



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 08:35 PM UTC

PDB ID : 7W9K / pdb_00007w9k
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)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

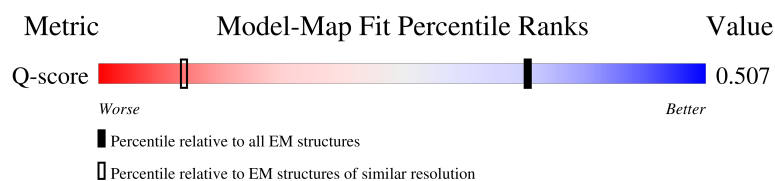
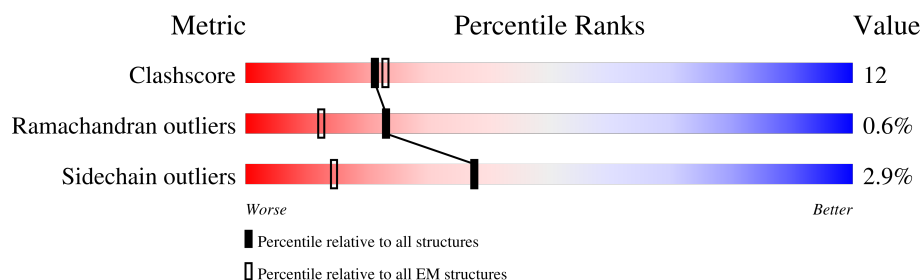
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.20 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3184 (1.71 - 2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2031	
2	B	218	
3	C	215	
4	D	2	

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Mol	Chain	Length	Quality of chain
4	E	2	 100%
4	F	2	 100%

2 Entry composition

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
1	A	1413	Total	C	N	O	S	1	0
			11412	7534	1796	1997	85		

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
2	B	173	Total	C	N	O	S	0	0
			1416	902	232	272	10		

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

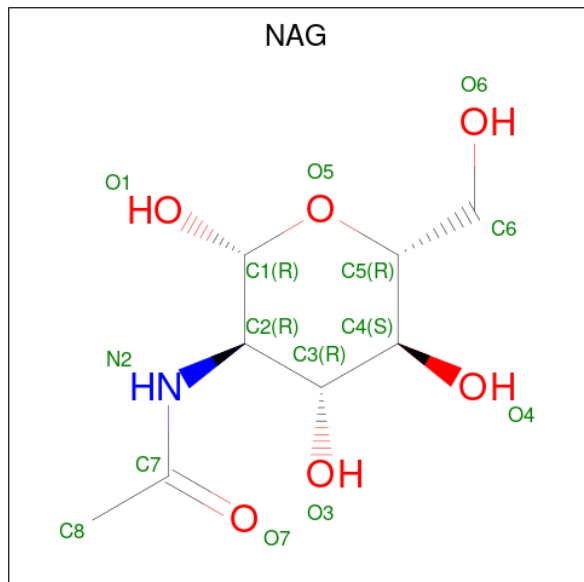
Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	119	Total	C	N	O	S	4	0
			980	615	172	183	10		

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



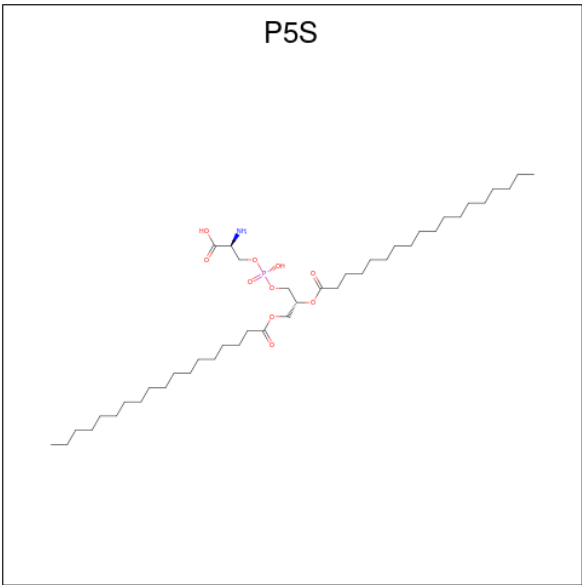
Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	2	Total	C	N	O		0	0
			28	16	2	10			
4	E	2	Total	C	N	O		0	0
			28	16	2	10			
4	F	2	Total	C	N	O		0	0
			28	16	2	10			

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



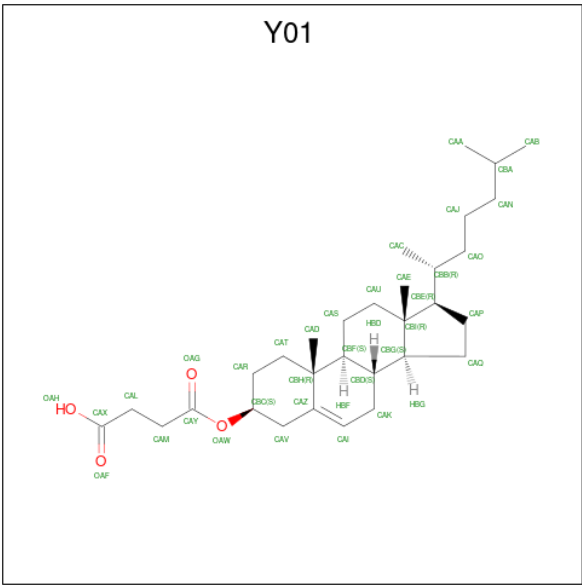
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	

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



Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			35	24	1	9	1	
6	A	1	Total	C	N	O	P	0
			41	31	1	8	1	
6	A	1	Total	C	N	O	P	0
			34	22	1	10	1	

- Molecule 7 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: C₃₁H₅₀O₄).



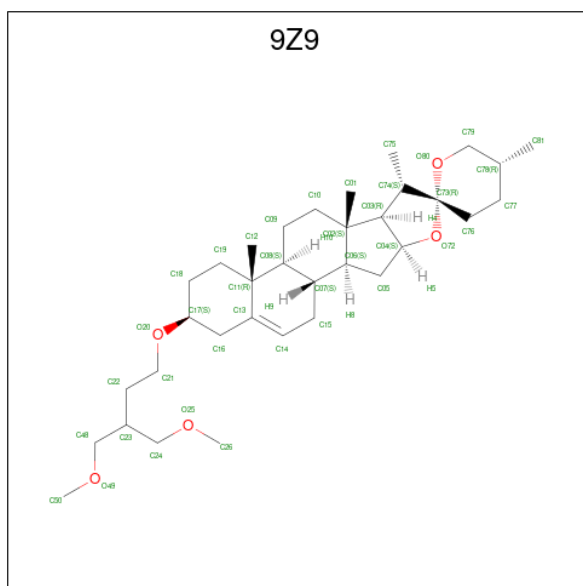
Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			35	31	4	

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

- Molecule 8 is (3beta,14beta,17beta,25R)-3-[4-methoxy-3-(methoxymethyl)butoxy]spirost-5-en (CCD ID: 9Z9) (formula: C₃₄H₅₆O₅).

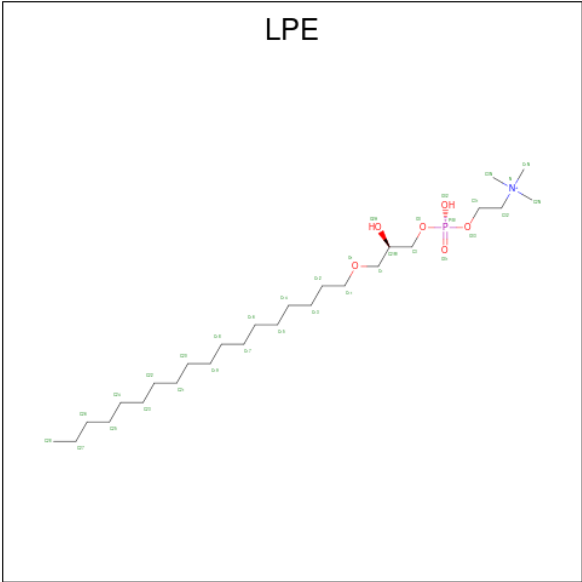


Mol	Chain	Residues	Atoms			AltConf
8	A	1	Total	C	O	0
			39	34	5	

- Molecule 9 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 10 is 1-O-OCTADECYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: LPE) (formula: C₂₆H₅₇NO₆P).



Mol	Chain	Residues	Atoms					AltConf
10	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
10	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
10	A	1	Total	C	N	O	P	0
			20	12	1	6	1	
10	A	1	Total	C	N	O	P	0
			22	14	1	6	1	
10	A	1	Total	C	N	O	P	0
			28	20	1	6	1	
10	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
10	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
10	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
10	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
10	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
10	A	1	Total	C	N	O	P	0
			17	9	1	6	1	
10	A	1	Total	C	N	O	P	0
			17	9	1	6	1	

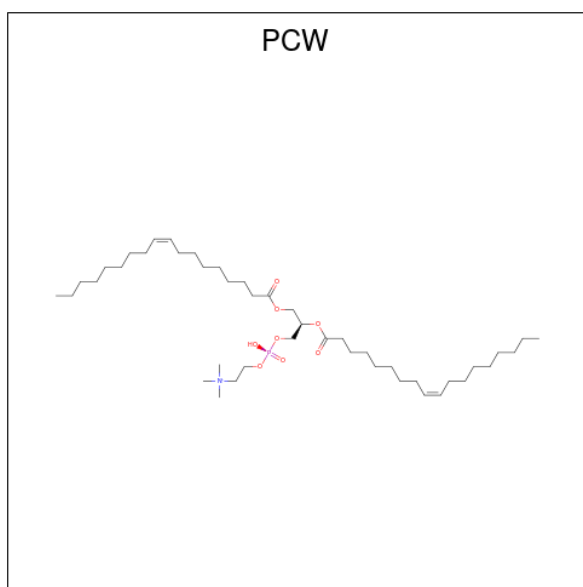
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Mol	Chain	Residues	Atoms				AltConf	
10	B	1	Total	C	N	O	P	0
			17	9	1	6	1	

- # 1PW

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

- 



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

- Molecule 13 is water.

