



## wwPDB EM Validation Summary Report ⓘ

Nov 29, 2022 – 12:31 AM JST

PDB ID : 7W9K  
EMDB ID : EMD-32368  
Title : Cryo-EM structure of human Nav1.7-beta1-beta2 complex at 2.2 angstrom resolution  
Authors : Yan, N.; Huang, G.; Liu, D.; Wei, P.; Shen, H.  
Deposited on : 2021-12-09  
Resolution : 2.20 Å(reported)

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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) : 2.31.3

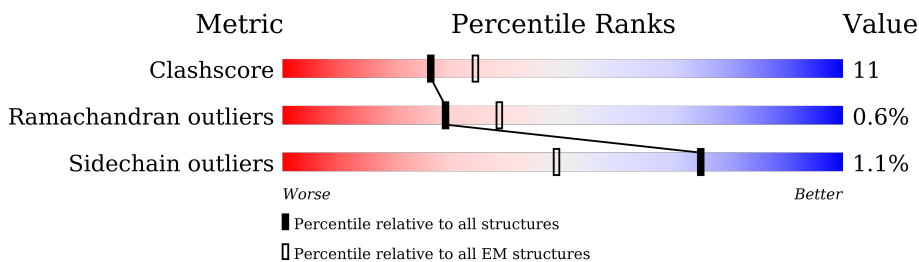
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.20 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	2031	
2	B	218	
3	C	215	
4	D	2	
4	E	2	
4	F	2	

## 2 Entry composition i

There are 13 unique types of molecules in this entry. The entry contains 14933 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	1413	11412	7534	1796	1997	85	1	0

There are 43 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-42	MET	-	initiating methionine	UNP Q15858
A	-41	ALA	-	expression tag	UNP Q15858
A	-40	SER	-	expression tag	UNP Q15858
A	-39	TRP	-	expression tag	UNP Q15858
A	-38	SER	-	expression tag	UNP Q15858
A	-37	HIS	-	expression tag	UNP Q15858
A	-36	PRO	-	expression tag	UNP Q15858
A	-35	GLN	-	expression tag	UNP Q15858
A	-34	PHE	-	expression tag	UNP Q15858
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

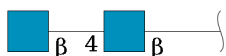
- Molecule 2 is a protein called Sodium channel subunit beta-1.

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

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

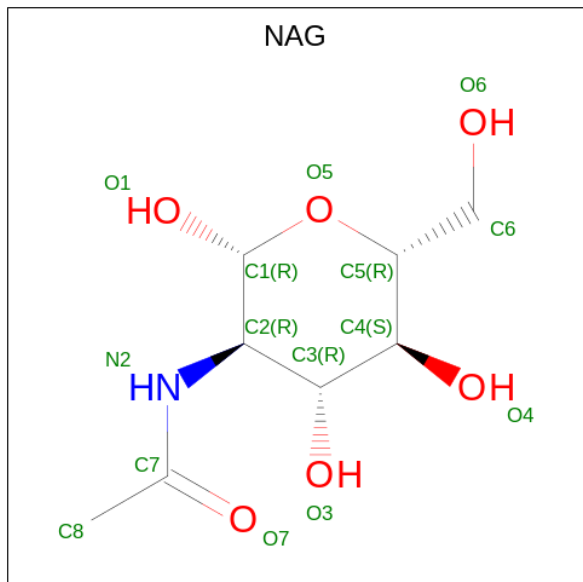
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	119	980	615	172	183	10	4	0

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



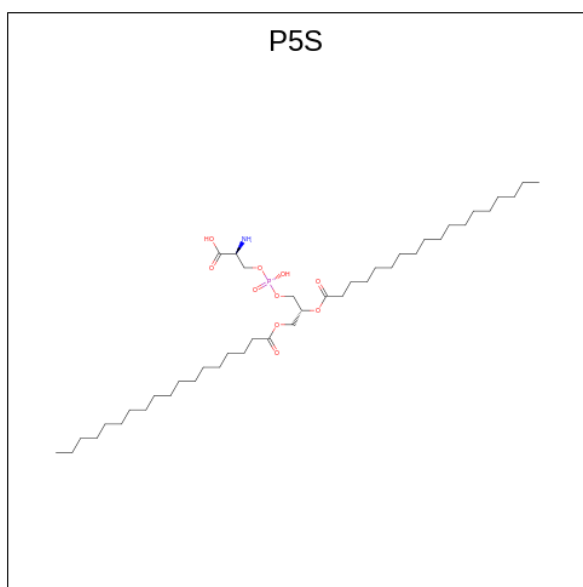
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	2	28	16	2	10	0	0
4	E	2	28	16	2	10	0	0
4	F	2	28	16	2	10	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ) (labeled as "Ligand of Interest" by depositor).



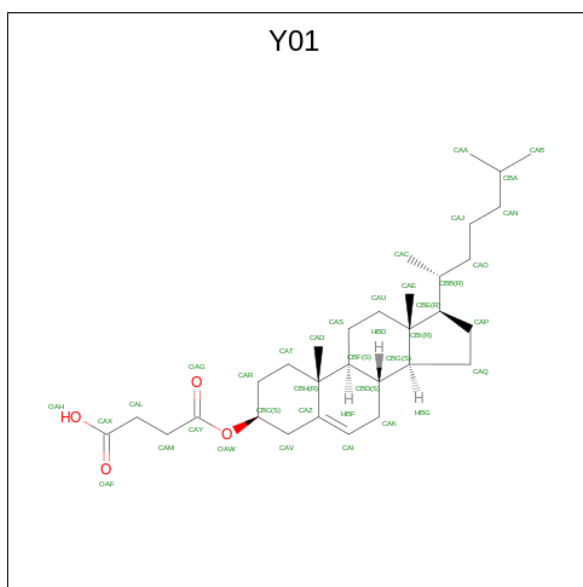
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	A	1	28	16	2	10	0
5	A	1	28	16	2	10	0
5	B	1	42	24	3	15	0
5	B	1	42	24	3	15	0
5	B	1	42	24	3	15	0

- Molecule 6 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (three-letter code: P5S) (formula:  $C_{42}H_{82}NO_{10}P$ ).



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		P
6	A	1	110	77	3	27	3	0
6	A	1	110	77	3	27	3	0
6	A	1	110	77	3	27	3	0

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



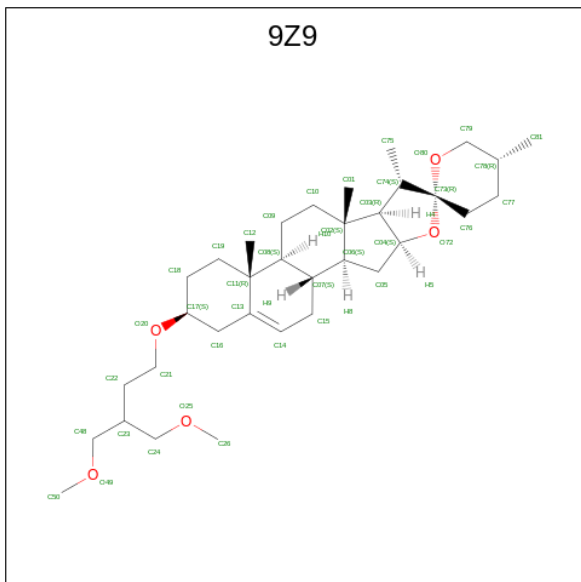
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
7	A	1	210	186	24	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
7	A	1	210	186	24	0
7	A	1	210	186	24	0
7	A	1	210	186	24	0
7	A	1	210	186	24	0
7	A	1	210	186	24	0

- Molecule 8 is (3beta,14beta,17beta,25R)-3-[4-methoxy-3-(methoxymethyl)butoxy]spirost-5-en (three-letter code: 9Z9) (formula: C<sub>34</sub>H<sub>56</sub>O<sub>5</sub>).

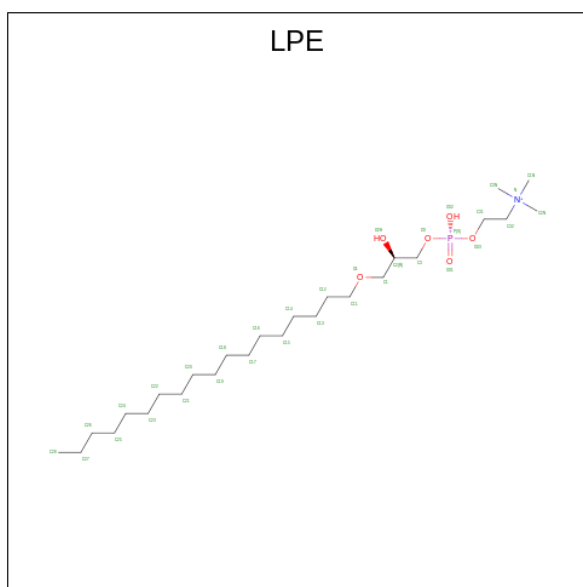


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
8	A	1	39	34	5	0

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
			Total	Na	
9	A	1	1	1	0

- Molecule 10 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	
10	A	1	Total 329	217	14	84	14	0
10	A	1	Total 329	217	14	84	14	0
10	A	1	Total 329	217	14	84	14	0
10	A	1	Total 329	217	14	84	14	0
10	A	1	Total 329	217	14	84	14	0
10	A	1	Total 329	217	14	84	14	0
10	A	1	Total 329	217	14	84	14	0
10	A	1	Total 329	217	14	84	14	0
10	A	1	Total 329	217	14	84	14	0
10	A	1	Total 329	217	14	84	14	0
10	A	1	Total 329	217	14	84	14	0
10	A	1	Total 329	217	14	84	14	0
10	A	1	Total 329	217	14	84	14	0
10	A	1	Total 329	217	14	84	14	0

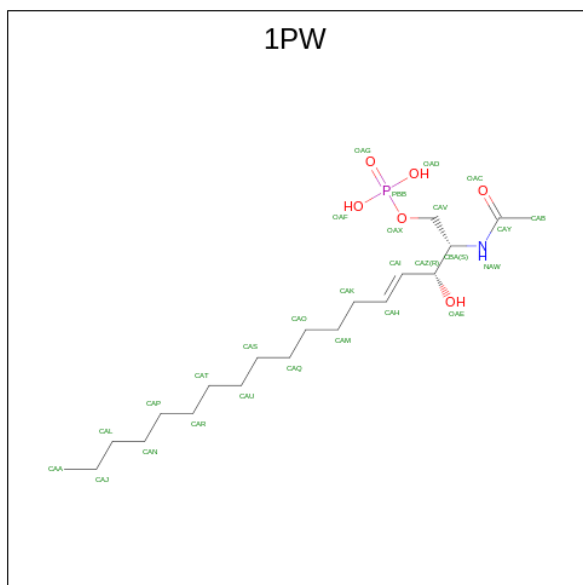
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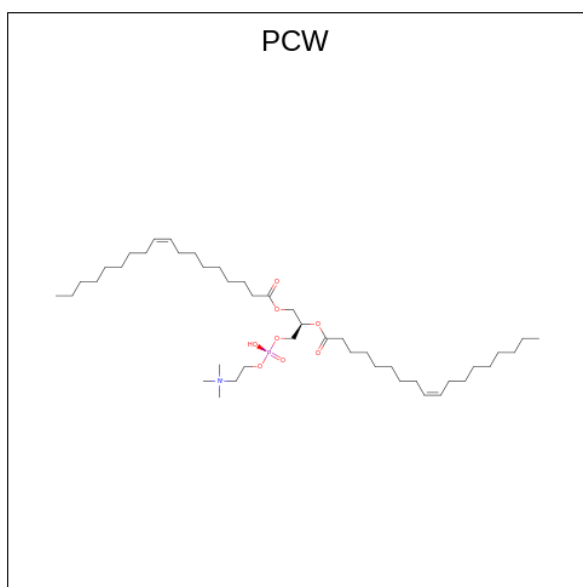
Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		P
10	B	1	17	9	1	6	1	0

- Molecule 11 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
			Total	C	O	P	
11	A	1	24	18	5	1	0

- Molecule 12 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	
12	A	1	Total	C	N	O	P	0
			232	182	5	40	5	
12	A	1	Total	C	N	O	P	0
			232	182	5	40	5	
12	A	1	Total	C	N	O	P	0
			232	182	5	40	5	
12	A	1	Total	C	N	O	P	0
			232	182	5	40	5	
12	A	1	Total	C	N	O	P	0
			232	182	5	40	5	

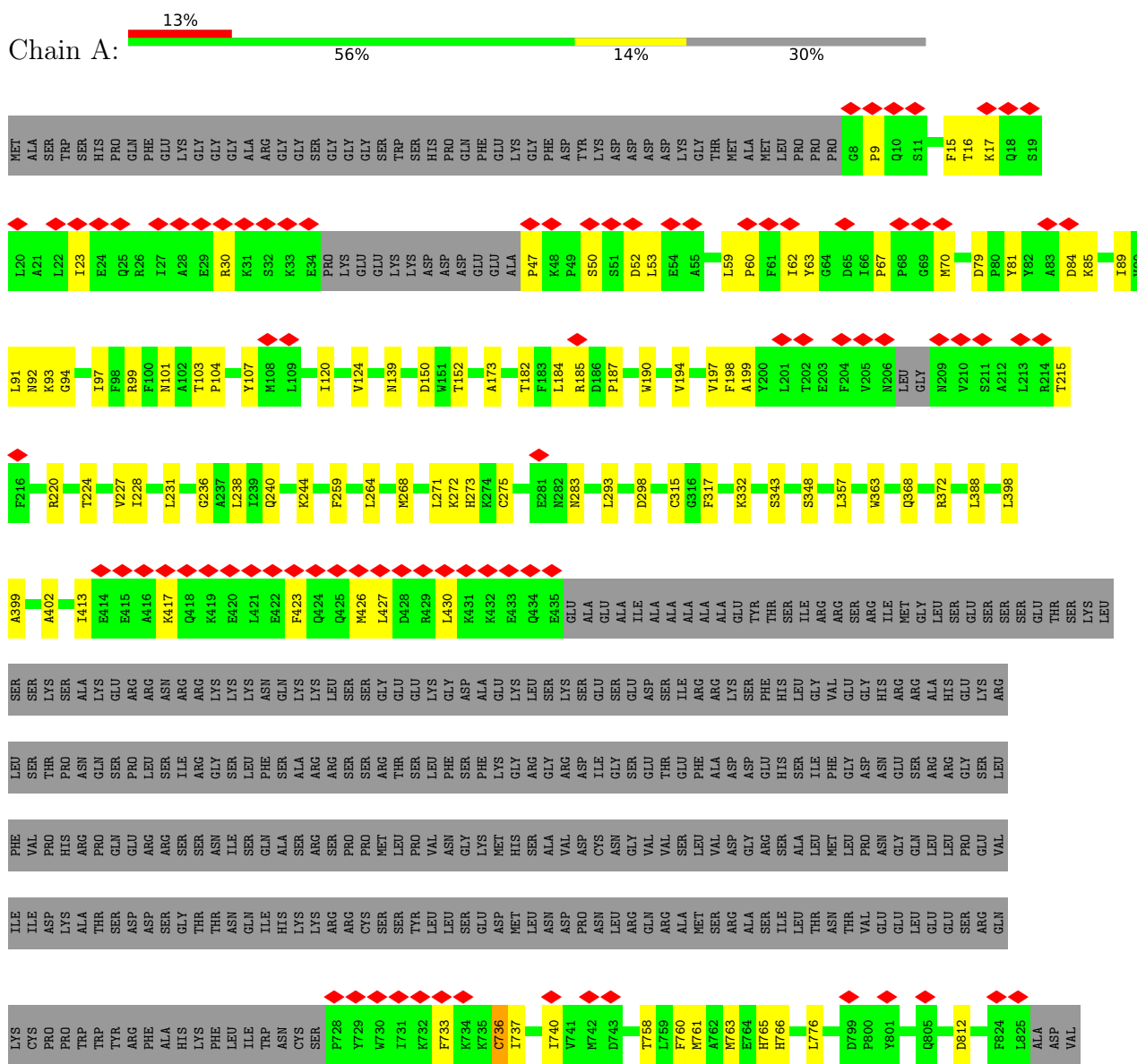
- Molecule 13 is water.

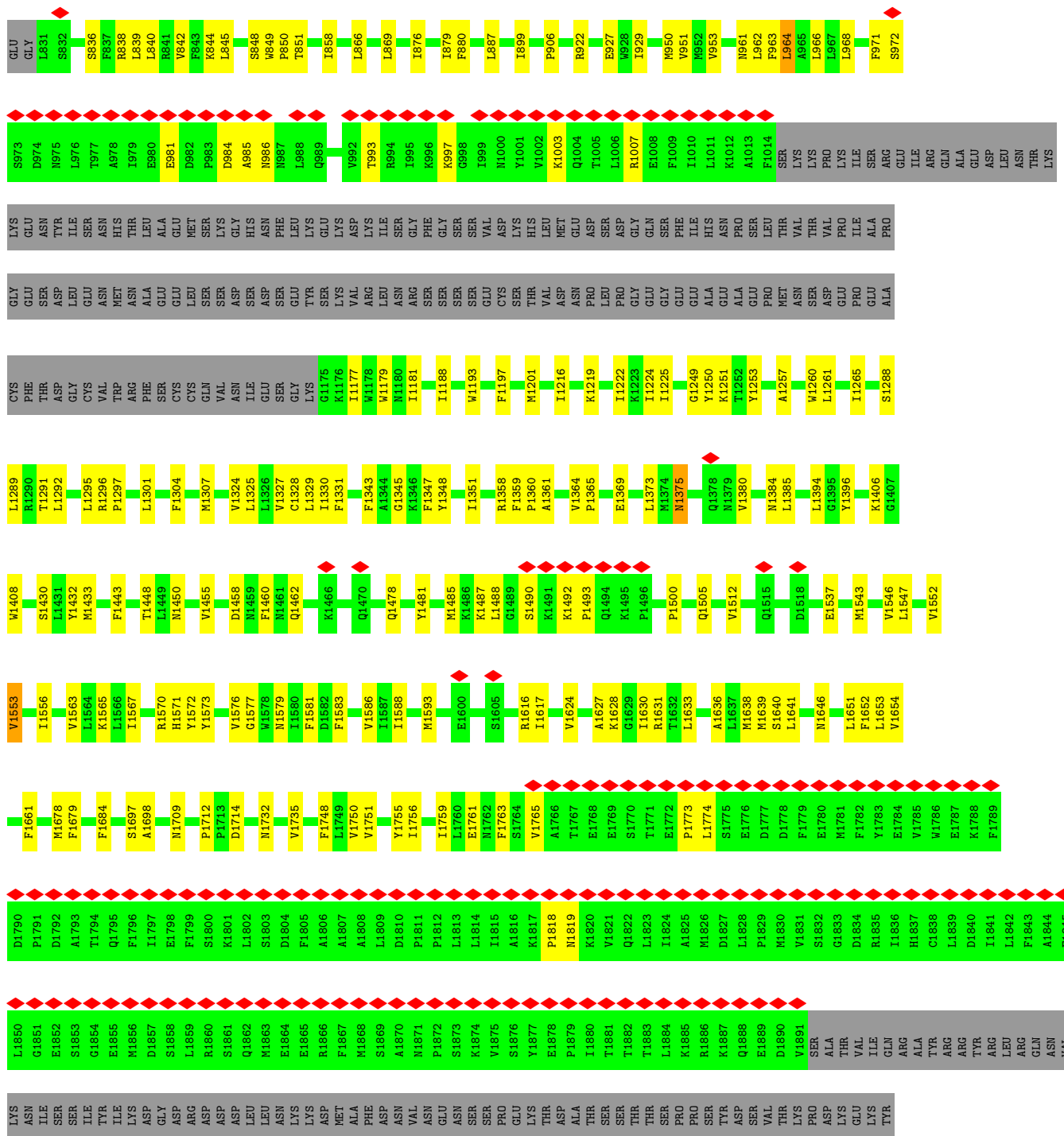
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
13	A	9	Total	O	0
			9	9	

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

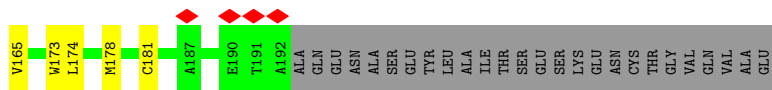
- Molecule 1: Sodium channel protein type 9 subunit alpha



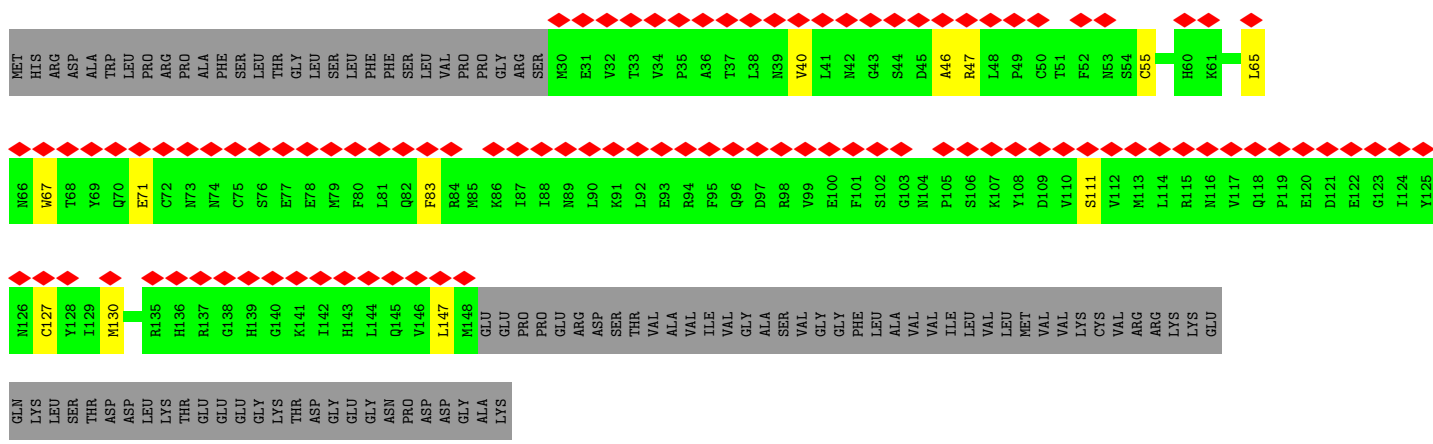


● Molecule 2: Sodium channel subunit beta-1





• Molecule 3: Sodium channel subunit beta-2



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



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



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



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	785228	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 (6k x 4k)	Depositor
Maximum map value	0.145	Depositor
Minimum map value	-0.060	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.022	Depositor
Map size ( $\text{\AA}$ )	421.59363, 421.59363, 421.59363	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.0979, 1.0979, 1.0979	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: P5S, NA, Y01, 1PW, 9Z9, PCW, NAG, LPE

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	0.85	0/11686	0.89	0/15823
2	B	1.03	0/1442	0.95	0/1949
3	C	0.35	0/1011	0.58	0/1367
All	All	0.85	0/14139	0.88	0/19139

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1712	PRO	Peptide

### 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	11412	0	11617	250	0
2	B	1416	0	1380	26	0
3	C	980	0	935	4	0
4	D	28	0	25	2	0
4	E	28	0	25	0	0
4	F	28	0	25	0	0
5	A	28	0	26	1	0
5	B	42	0	39	7	0
6	A	110	0	130	9	0
7	A	210	0	294	71	0
8	A	39	0	0	14	0
9	A	1	0	0	0	0
10	A	329	0	445	34	0
10	B	17	0	19	0	0
11	A	24	0	33	2	0
12	A	232	0	323	29	0
13	A	9	0	0	0	0
All	All	14933	0	15316	337	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 11.

