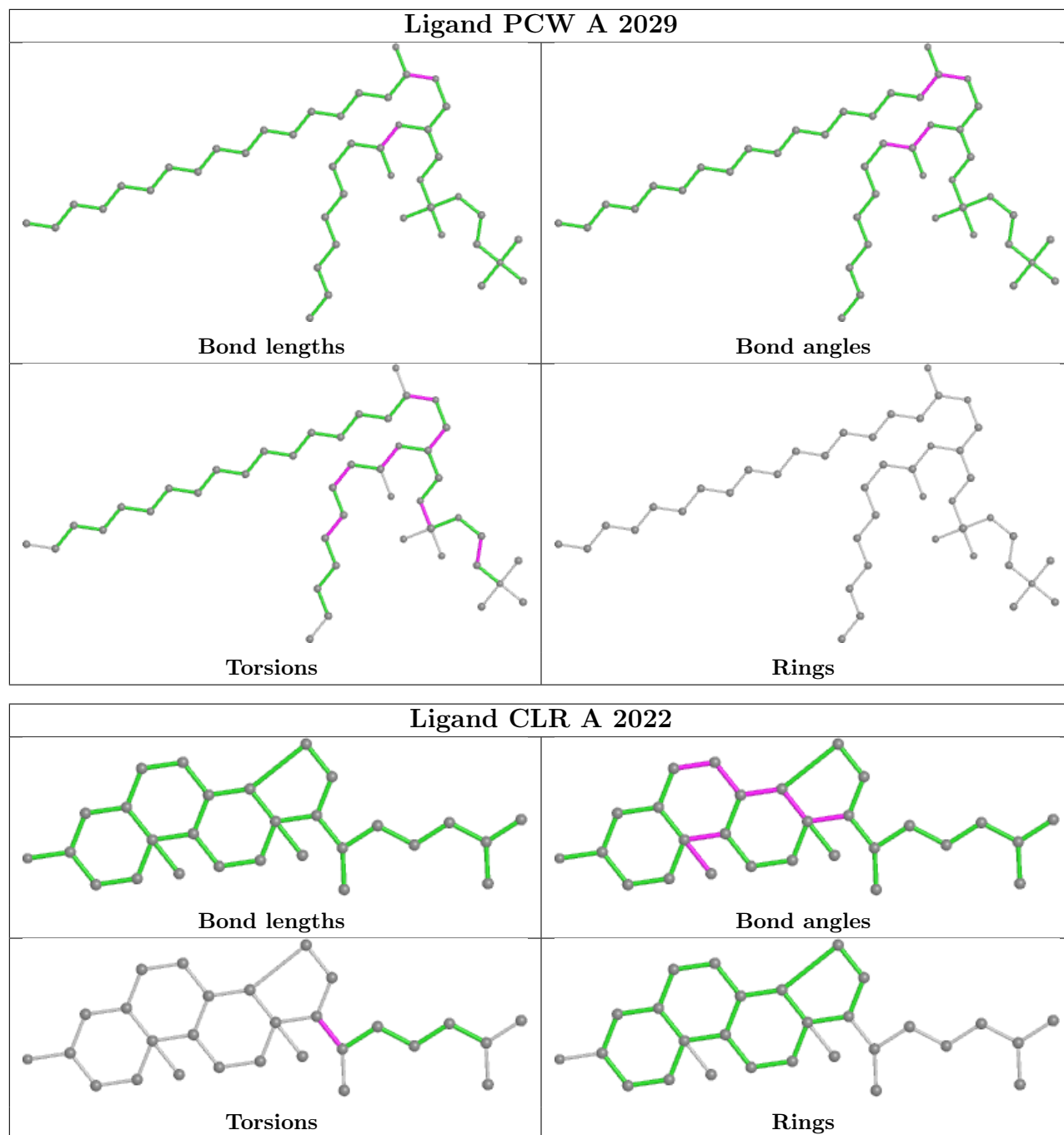
*Continued on next page...*

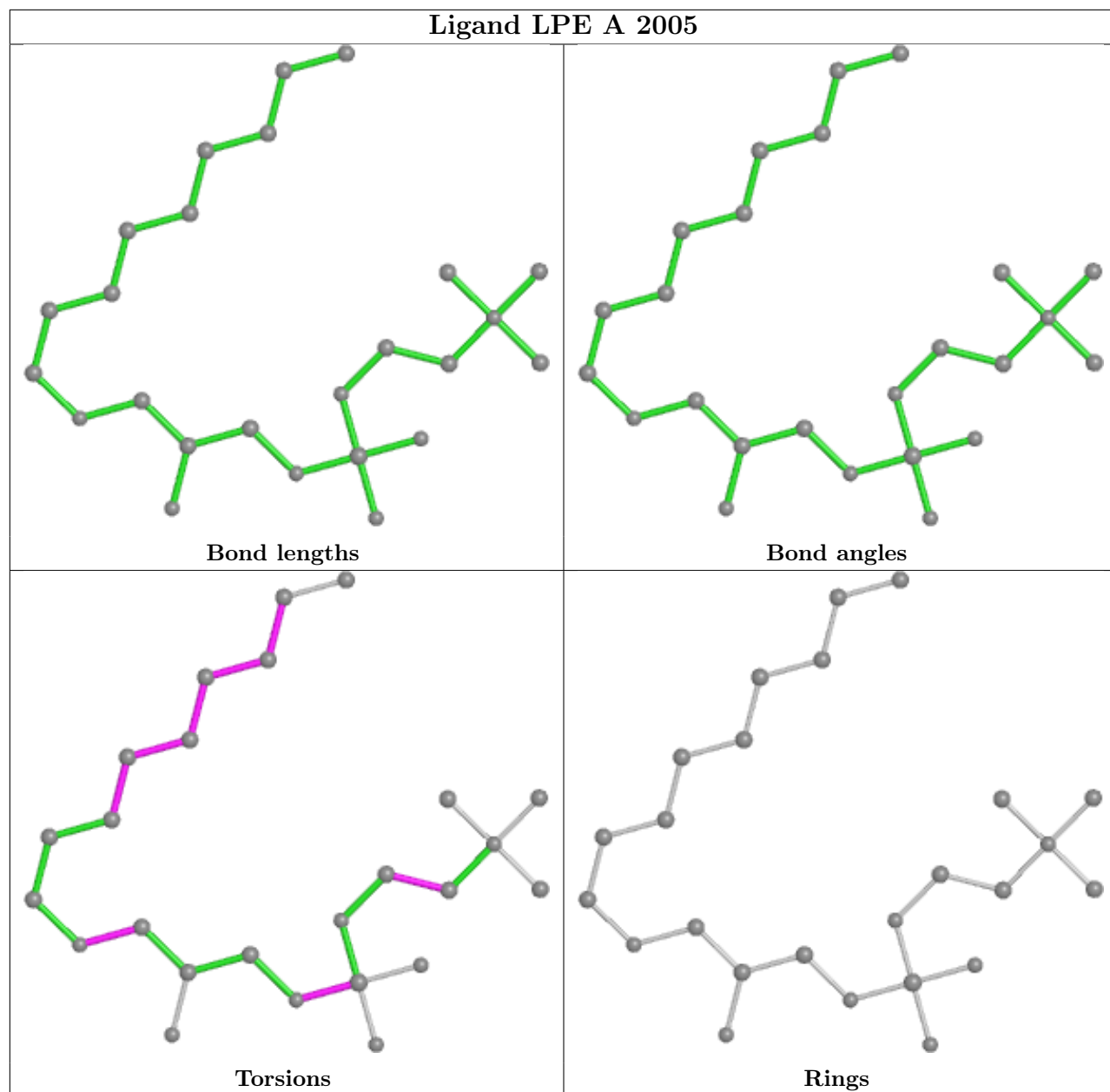
*Continued from previous page...*

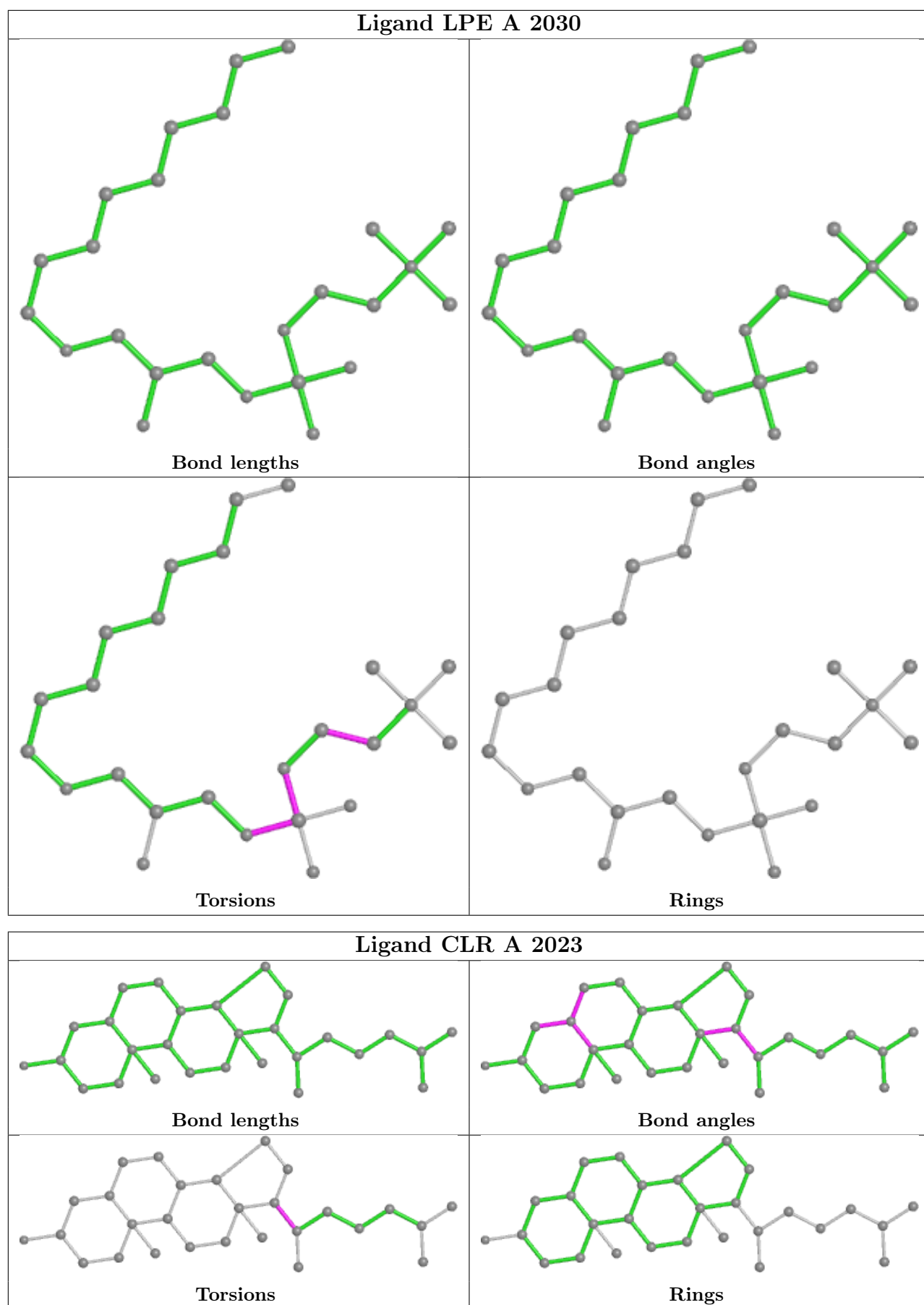
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	2032	LPE	2	0
8	A	2026	LPE	7	0
5	B	305	NAG	1	0
8	A	2025	LPE	1	0
7	A	2021	CLR	4	0
8	A	2016	LPE	1	0
8	A	2018	LPE	3	0
10	A	2013	PCW	2	0
8	A	2006	LPE	2	0
8	B	301	LPE	2	0
10	A	2028	PCW	1	0
10	A	2009	PCW	3	0
7	A	2004	CLR	20	0
8	A	2017	LPE	2	0
6	A	2003	Y01	13	0
8	A	2024	LPE	2	0
5	C	301	NAG	2	0
8	A	2019	LPE	3	0
10	A	2012	PCW	4	0

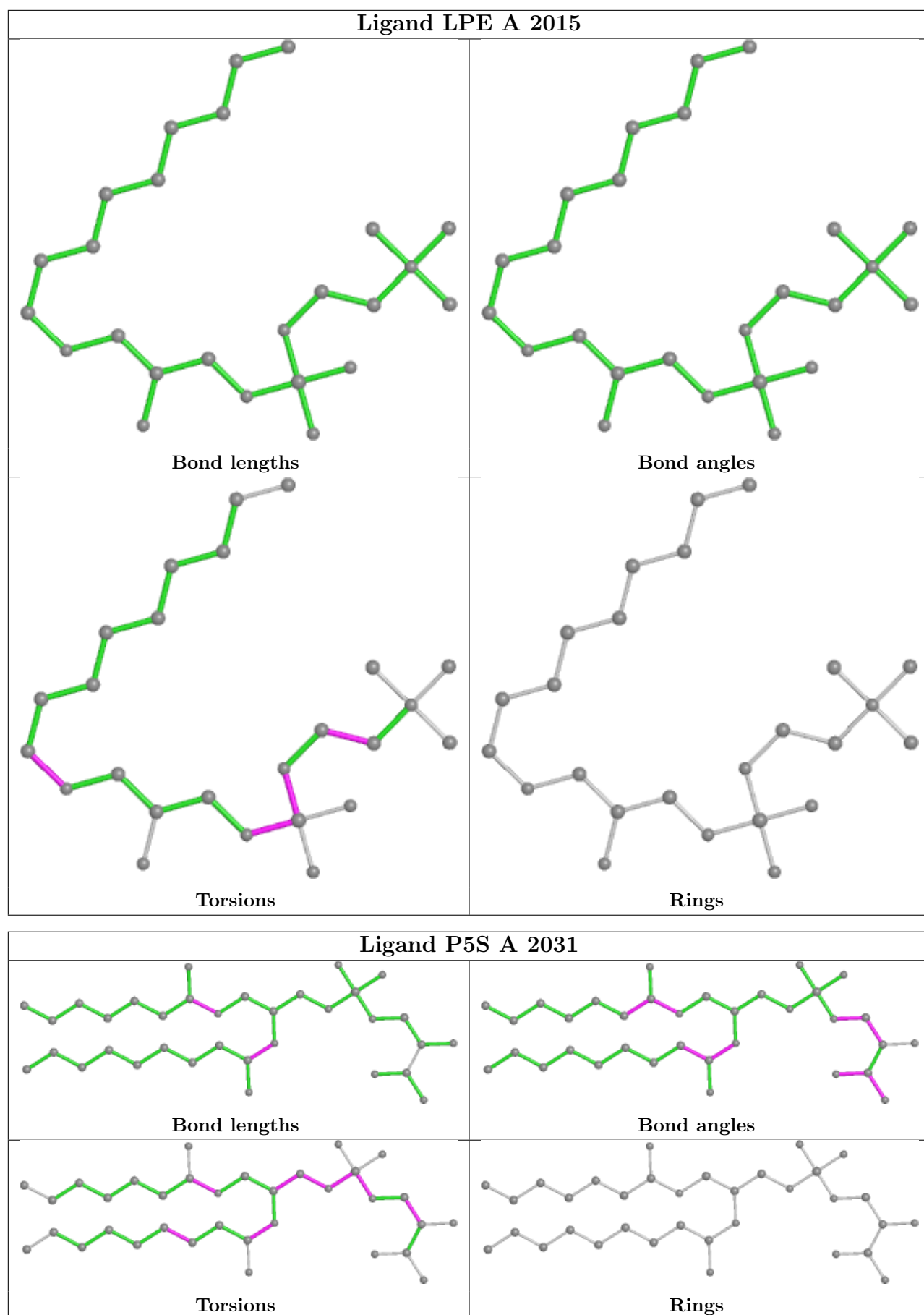
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