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



Chain E:  100%

MAG1
MAG2

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

Chain F:  100%

MAG1
MAG2

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 (Å)	421.59363, 421.59363, 421.59363	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0979, 1.0979, 1.0979	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: Y01, 1PW, NAG, NA, PCW, P5S, LPE, 9Z9

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	1.34	115/11686 (1.0%)	1.30	106/15823 (0.7%)
2	B	1.59	24/1442 (1.7%)	1.34	16/1949 (0.8%)
3	C	0.34	0/1011	0.59	1/1367 (0.1%)
All	All	1.32	139/14139 (1.0%)	1.27	123/19139 (0.6%)

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

The worst 5 of 139 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1388	ASN	C-O	-9.26	1.17	1.24
1	A	1437	PHE	C-O	-8.38	1.14	1.24
1	A	1442	ILE	C-O	-8.34	1.14	1.24
1	A	1416	VAL	CA-CB	8.29	1.65	1.54
1	A	919	ILE	CA-CB	8.26	1.64	1.54

The worst 5 of 123 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	955	GLY	N-CA-C	10.28	125.08	112.64
1	A	1353	THR	N-CA-C	10.12	122.31	111.28
1	A	388	LEU	N-CA-C	9.97	122.10	111.03
2	B	99	LYS	N-CA-C	-8.85	102.49	113.38
2	B	47	SER	N-CA-C	8.77	120.84	111.28

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 ⓘ

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	268	0
2	B	1416	0	1380	27	0
3	C	980	0	935	5	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	72	0
8	A	39	0	0	14	0
9	A	1	0	0	0	0
10	A	329	0	445	37	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	357	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.

The worst 5 of 357 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1485:MET:HB3	1:A:1639:MET:HE1	1.43	0.98
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%)	21	23
2	B	171/218 (78%)	167 (98%)	3 (2%)	1 (1%)	21	23
3	C	120/215 (56%)	117 (98%)	3 (2%)	0	100	100
All	All	1693/2464 (69%)	1602 (95%)	81 (5%)	10 (1%)	23	23

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%)	1232 (97%)	33 (3%)	40	55
2	B	157/190 (83%)	150 (96%)	7 (4%)	24	33
3	C	114/193 (59%)	109 (96%)	5 (4%)	25	34
All	All	1536/2192 (70%)	1491 (97%)	45 (3%)	38	51

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1599	ILE
2	B	90	VAL
1	A	1620	ILE
1	A	1711	LYS
2	B	104	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	143	HIS
3	C	53	ASN
1	A	1323	ASN
1	A	1276	ASN
3	C	82	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

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	0.53	0
4	NAG	D	2	4	14,14,15	0.28	0	17,19,21	0.73	0
4	NAG	E	1	1,4	14,14,15	0.18	0	17,19,21	0.47	0
4	NAG	E	2	4	14,14,15	0.45	0	17,19,21	0.67	0
4	NAG	F	1	2,4	14,14,15	0.55	0	17,19,21	1.18	2 (11%)
4	NAG	F	2	4	14,14,15	0.66	0	17,19,21	1.21	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	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	2.78	115.92	112.19
4	F	1	NAG	C3-C4-C5	-2.60	105.52	110.23
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:

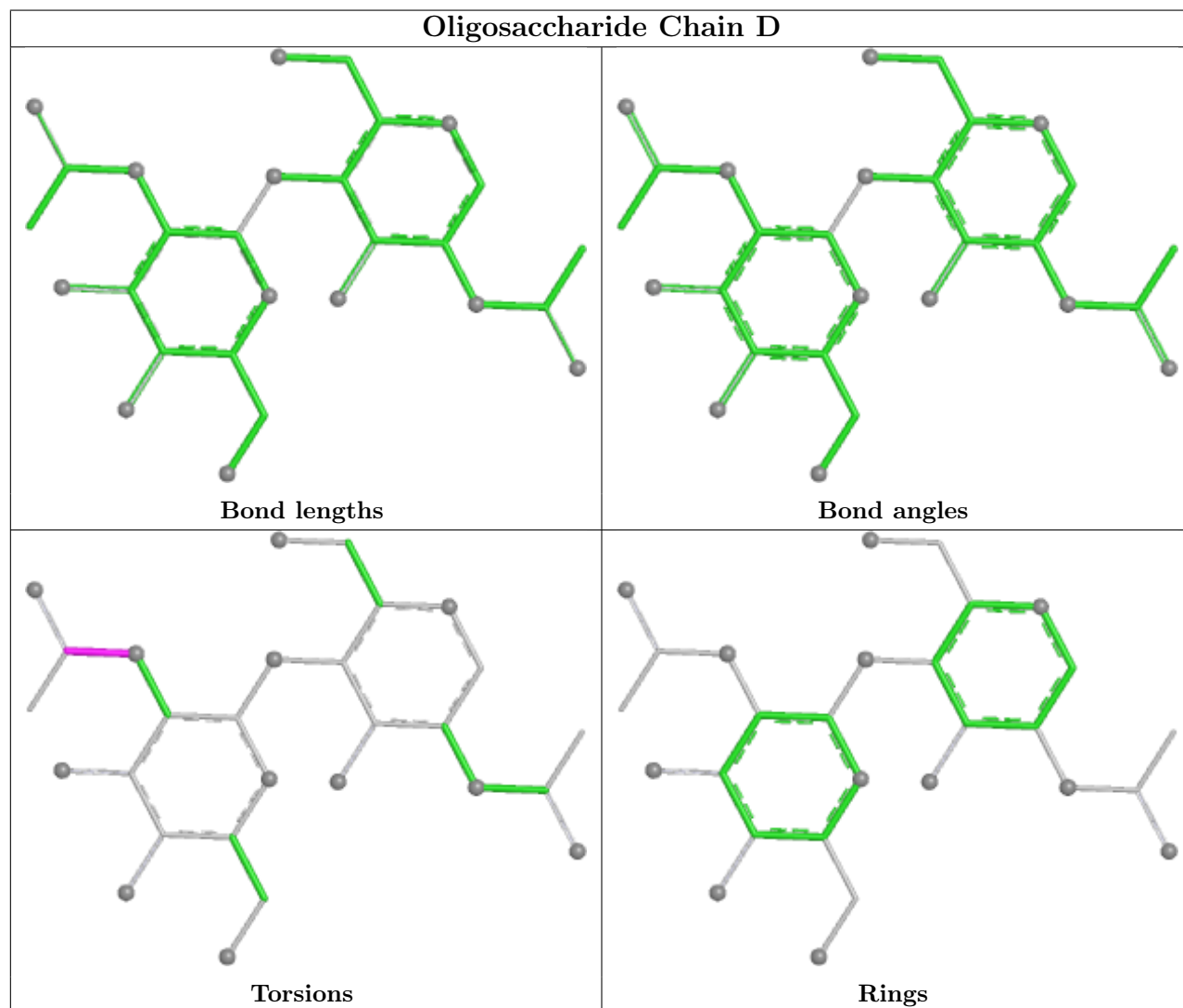
Mol	Chain	Res	Type	Atoms
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
4	F	2	NAG	C4-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6