The worst 5 of 337 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ILE:HD11	1:A:99:ARG:NH1	1.60	1.16
2:B:112:THR:HG21	5:B:303:NAG:C8	1.84	1.06
1:A:1250:TYR:HB3	7:A:2004:Y01:HAU1	1.36	1.03
1:A:950:MET:HE3	7:A:2007:Y01:HAU2	1.40	1.02
1:A:1324:VAL:HG21	1:A:1455:VAL:HG21	1.47	0.96

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	1402/2031 (69%)	1318 (94%)	75 (5%)	9 (1%)	25	26
2	B	171/218 (78%)	167 (98%)	3 (2%)	1 (1%)	25	26
3	C	120/215 (56%)	117 (98%)	3 (2%)	0	100	100
All	All	1693/2464 (69%)	1602 (95%)	81 (5%)	10 (1%)	29	26

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1773	PRO
2	B	150	ALA
1	A	15	PHE
1	A	93	LYS
1	A	953	VAL

### 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	1265/1809 (70%)	1253 (99%)	12 (1%)	78	88
2	B	157/190 (83%)	156 (99%)	1 (1%)	86	93
3	C	114/193 (59%)	110 (96%)	4 (4%)	36	46
All	All	1536/2192 (70%)	1519 (99%)	17 (1%)	74	85

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	71	GLU
3	C	147	LEU
1	A	1547	LEU
1	A	1553	VAL
1	A	1616	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1378	GLN
3	C	53	ASN
1	A	1461	ASN
3	C	118	GLN
1	A	1732	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](#)

6 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	NAG	D	1	1,4	14,14,15	0.35	0	17,19,21	0.55	0
4	NAG	D	2	4	14,14,15	0.28	0	17,19,21	0.76	0
4	NAG	E	1	1,4	14,14,15	0.19	0	17,19,21	0.45	0
4	NAG	E	2	4	14,14,15	0.45	0	17,19,21	0.66	0
4	NAG	F	1	2,4	14,14,15	0.57	0	17,19,21	1.19	2 (11%)
4	NAG	F	2	4	14,14,15	0.65	0	17,19,21	1.20	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	NAG	E	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	NAG	F	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1	NAG	C1-O5-C5	2.75	115.92	112.19
4	F	1	NAG	C3-C4-C5	-2.64	105.52	110.24
4	F	2	NAG	C4-C3-C2	-2.40	107.50	111.02

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

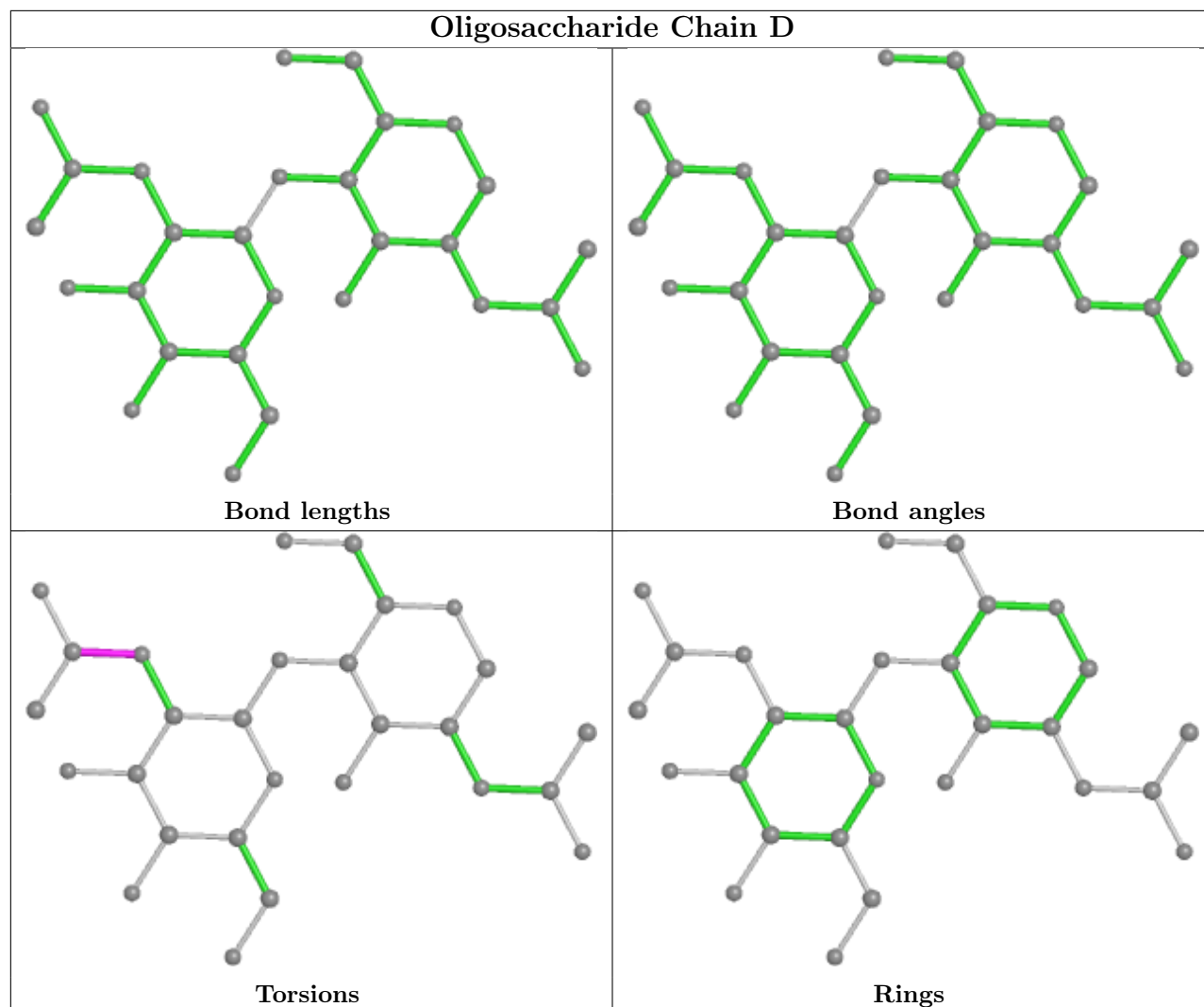
Mol	Chain	Res	Type	Atoms
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
4	E	1	NAG	O5-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6

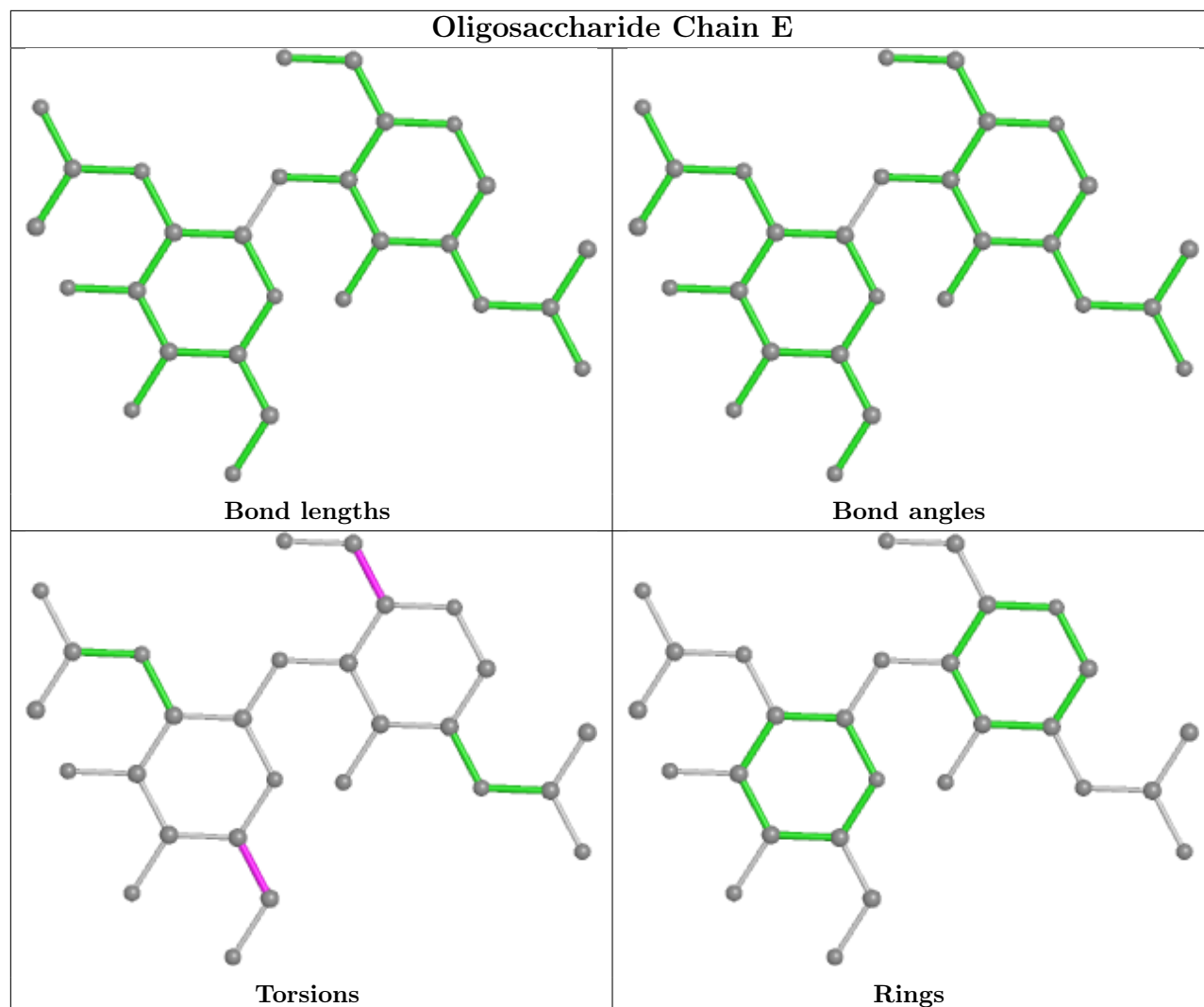
There are no ring outliers.

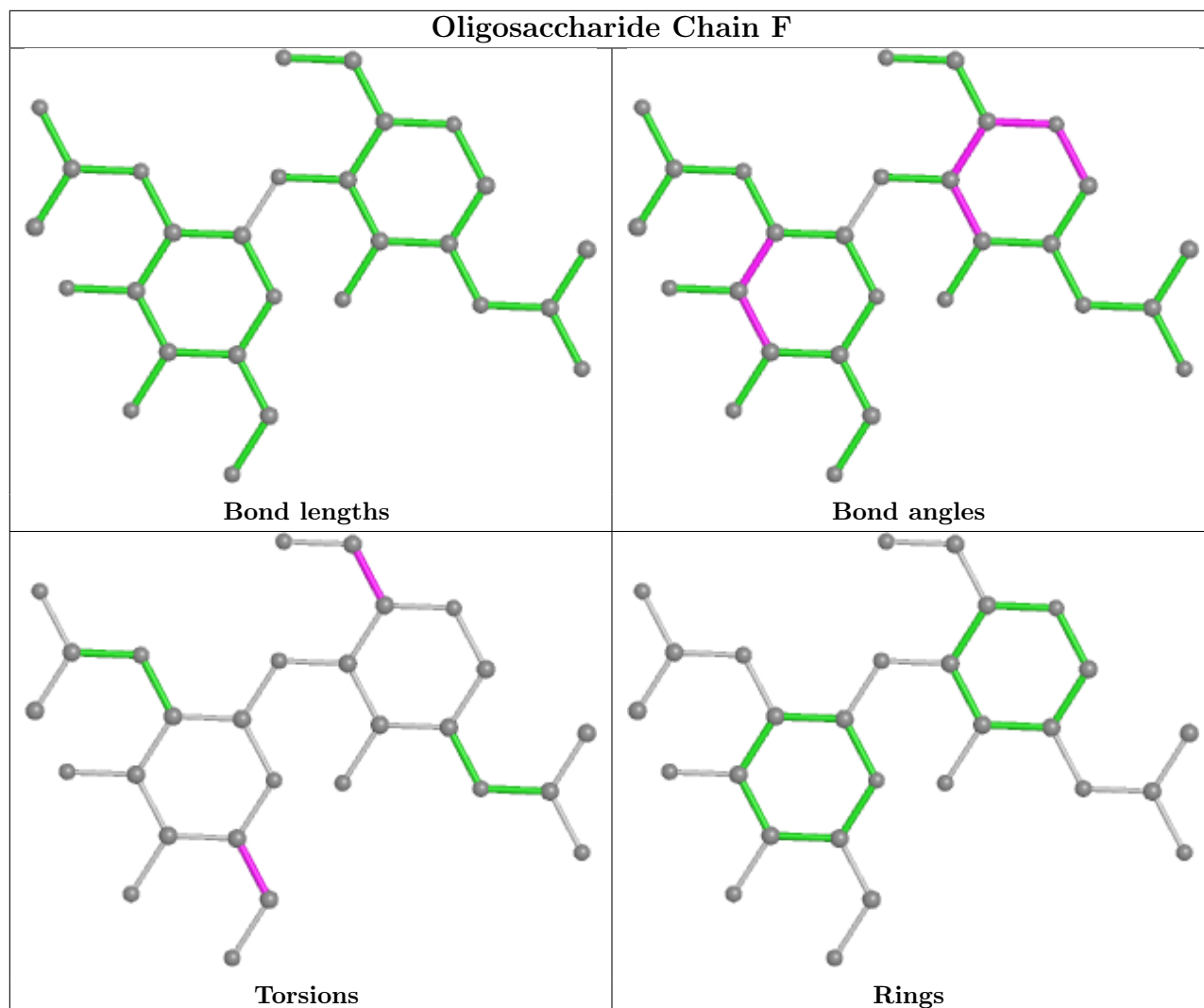
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	2	NAG	2	0
4	D	1	NAG	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 oligosaccharide.







## 5.6 Ligand geometry [i](#)

Of 37 ligands modelled in this entry, 1 is monoatomic - leaving 36 for Mogul analysis.

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	$\# Z  > 2$
7	Y01	A	2032	-	38,38,38	1.62	7 (18%)	57,57,57	1.63	9 (15%)
5	NAG	A	2008	1	14,14,15	0.38	0	17,19,21	0.90	1 (5%)
5	NAG	B	301	2	14,14,15	0.64	0	17,19,21	0.98	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	LPE	A	2017	-	27,27,33	0.54	0	31,33,39	0.61	0
10	LPE	A	2016	-	21,21,33	0.68	0	25,27,39	1.03	2 (8%)
5	NAG	A	2001	1	14,14,15	0.35	0	17,19,21	0.44	0
7	Y01	A	2007	-	38,38,38	0.66	1 (2%)	57,57,57	1.78	10 (17%)
6	P5S	A	2031	-	32,33,53	1.17	4 (12%)	36,40,60	1.04	3 (8%)
10	LPE	A	2025	-	24,24,33	0.53	0	28,30,39	0.53	0
5	NAG	B	302	2	14,14,15	0.18	0	17,19,21	0.41	0
6	P5S	A	2002	-	33,34,53	0.76	1 (3%)	36,40,60	1.81	5 (13%)
10	LPE	A	2021	-	24,24,33	0.60	0	28,30,39	0.89	1 (3%)
10	LPE	A	2024	-	24,24,33	0.53	0	28,30,39	0.63	0
10	LPE	A	2033	-	16,16,33	0.67	0	20,22,39	0.67	0
10	LPE	A	2023	-	24,24,33	0.54	0	28,30,39	0.68	1 (3%)
10	LPE	A	2014	-	19,19,33	0.62	0	23,25,39	0.51	0
12	PCW	A	2020	-	43,43,53	1.01	2 (4%)	49,51,61	1.12	5 (10%)
10	LPE	A	2022	-	24,24,33	0.85	0	28,30,39	0.92	1 (3%)
10	LPE	A	2011	-	24,24,33	0.51	0	28,30,39	0.60	0
7	Y01	A	2005	-	38,38,38	1.15	4 (10%)	57,57,57	1.74	12 (21%)
7	Y01	A	2003	-	38,38,38	0.66	1 (2%)	57,57,57	1.79	11 (19%)
12	PCW	A	2029	-	43,43,53	1.03	2 (4%)	49,51,61	0.94	2 (4%)
12	PCW	A	2018	-	46,46,53	0.99	3 (6%)	52,54,61	1.18	4 (7%)
12	PCW	A	2030	-	43,43,53	1.03	2 (4%)	49,51,61	1.00	2 (4%)
8	9Z9	A	2006	-	44,44,44	0.70	1 (2%)	66,68,68	1.45	12 (18%)
10	LPE	A	2026	-	24,24,33	0.51	0	28,30,39	0.62	0
10	LPE	A	2028	-	16,16,33	0.69	0	20,22,39	0.67	0
11	1PW	A	2013	-	23,23,27	0.44	0	24,26,32	0.61	0
10	LPE	B	304	-	16,16,33	0.67	0	20,22,39	0.60	0
10	LPE	A	2027	-	24,24,33	0.54	0	28,30,39	0.50	0
12	PCW	A	2015	-	52,52,53	0.93	2 (3%)	58,60,61	0.97	2 (3%)
5	NAG	B	303	2	14,14,15	0.25	0	17,19,21	0.42	0
6	P5S	A	2019	-	40,40,53	1.13	3 (7%)	43,45,60	1.37	3 (6%)
7	Y01	A	2004	-	38,38,38	0.65	1 (2%)	57,57,57	1.79	11 (19%)
10	LPE	A	2012	-	24,24,33	0.33	0	25,27,39	0.60	0
7	Y01	A	2009	-	38,38,38	1.15	4 (10%)	57,57,57	1.74	11 (19%)

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
7	Y01	A	2032	-	-	7/19/77/77	0/4/4/4
5	NAG	A	2008	1	-	2/6/23/26	0/1/1/1
5	NAG	B	301	2	-	0/6/23/26	0/1/1/1
10	LPE	A	2017	-	-	10/28/28/34	-
10	LPE	A	2016	-	-	15/22/22/34	-
5	NAG	A	2001	1	-	2/6/23/26	0/1/1/1
7	Y01	A	2007	-	-	0/19/77/77	0/4/4/4
6	P5S	A	2031	-	-	16/39/39/59	-
10	LPE	A	2025	-	-	8/25/25/34	-
5	NAG	B	302	2	-	0/6/23/26	0/1/1/1
6	P5S	A	2002	-	-	28/39/39/59	-
10	LPE	A	2021	-	-	7/25/25/34	-
10	LPE	A	2024	-	-	3/25/25/34	-
10	LPE	A	2033	-	-	8/17/17/34	-
10	LPE	A	2023	-	-	3/25/25/34	-
10	LPE	A	2014	-	-	10/20/20/34	-
12	PCW	A	2020	-	-	12/47/47/57	-
10	LPE	A	2022	-	-	12/25/25/34	-
10	LPE	A	2011	-	-	10/25/25/34	-
7	Y01	A	2005	-	-	4/19/77/77	0/4/4/4
7	Y01	A	2003	-	-	0/19/77/77	0/4/4/4
12	PCW	A	2029	-	-	16/47/47/57	-
12	PCW	A	2018	-	-	13/50/50/57	-
12	PCW	A	2030	-	-	11/47/47/57	-
8	9Z9	A	2006	-	-	0/12/100/100	0/6/6/6
10	LPE	A	2026	-	-	6/25/25/34	-
10	LPE	A	2028	-	-	7/17/17/34	-
11	1PW	A	2013	-	-	4/22/22/29	-
10	LPE	B	304	-	-	9/17/17/34	-
10	LPE	A	2027	-	-	10/25/25/34	-
12	PCW	A	2015	-	-	16/56/56/57	-
5	NAG	B	303	2	-	0/6/23/26	0/1/1/1
6	P5S	A	2019	-	-	8/44/44/59	-
7	Y01	A	2004	-	-	0/19/77/77	0/4/4/4
10	LPE	A	2012	-	-	8/25/25/34	-
7	Y01	A	2009	-	-	4/19/77/77	0/4/4/4



The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	2029	PCW	O3-C11	4.40	1.46	1.33
6	A	2019	P5S	O37-C38	4.40	1.46	1.34
7	A	2032	Y01	CBB-CBE	-4.36	1.46	1.54
12	A	2030	PCW	O3-C11	4.26	1.45	1.33
12	A	2030	PCW	O2-C31	4.20	1.46	1.34

The worst 5 of 108 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	2002	P5S	OG-CB-CA	7.10	114.25	108.06
7	A	2009	Y01	CBI-CBE-CBB	-5.94	110.19	119.49
7	A	2005	Y01	CBI-CBE-CBB	-5.92	110.21	119.49
7	A	2004	Y01	CBI-CBE-CBB	-5.91	110.23	119.49
7	A	2007	Y01	CBI-CBE-CBB	-5.91	110.23	119.49

There are no chirality outliers.

5 of 269 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	2002	P5S	C-CA-CB-OG
6	A	2002	P5S	N-CA-CB-OG
6	A	2002	P5S	CB-OG-P12-O13
6	A	2002	P5S	C3-O16-P12-OG
6	A	2002	P5S	C3-O16-P12-O13

There are no ring outliers.