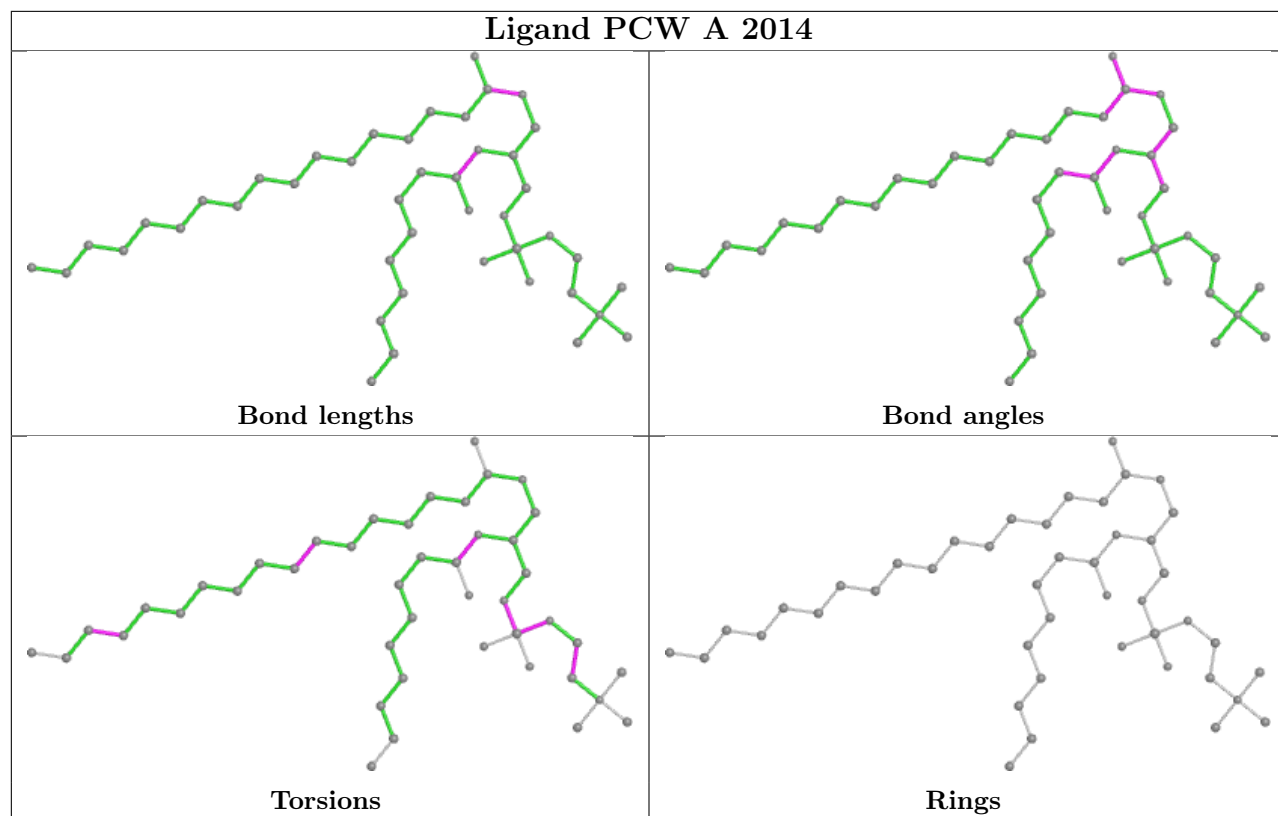


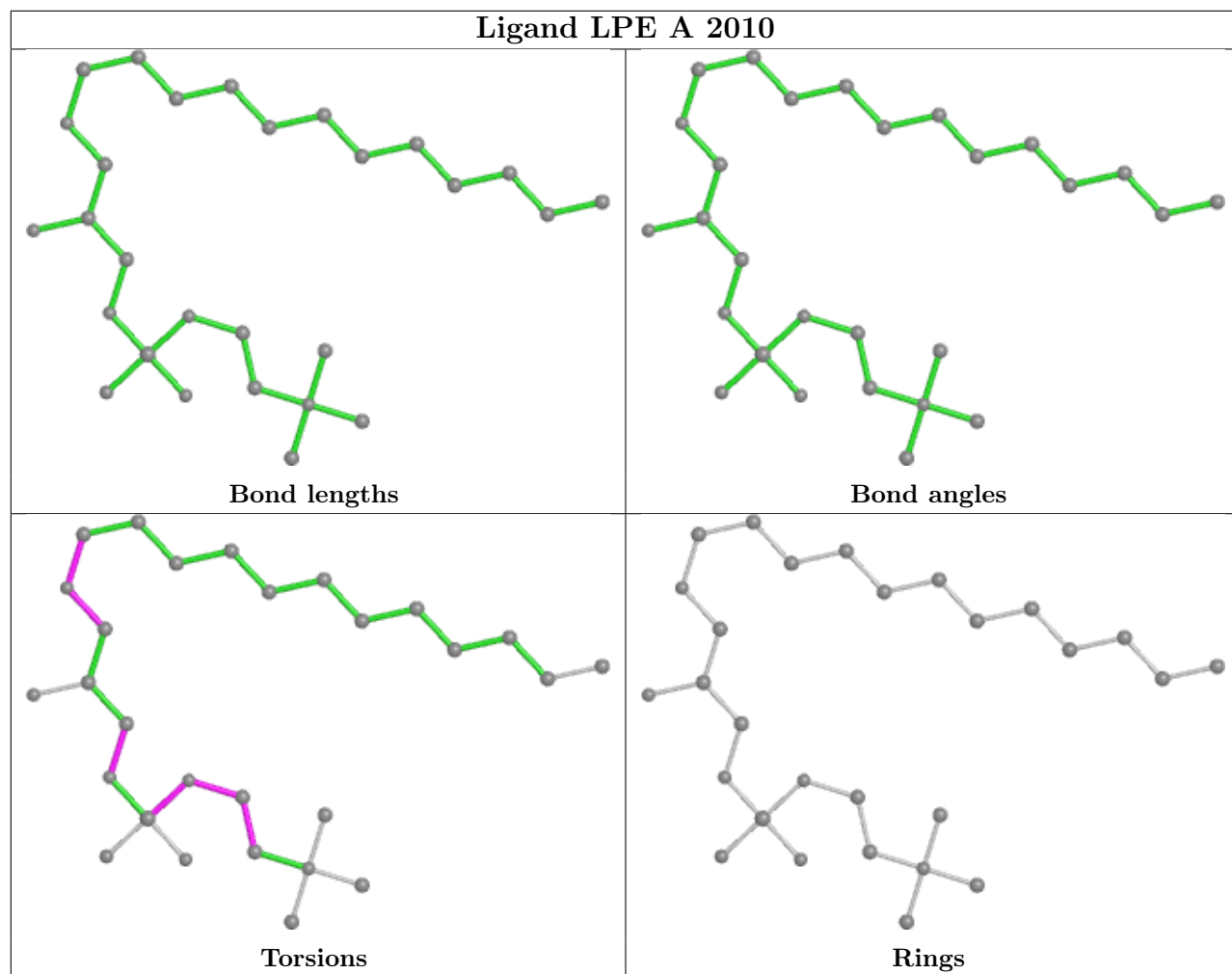


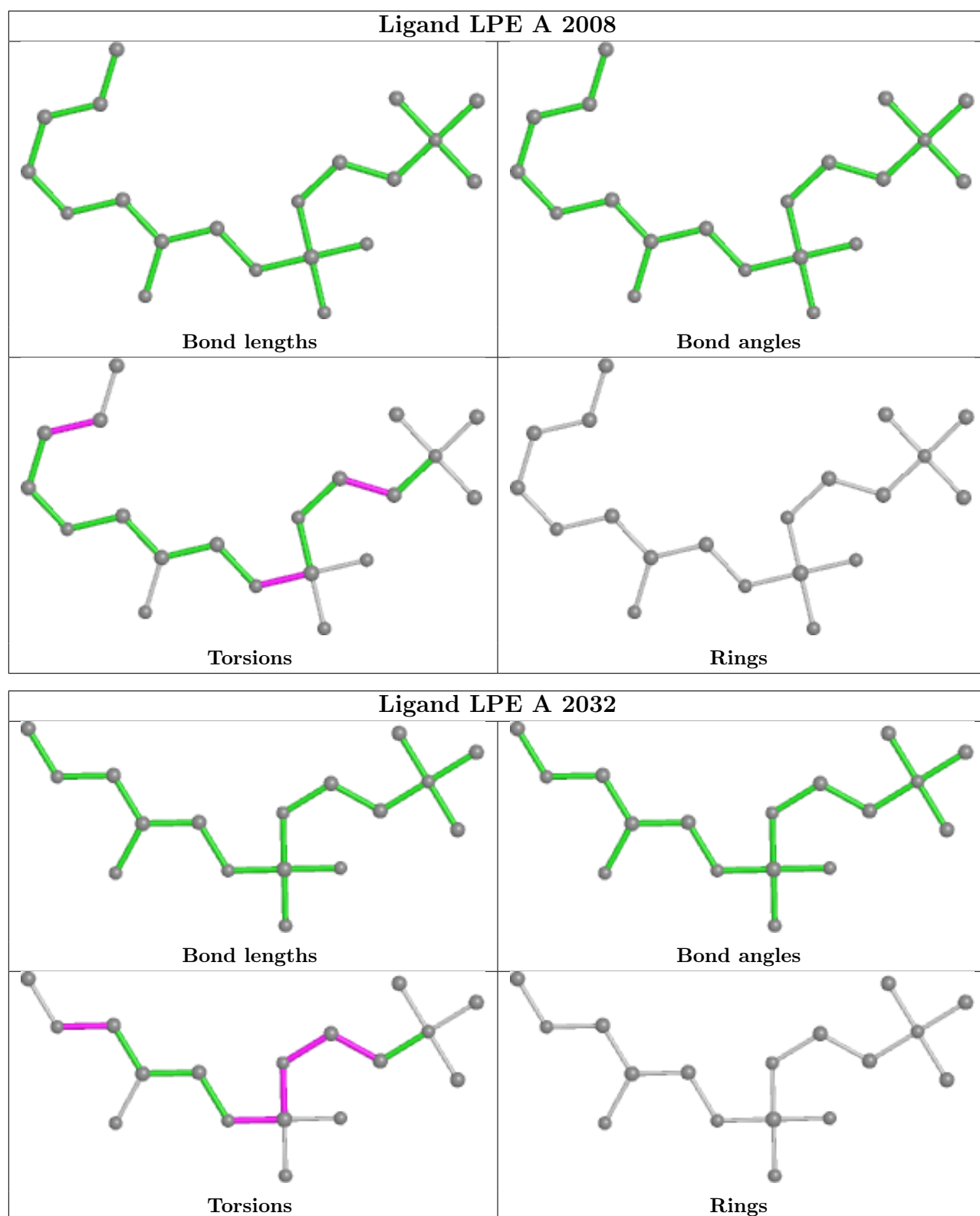


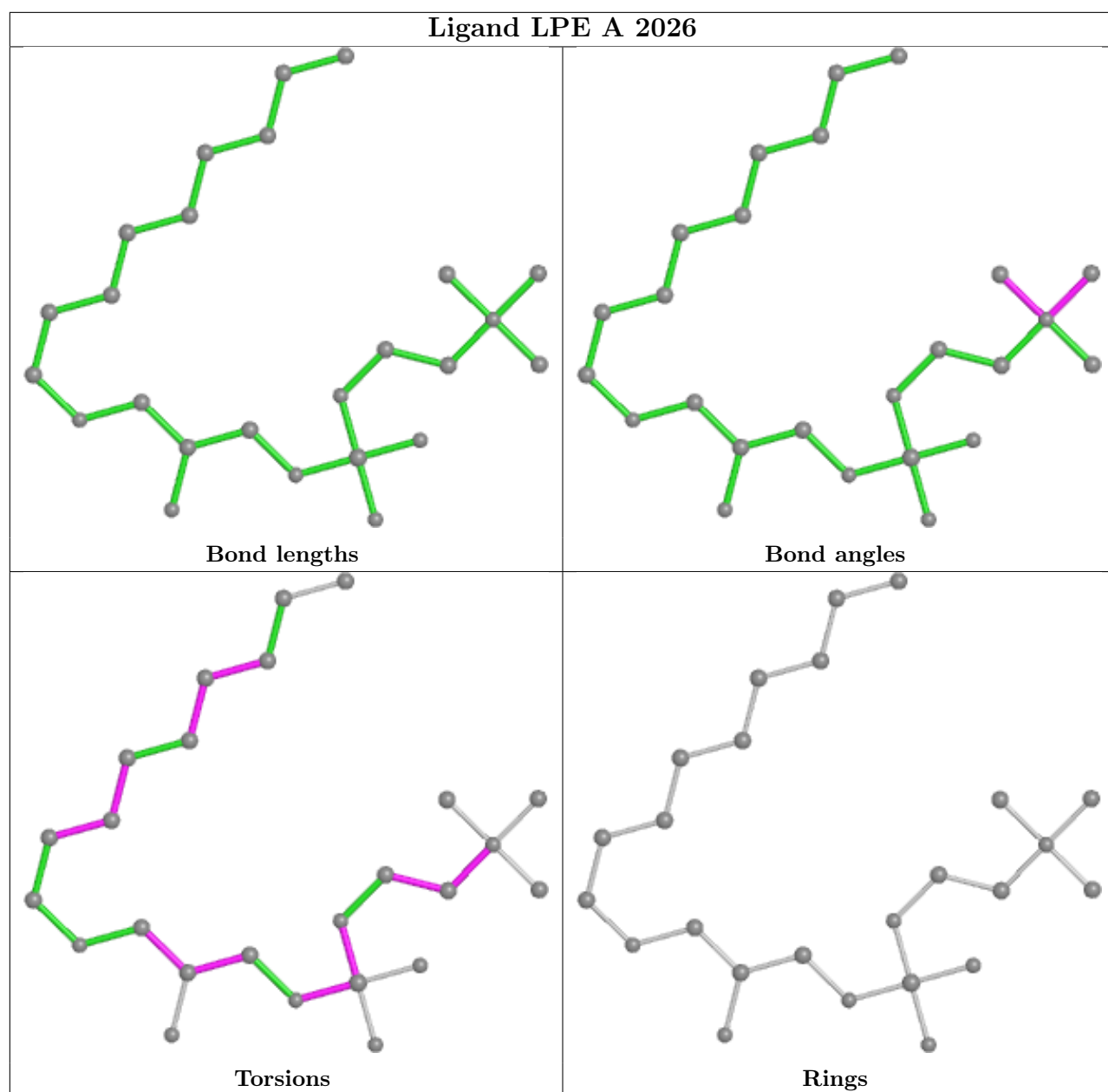