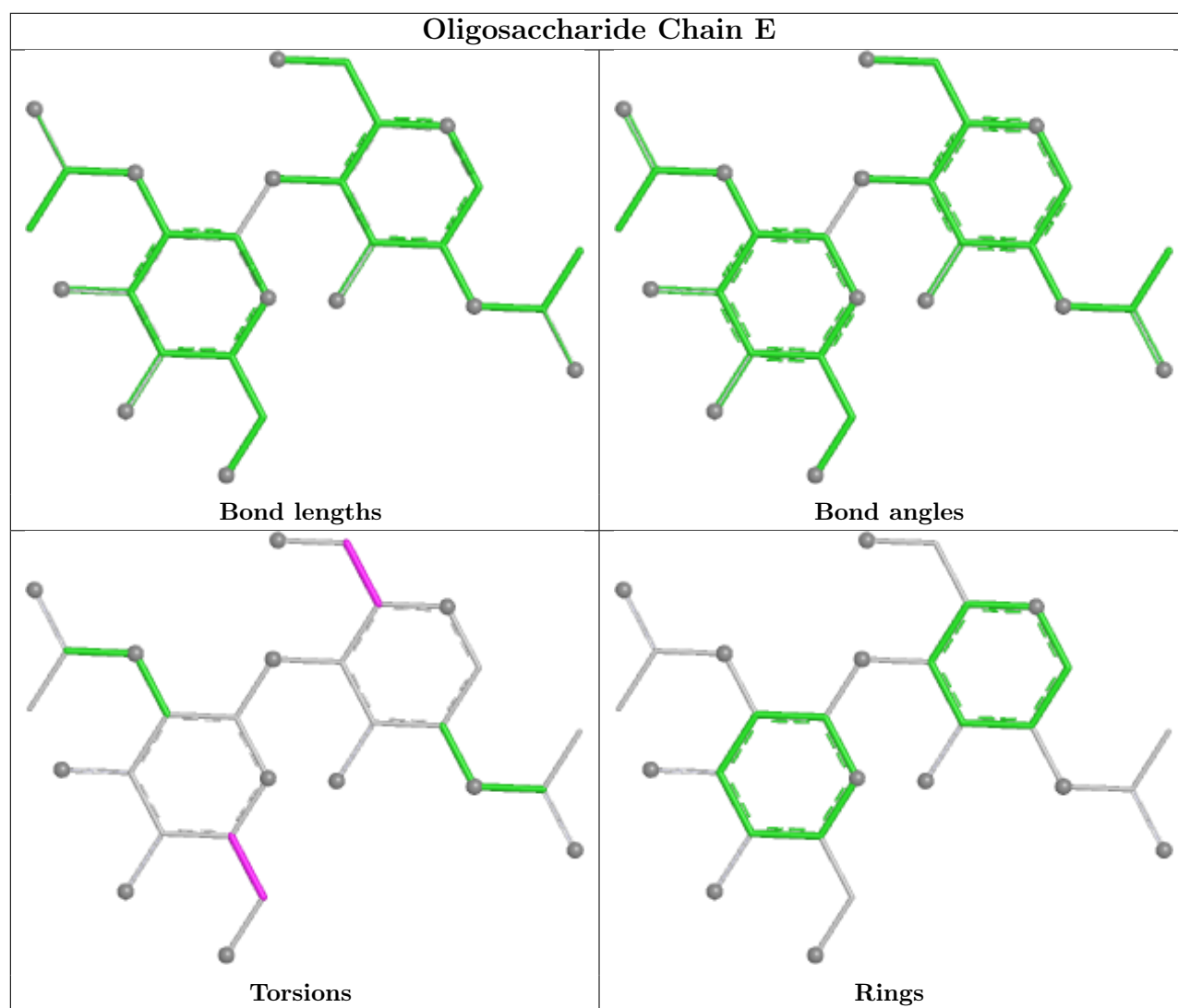
There are no ring outliers.

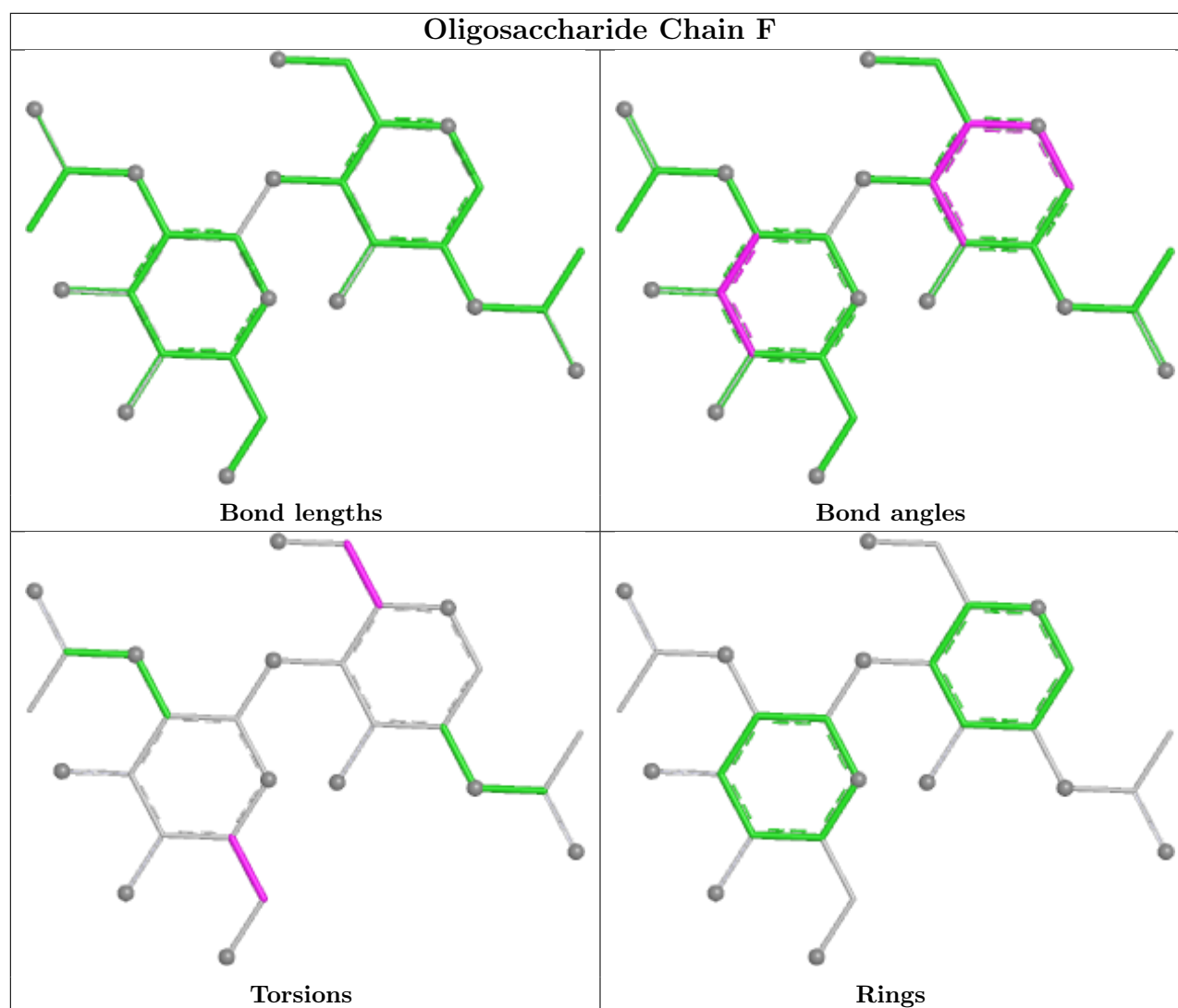
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	NAG	2	0
4	D	2	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	2004	-	38,38,38	0.68	1 (2%)	57,57,57	1.83	13 (22%)
7	Y01	A	2005	-	38,38,38	1.17	4 (10%)	57,57,57	1.79	12 (21%)
5	NAG	B	302	2	14,14,15	0.19	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	301	2	14,14,15	0.64	0	17,19,21	0.97	0
7	Y01	A	2009	-	38,38,38	1.17	4 (10%)	57,57,57	1.79	12 (21%)
11	1PW	A	2013	-	23,23,27	0.44	0	24,26,32	0.54	0
10	LPE	A	2011	-	24,24,33	0.52	0	28,30,39	0.61	0
10	LPE	A	2016	-	21,21,33	0.70	0	25,27,39	1.05	2 (8%)
10	LPE	A	2024	-	24,24,33	0.54	0	28,30,39	0.65	0
10	LPE	A	2014	-	19,19,33	0.63	0	23,25,39	0.53	0
10	LPE	A	2025	-	24,24,33	0.54	0	28,30,39	0.54	0
5	NAG	B	303	2	14,14,15	0.26	0	17,19,21	0.44	0
10	LPE	A	2023	-	24,24,33	0.55	0	28,30,39	0.69	1 (3%)
7	Y01	A	2007	-	38,38,38	0.69	1 (2%)	57,57,57	1.83	12 (21%)
12	PCW	A	2030	-	43,43,53	1.04	2 (4%)	49,51,61	1.01	2 (4%)
12	PCW	A	2018	-	46,46,53	1.00	3 (6%)	52,54,61	1.19	4 (7%)
7	Y01	A	2032	-	38,38,38	1.66	7 (18%)	57,57,57	1.68	12 (21%)
12	PCW	A	2029	-	43,43,53	1.04	2 (4%)	49,51,61	0.95	2 (4%)
10	LPE	A	2021	-	24,24,33	0.61	0	28,30,39	0.91	1 (3%)
5	NAG	A	2008	1	14,14,15	0.40	0	17,19,21	0.88	1 (5%)
10	LPE	A	2033	-	16,16,33	0.69	0	20,22,39	0.68	0
6	P5S	A	2031	-	32,33,53	1.19	4 (12%)	34,40,60	1.02	2 (5%)
12	PCW	A	2020	-	43,43,53	1.02	2 (4%)	49,51,61	1.13	5 (10%)
7	Y01	A	2003	-	38,38,38	0.69	1 (2%)	57,57,57	1.83	12 (21%)
10	LPE	A	2022	-	24,24,33	0.88	0	28,30,39	0.91	1 (3%)
10	LPE	A	2012	-	24,24,33	0.33	0	25,27,39	0.61	0
10	LPE	A	2027	-	24,24,33	0.56	0	28,30,39	0.50	0
10	LPE	A	2017	-	27,27,33	0.55	0	31,33,39	0.62	0
5	NAG	A	2001	1	14,14,15	0.36	0	17,19,21	0.46	0
12	PCW	A	2015	-	52,52,53	0.94	2 (3%)	58,60,61	0.99	2 (3%)
6	P5S	A	2019	-	40,40,53	1.17	3 (7%)	43,45,60	1.38	3 (6%)
10	LPE	A	2028	-	16,16,33	0.71	0	20,22,39	0.69	0
8	9Z9	A	2006	-	44,44,44	0.73	1 (2%)	64,68,68	1.51	11 (17%)
10	LPE	B	304	-	16,16,33	0.68	0	20,22,39	0.61	0
10	LPE	A	2026	-	24,24,33	0.52	0	28,30,39	0.63	0
6	P5S	A	2002	-	33,34,53	0.77	1 (3%)	34,40,60	1.80	4 (11%)