31 monomers are involved in 149 short contacts:

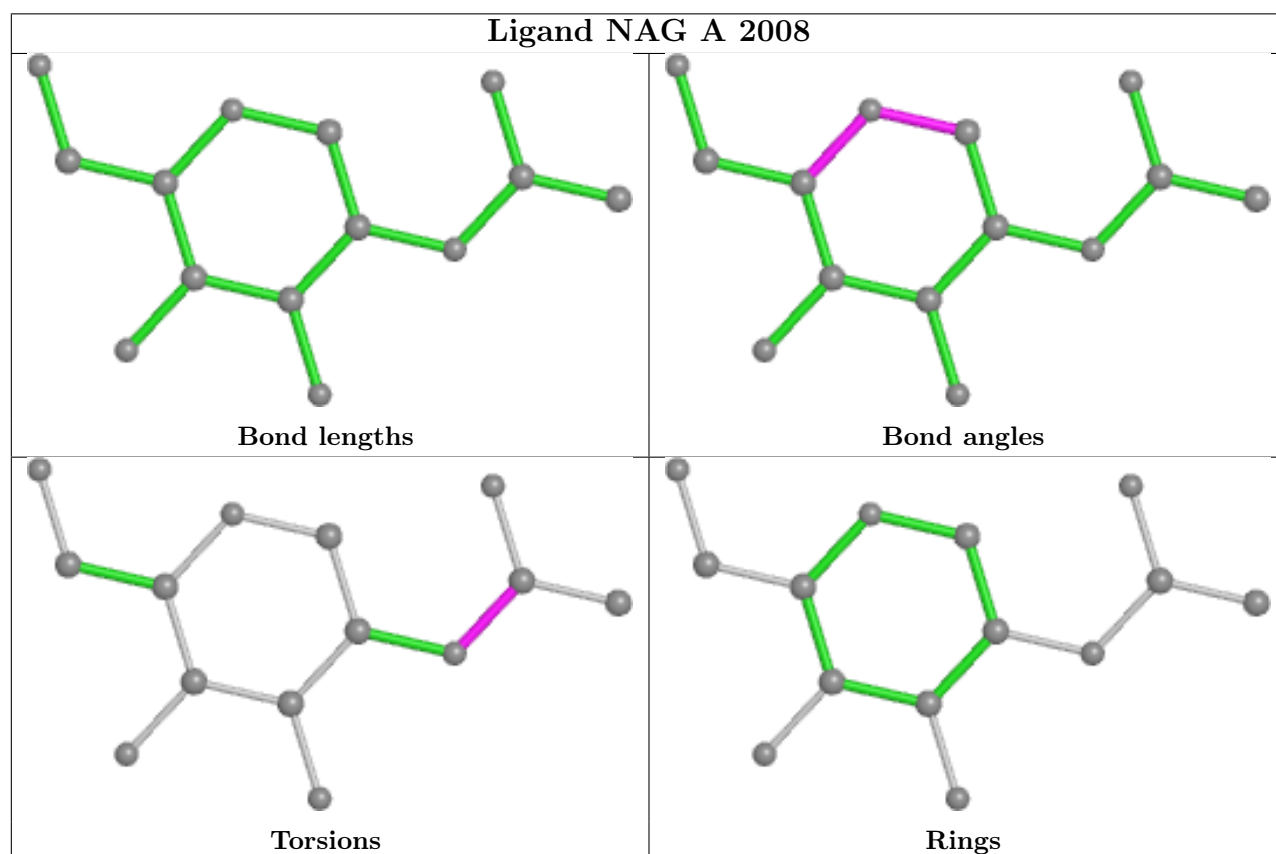
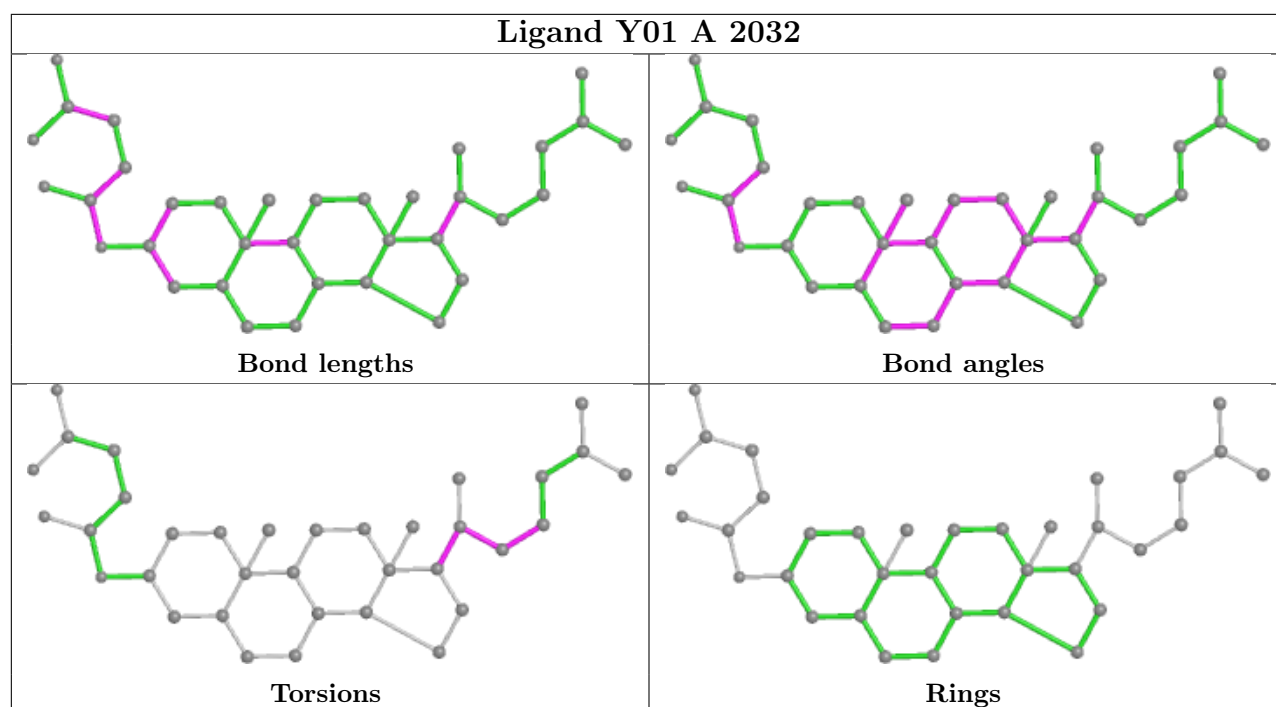
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	2032	Y01	20	0
10	A	2017	LPE	3	0
10	A	2016	LPE	5	0
5	A	2001	NAG	1	0
7	A	2007	Y01	13	0
6	A	2031	P5S	3	0
10	A	2025	LPE	2	0
5	B	302	NAG	1	0
6	A	2002	P5S	2	0
10	A	2021	LPE	7	0
10	A	2024	LPE	2	0

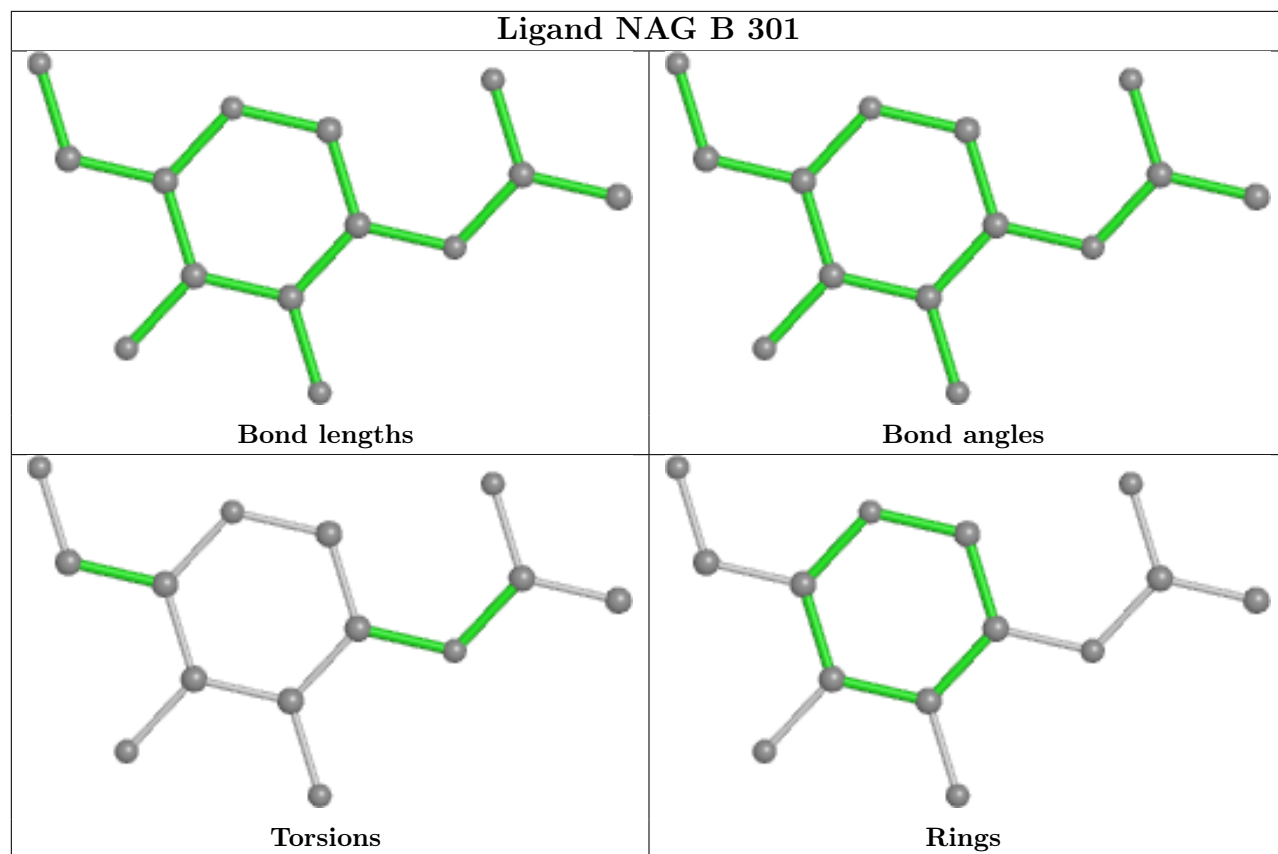
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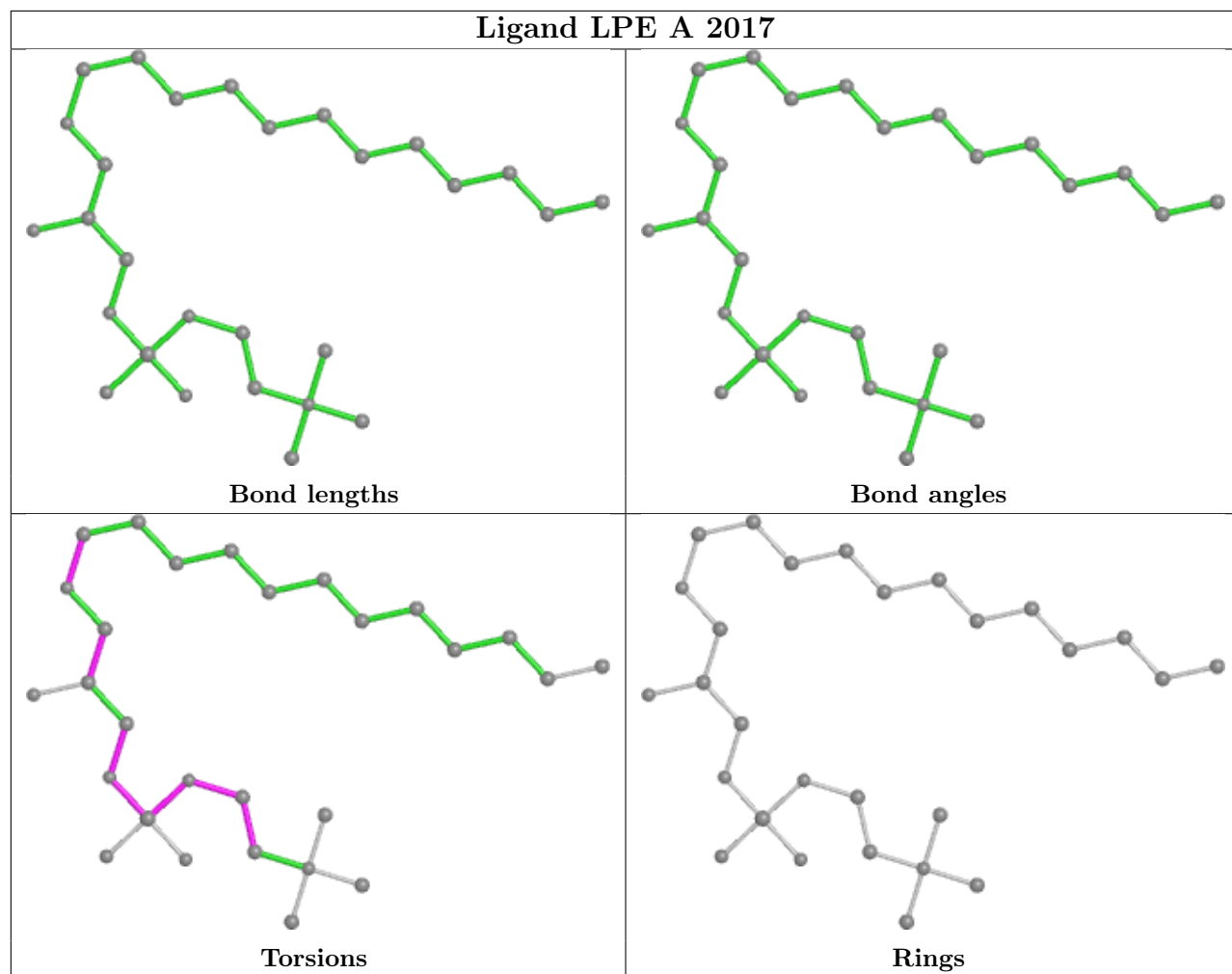
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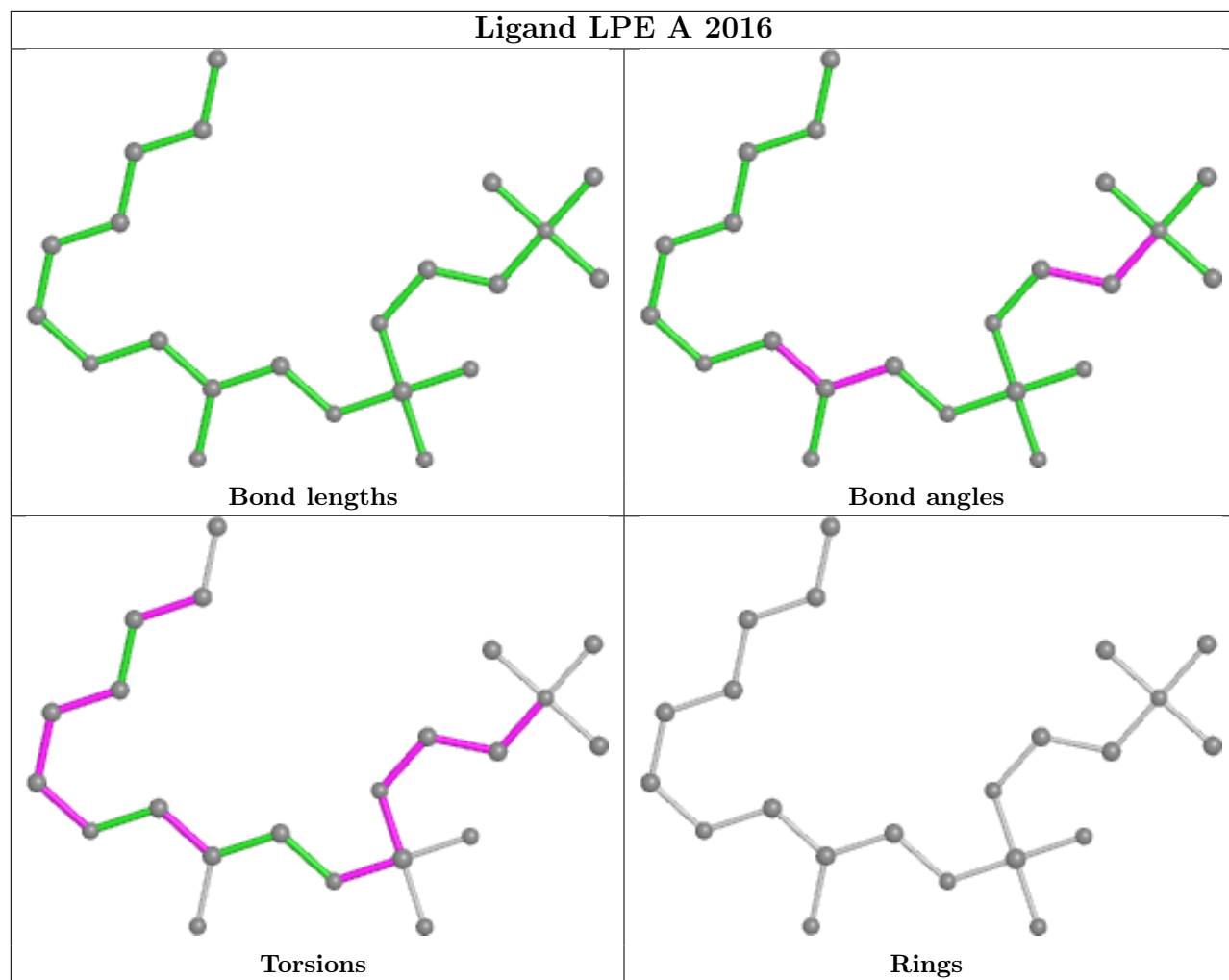
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	2033	LPE	3	0
10	A	2023	LPE	3	0
10	A	2014	LPE	2	0
12	A	2020	PCW	7	0
10	A	2022	LPE	1	0
7	A	2005	Y01	19	0
7	A	2003	Y01	4	0
12	A	2029	PCW	3	0
12	A	2018	PCW	1	0
8	A	2006	9Z9	14	0
10	A	2026	LPE	2	0
10	A	2028	LPE	1	0
11	A	2013	1PW	2	0
10	A	2027	LPE	3	0
12	A	2015	PCW	19	0
5	B	303	NAG	6	0
6	A	2019	P5S	4	0
7	A	2004	Y01	6	0
10	A	2012	LPE	1	0
7	A	2009	Y01	9	0

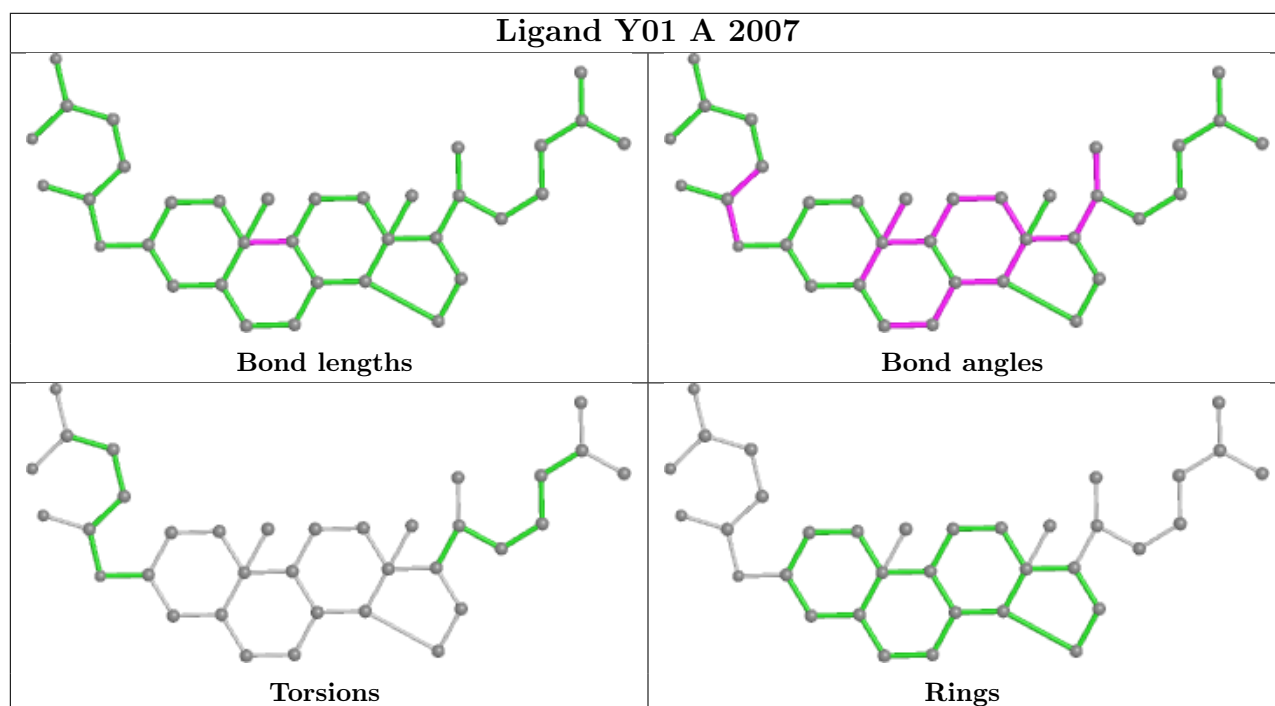
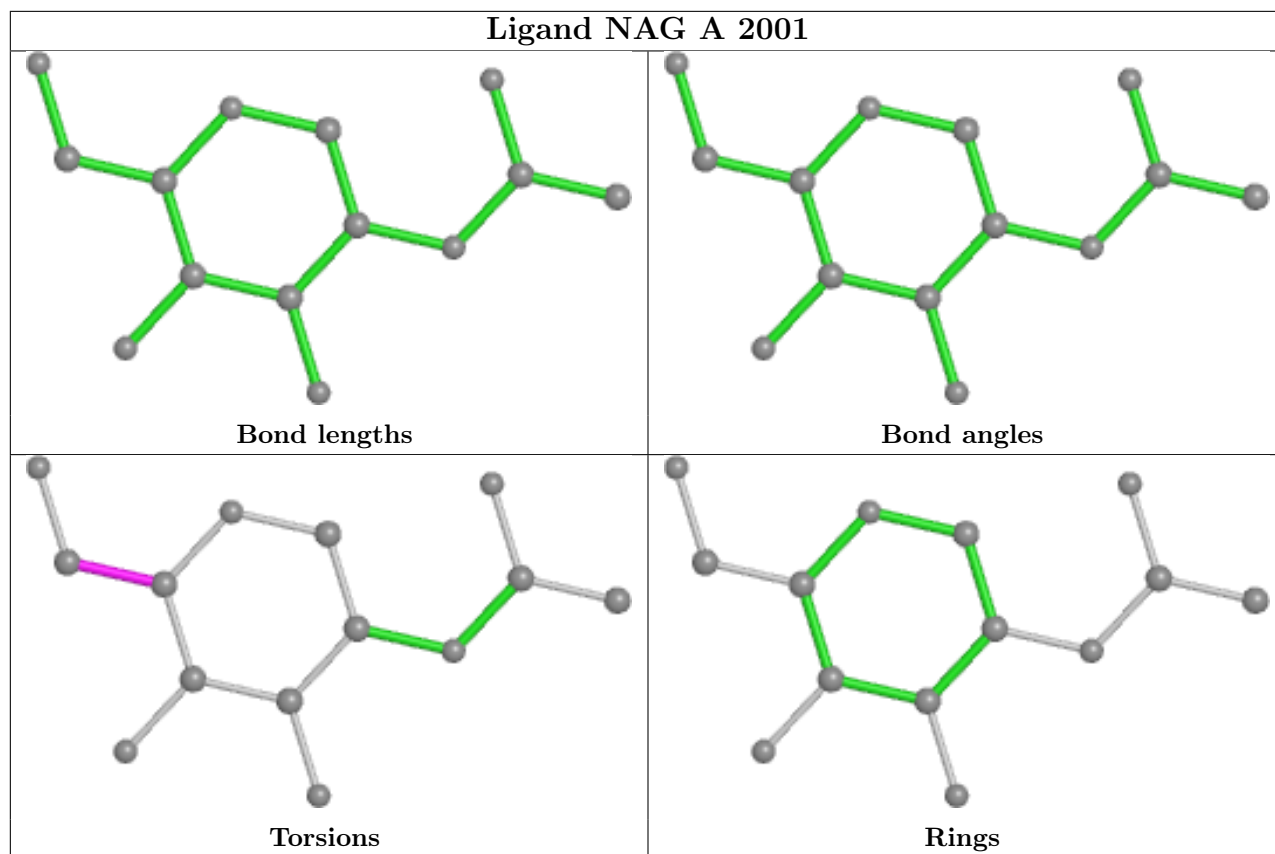
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