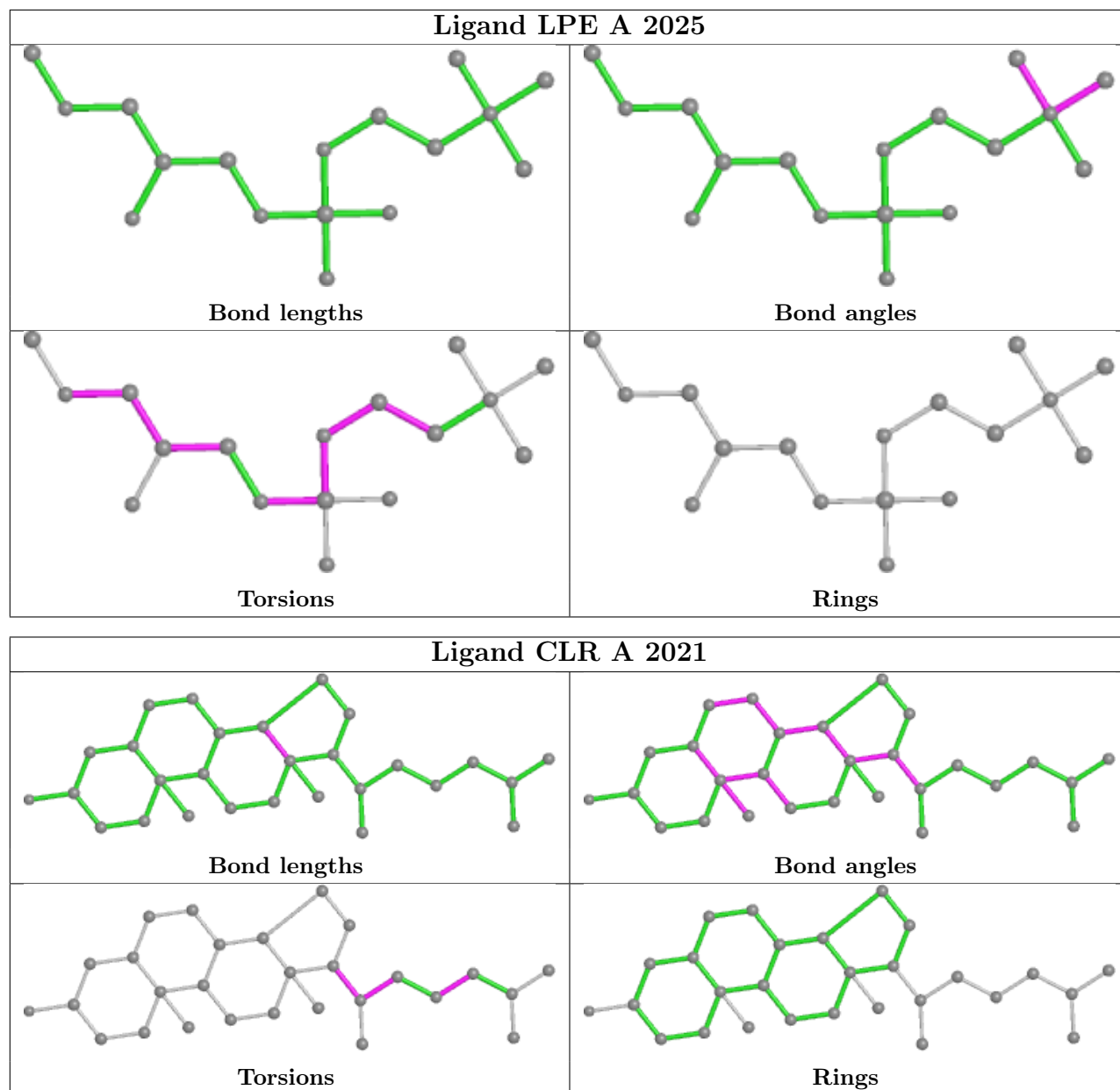


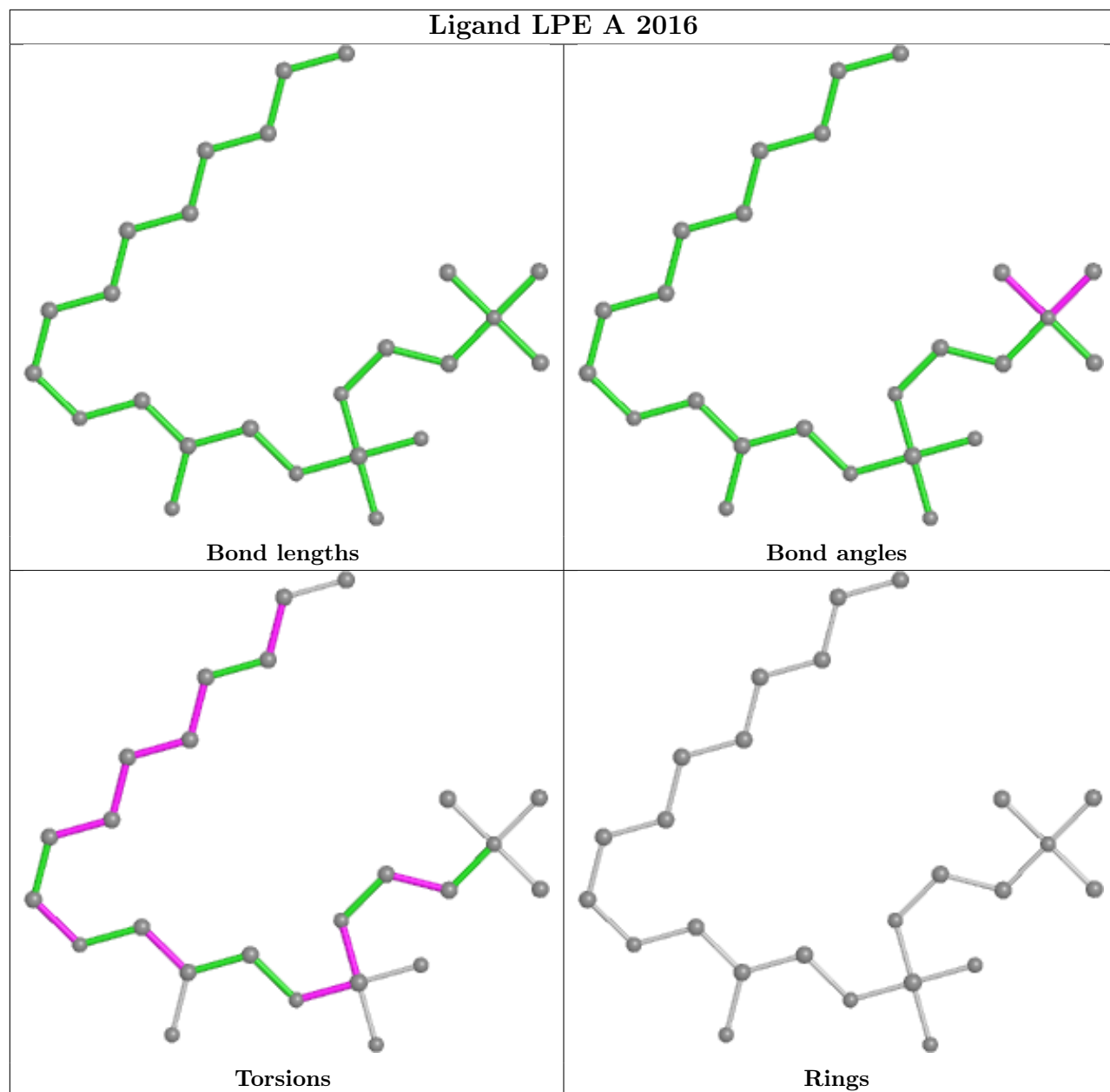


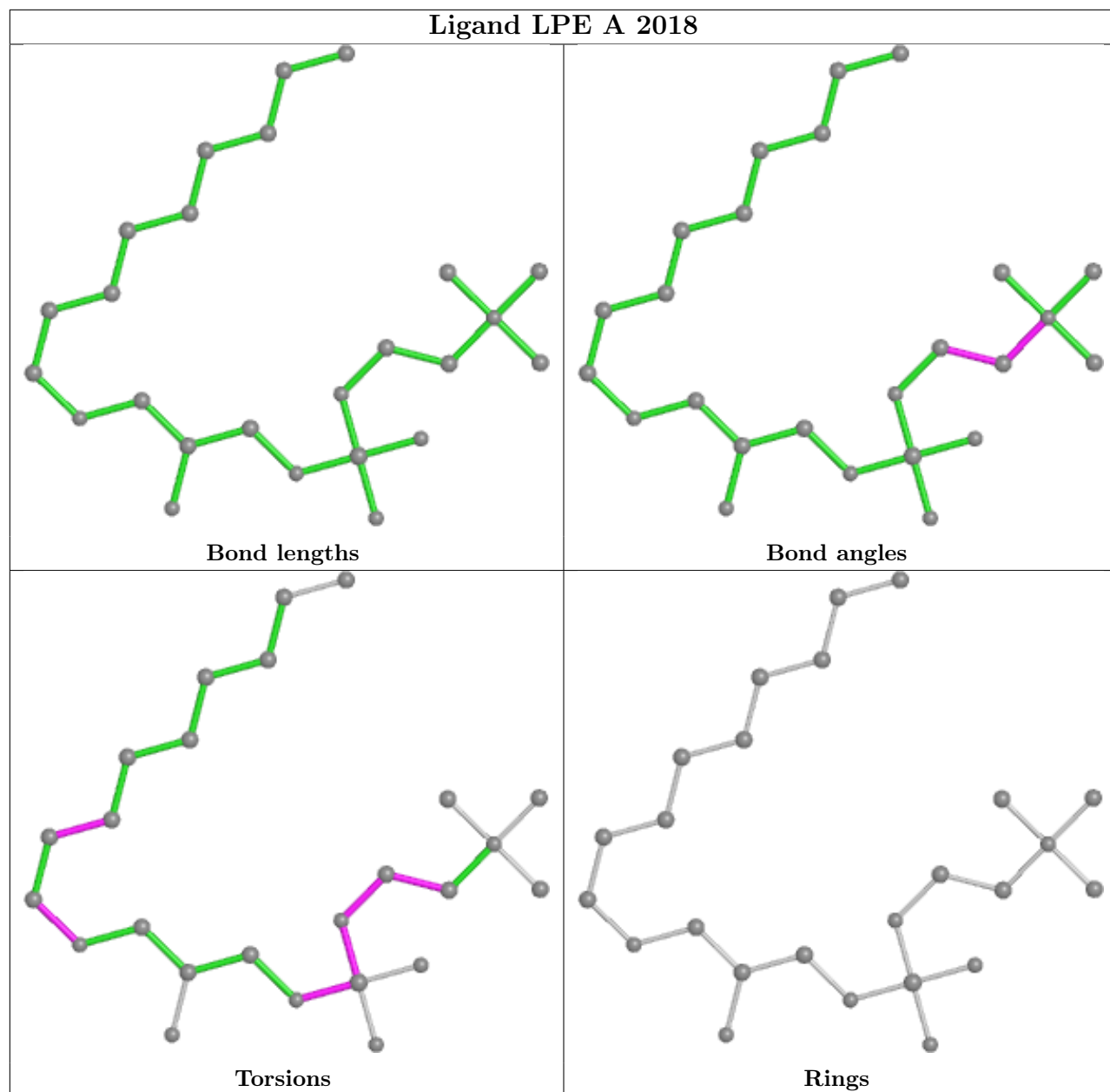


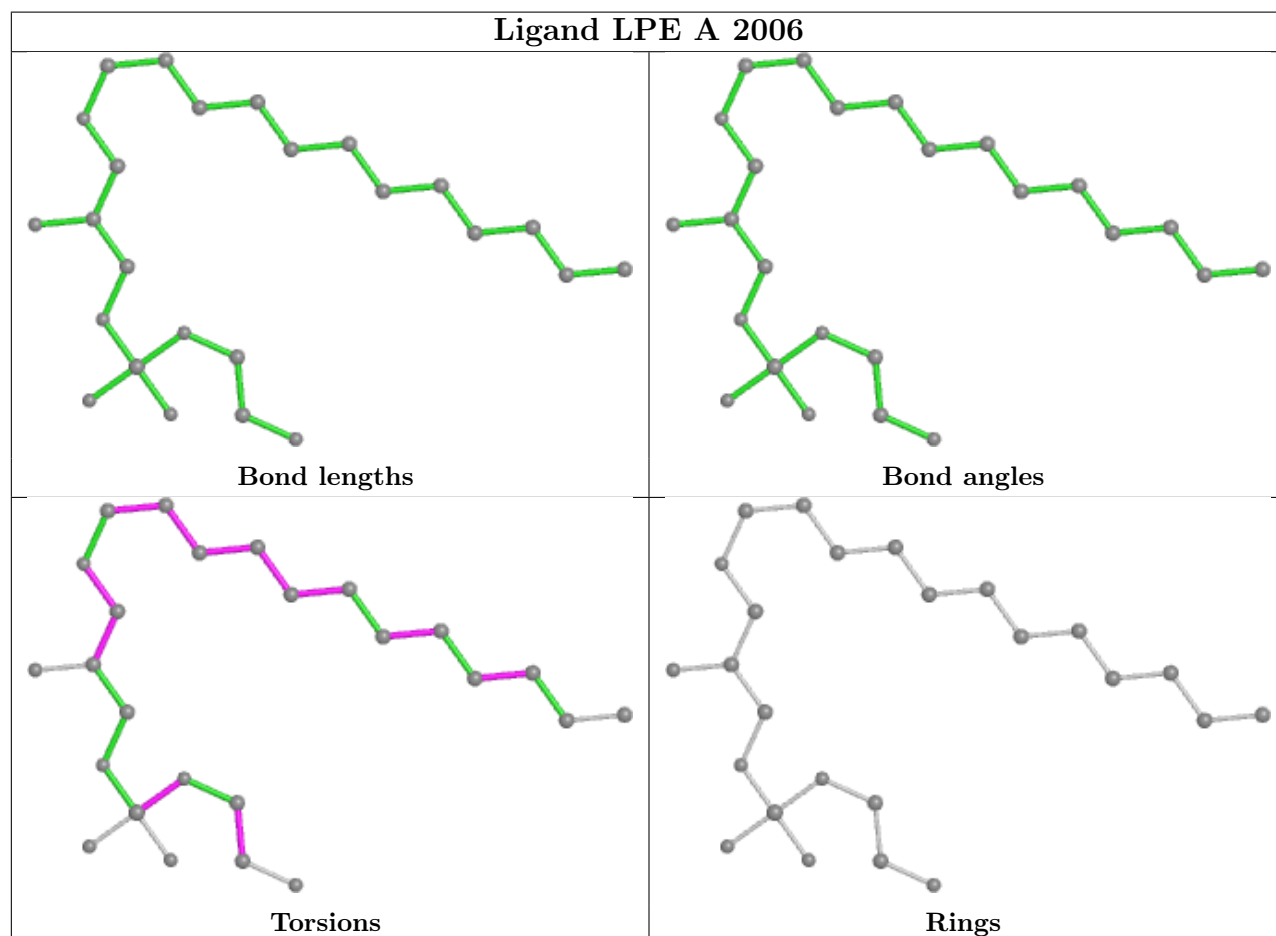
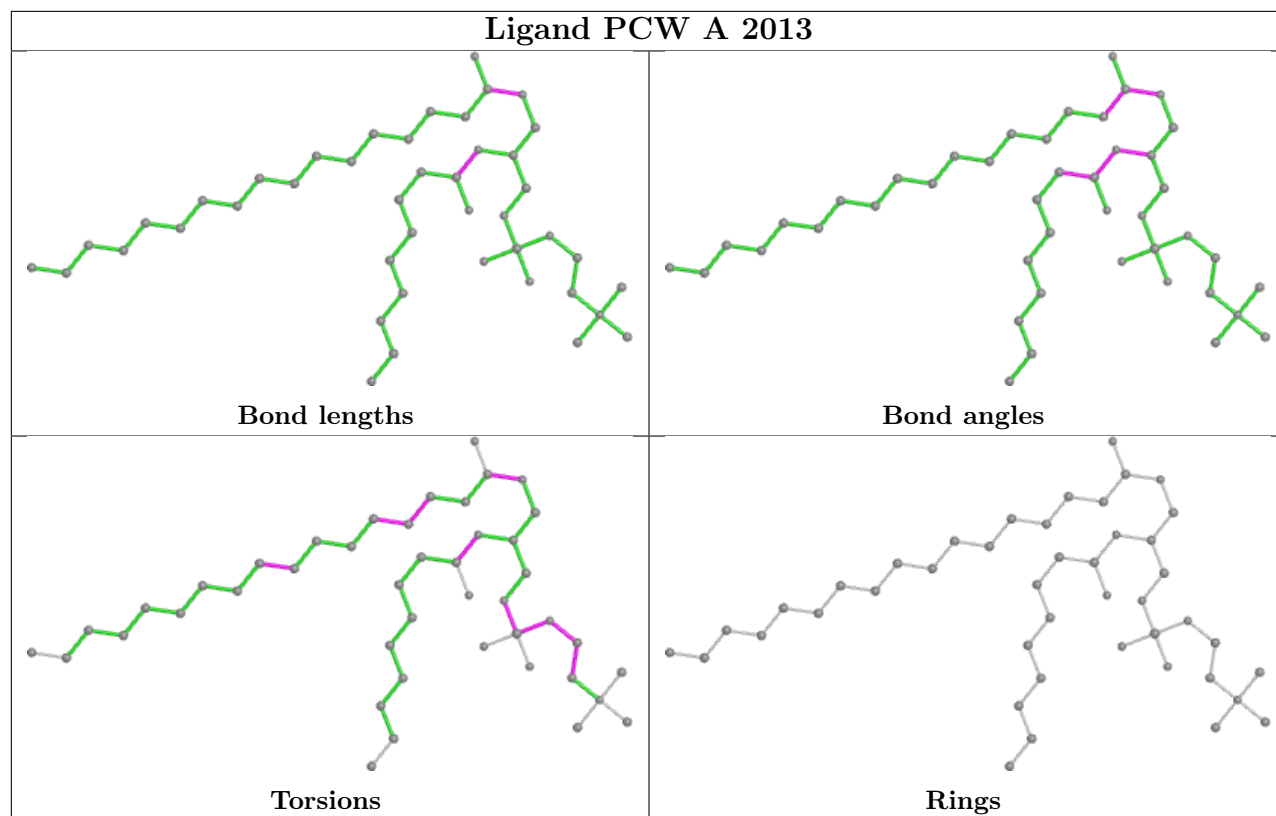