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	2004	-	-	0/19/77/77	0/4/4/4
7	Y01	A	2005	-	-	4/19/77/77	0/4/4/4
5	NAG	B	302	2	-	0/6/23/26	0/1/1/1
5	NAG	B	301	2	-	0/6/23/26	0/1/1/1
7	Y01	A	2009	-	-	4/19/77/77	0/4/4/4
11	1PW	A	2013	-	-	4/22/22/29	-
10	LPE	A	2011	-	-	8/25/25/34	-
10	LPE	A	2016	-	-	15/22/22/34	-
10	LPE	A	2024	-	-	3/25/25/34	-
10	LPE	A	2014	-	-	8/20/20/34	-
10	LPE	A	2025	-	-	7/25/25/34	-
5	NAG	B	303	2	-	0/6/23/26	0/1/1/1
10	LPE	A	2023	-	-	2/25/25/34	-
7	Y01	A	2007	-	-	0/19/77/77	0/4/4/4
12	PCW	A	2030	-	-	11/47/47/57	-
12	PCW	A	2018	-	-	12/50/50/57	-
7	Y01	A	2032	-	-	7/19/77/77	0/4/4/4
12	PCW	A	2029	-	-	15/47/47/57	-
10	LPE	A	2021	-	-	5/25/25/34	-
5	NAG	A	2008	1	-	2/6/23/26	0/1/1/1
10	LPE	A	2033	-	-	8/17/17/34	-
6	P5S	A	2031	-	-	18/39/39/59	-
12	PCW	A	2020	-	-	10/47/47/57	-
7	Y01	A	2003	-	-	0/19/77/77	0/4/4/4
10	LPE	A	2022	-	-	11/25/25/34	-
10	LPE	A	2012	-	-	8/25/25/34	-
10	LPE	A	2027	-	-	10/25/25/34	-
10	LPE	A	2017	-	-	8/28/28/34	-
5	NAG	A	2001	1	-	2/6/23/26	0/1/1/1
12	PCW	A	2015	-	-	16/56/56/57	-
6	P5S	A	2019	-	-	8/44/44/59	-
10	LPE	A	2028	-	-	6/17/17/34	-
8	9Z9	A	2006	-	-	0/12/100/100	0/6/6/6
10	LPE	B	304	-	-	9/17/17/34	-
10	LPE	A	2026	-	-	4/25/25/34	-
6	P5S	A	2002	-	-	27/39/39/59	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2032	Y01	CBB-CBE	-4.44	1.46	1.54
12	A	2029	PCW	O3-C11	4.41	1.46	1.33
6	A	2019	P5S	O37-C38	4.40	1.46	1.34
12	A	2030	PCW	O3-C11	4.27	1.45	1.33
7	A	2032	Y01	CAR-CBC	-4.24	1.39	1.51

The worst 5 of 114 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	-6.03	110.19	119.50
7	A	2005	Y01	CBI-CBE-CBB	-6.01	110.21	119.50
7	A	2004	Y01	CBI-CBE-CBB	-6.00	110.23	119.50
7	A	2007	Y01	CBI-CBE-CBB	-6.00	110.23	119.50

There are no chirality outliers.

5 of 252 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	CB-OG-P12-O16
6	A	2002	P5S	C3-O16-P12-OG

There are no ring outliers.

31 monomers are involved in 153 short contacts:

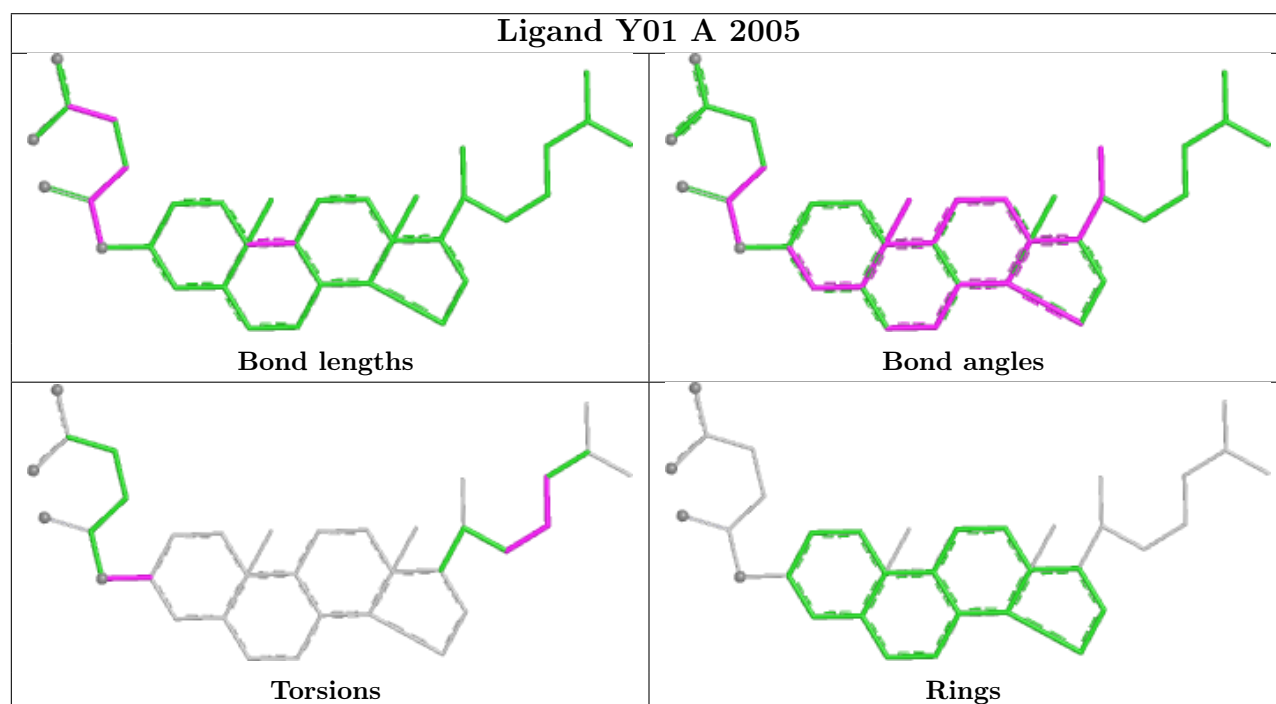
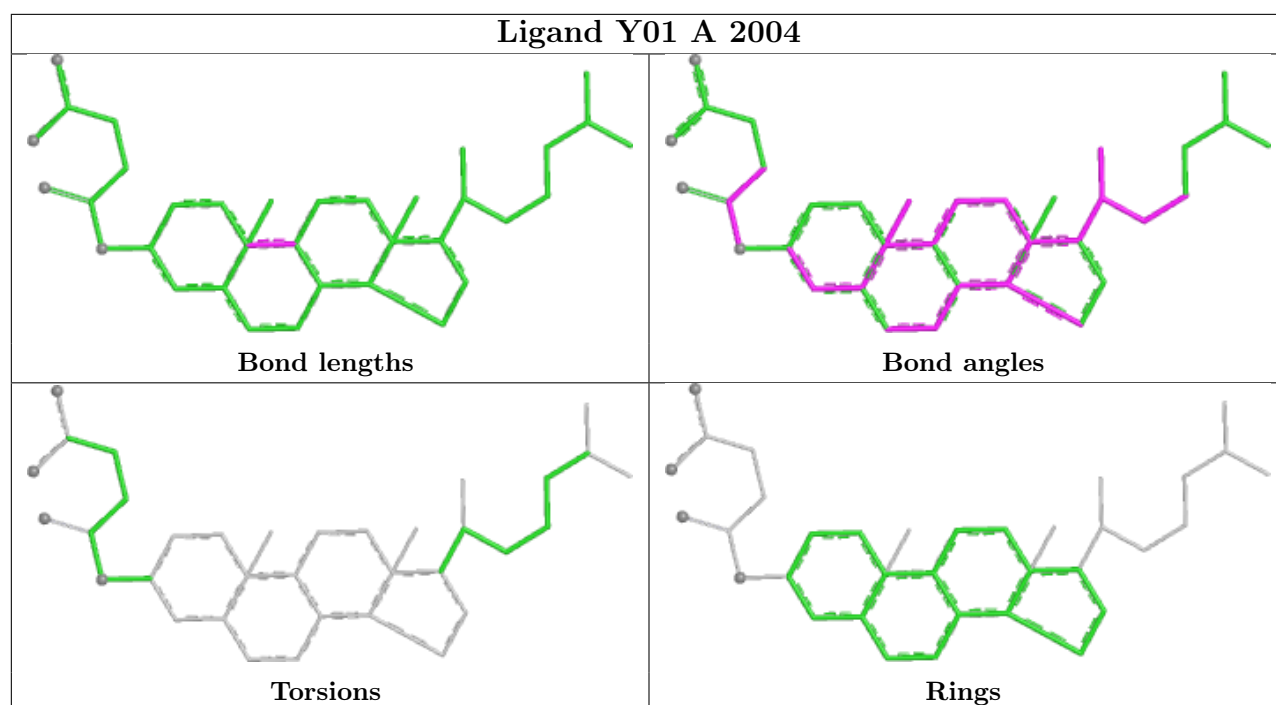
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	2004	Y01	6	0
7	A	2005	Y01	19	0
5	B	302	NAG	1	0
7	A	2009	Y01	9	0
11	A	2013	1PW	2	0
10	A	2016	LPE	5	0
10	A	2024	LPE	2	0
10	A	2014	LPE	2	0
10	A	2025	LPE	2	0
5	B	303	NAG	6	0
10	A	2023	LPE	4	0