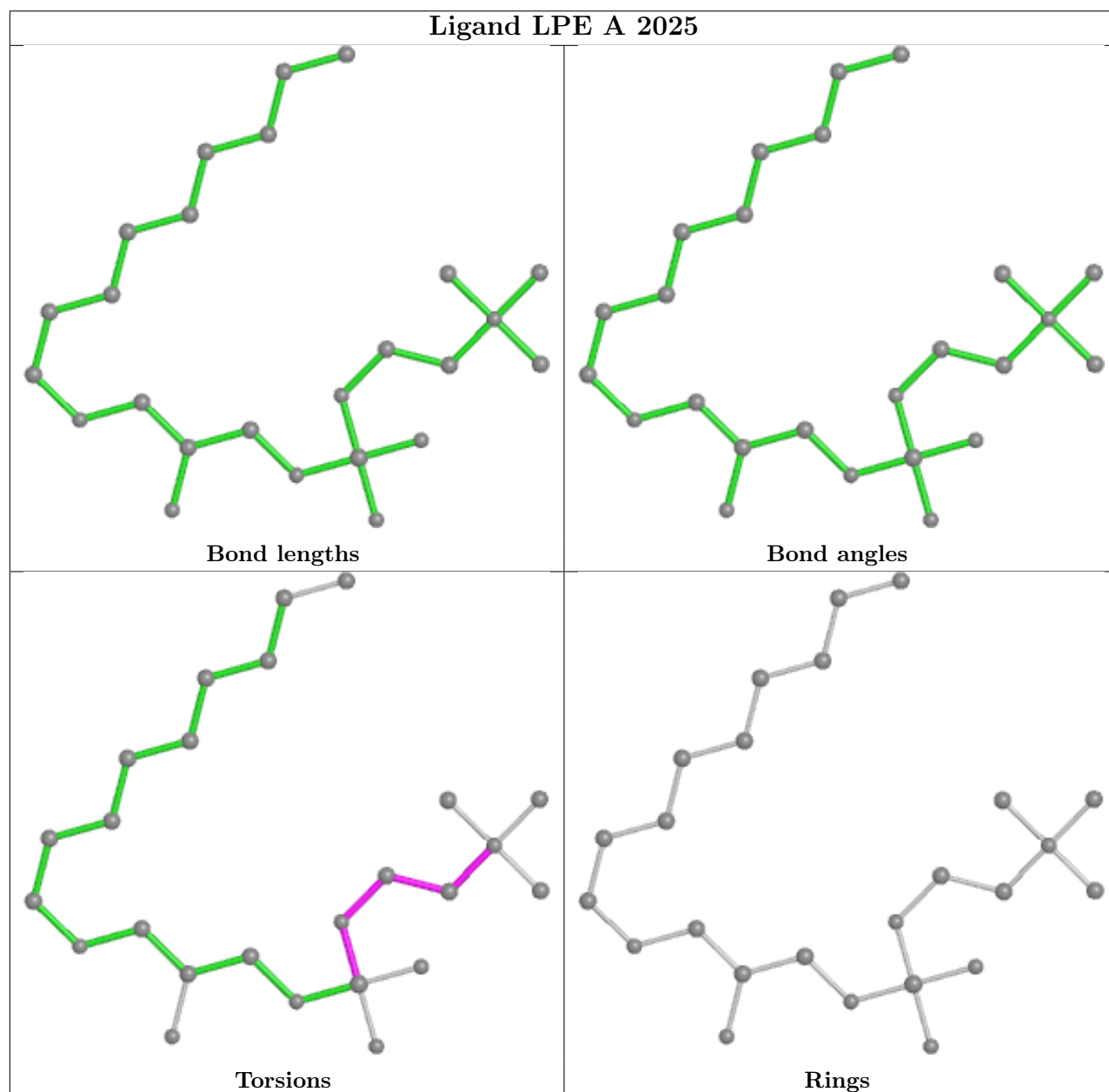
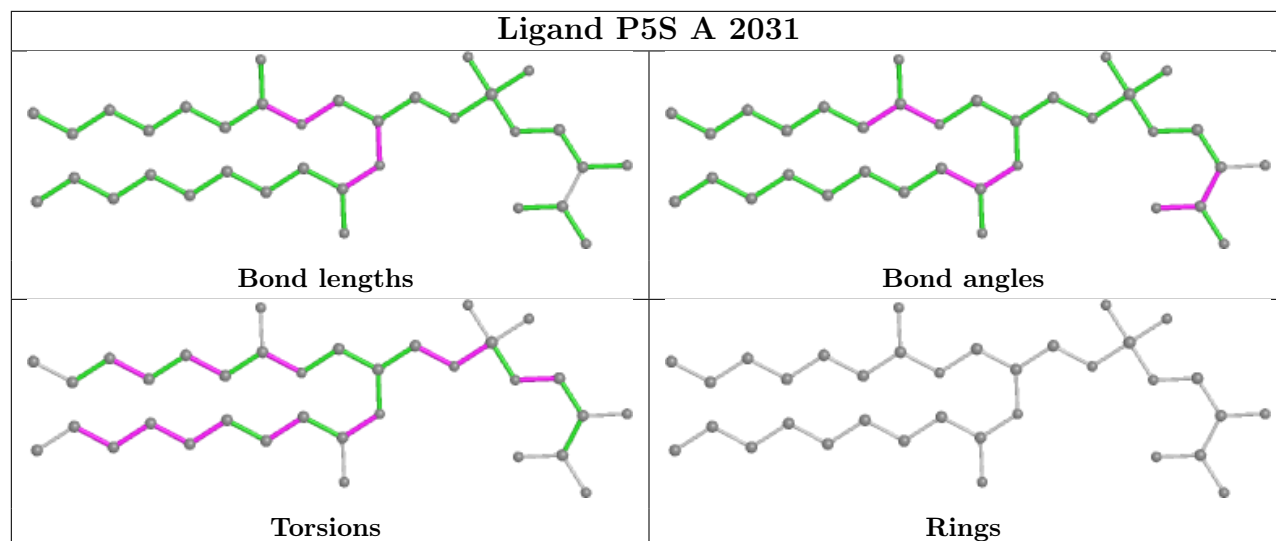




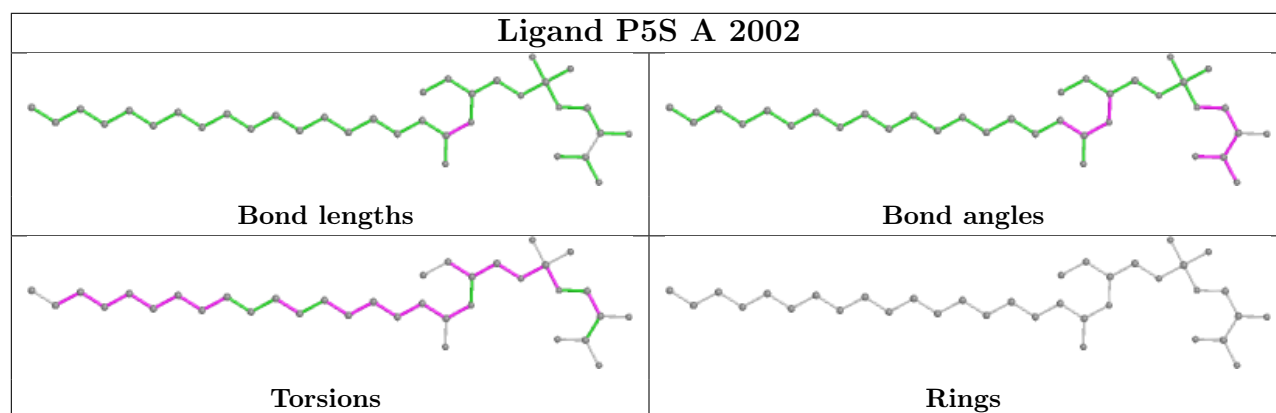
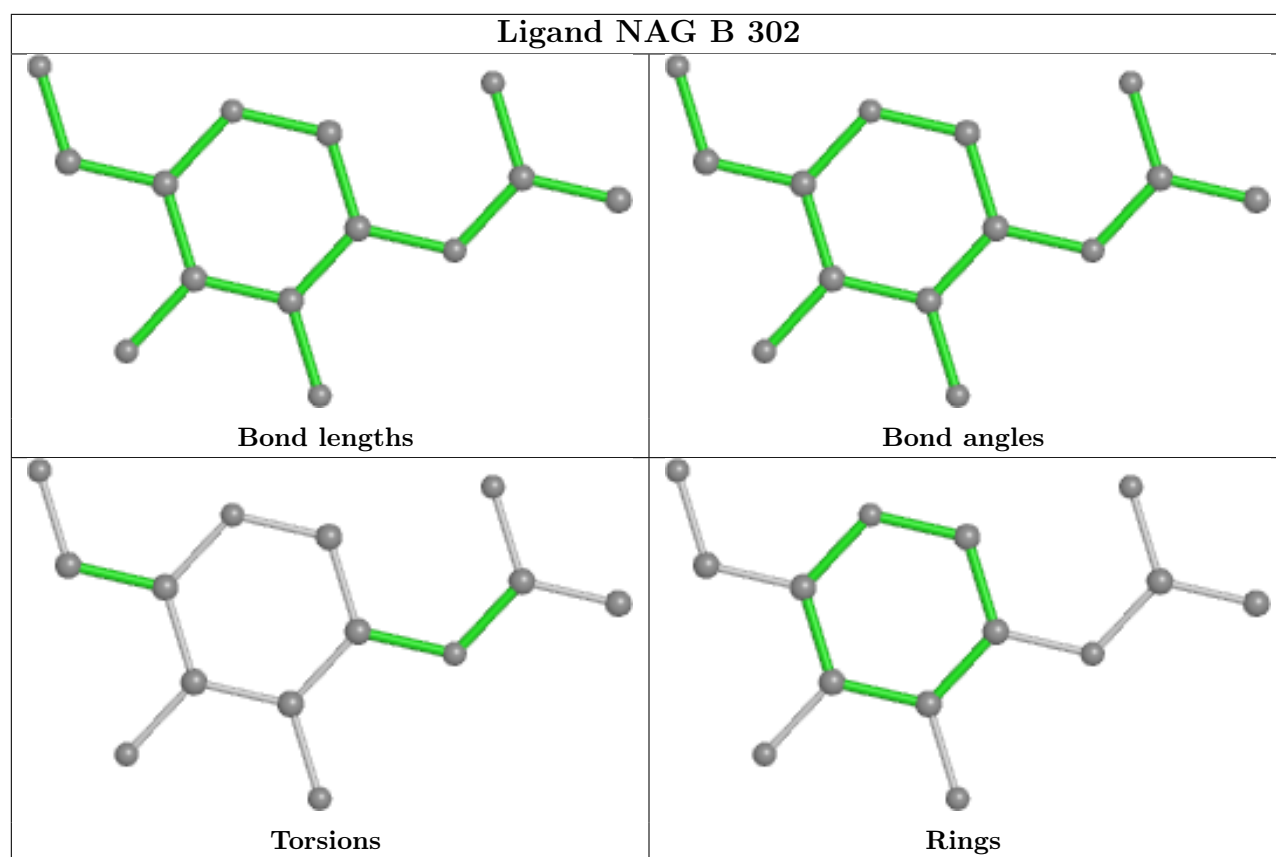