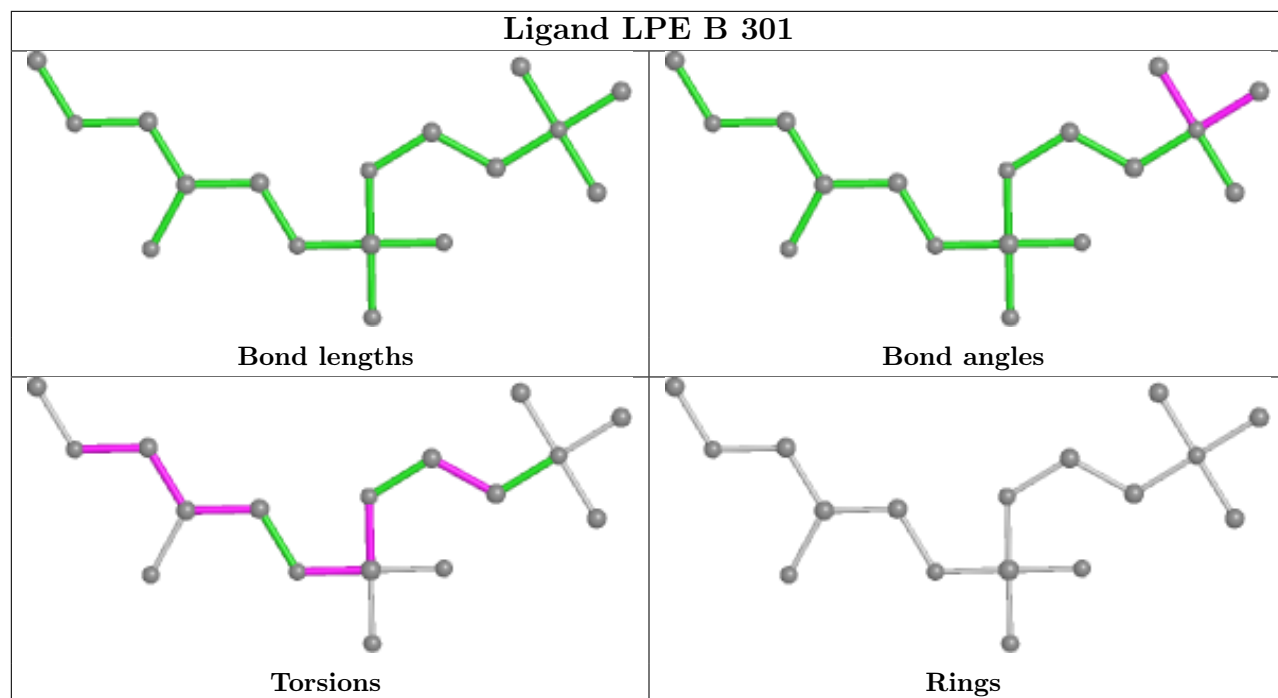


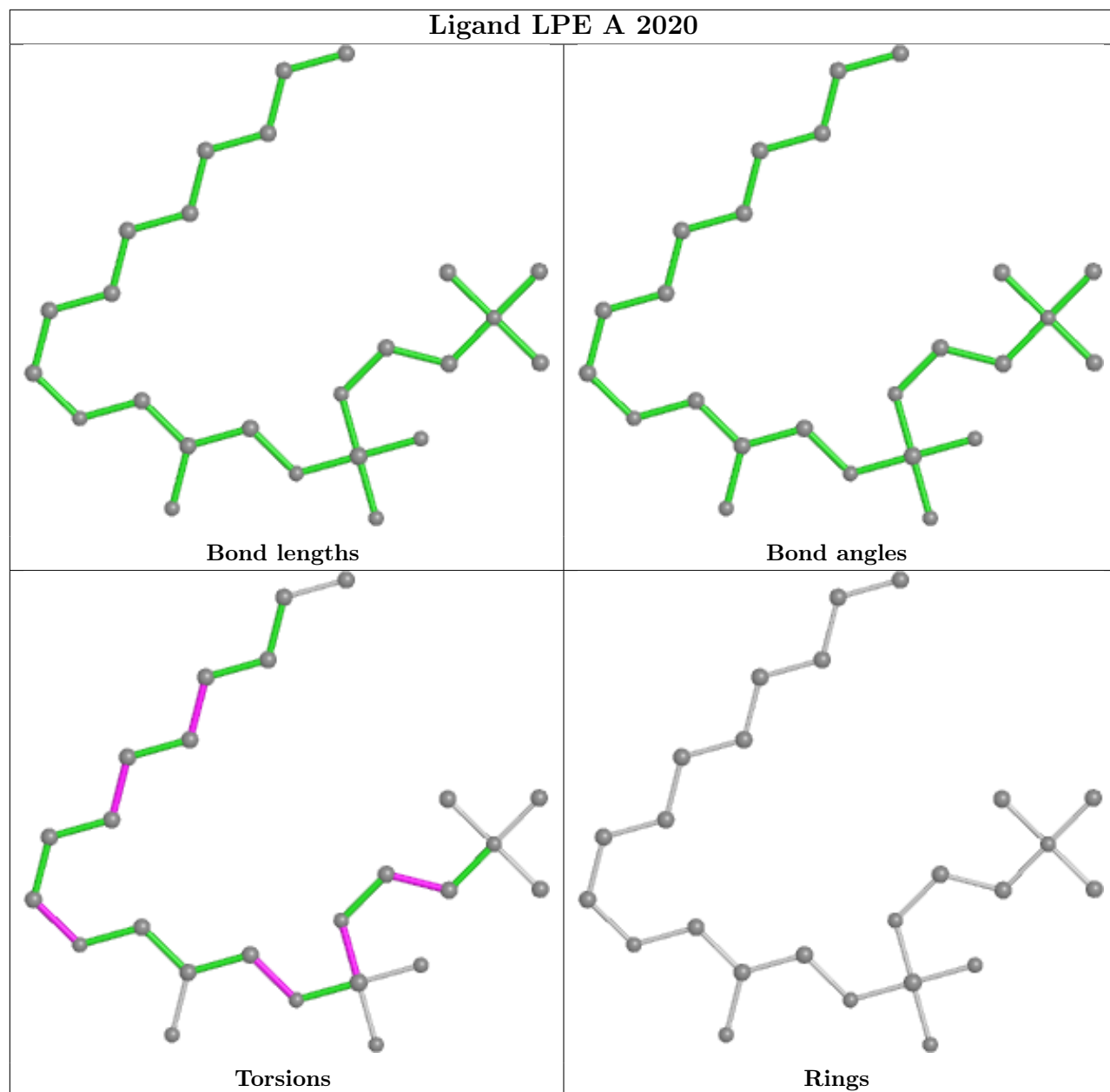


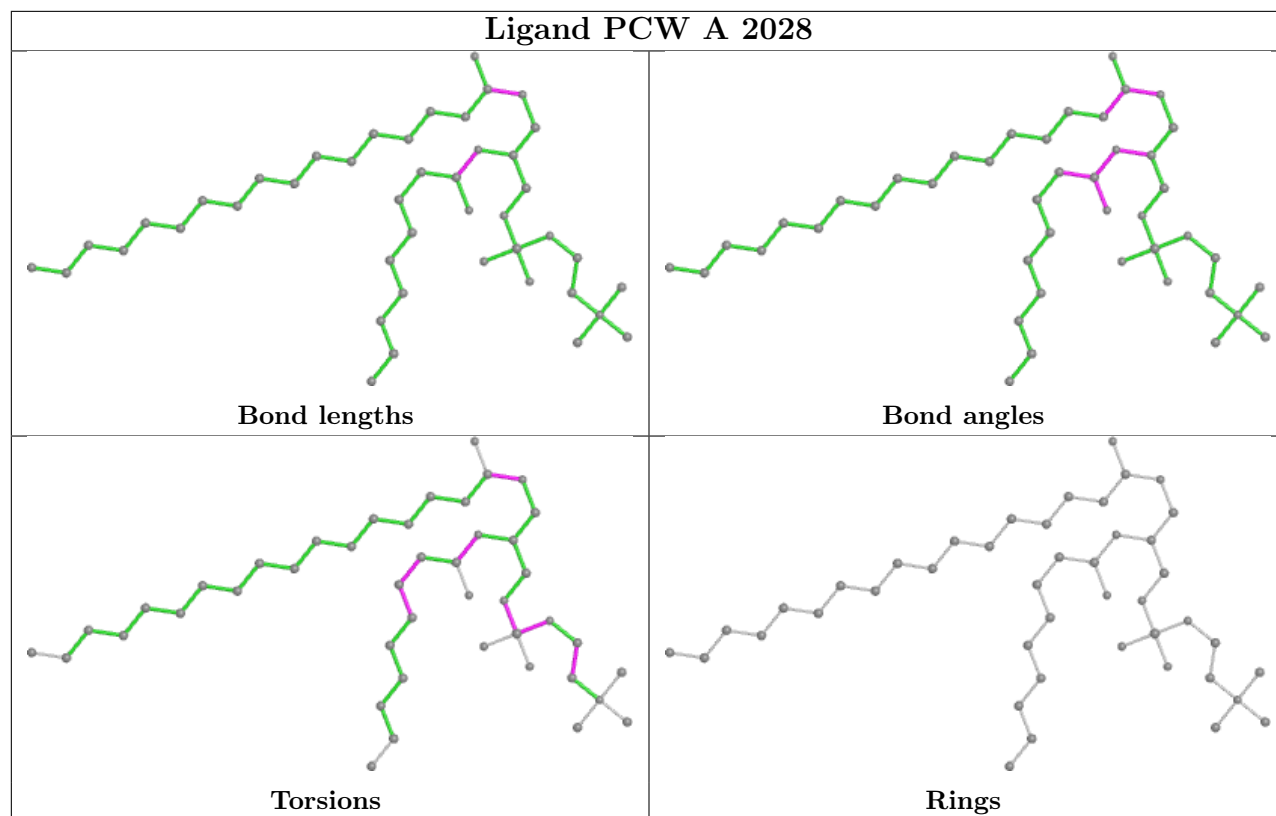


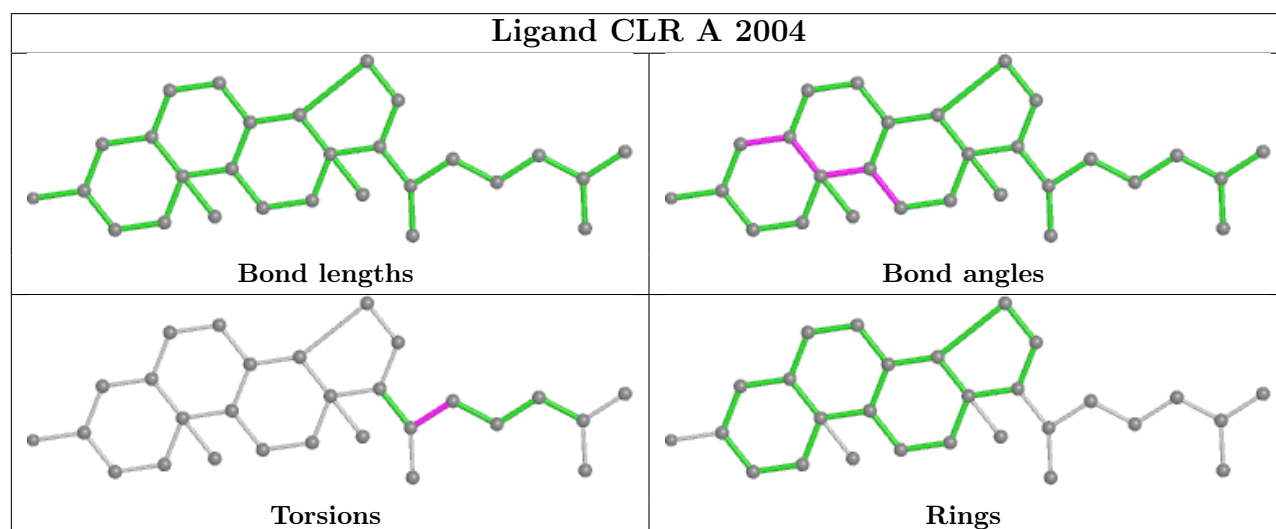
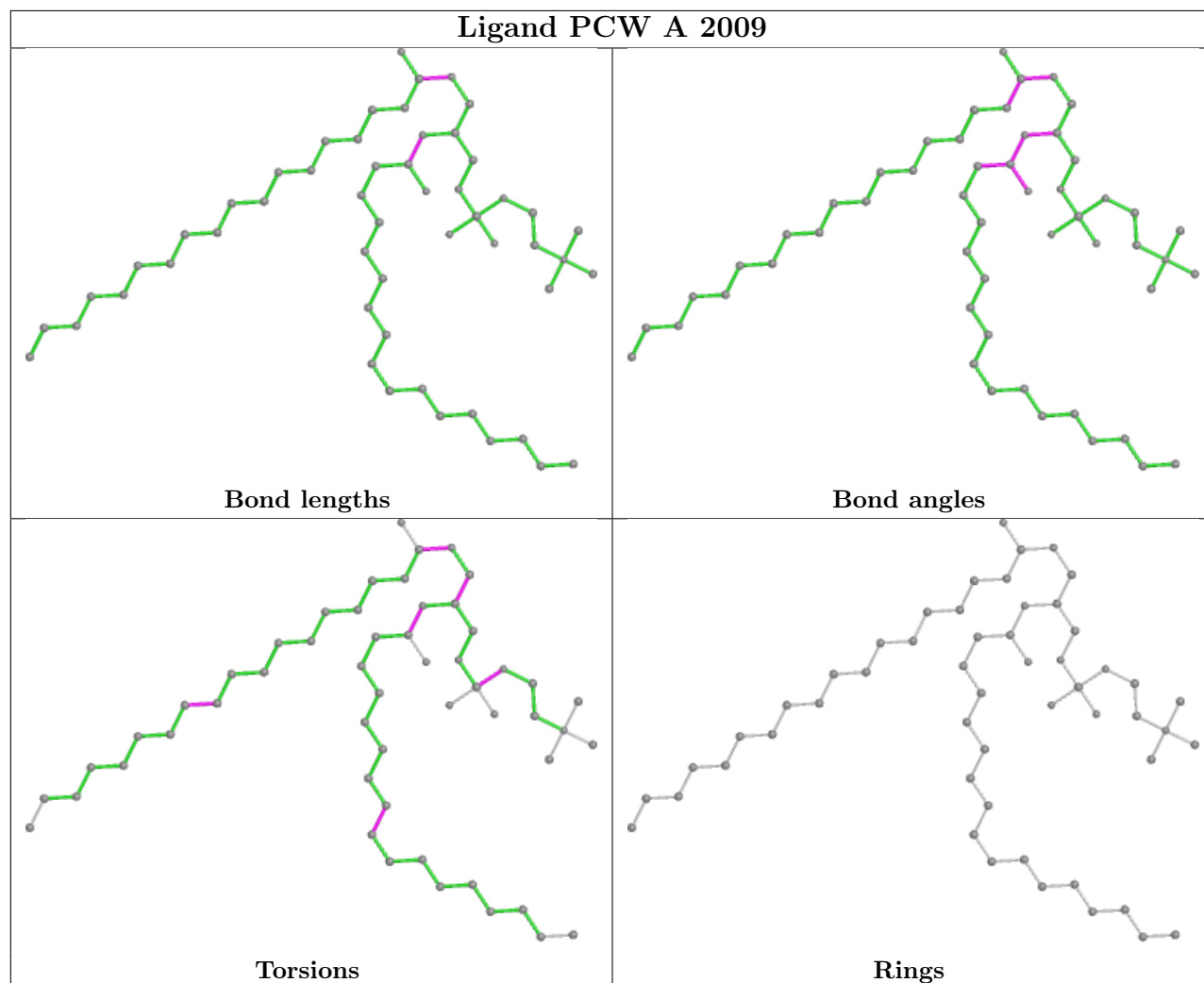