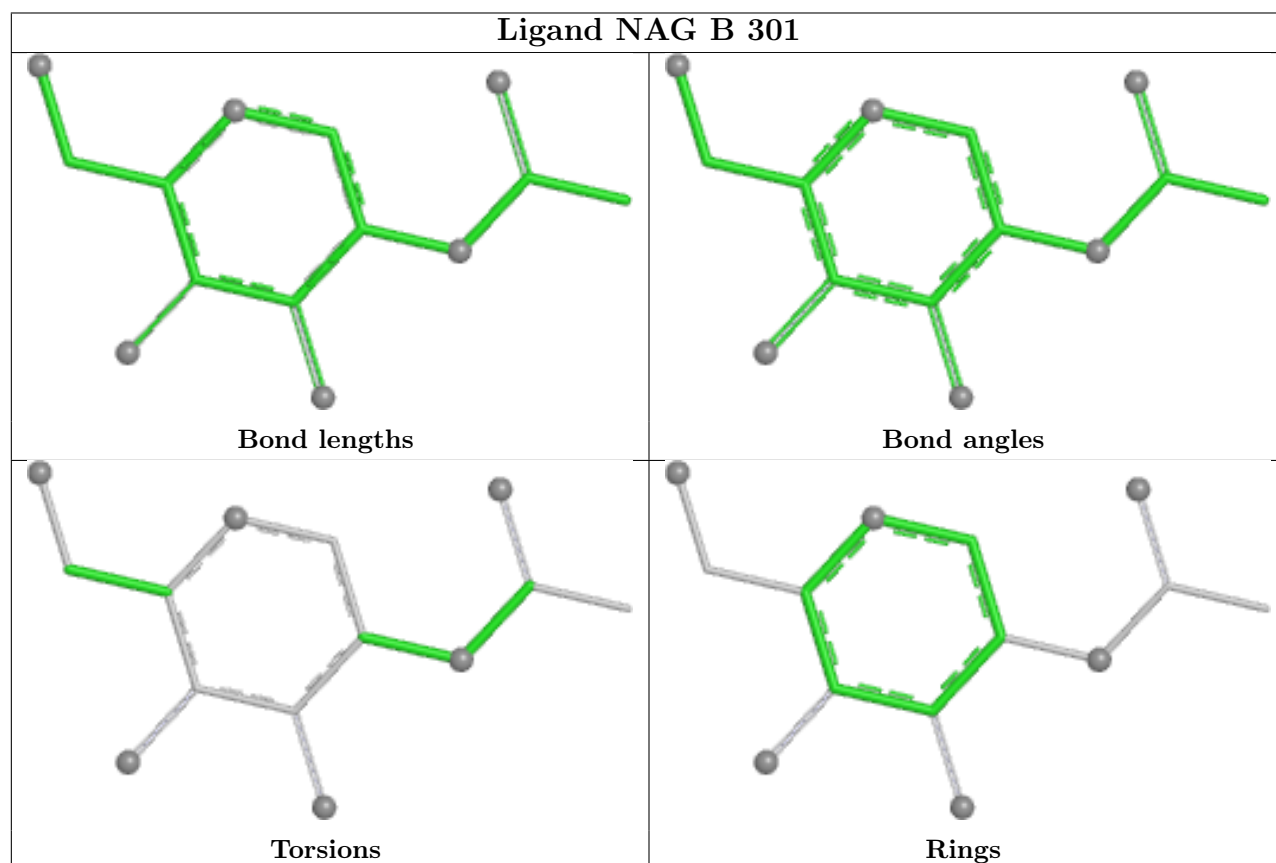
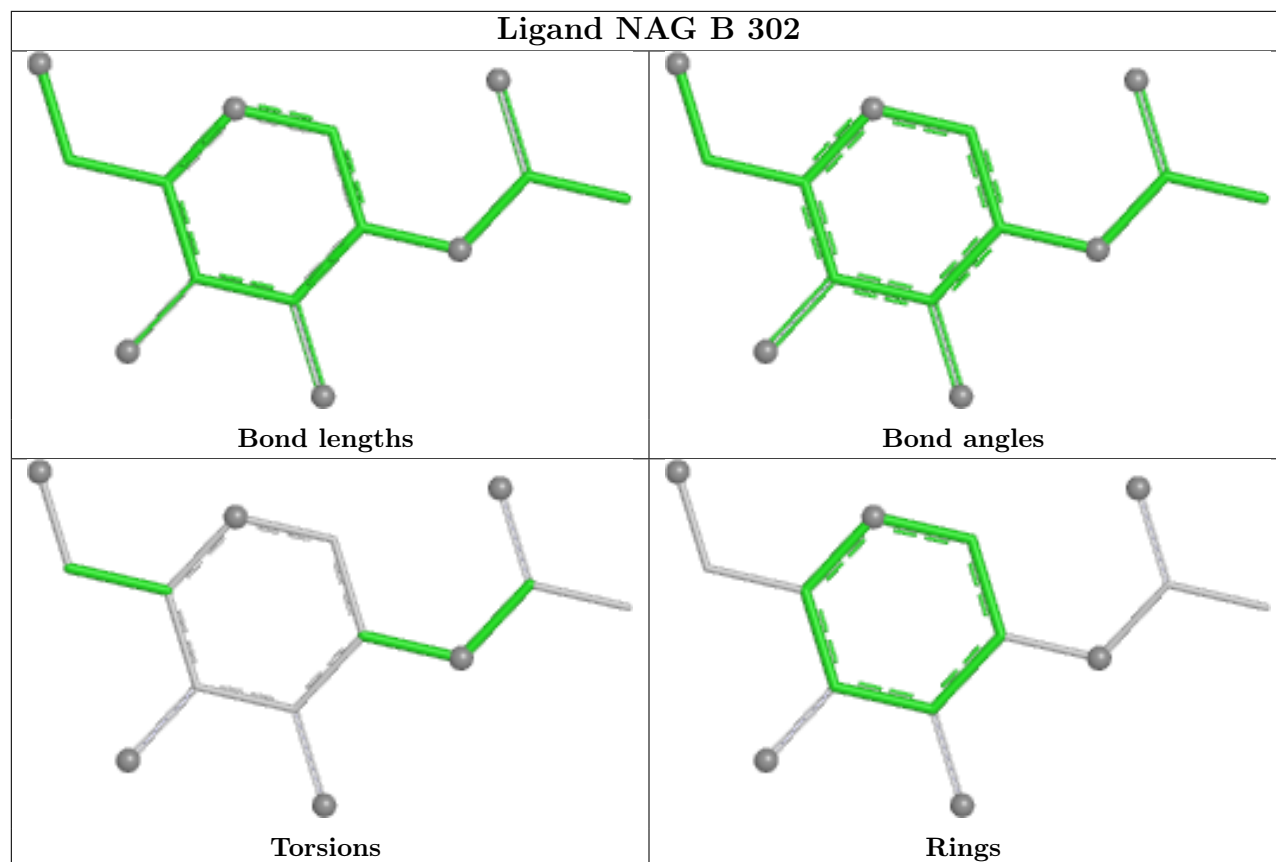
Continued on next page...