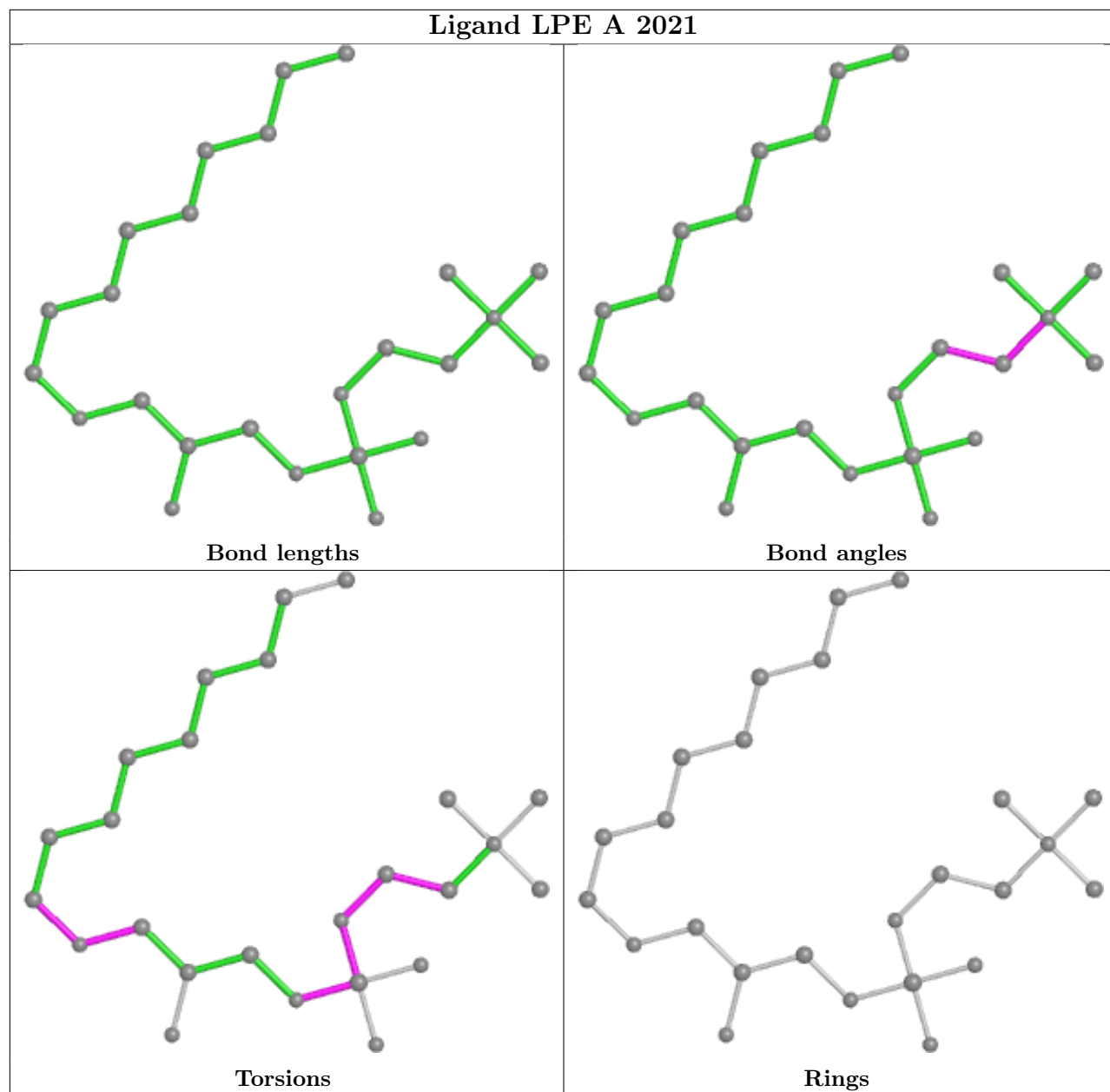


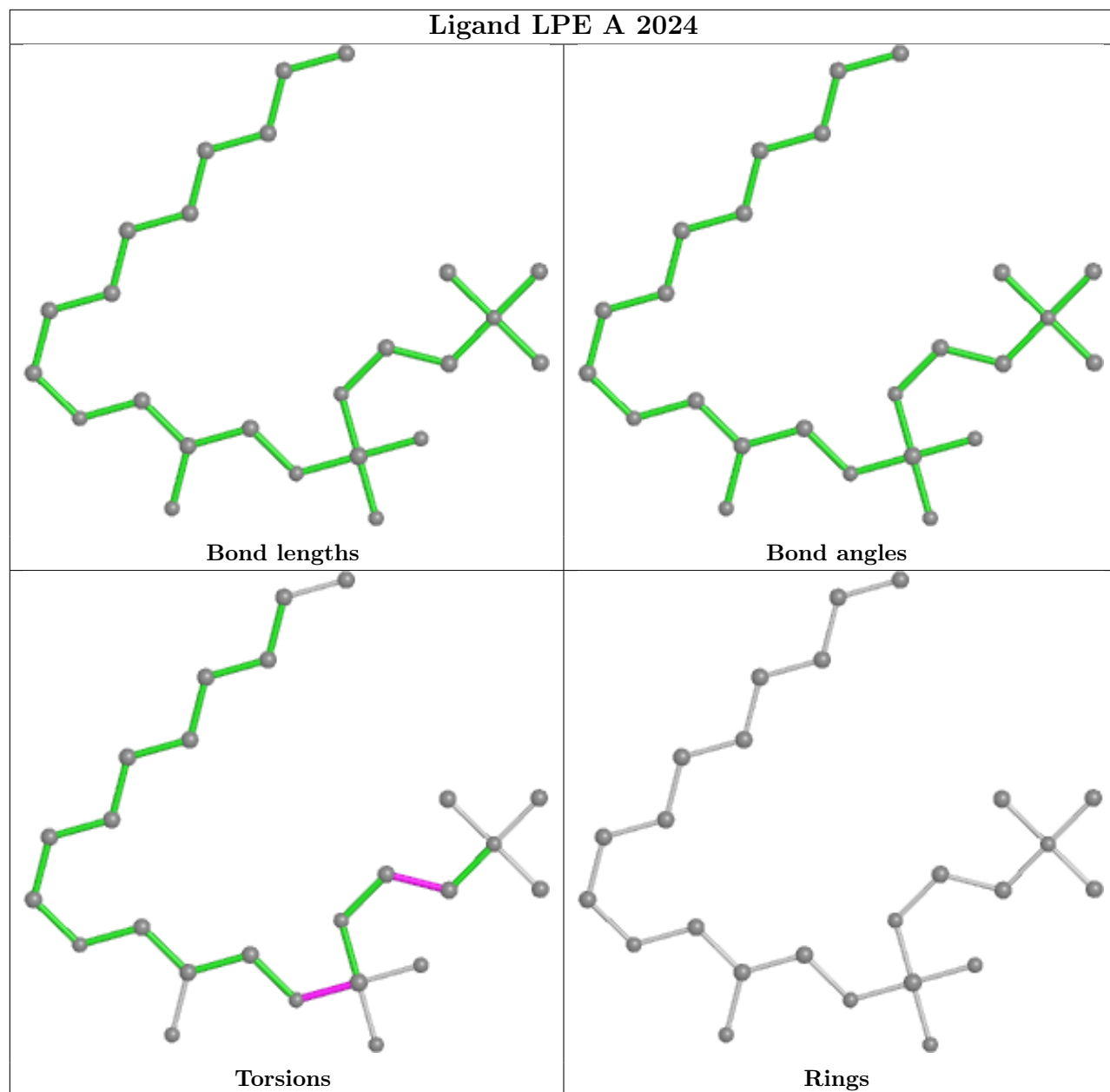


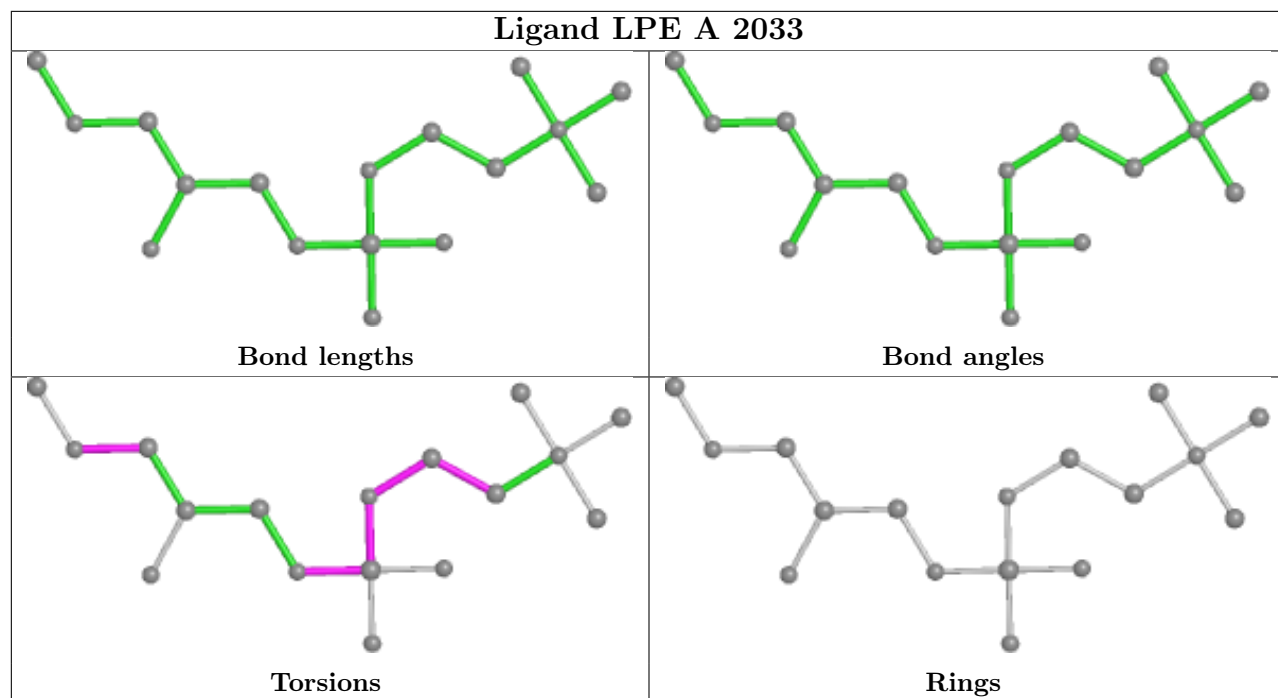


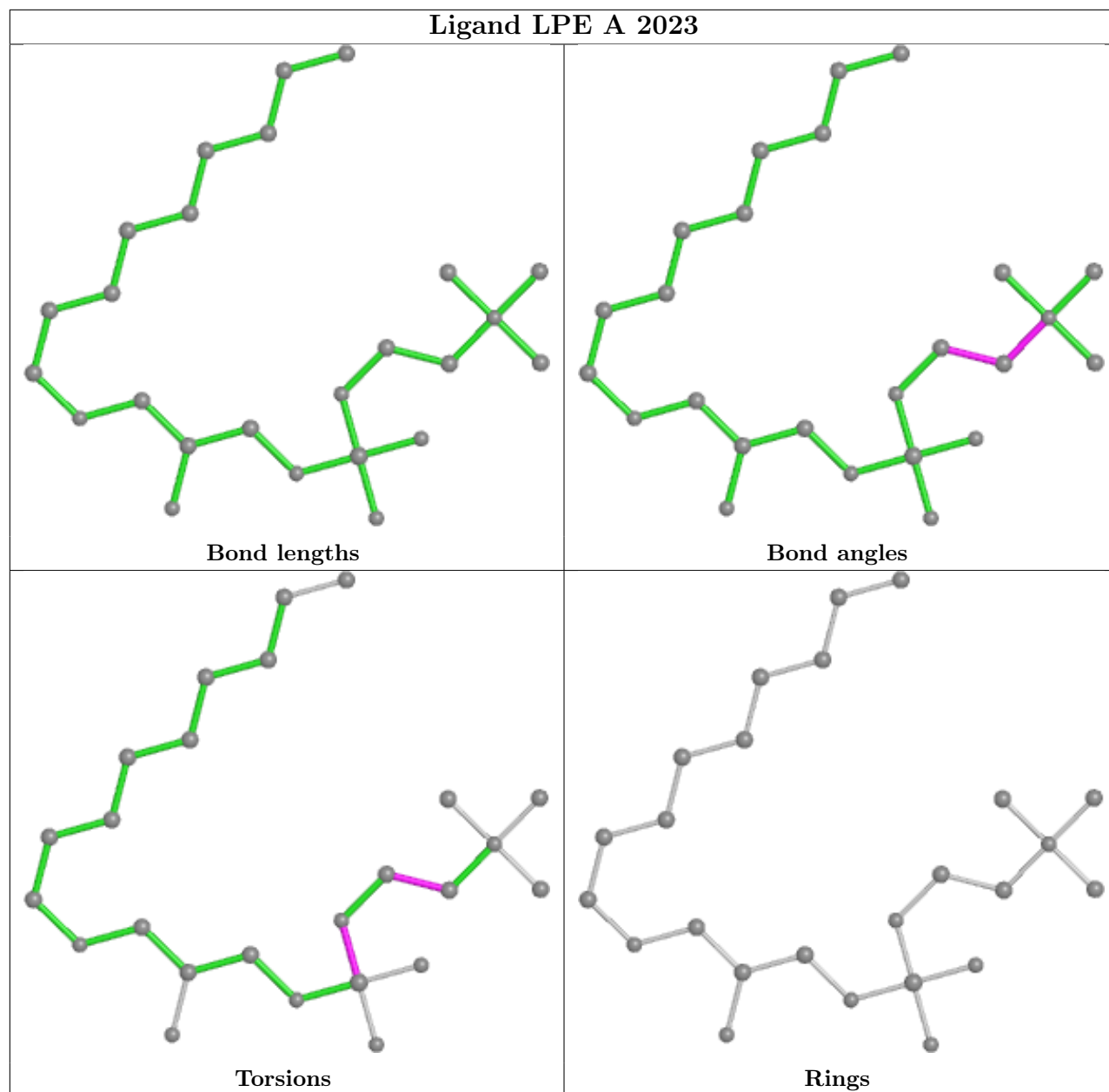


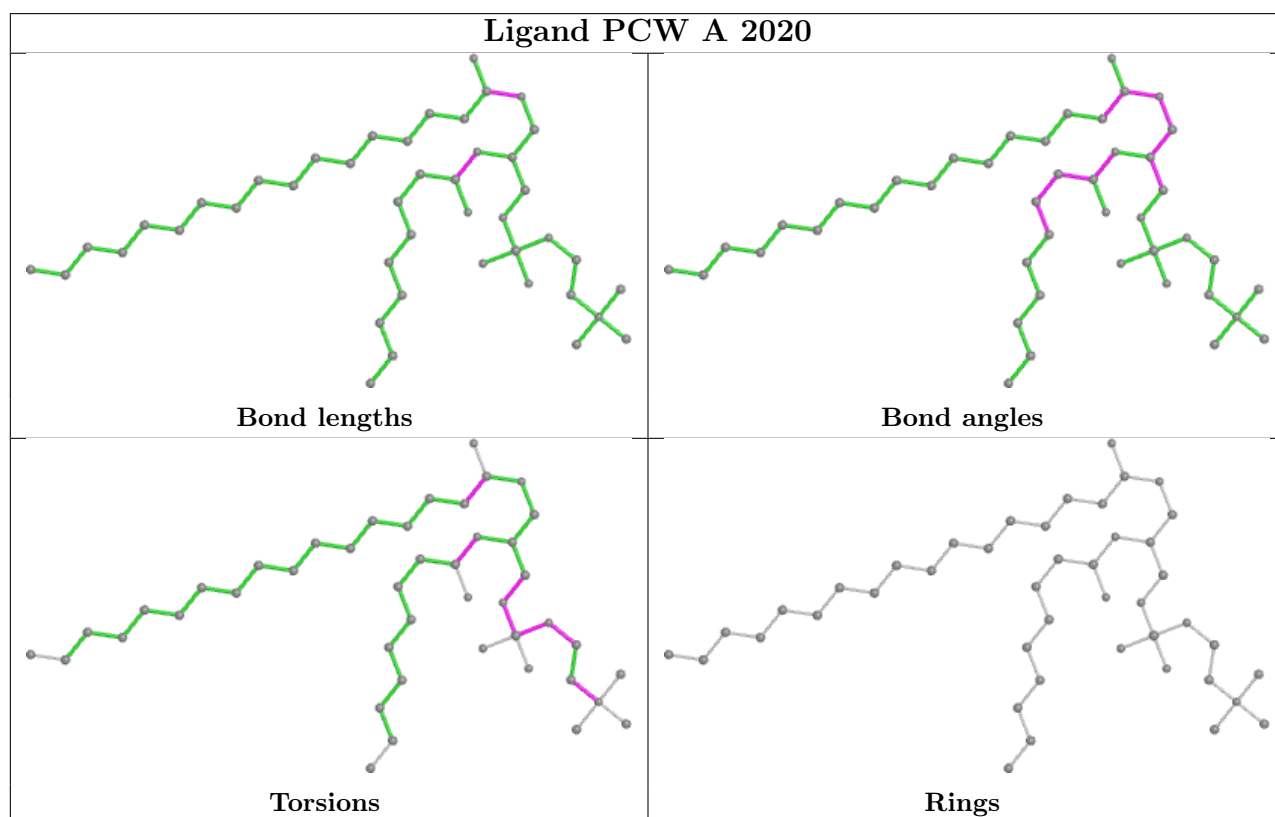
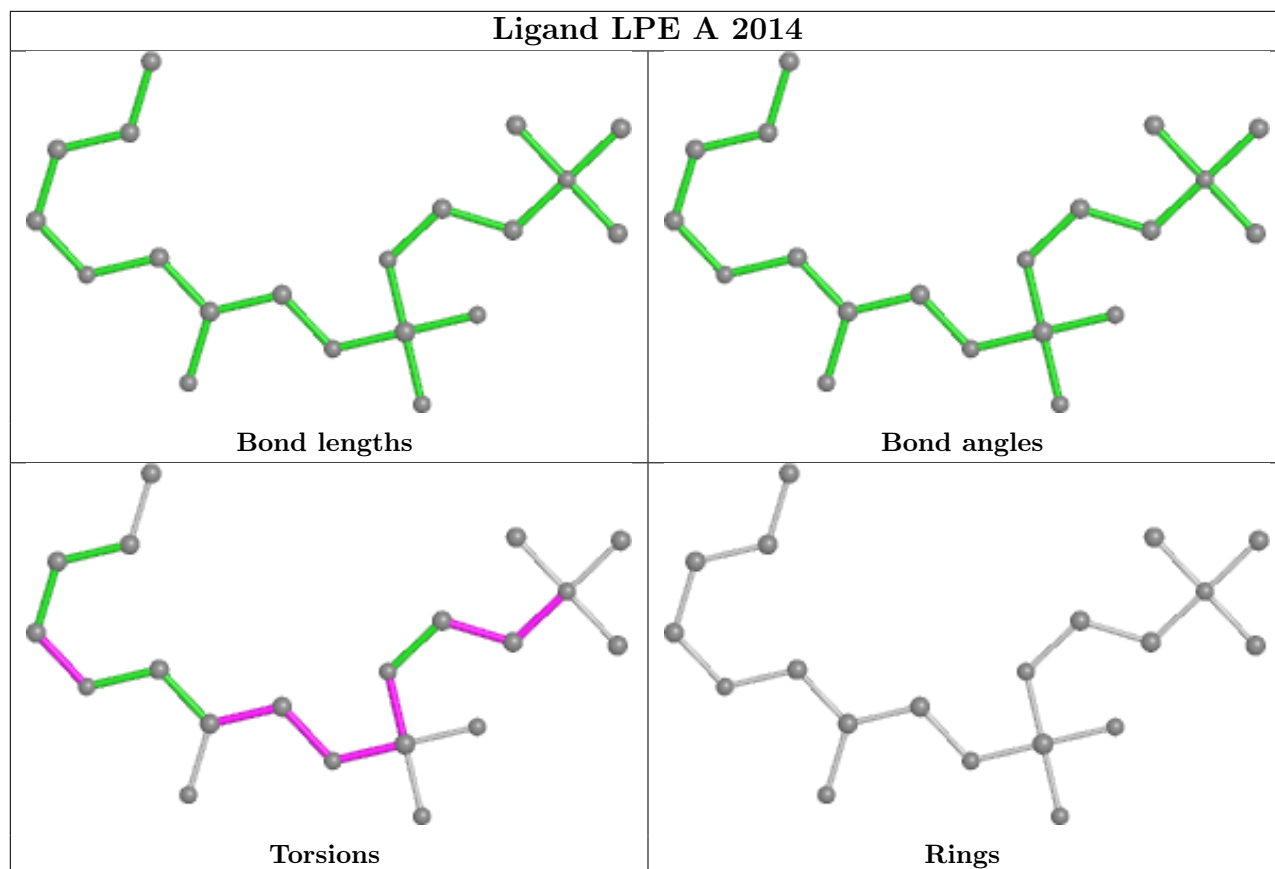


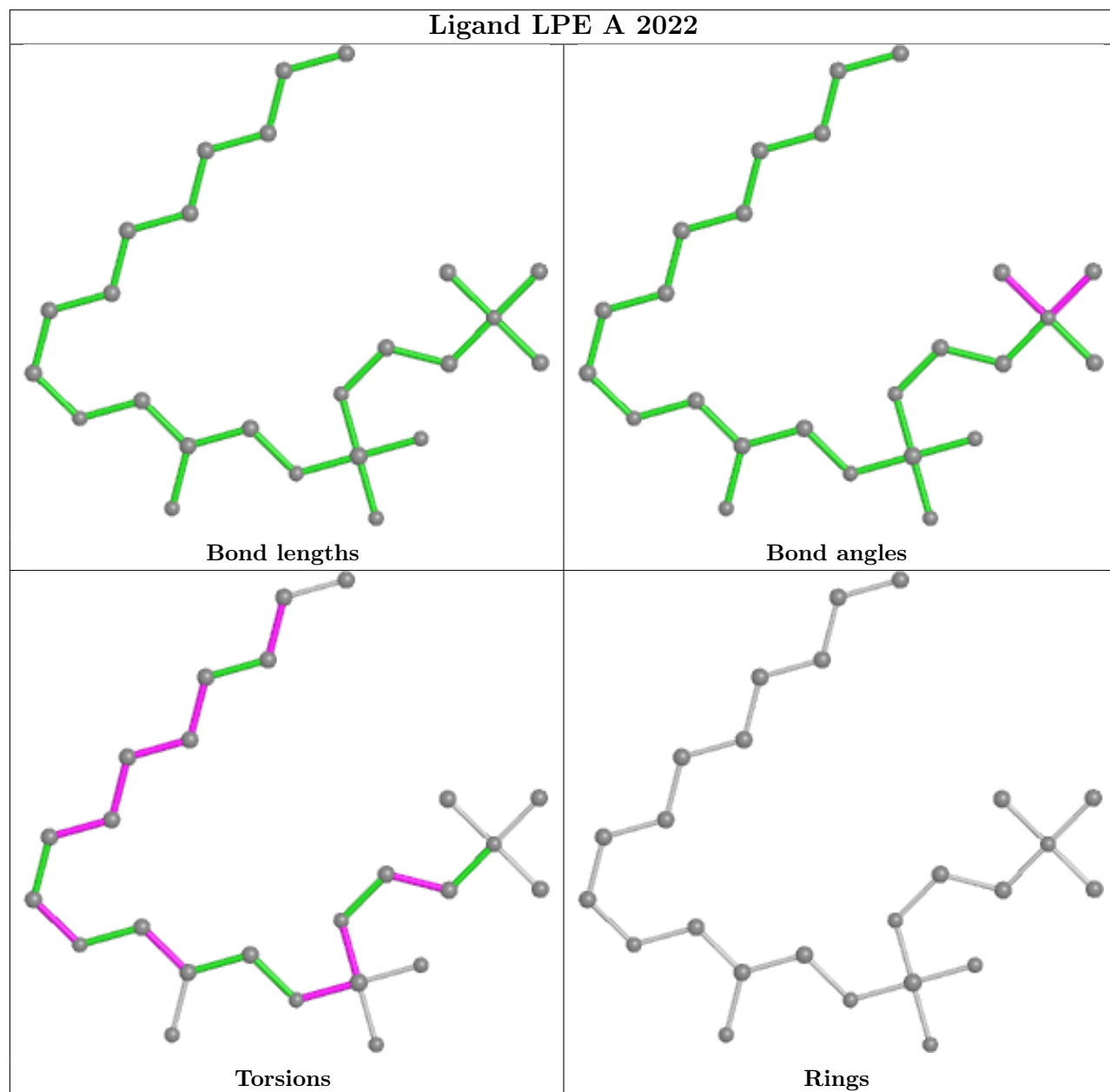


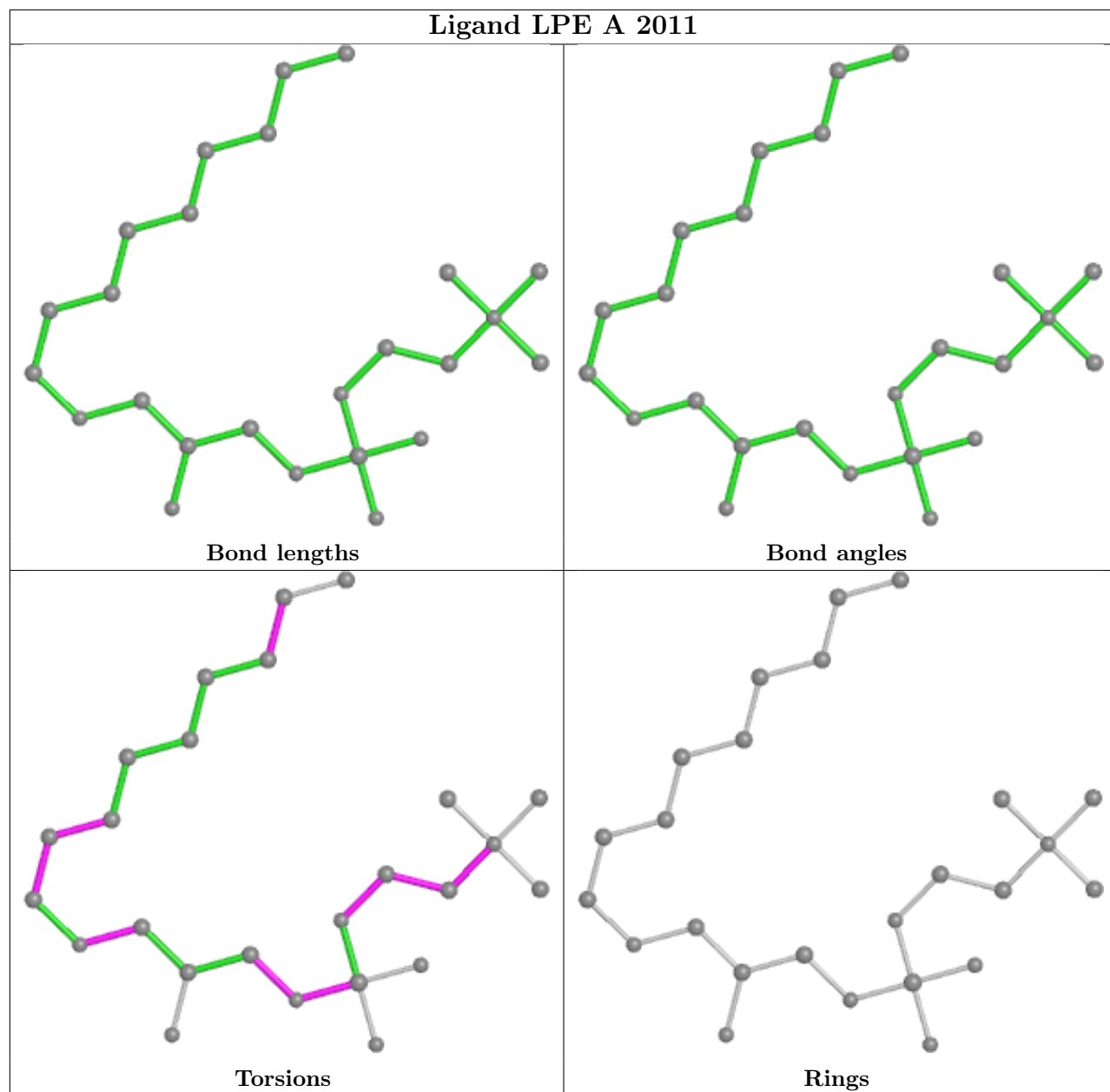




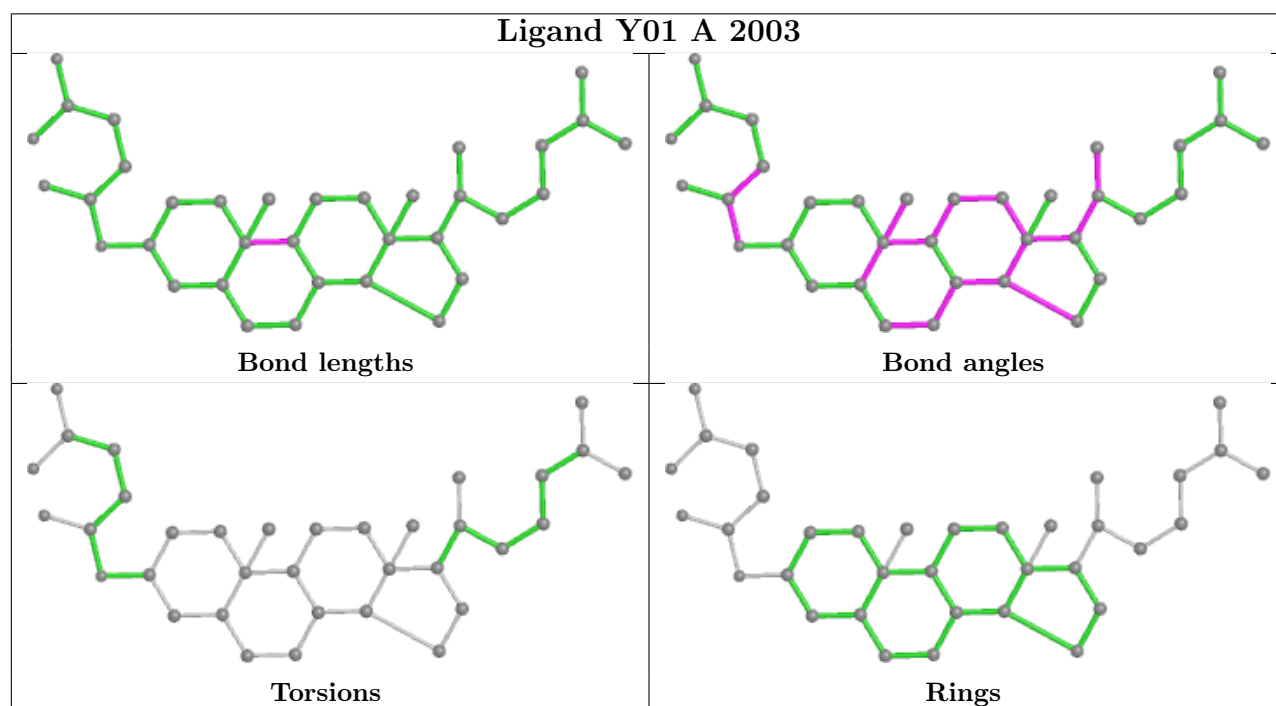
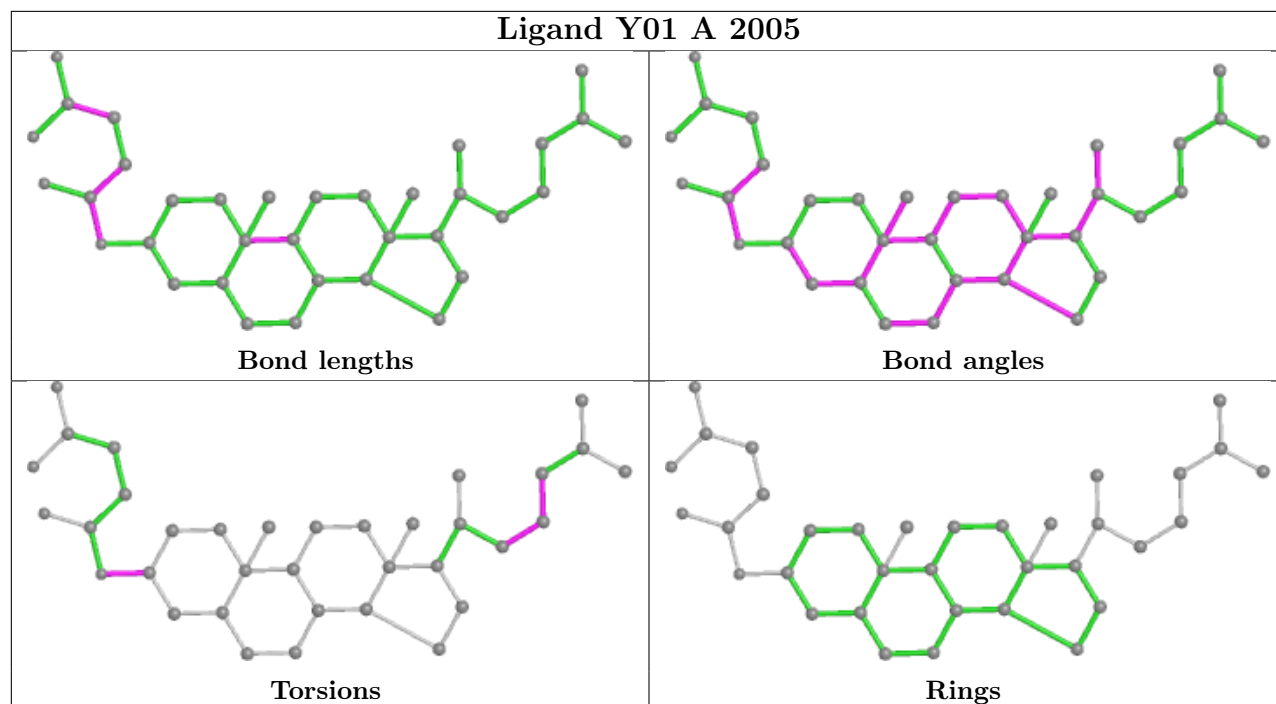