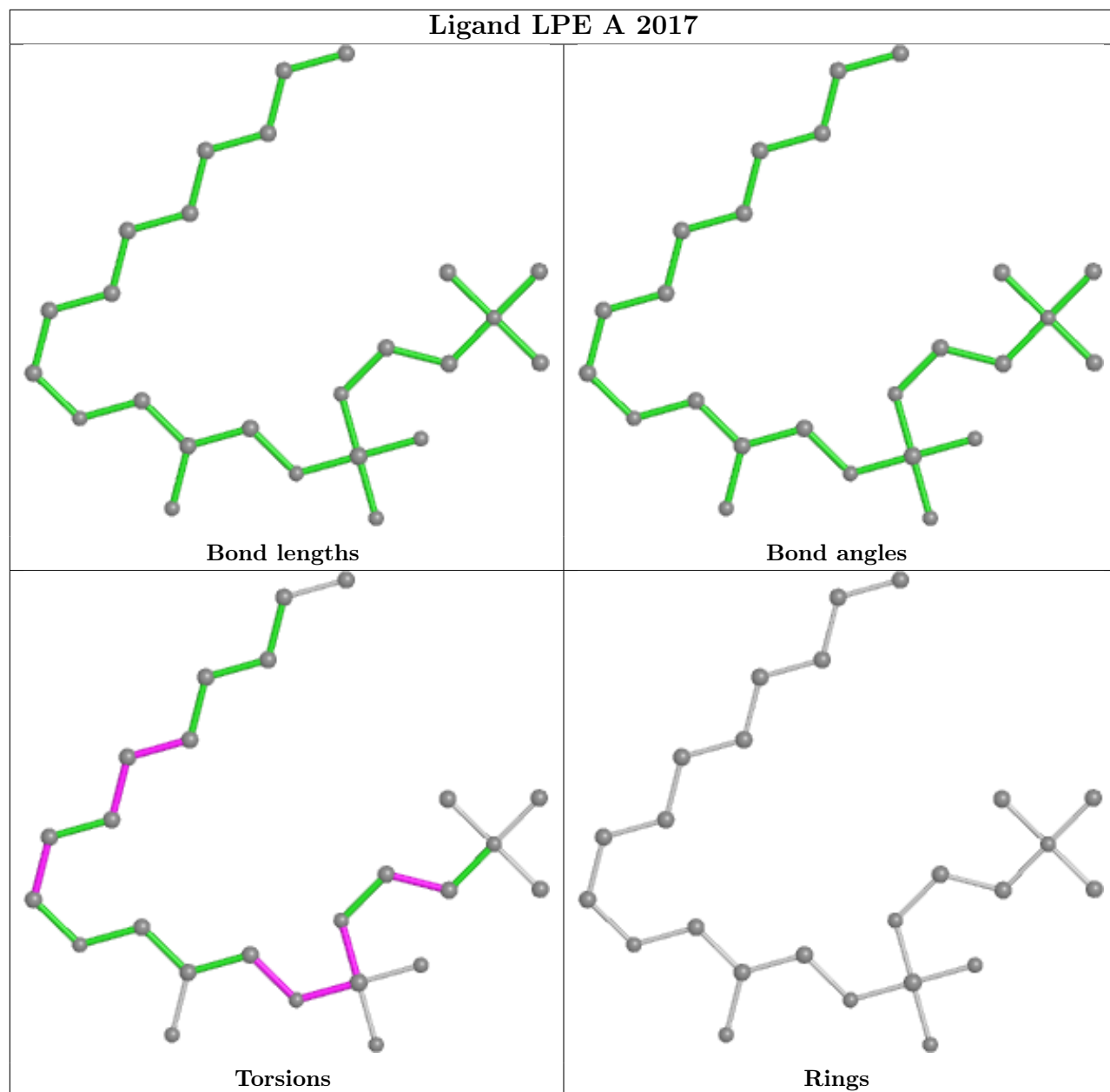


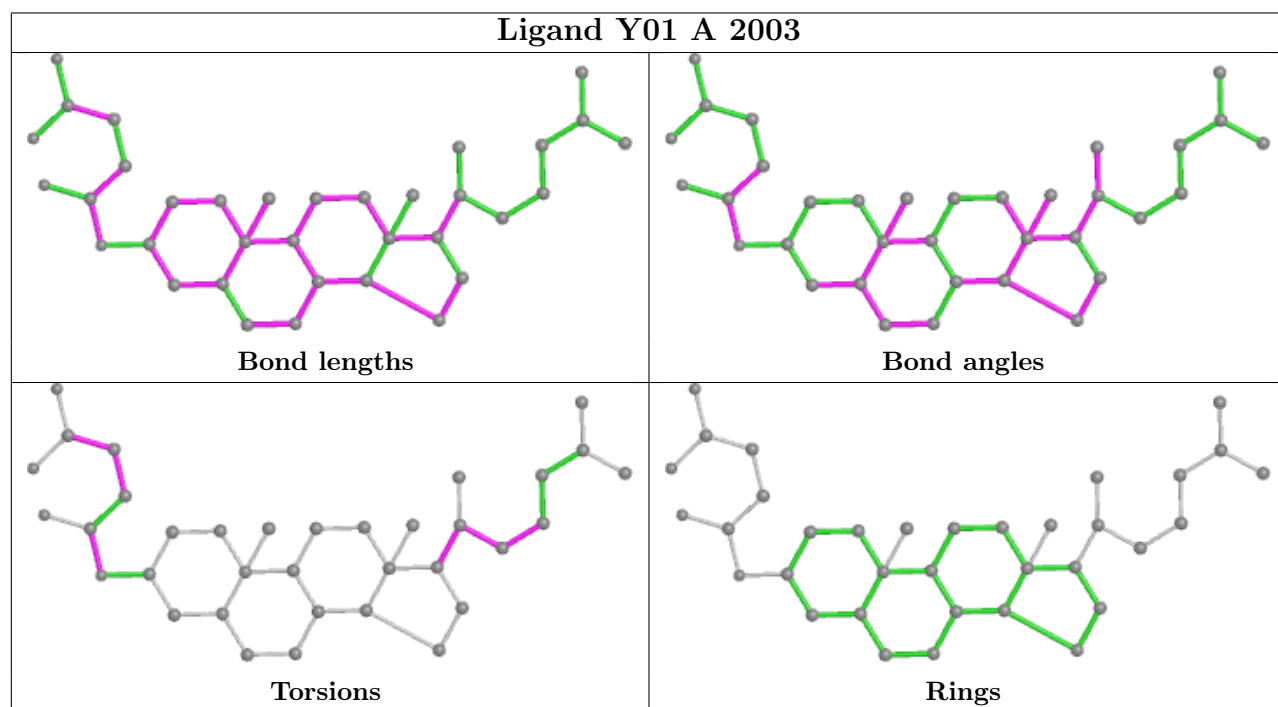
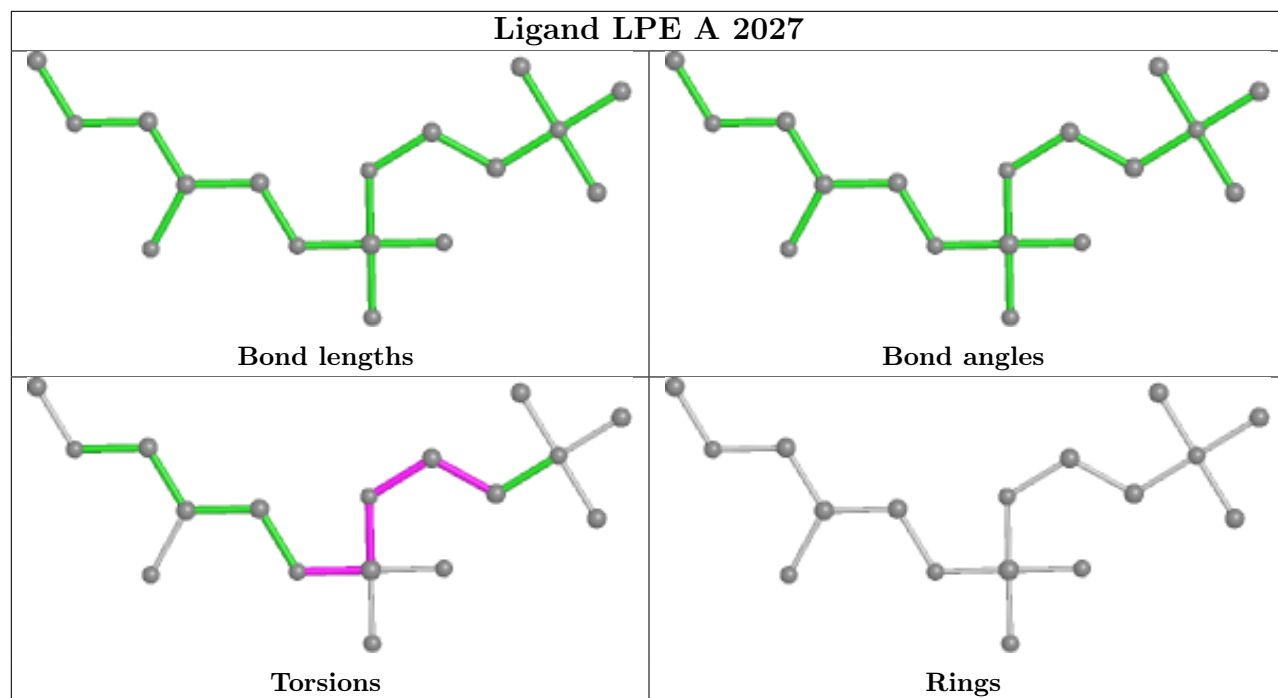