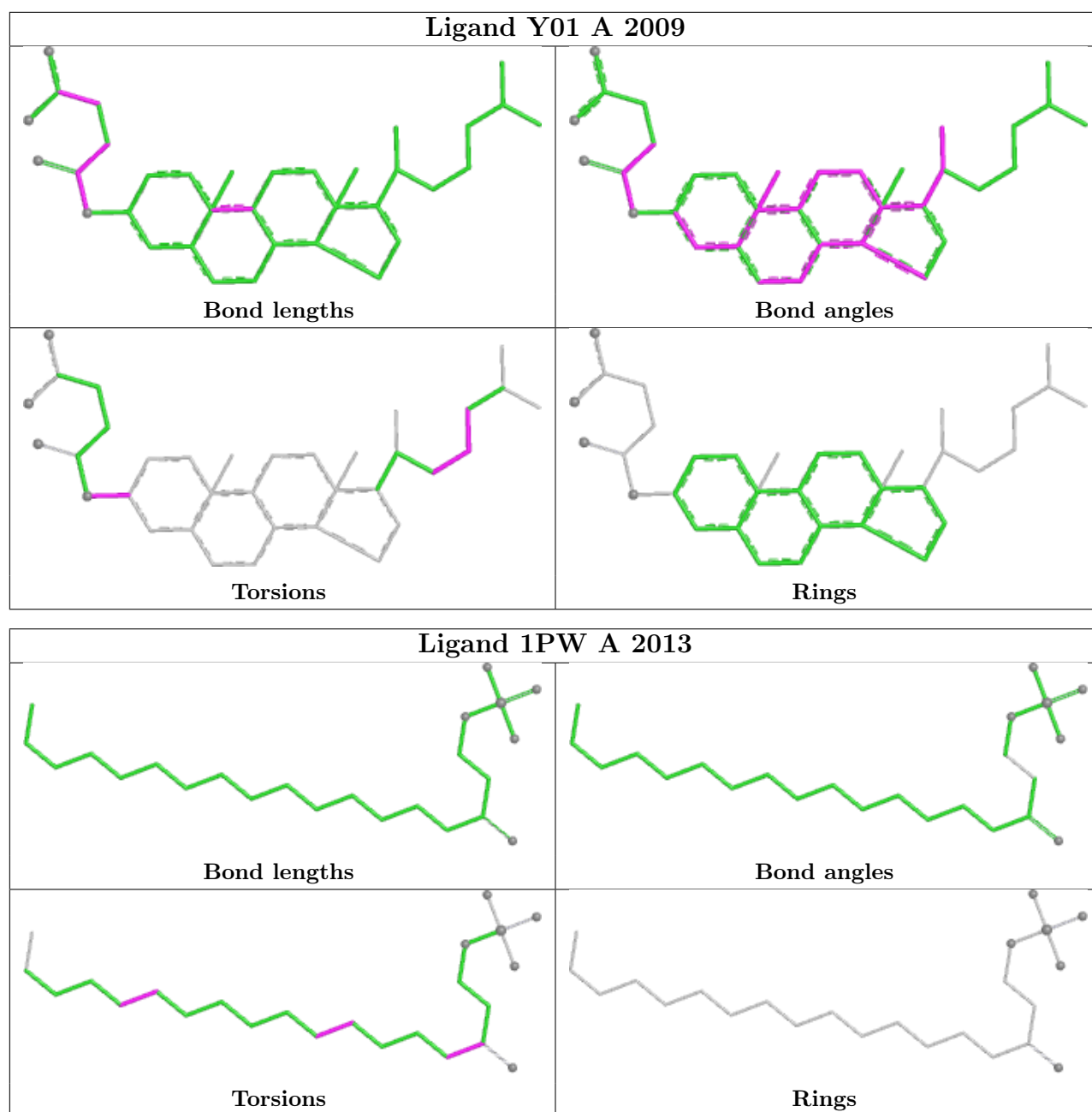
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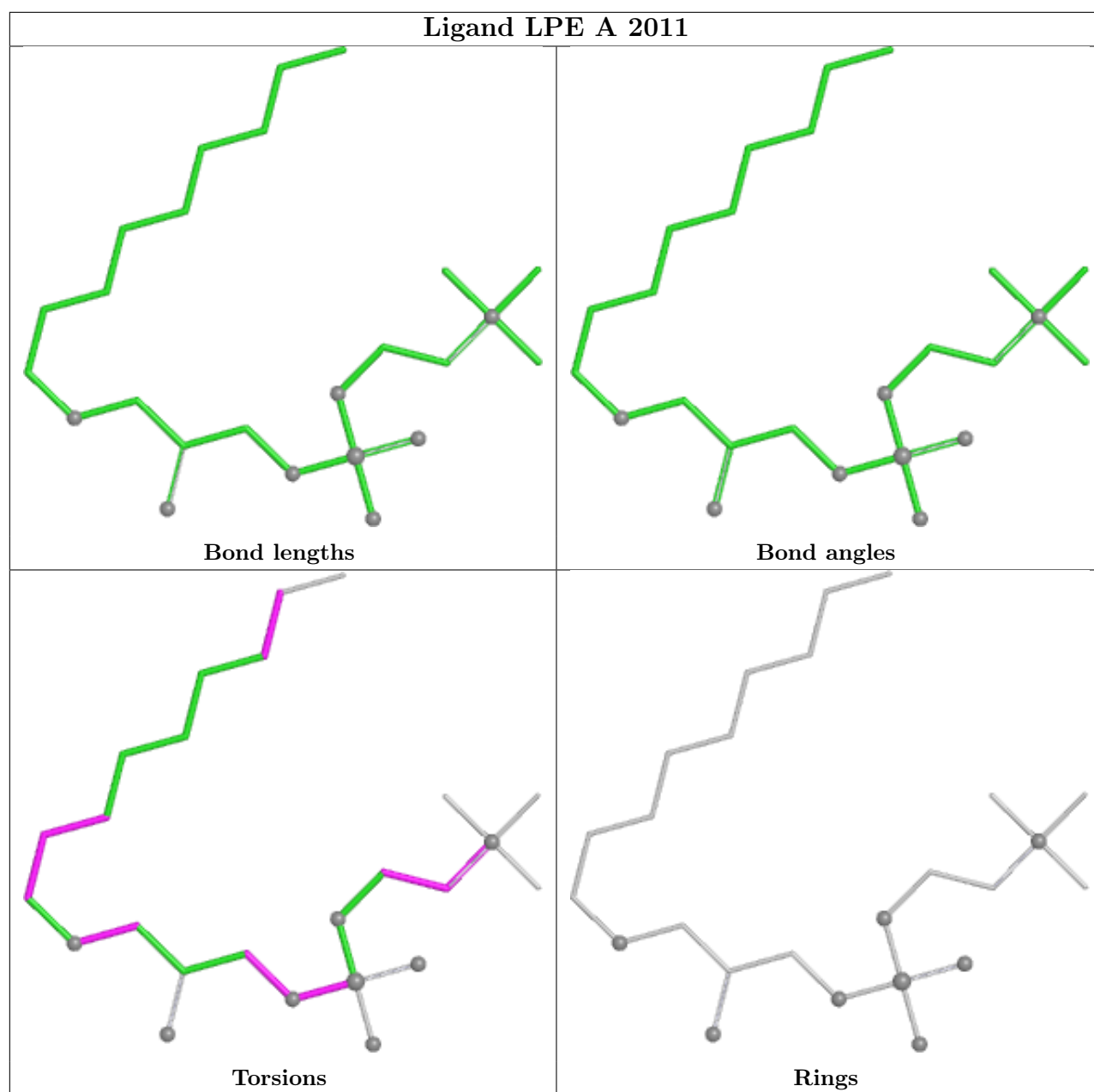
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	2007	Y01	14	0
12	A	2018	PCW	1	0
7	A	2032	Y01	20	0
12	A	2029	PCW	3	0
10	A	2021	LPE	7	0
10	A	2033	LPE	3	0
6	A	2031	P5S	3	0
12	A	2020	PCW	7	0
7	A	2003	Y01	4	0
10	A	2022	LPE	1	0
10	A	2012	LPE	1	0
10	A	2027	LPE	3	0
10	A	2017	LPE	3	0
5	A	2001	NAG	1	0
12	A	2015	PCW	19	0
6	A	2019	P5S	4	0
10	A	2028	LPE	1	0
8	A	2006	9Z9	14	0
10	A	2026	LPE	4	0
6	A	2002	P5S	2	0

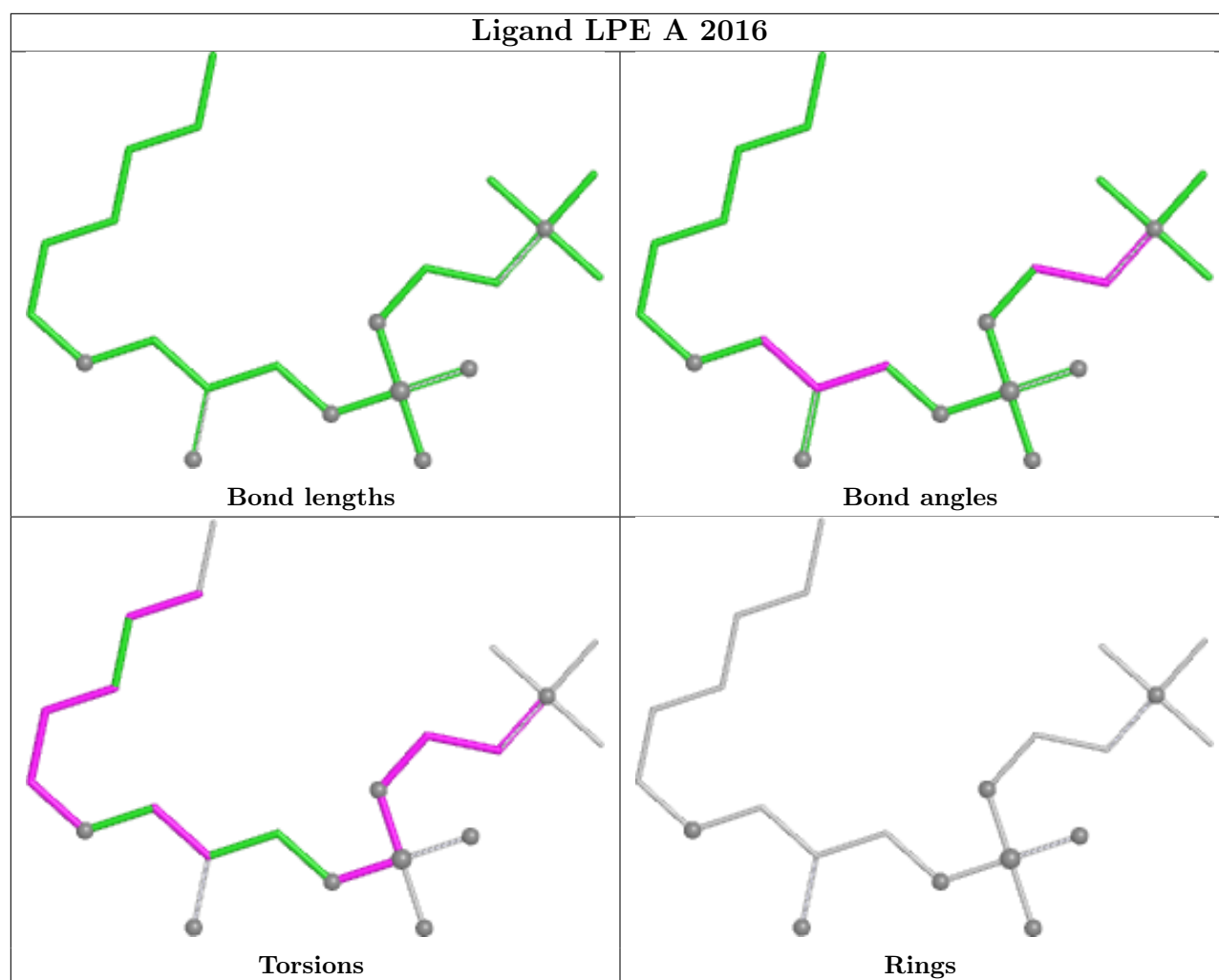
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