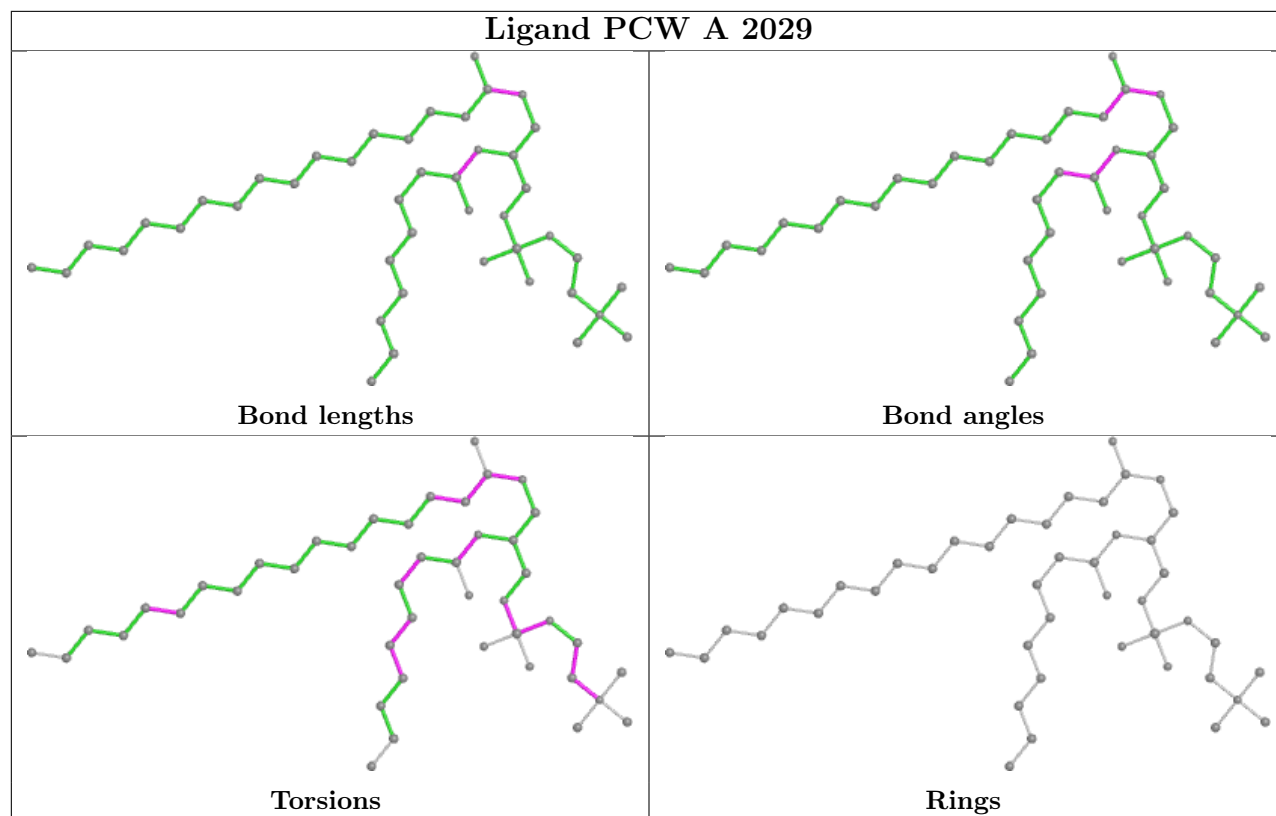


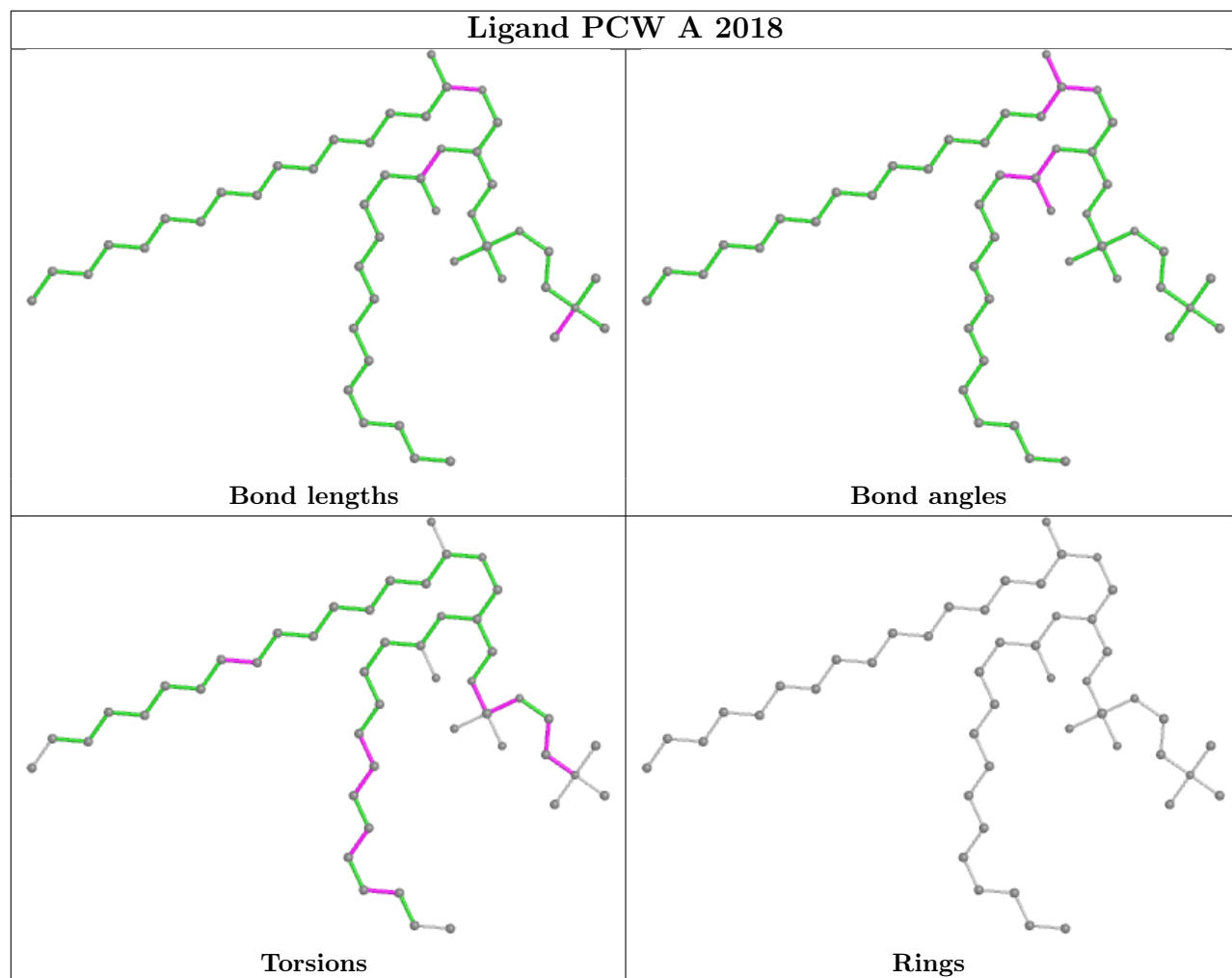


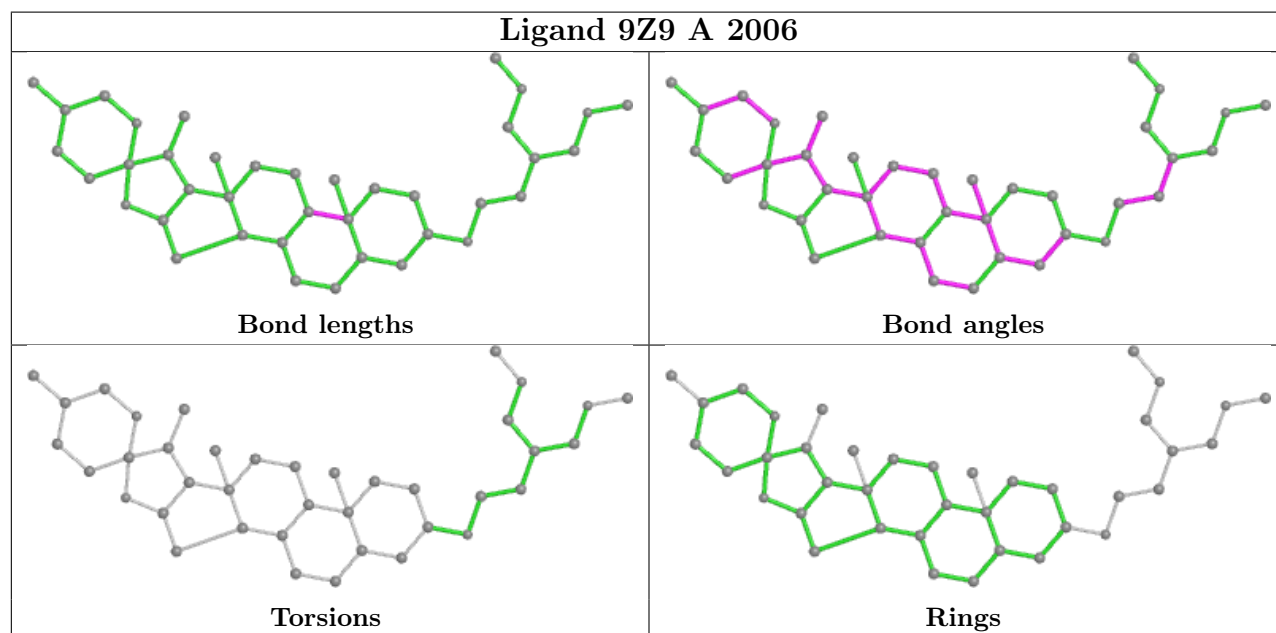
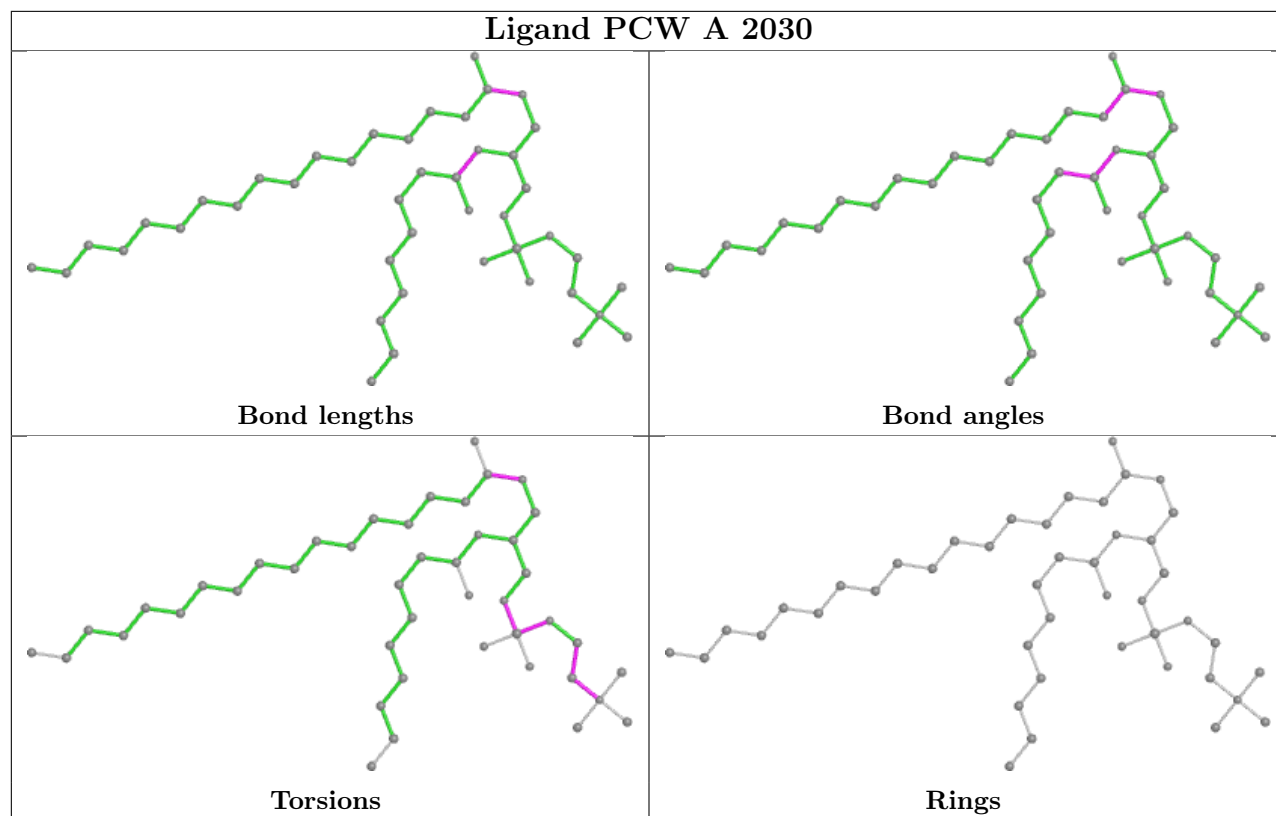