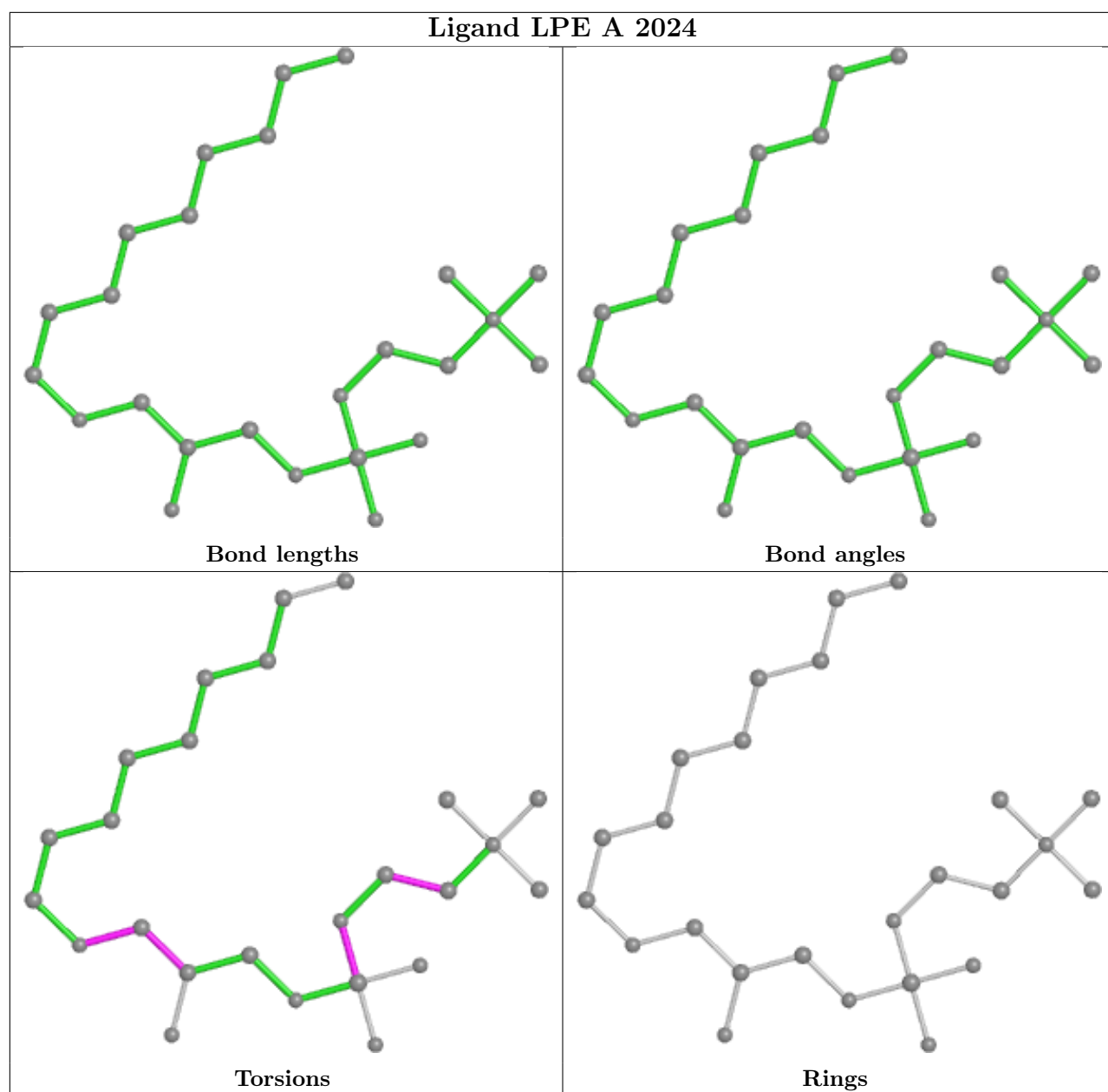


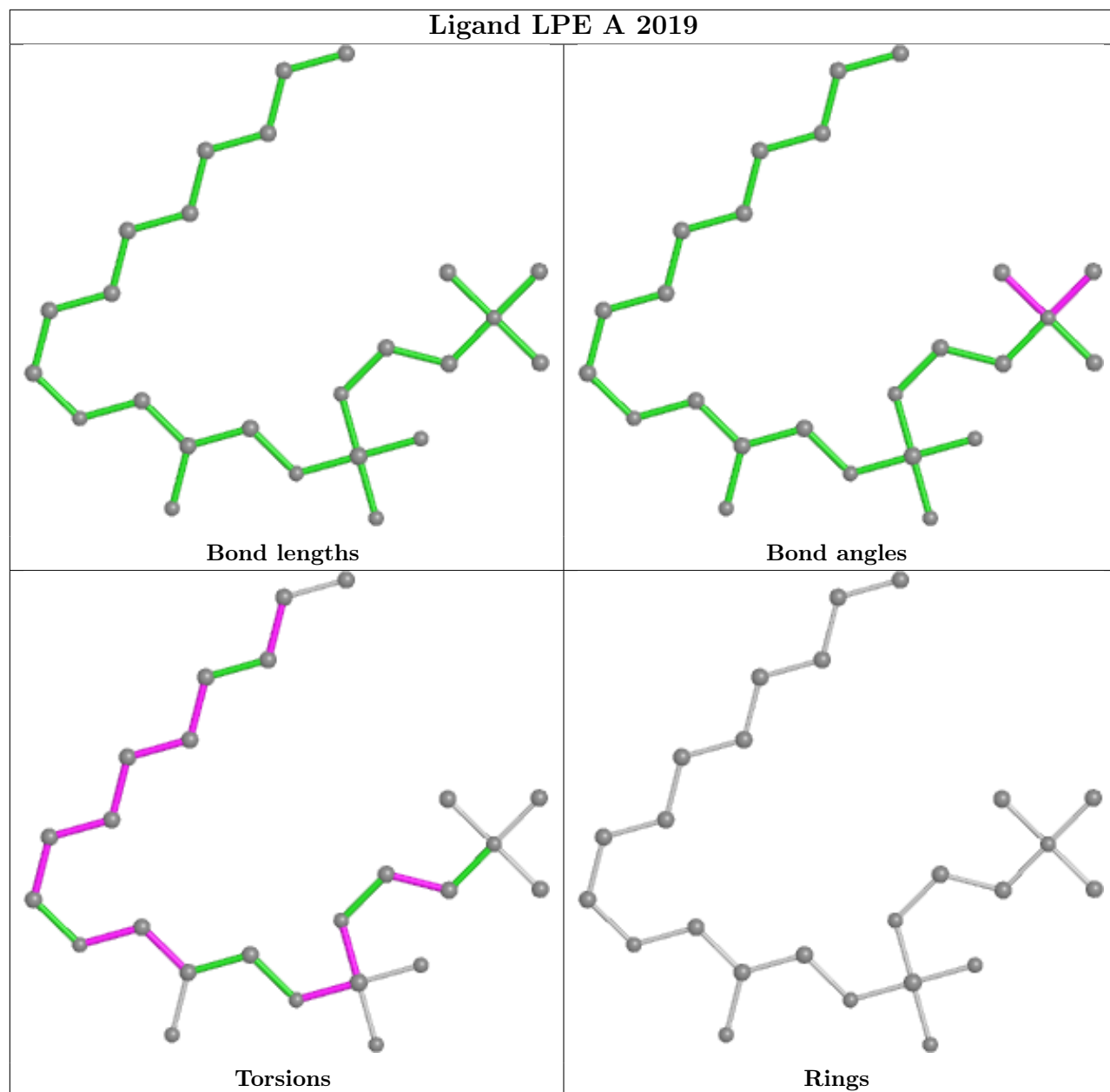




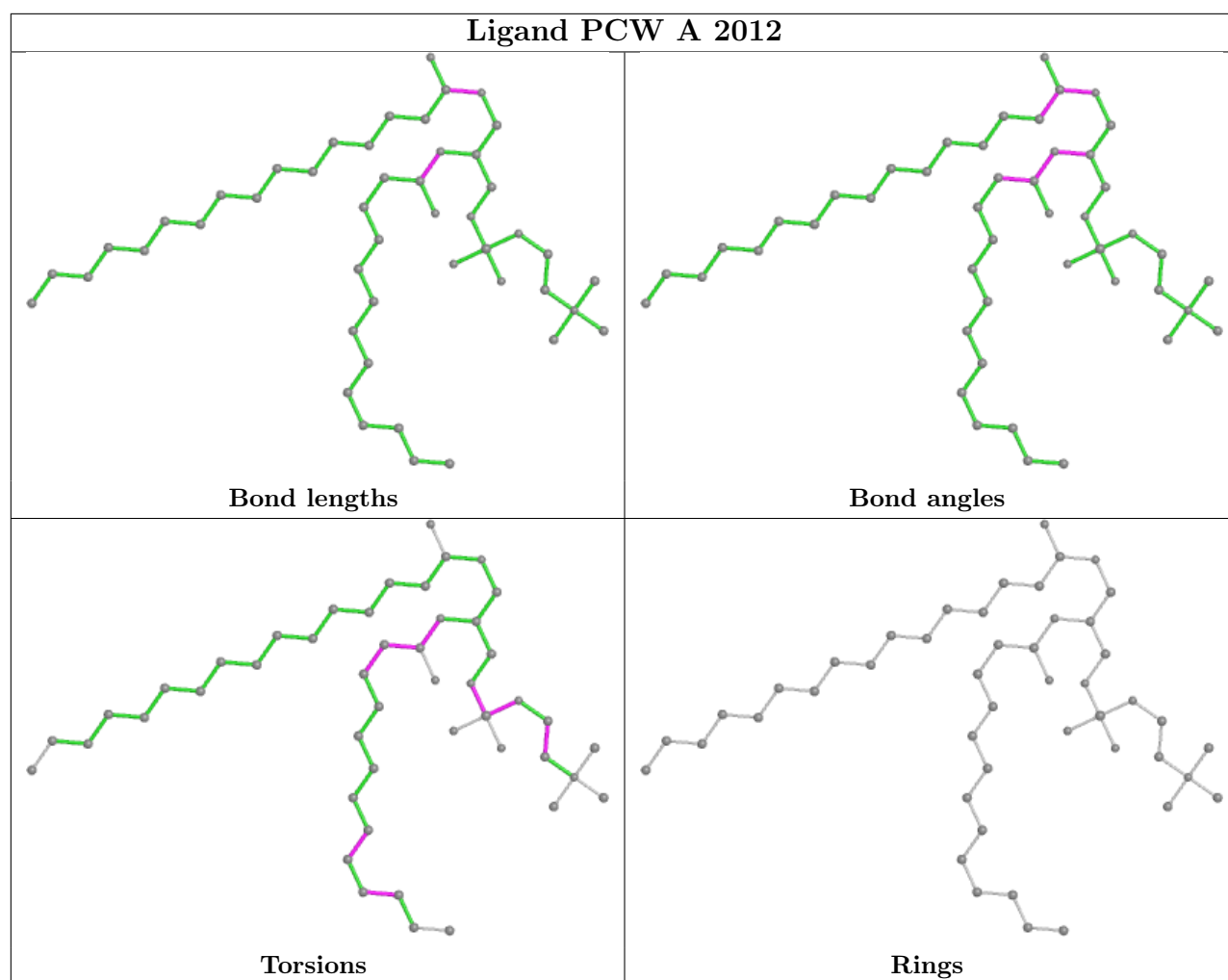












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

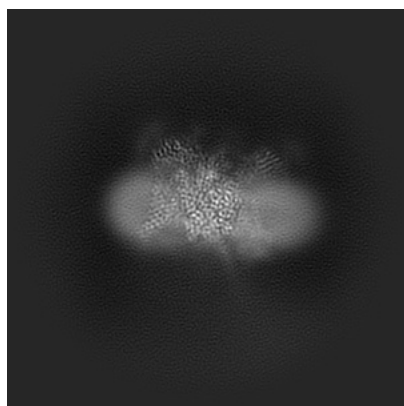
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33484. These allow visual inspection of the internal detail of the map and identification of artifacts.

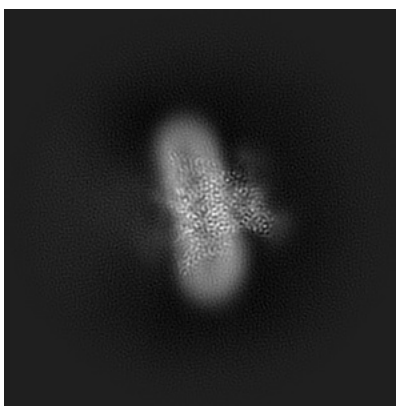
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

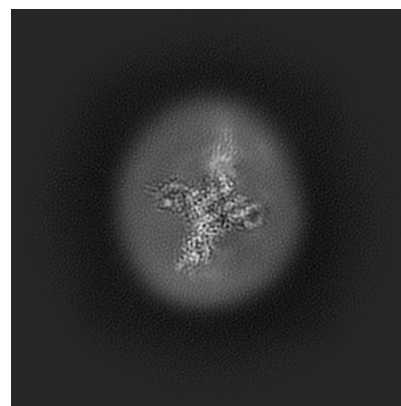
#### 6.1.1 Primary map



X

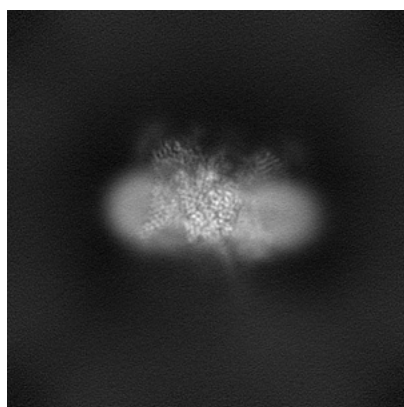


Y

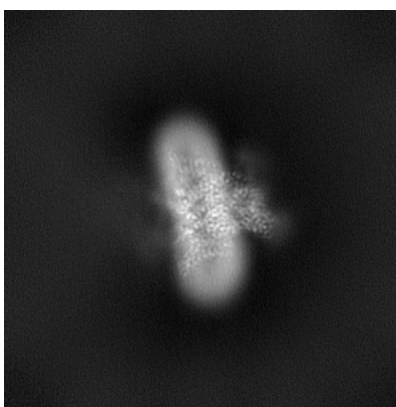


Z

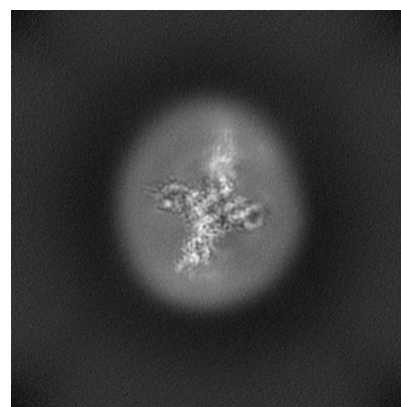
#### 6.1.2 Raw map



X



Y

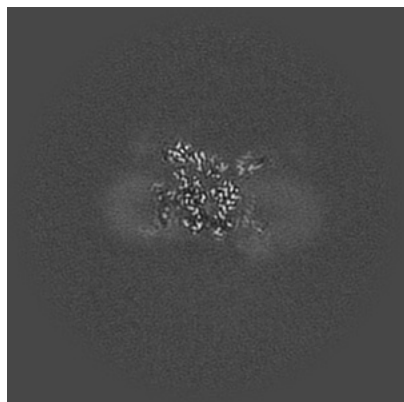


Z

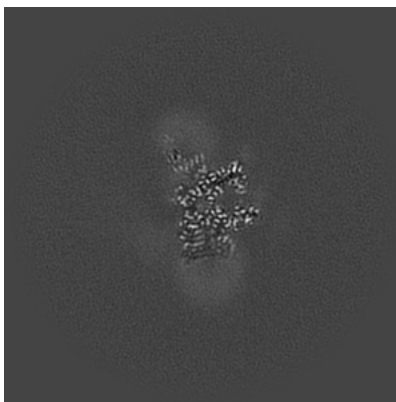
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

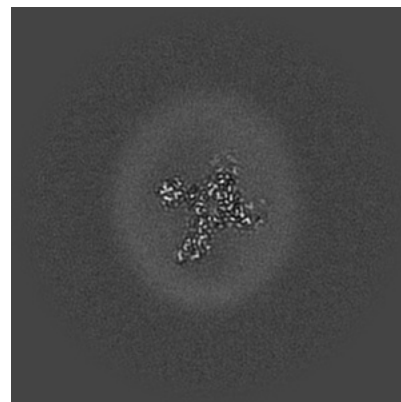
### 6.2.1 Primary map



X Index: 160

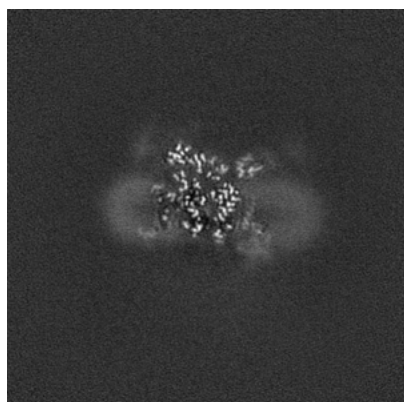


Y Index: 160

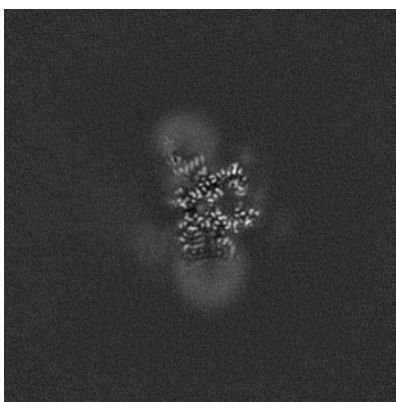


Z Index: 160

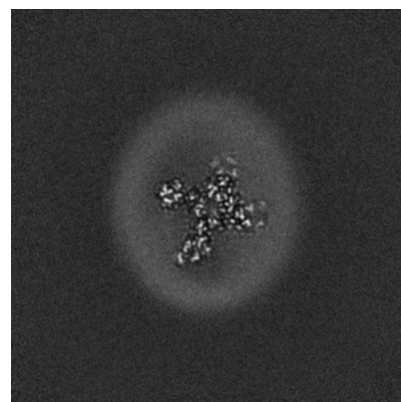
### 6.2.2 Raw map



X Index: 160



Y Index: 160

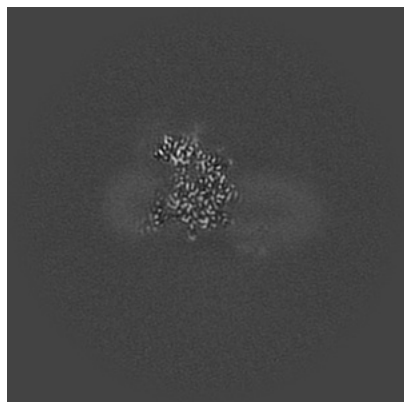


Z Index: 160

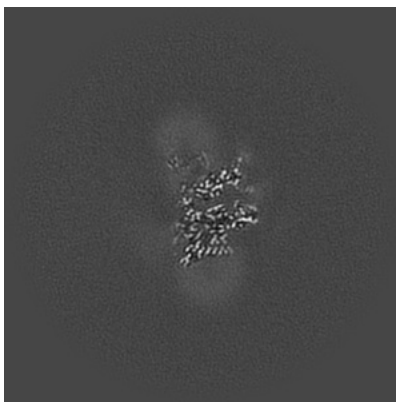
The images above show central slices of the map in three orthogonal directions.