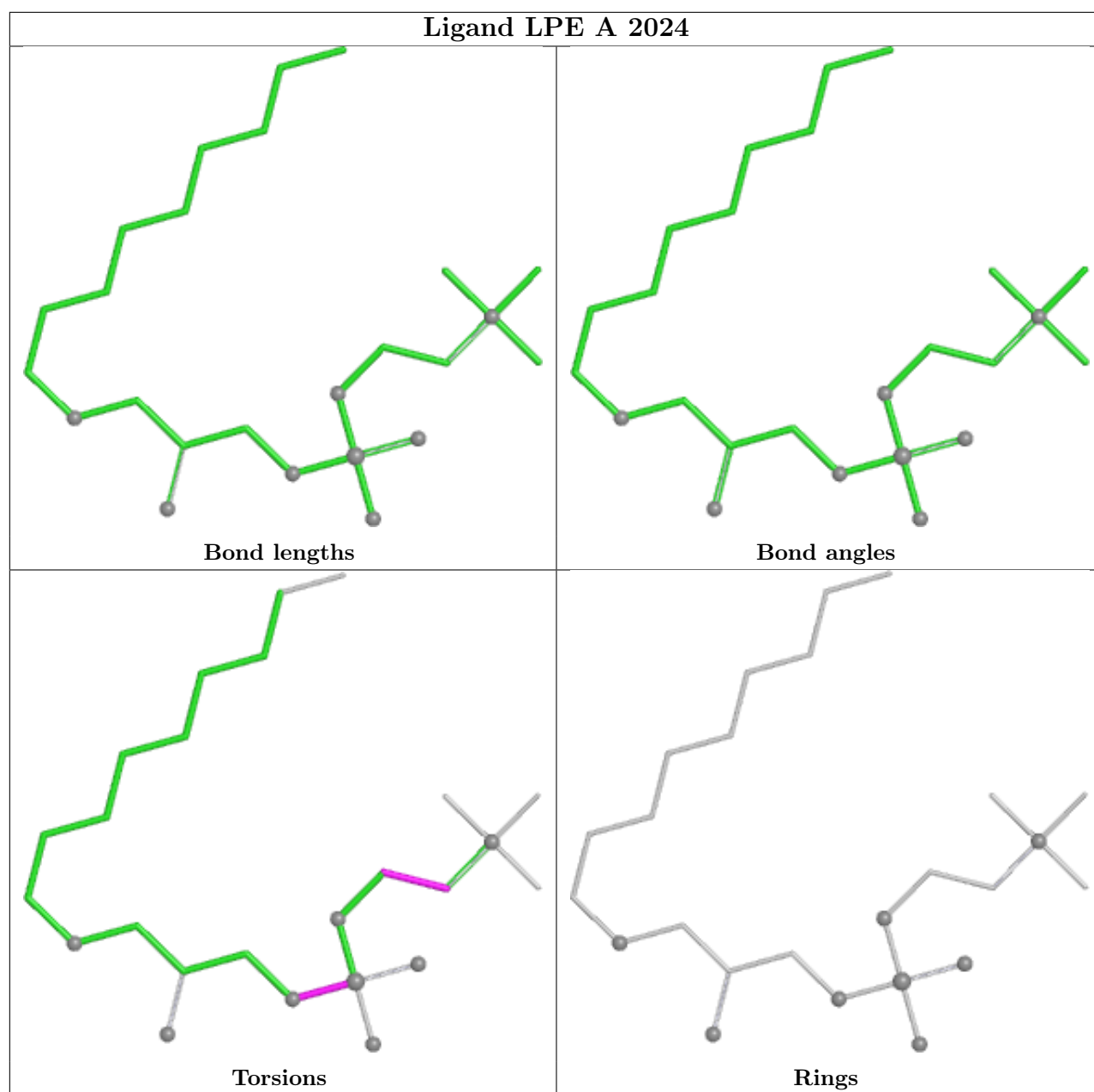


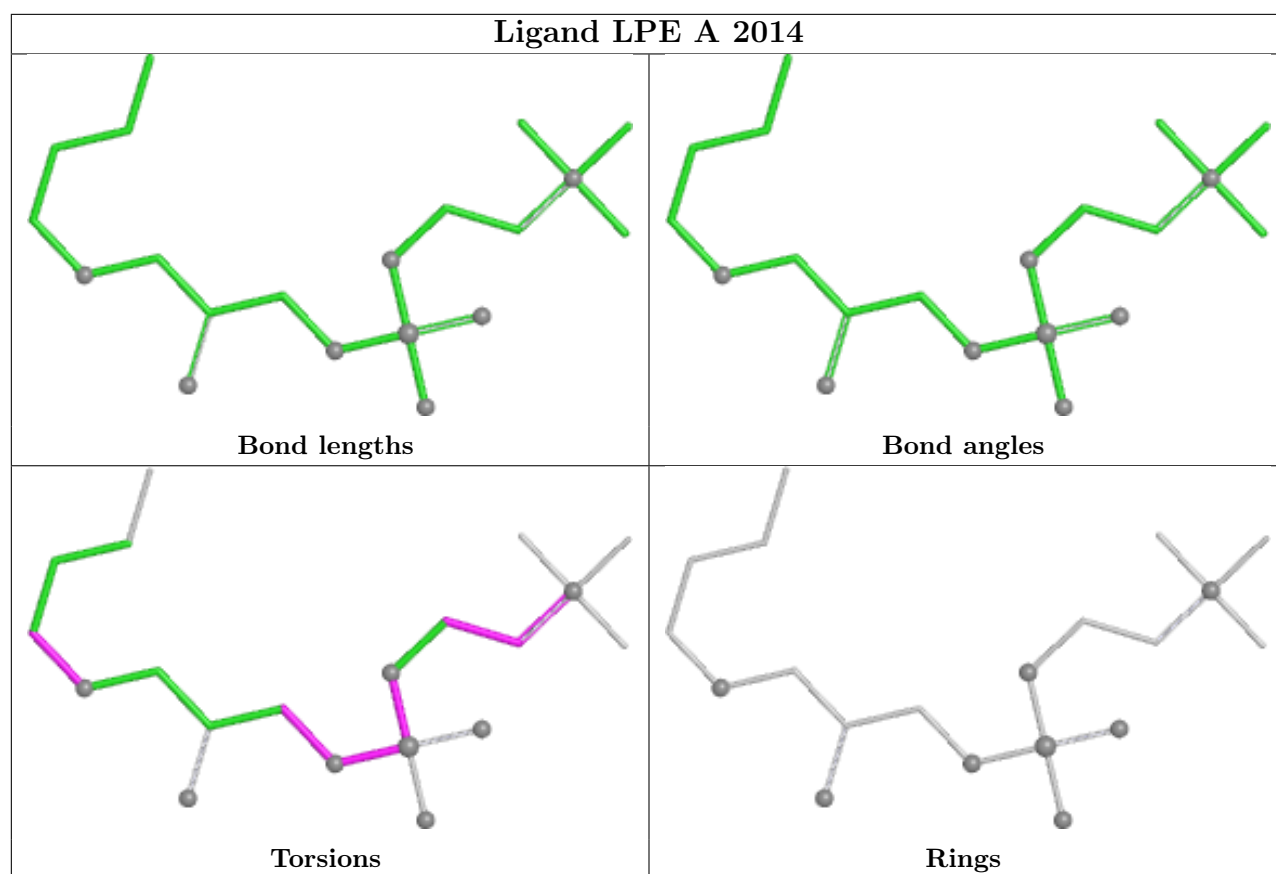


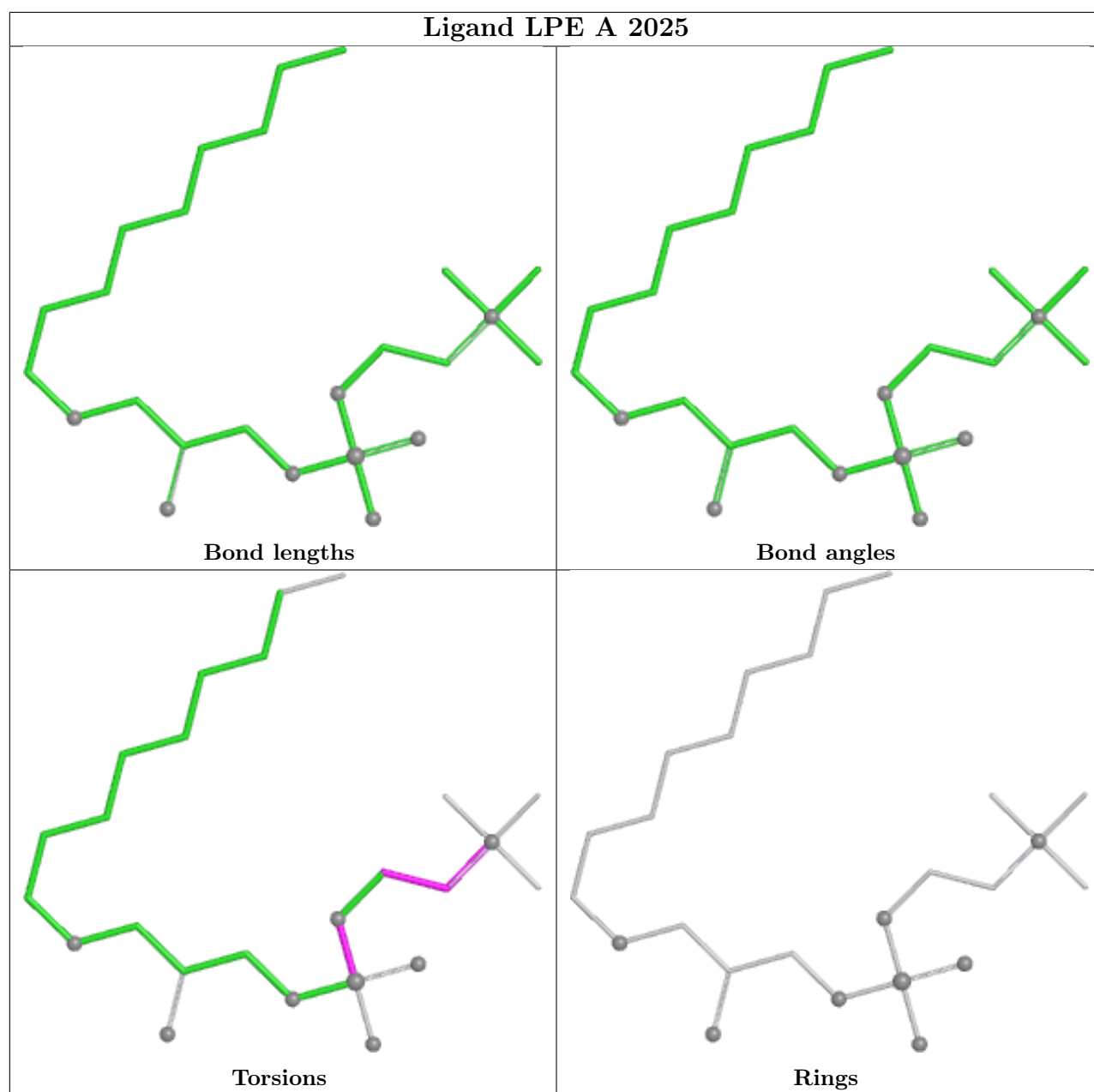