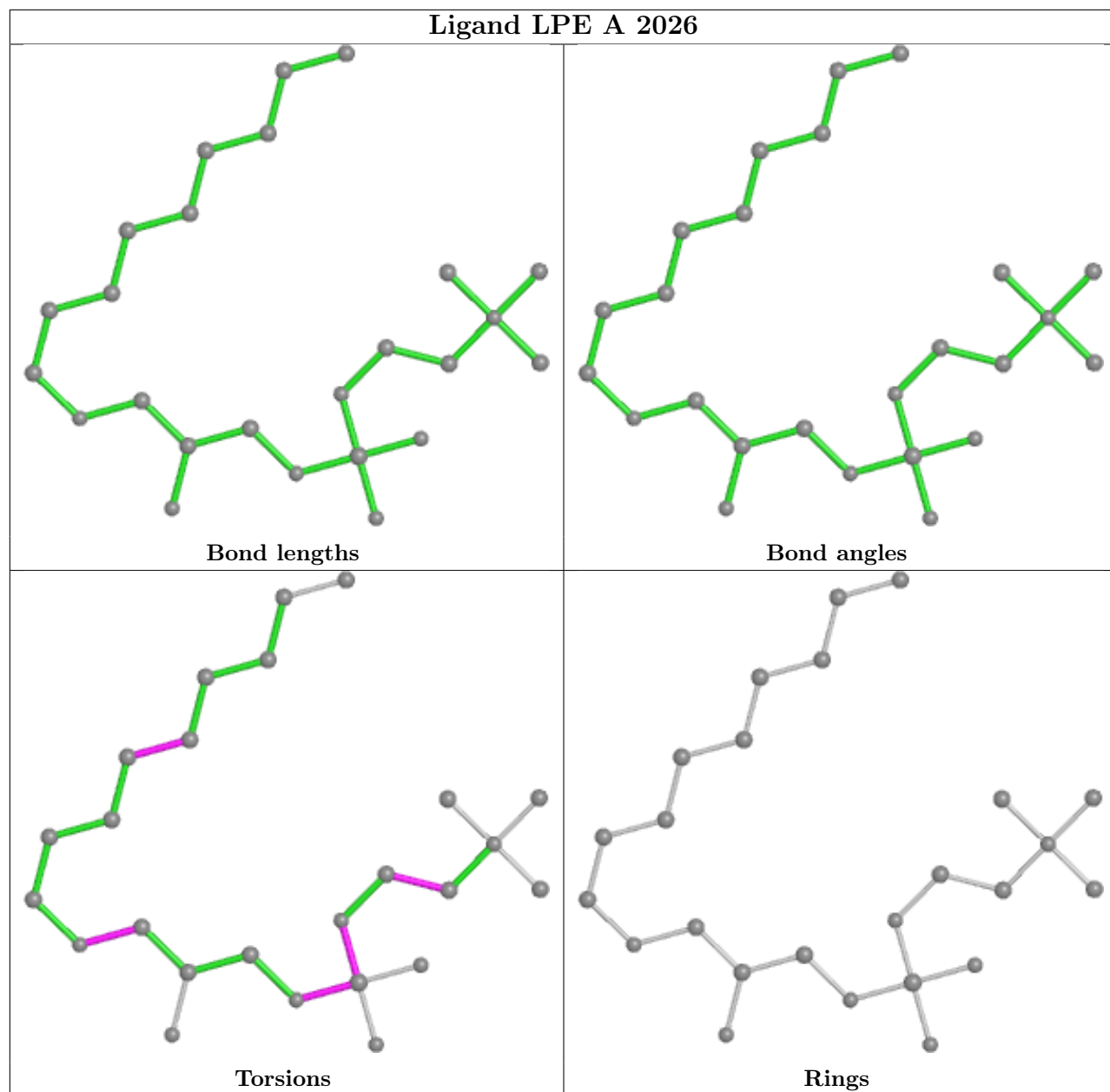


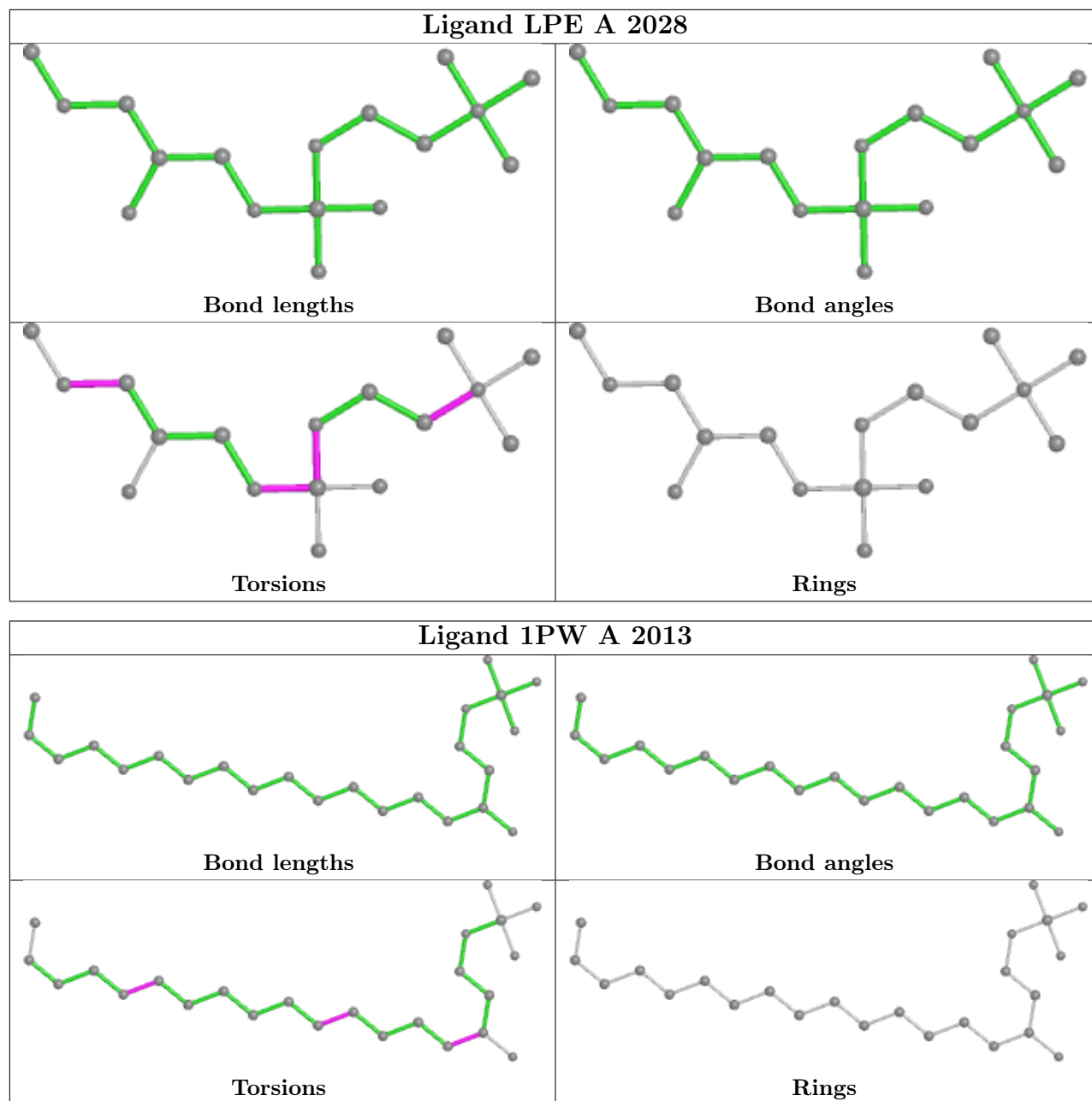


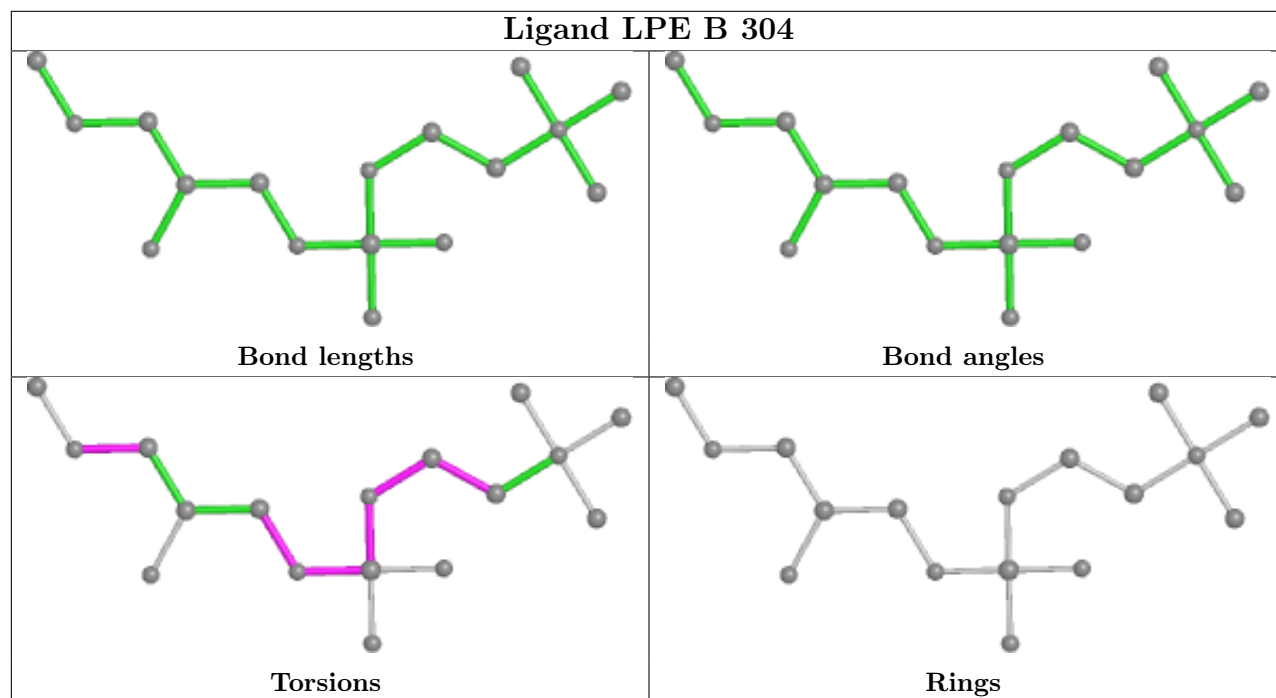


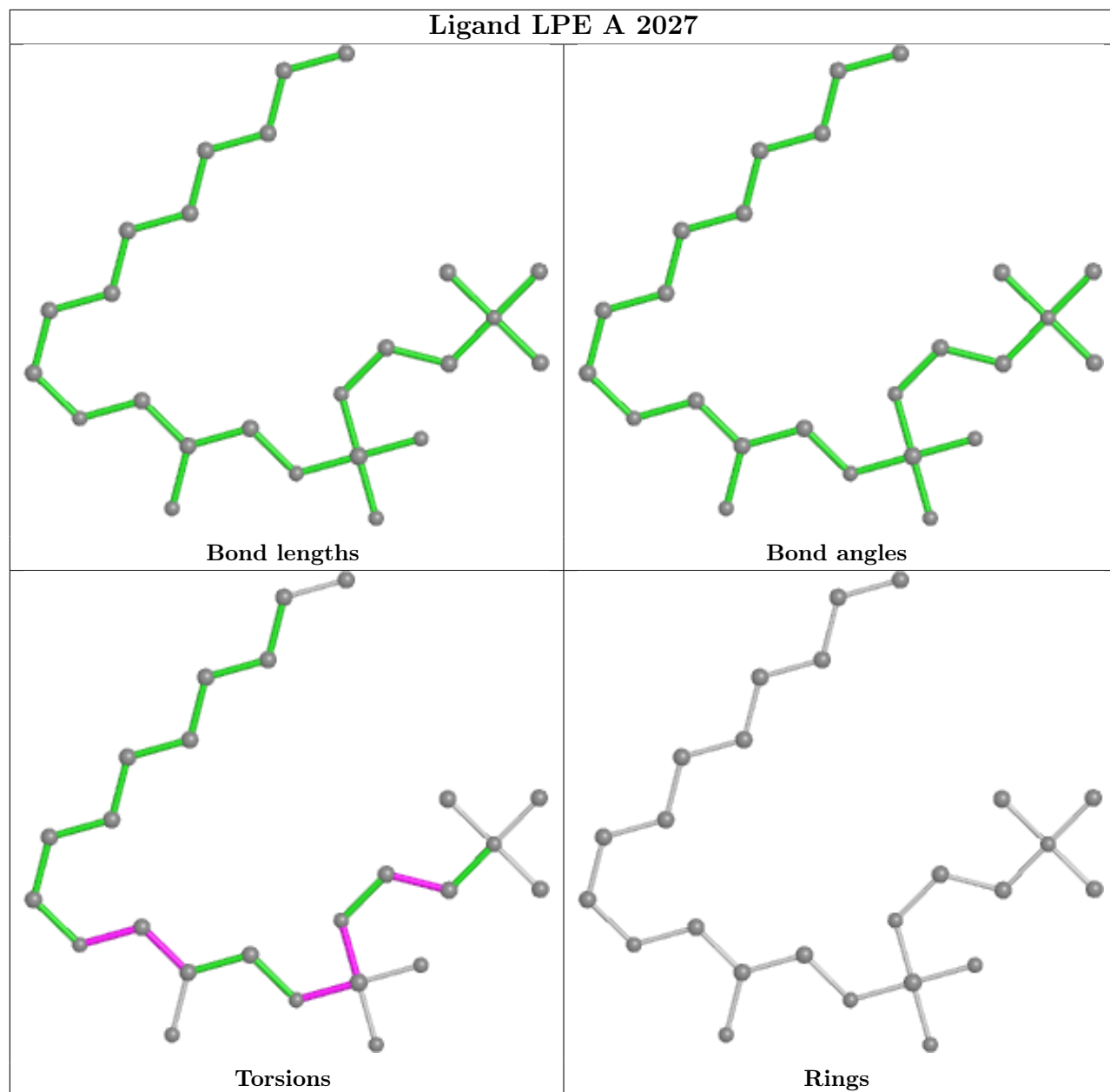




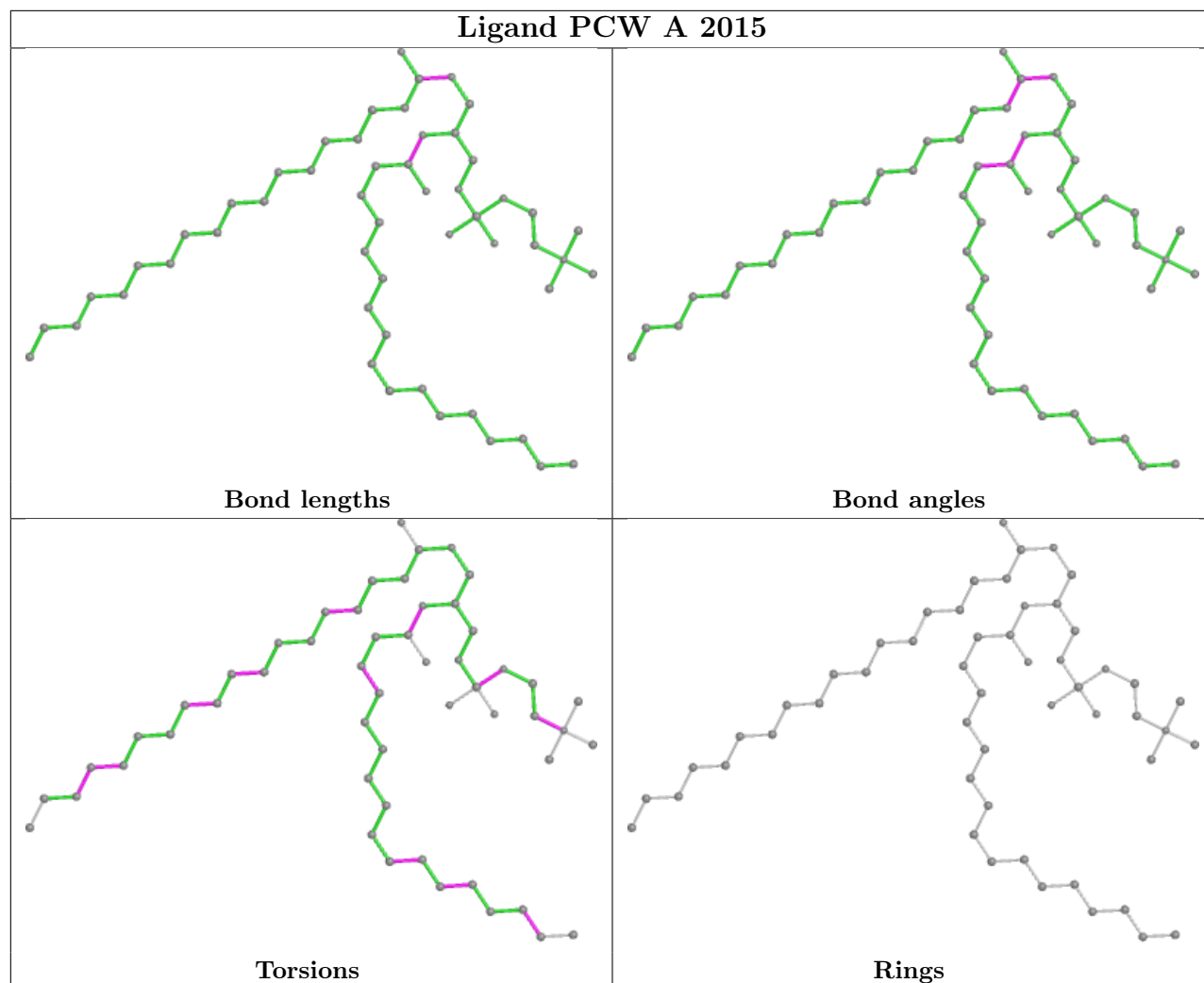


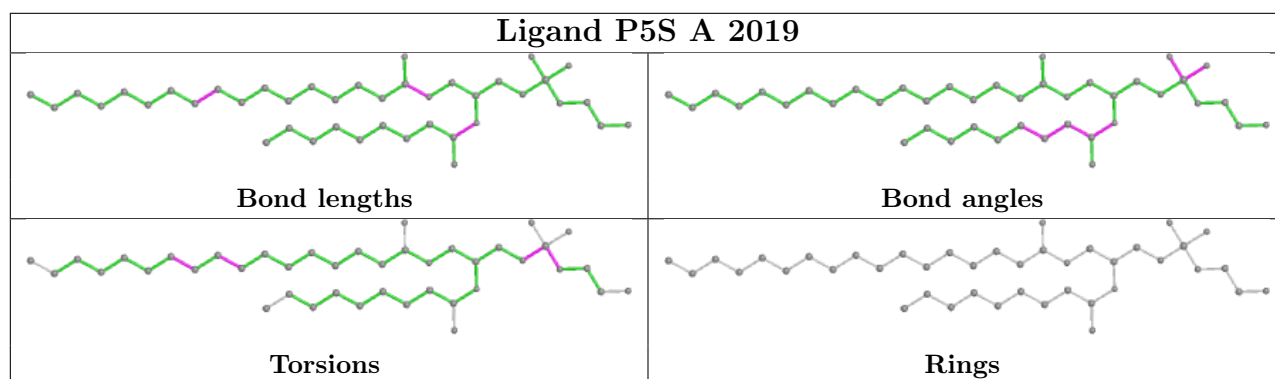
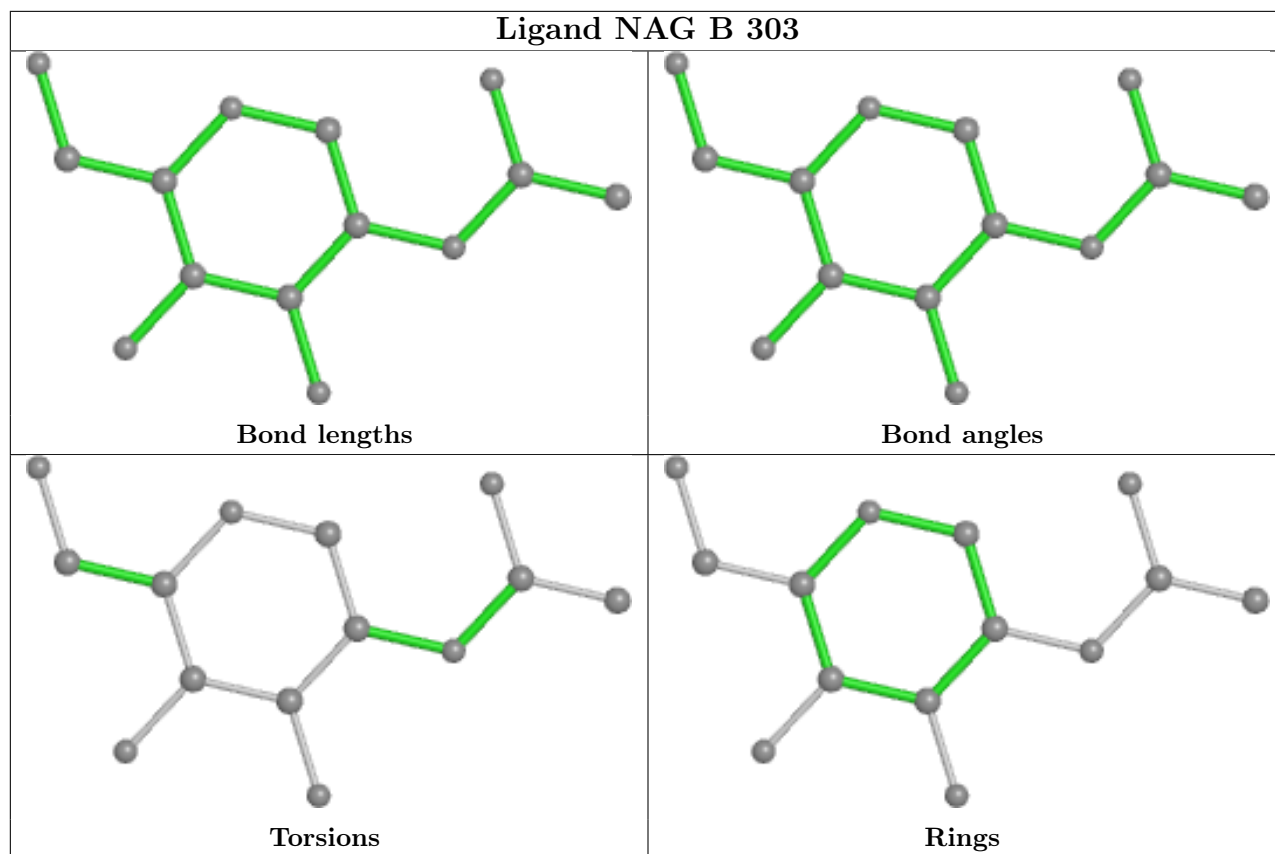


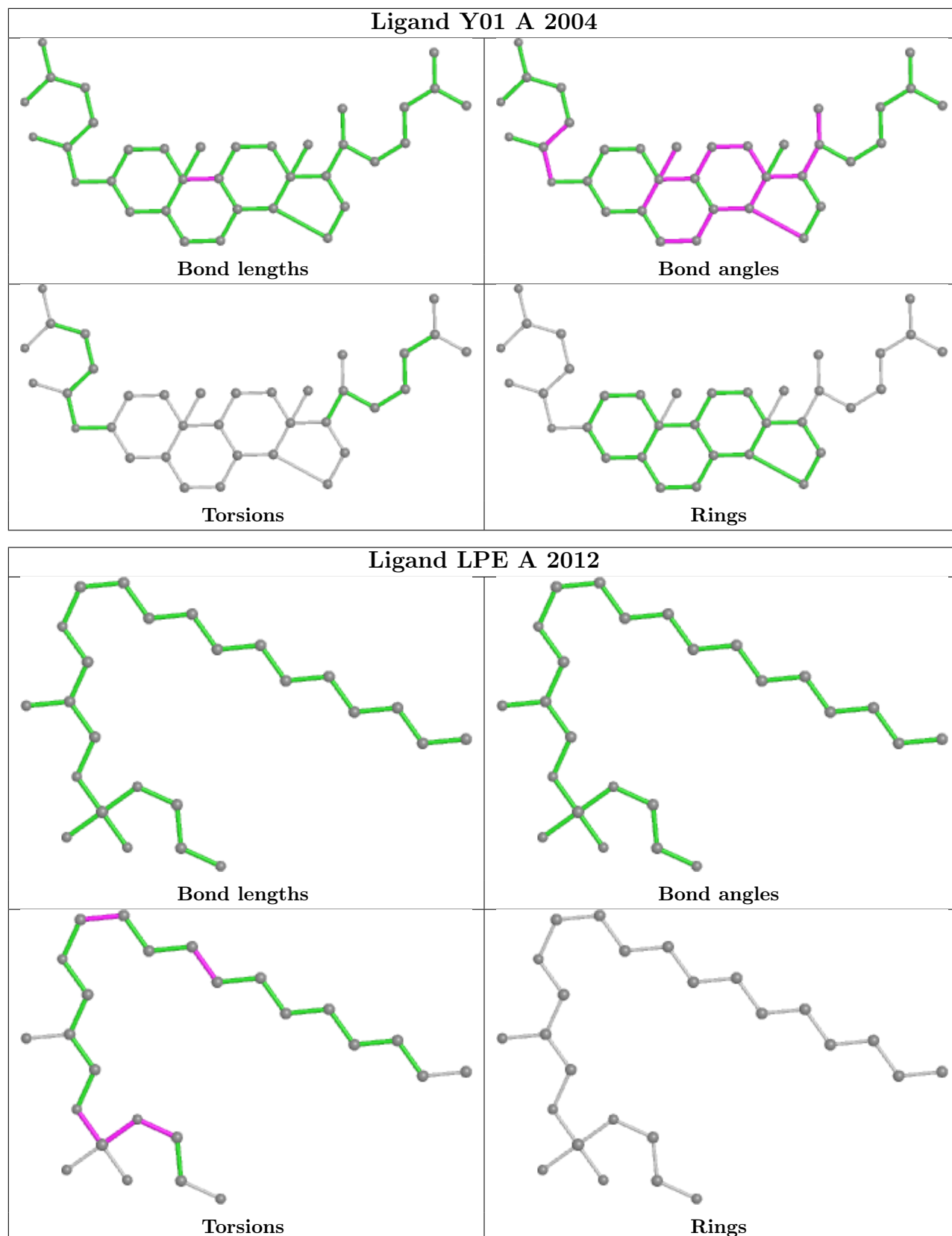


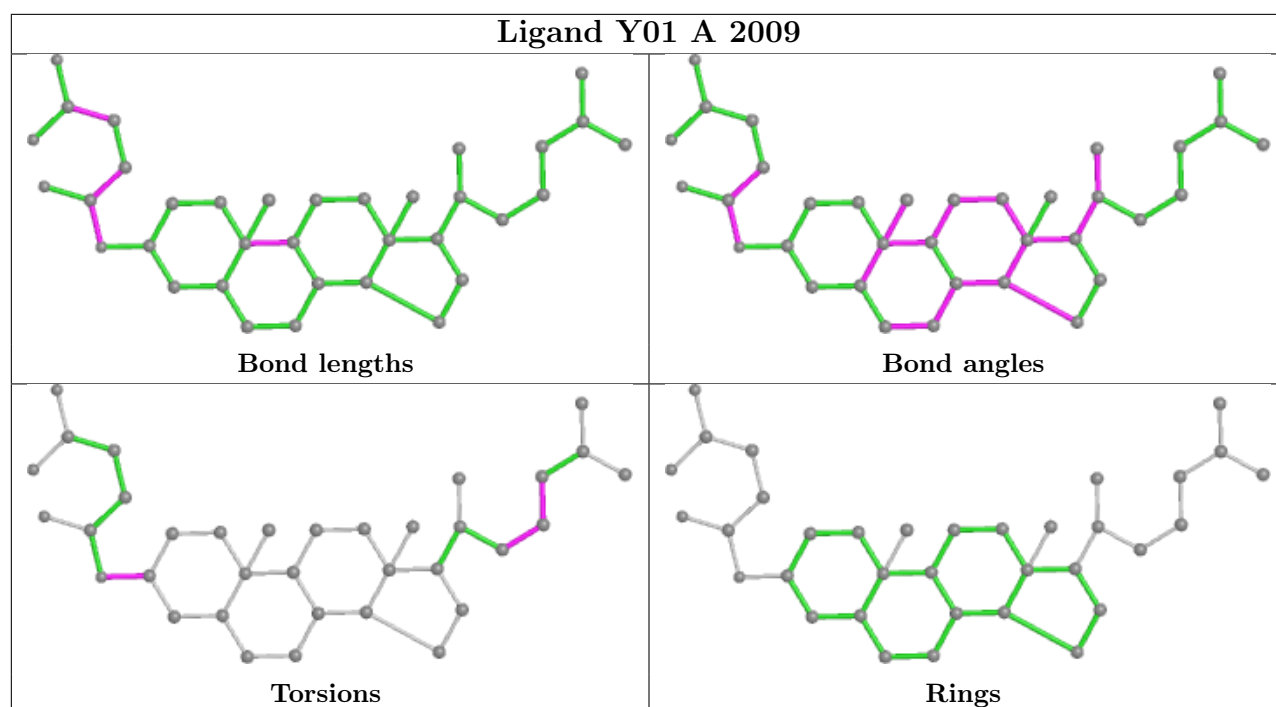












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

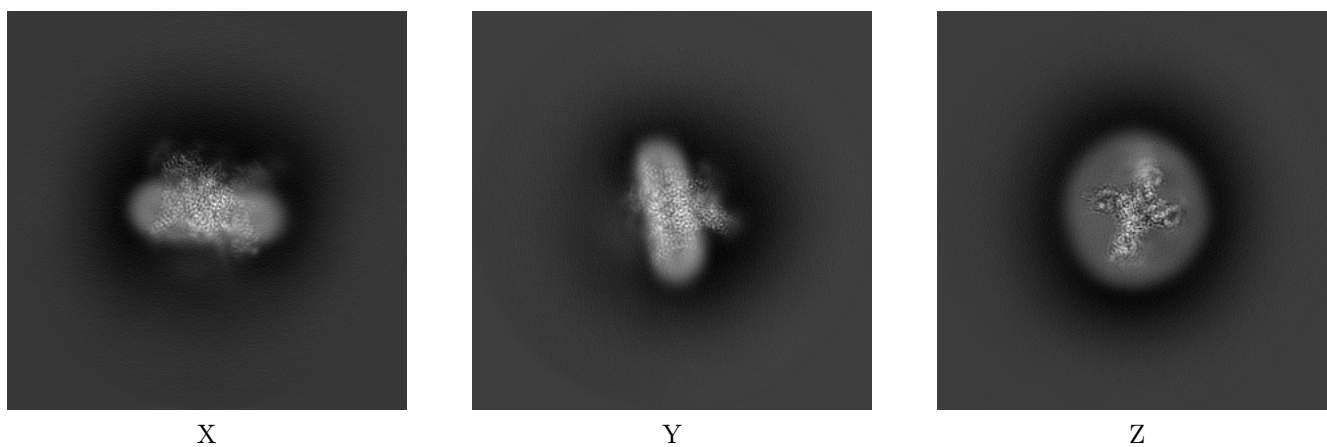
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32368. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

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

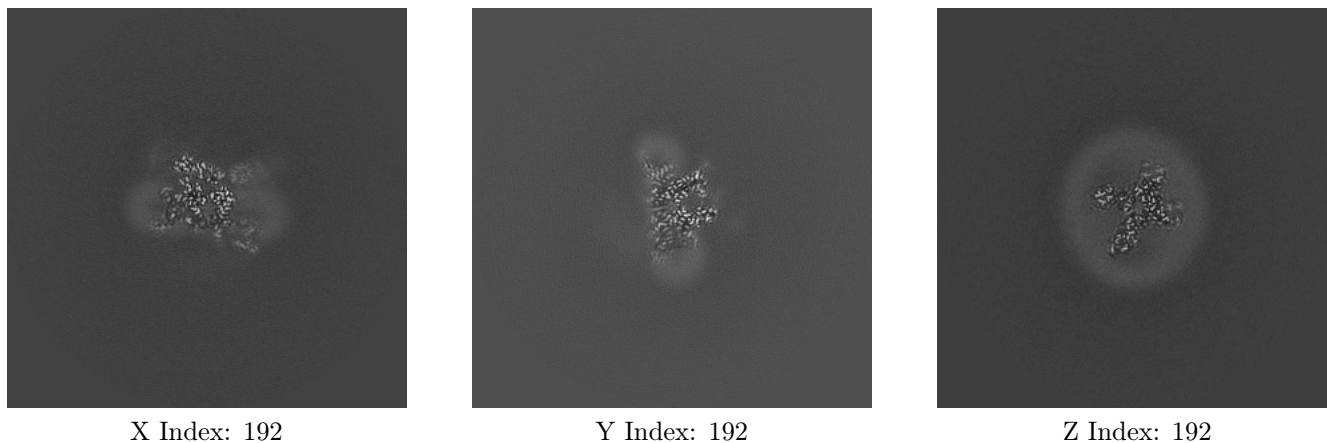
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

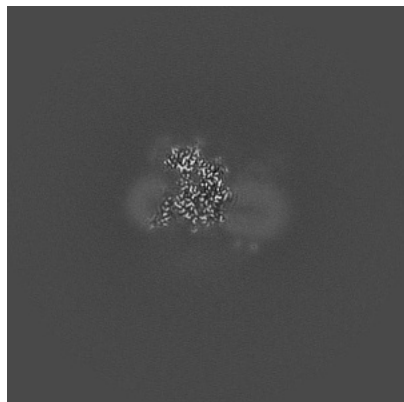
#### 6.2.1 Primary map



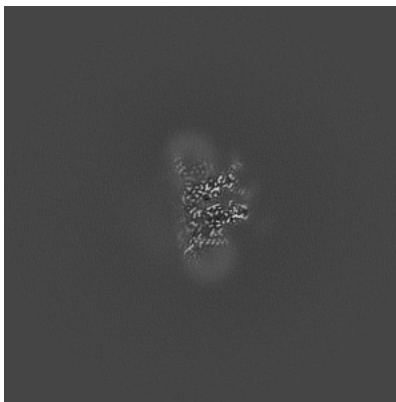
The images above show central slices of the map in three orthogonal directions.