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

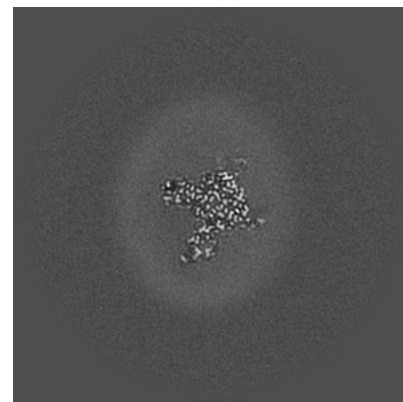
### 6.3.1 Primary map



X Index: 151

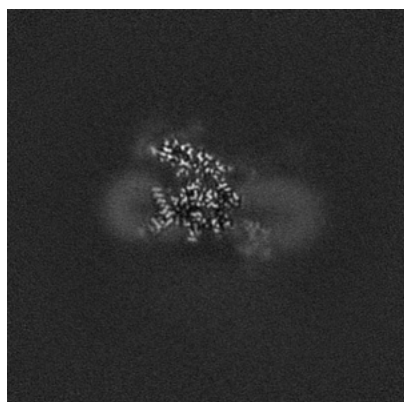


Y Index: 164

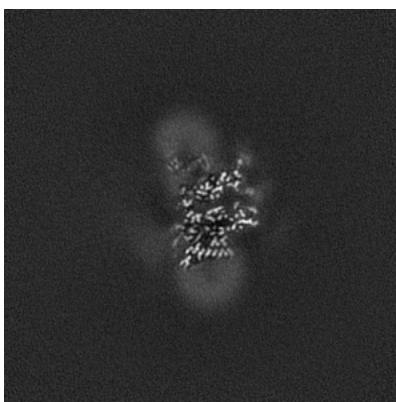


Z Index: 166

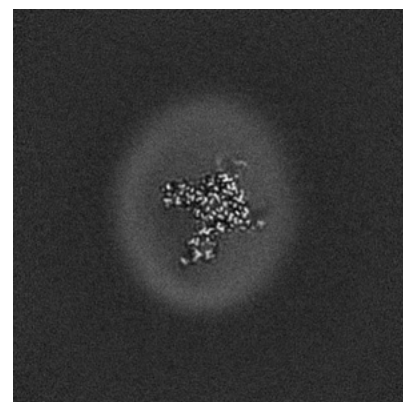
### 6.3.2 Raw map



X Index: 156



Y Index: 164

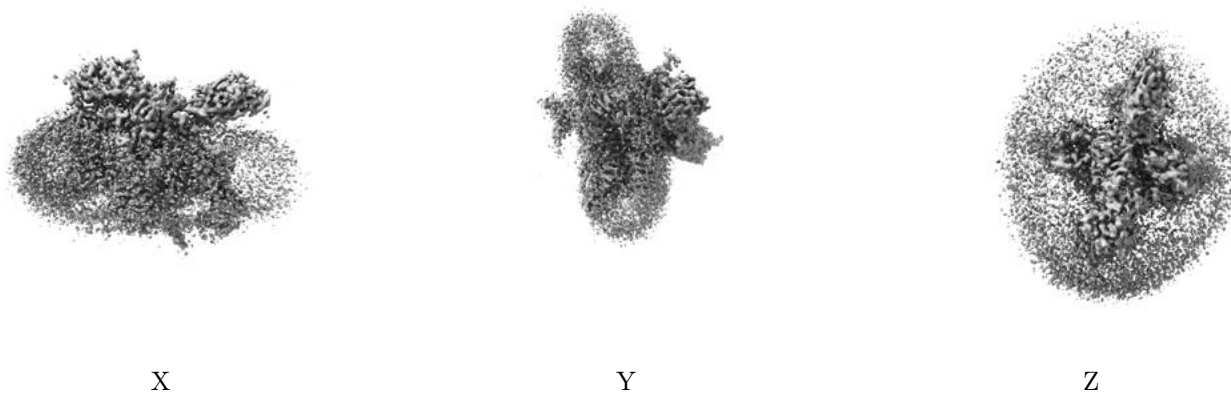


Z Index: 166

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

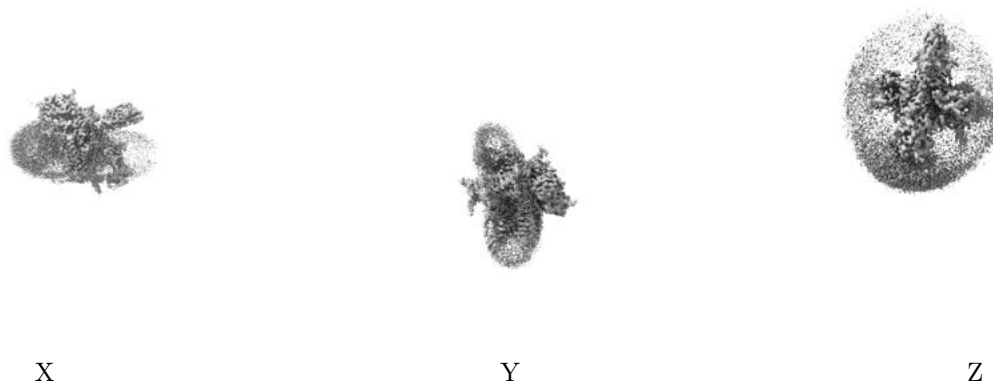
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.36. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 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.

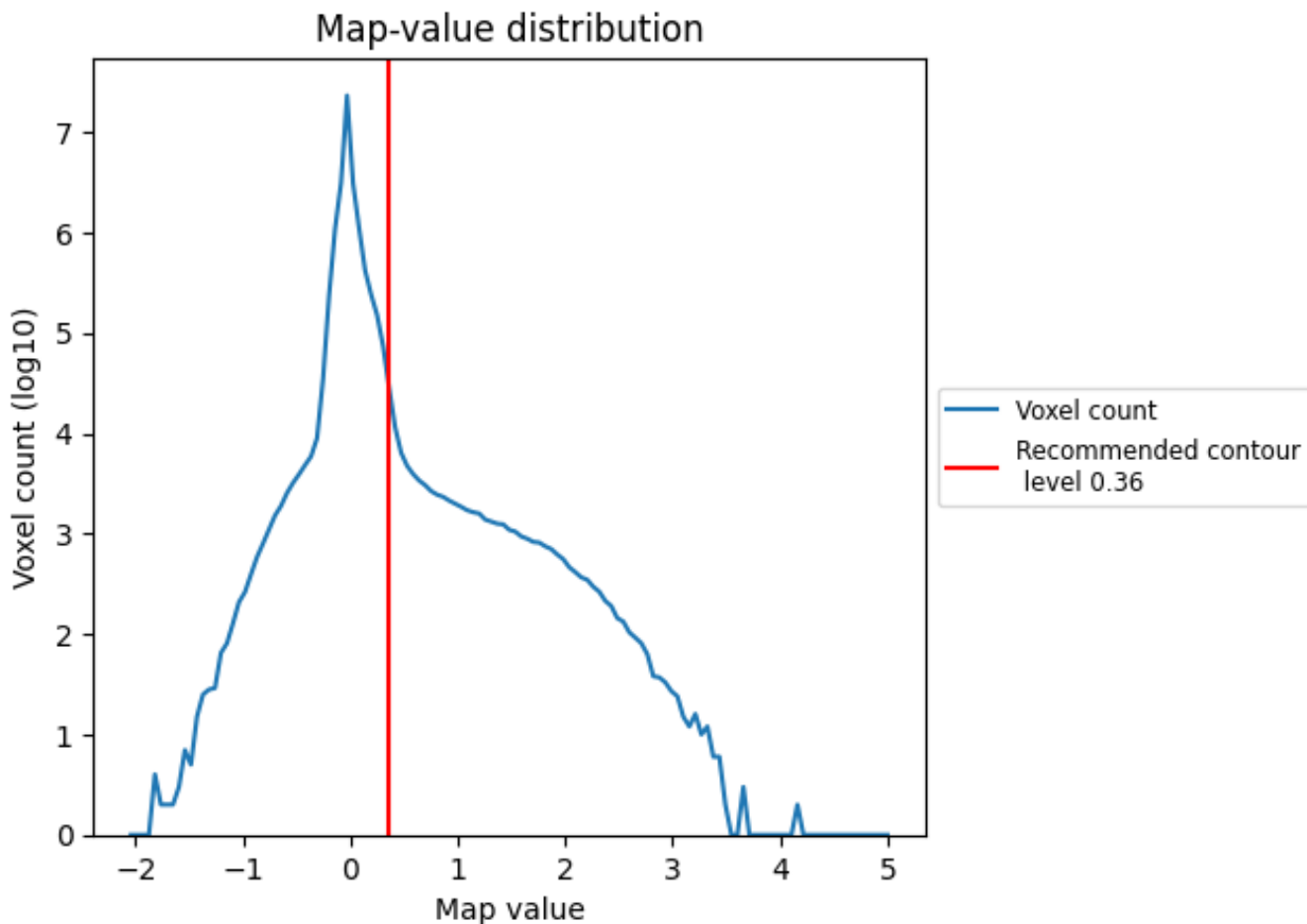
## 6.5 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

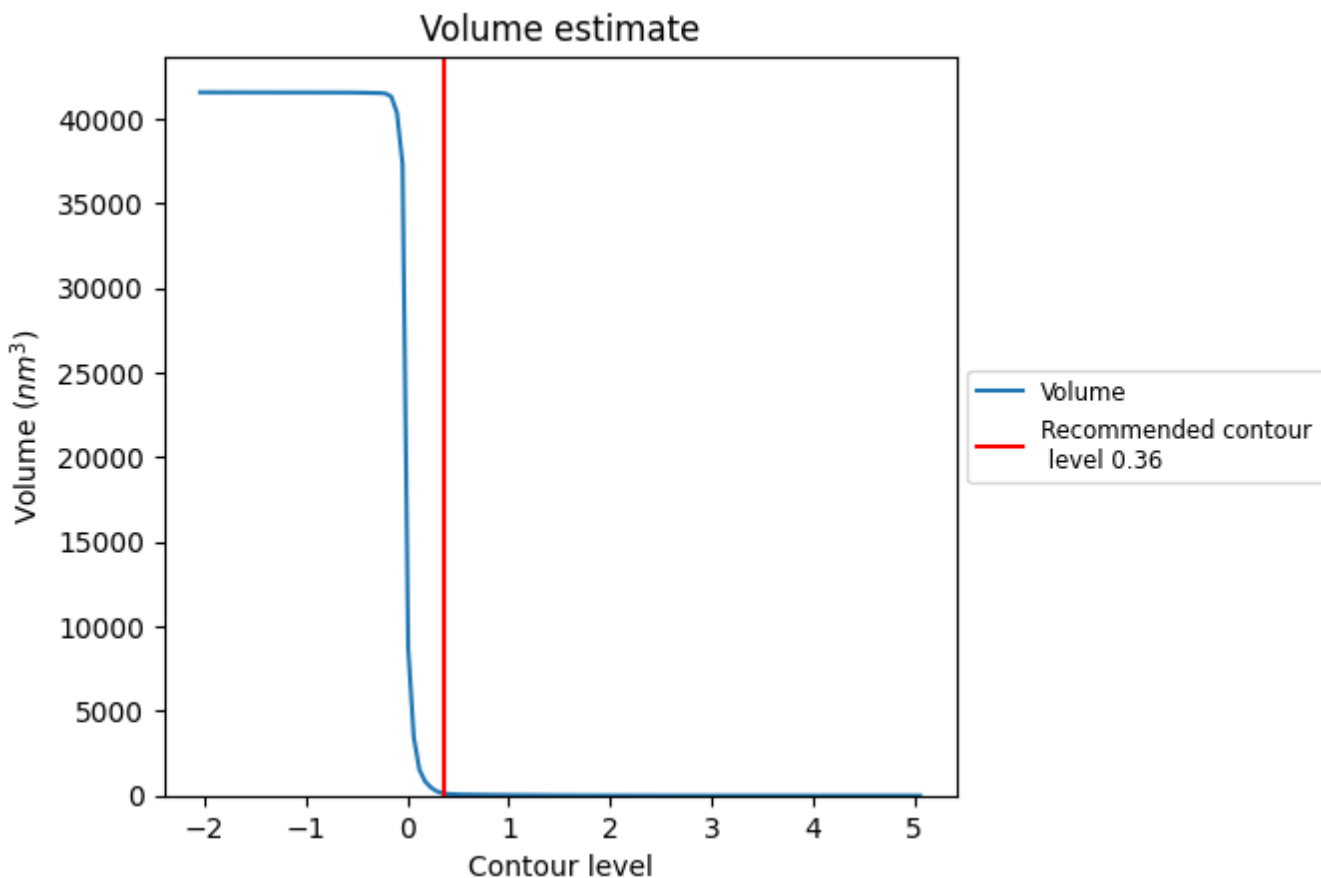
This section contains the results of statistical analysis of the map.