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

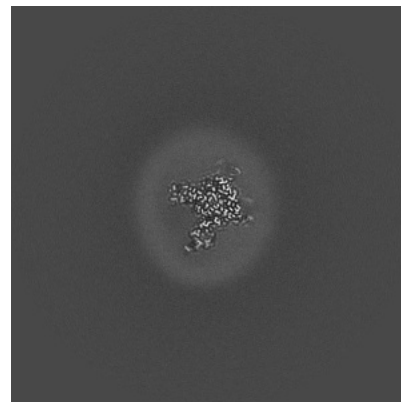
### 6.3.1 Primary map



X Index: 183



Y Index: 196



Z Index: 198

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

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

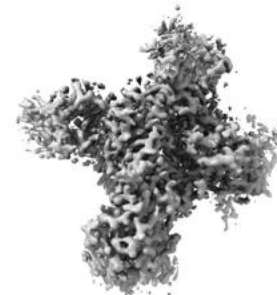
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

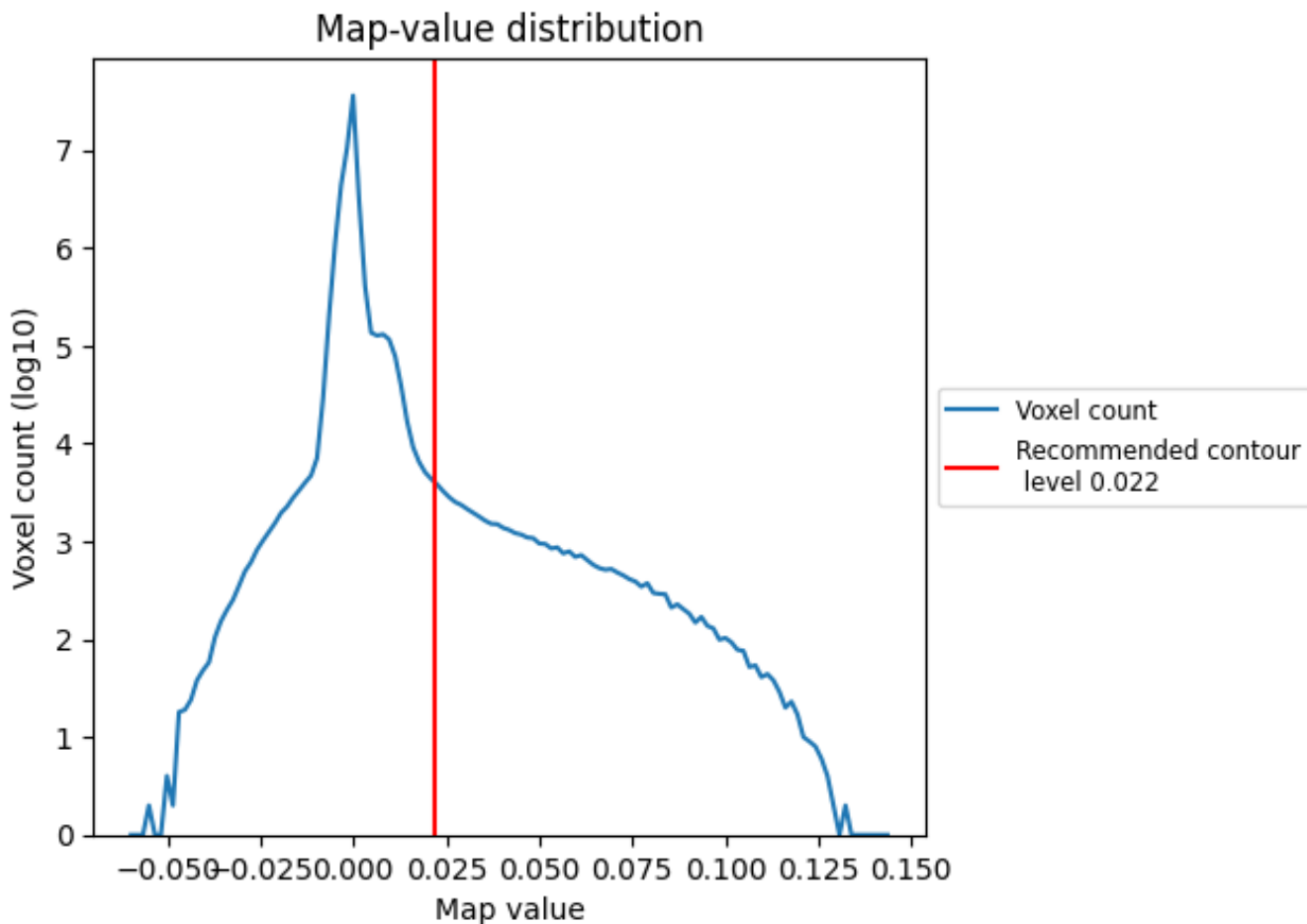
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

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

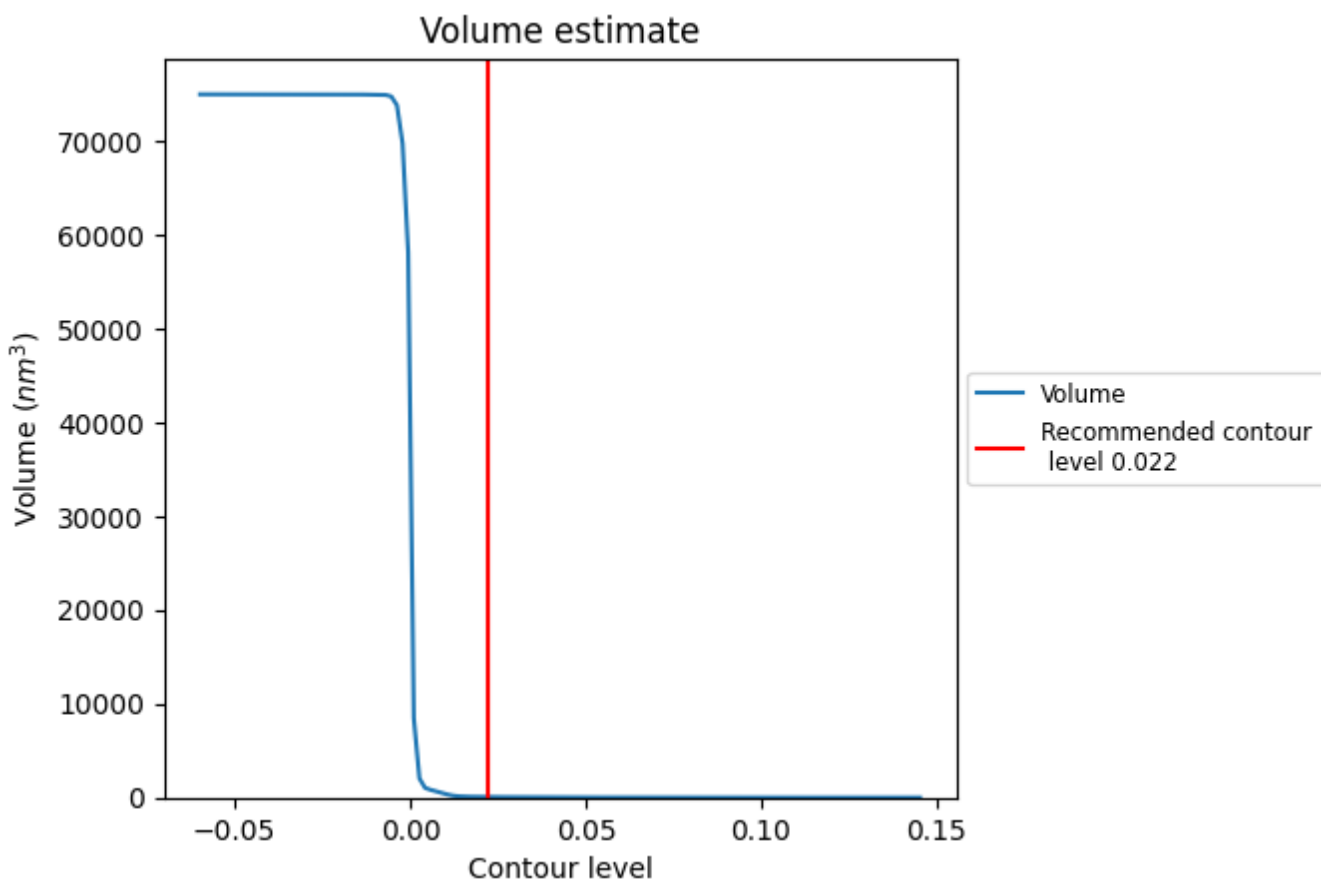
### 7.1 Map-value distribution [i](#)



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



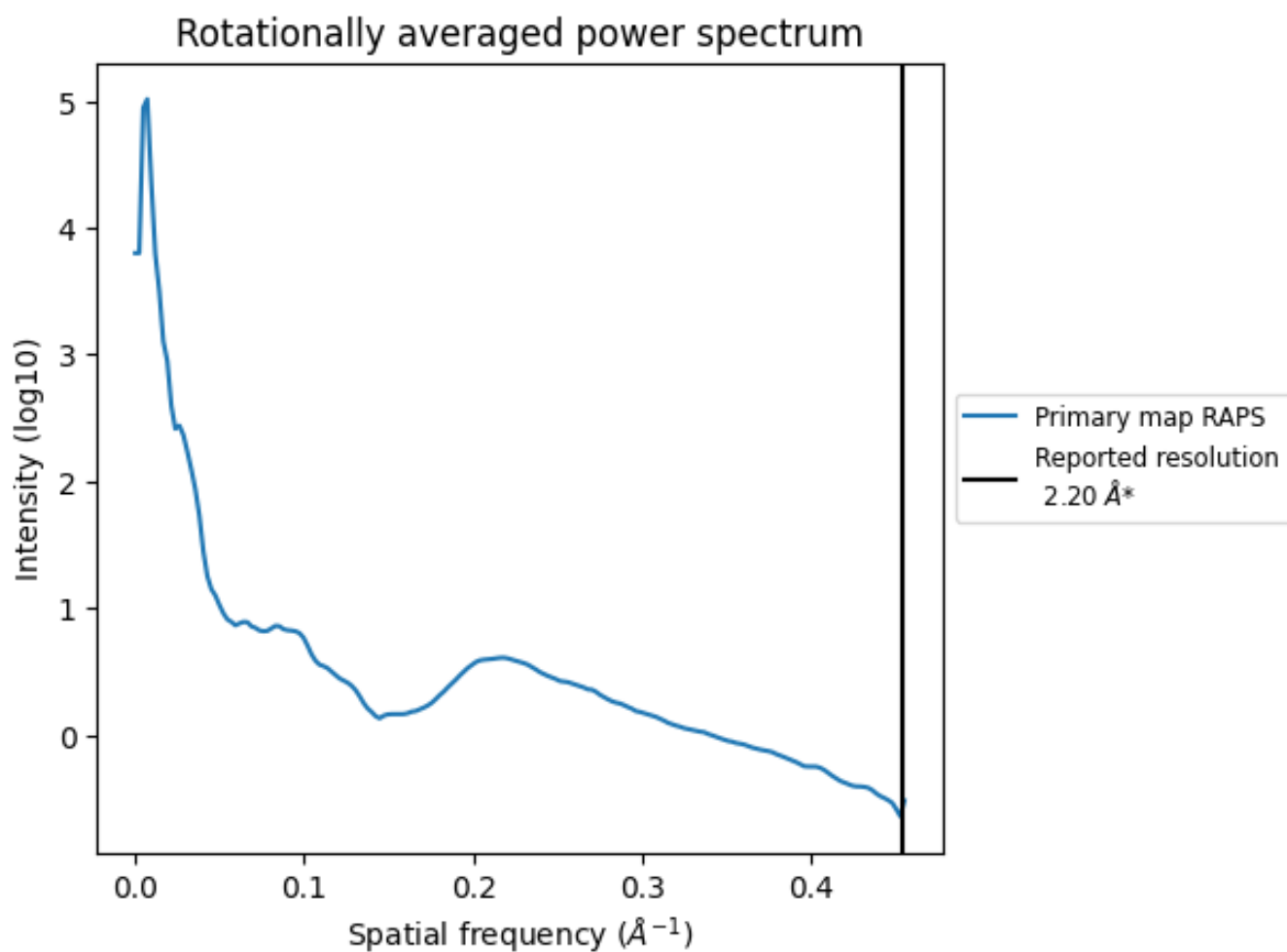
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 65  $\text{nm}^3$ ; this corresponds to an approximate mass of 58 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  $0.455 \text{ \AA}^{-1}$

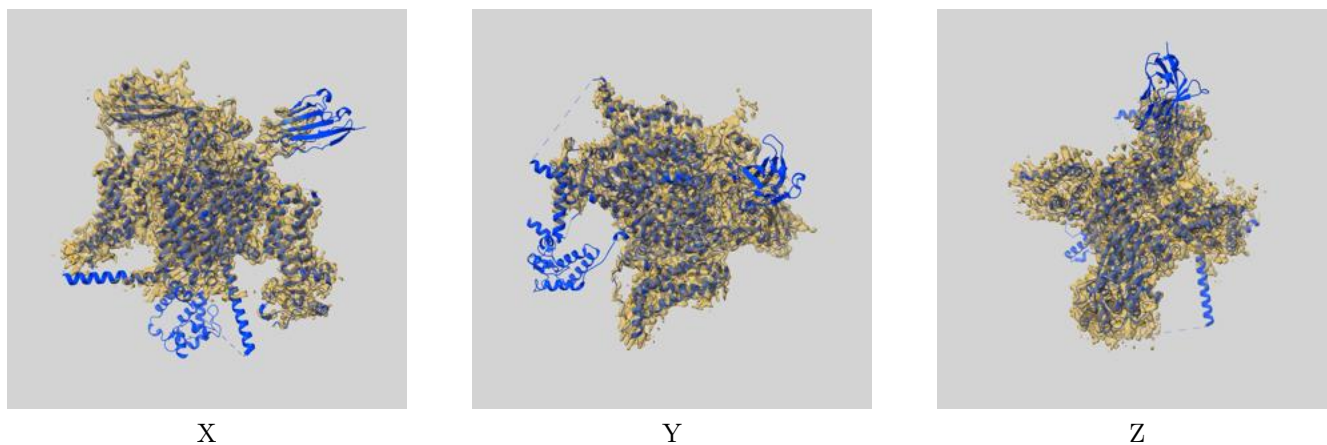
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

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

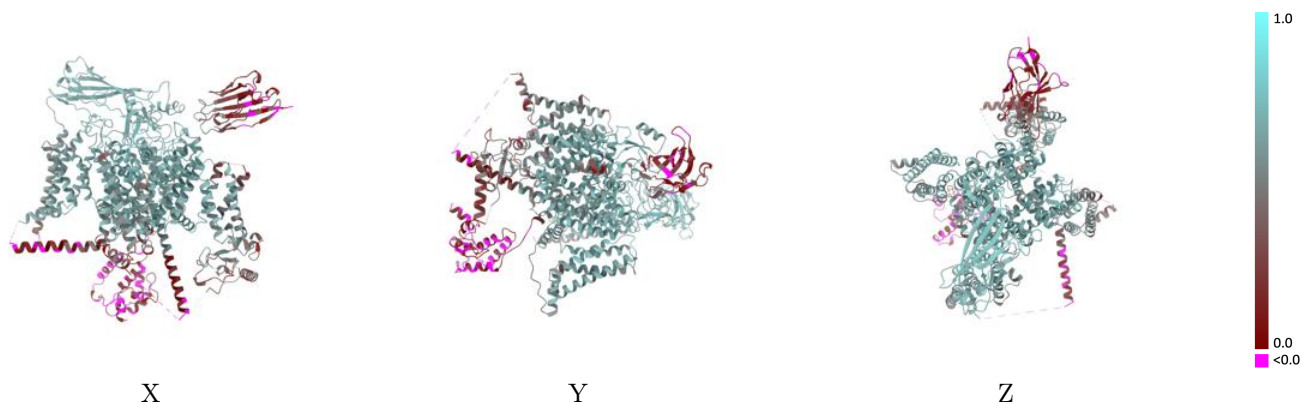
This section contains information regarding the fit between EMDB map EMD-32368 and PDB model 7W9K. Per-residue inclusion information can be found in section [3](#) on page [11](#).

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



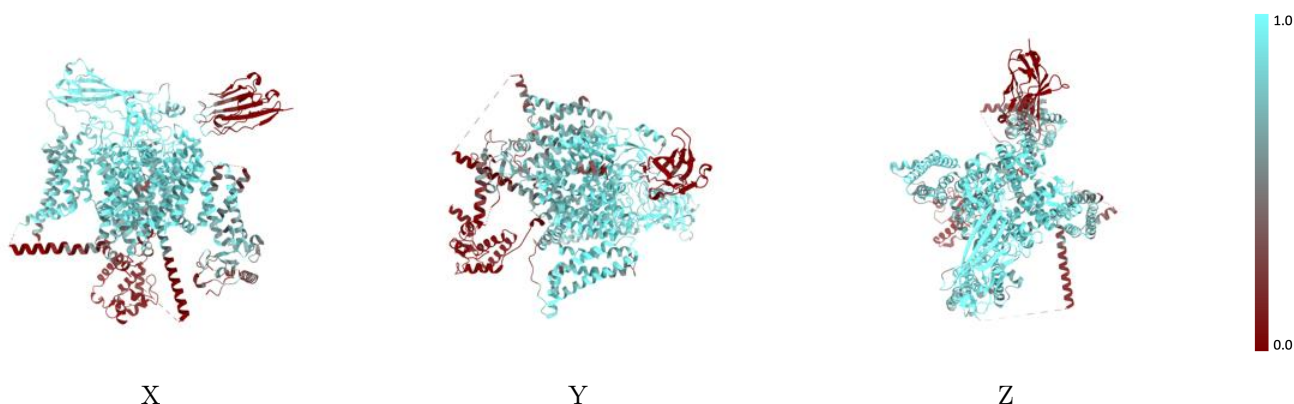
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



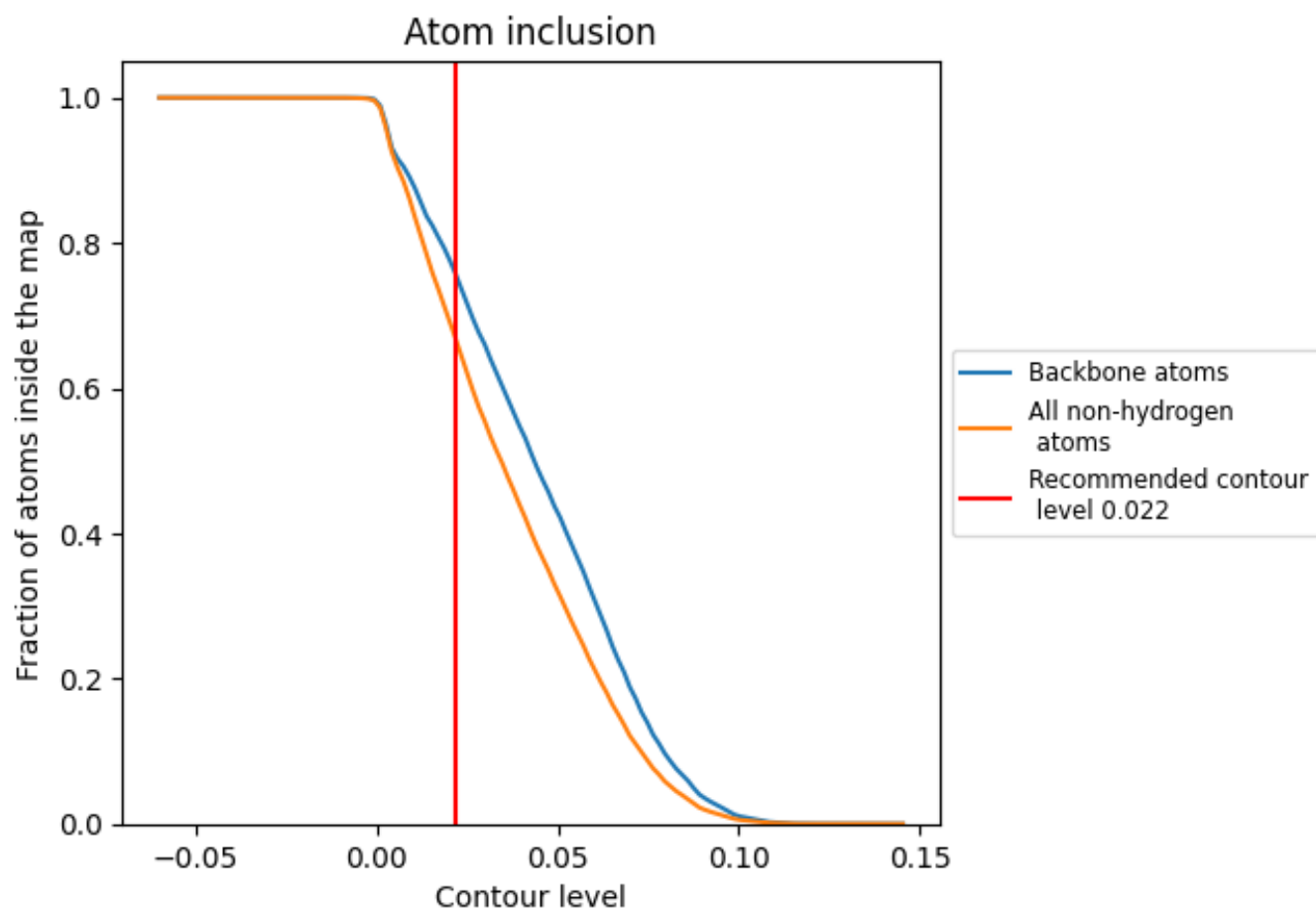
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.022).















## 9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 67% 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 (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6660	 0.5070
A	 0.6842	 0.5180
B	 0.8587	 0.6100
C	 0.1441	 0.2110
D	 0.5000	 0.4100
E	 0.7143	 0.4790
F	 0.9286	 0.6380