### 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.

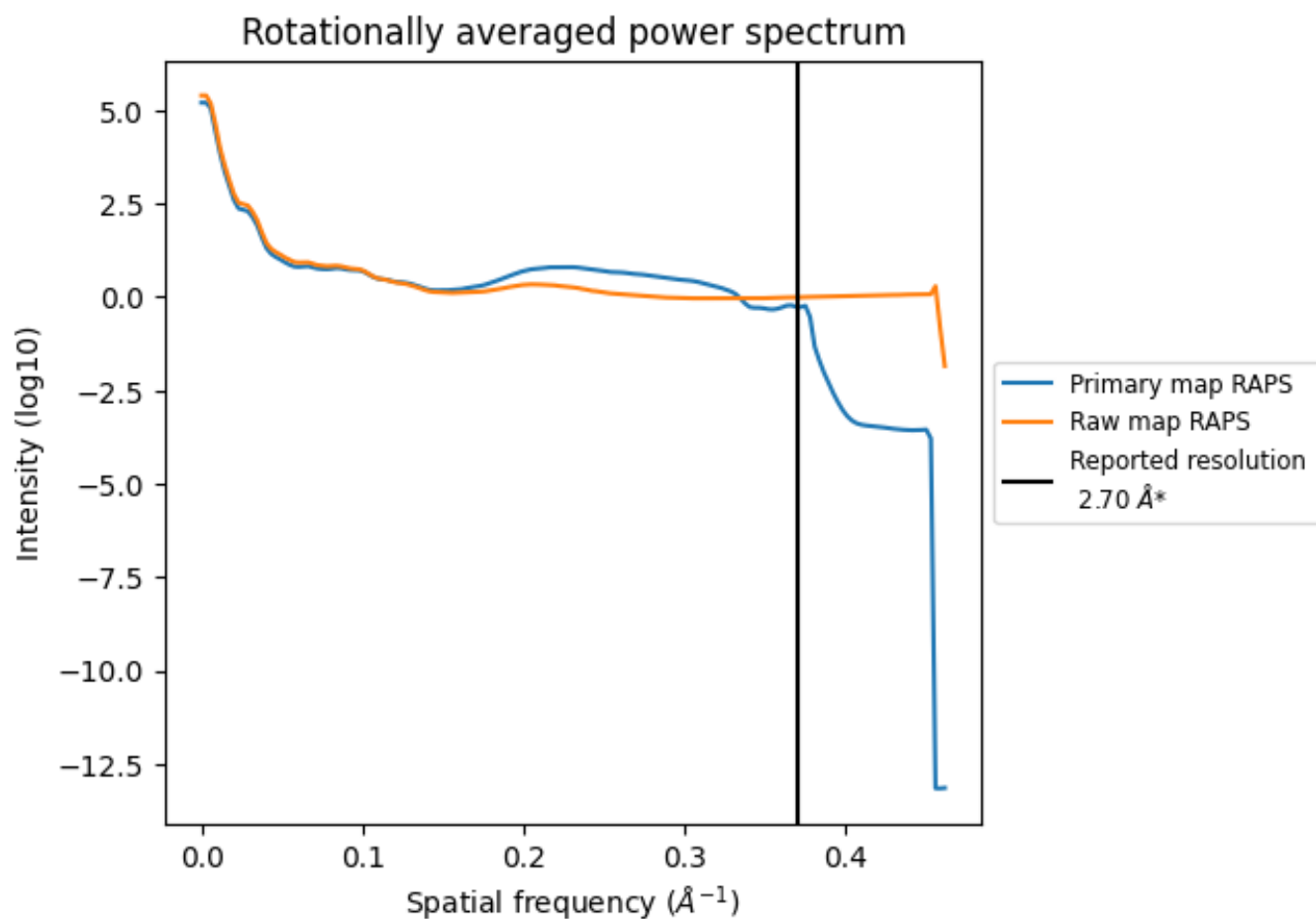
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 129 nm<sup>3</sup>; this corresponds to an approximate mass of 116 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](#)



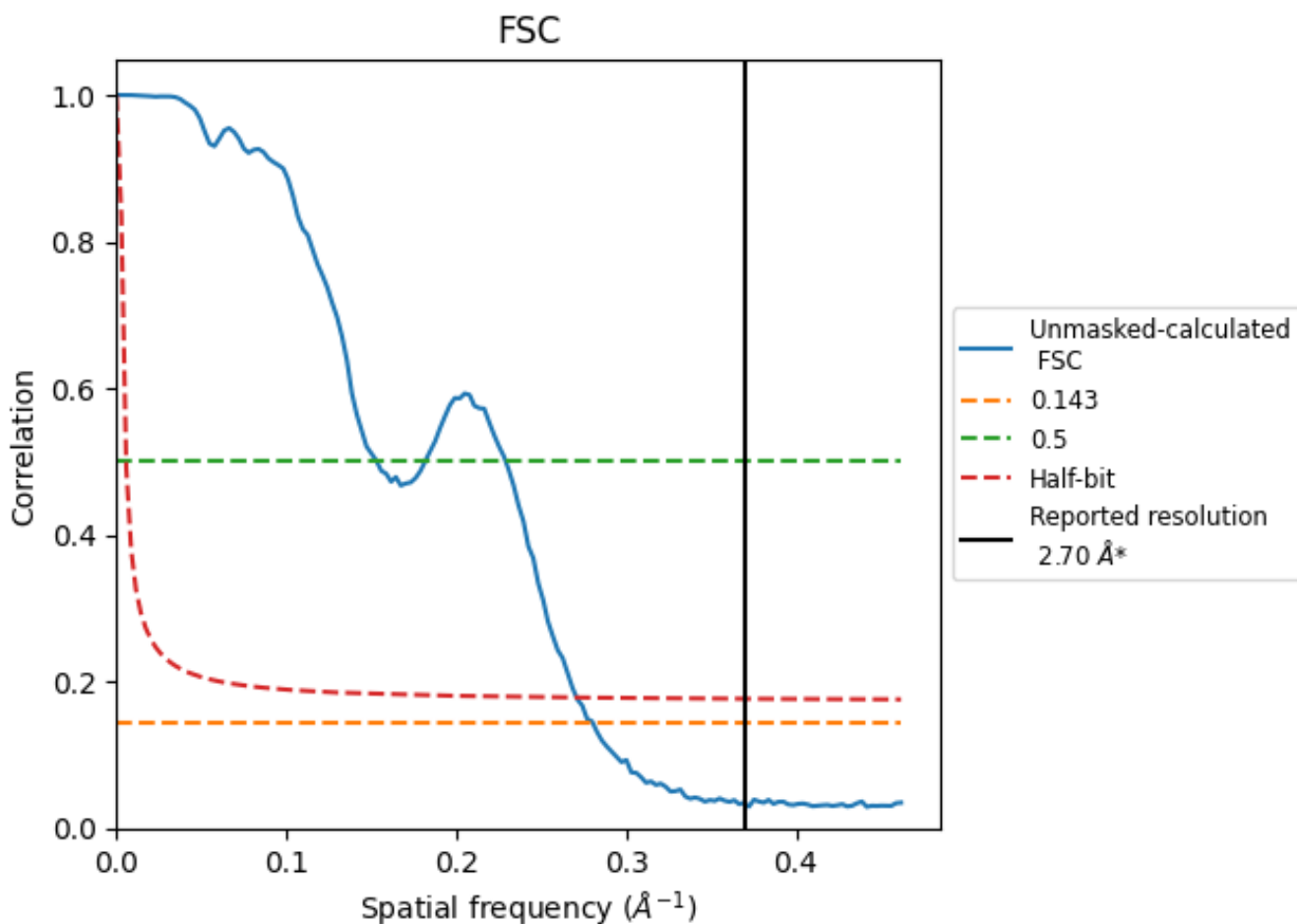
\*Reported resolution corresponds to spatial frequency of  $0.370 \text{ \AA}^{-1}$



## 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 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

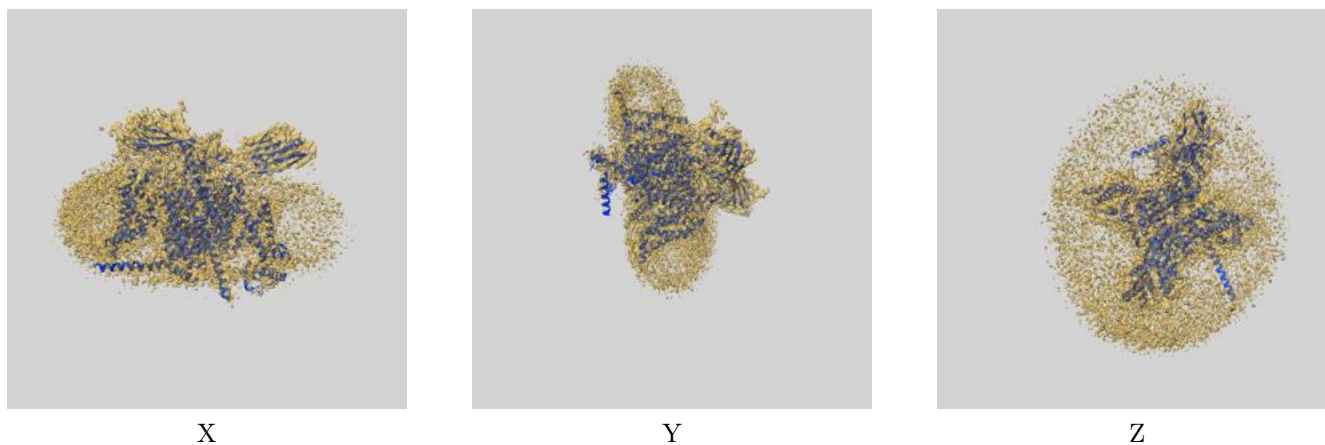
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.57	6.53	3.69

\*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 3.57 differs from the reported value 2.7 by more than 10 %

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

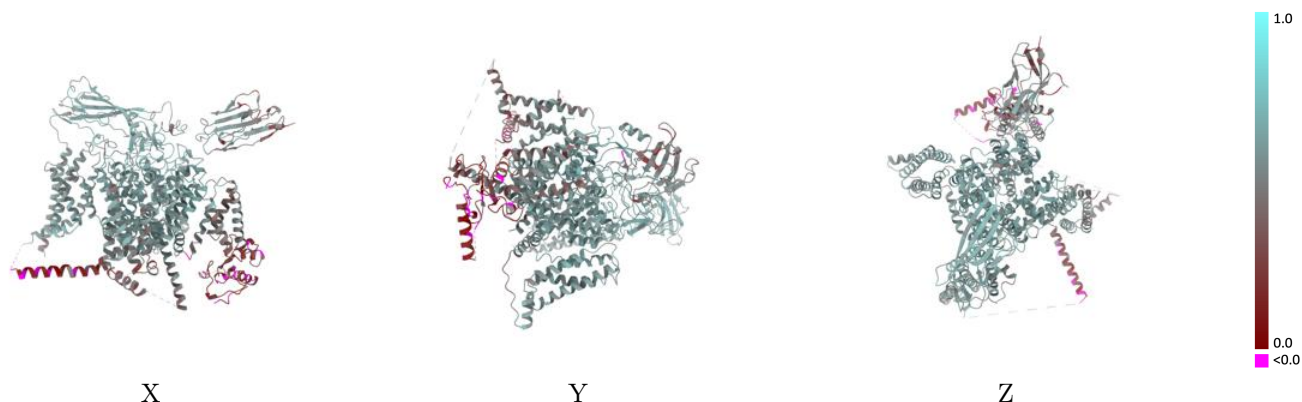
This section contains information regarding the fit between EMDB map EMD-33484 and PDB model 7XVE. Per-residue inclusion information can be found in section 3 on page 11.

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



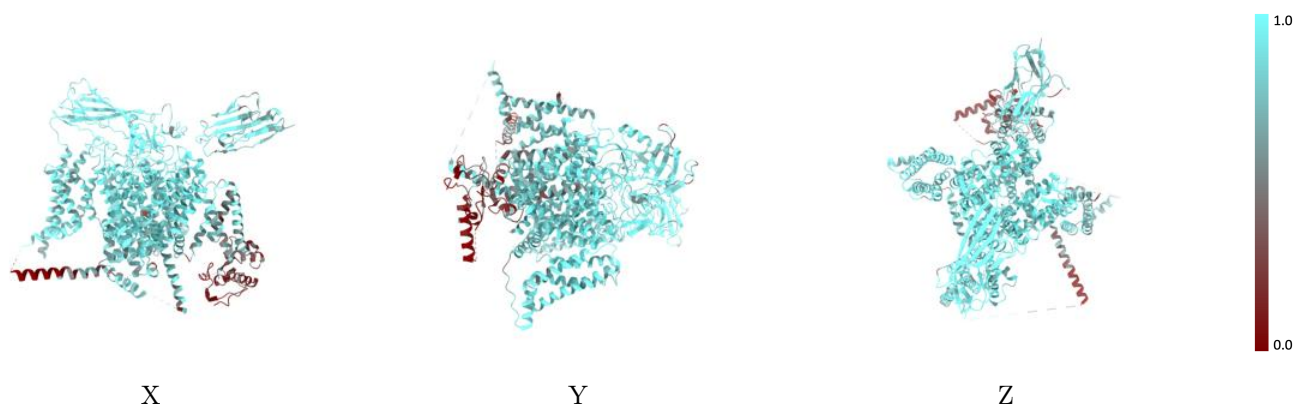
The images above show the 3D surface view of the map at the recommended contour level 0.36 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



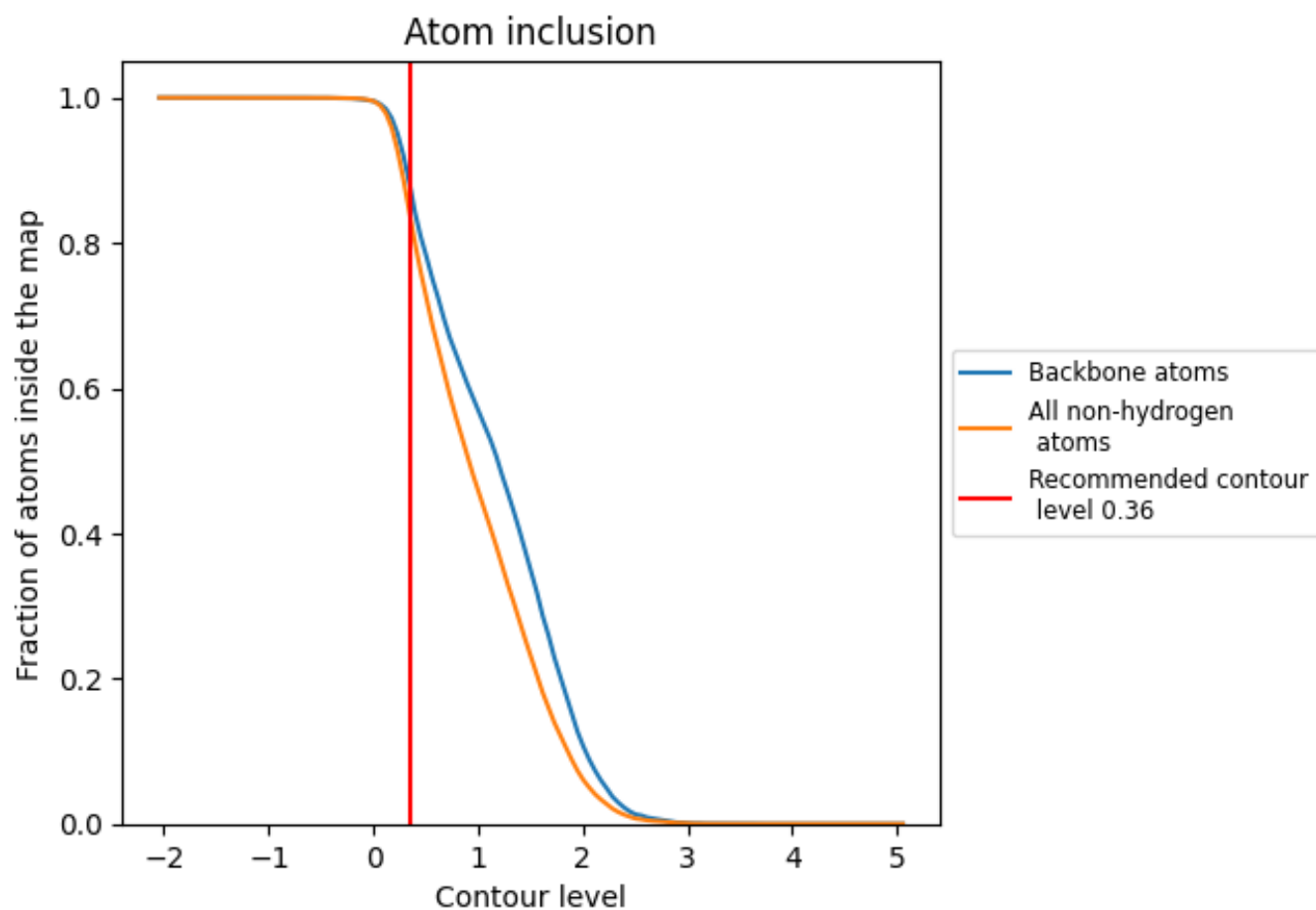
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.36).













## 9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 83% 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 (0.36) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8295	 0.5260
A	 0.8216	 0.5240
B	 0.9136	 0.5700
C	 0.7895	 0.4750
D	 0.9286	 0.5210
E	 0.8571	 0.4830