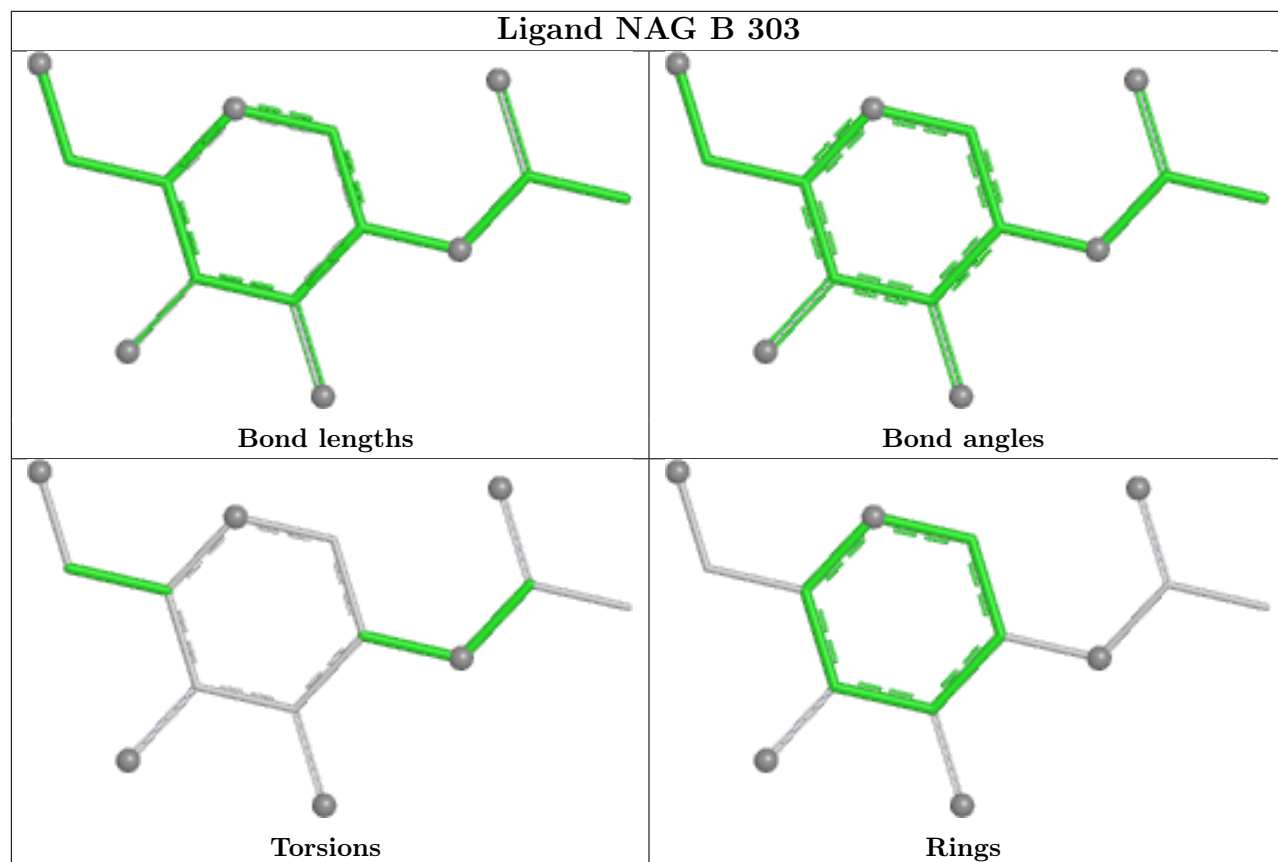


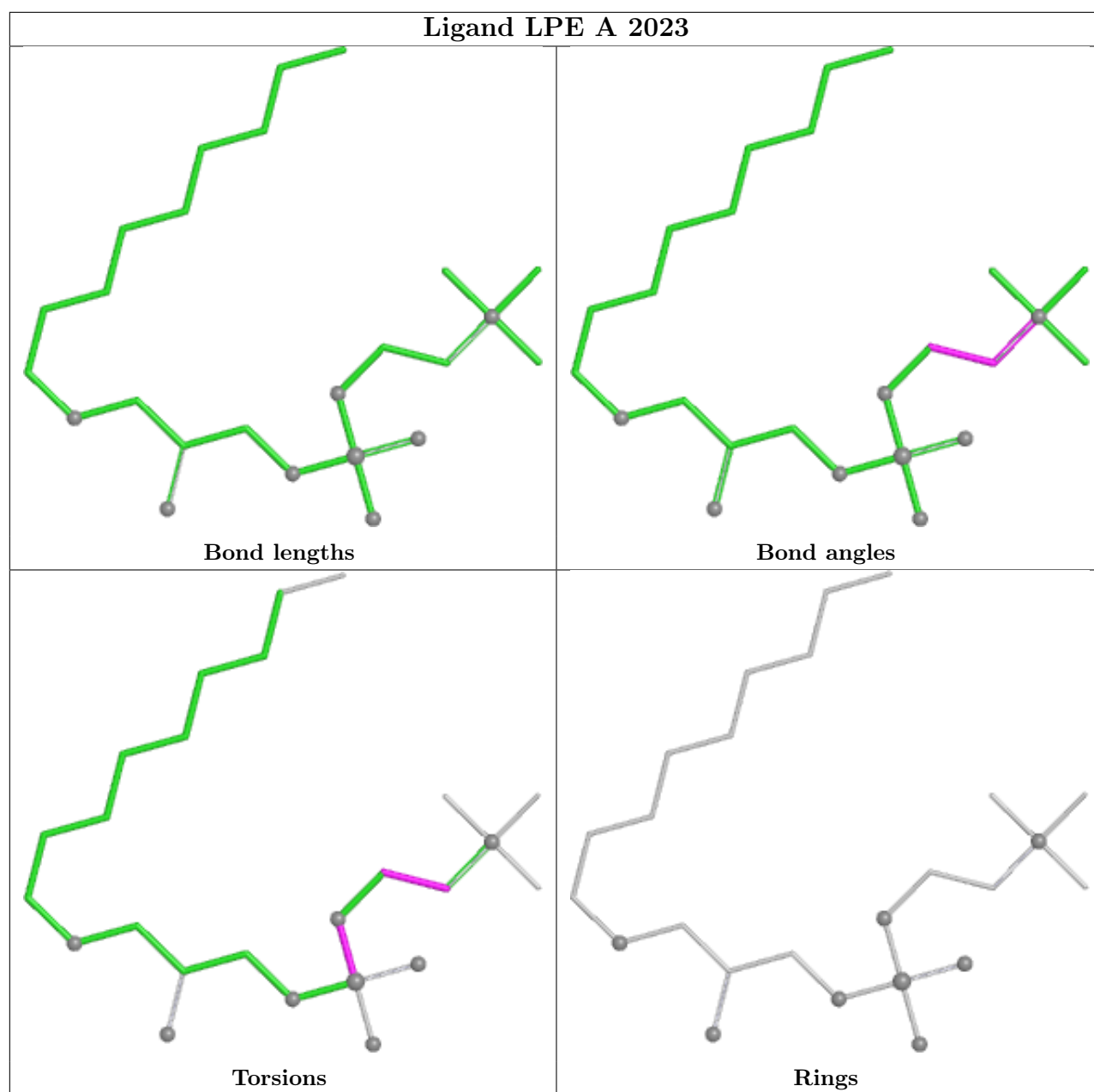


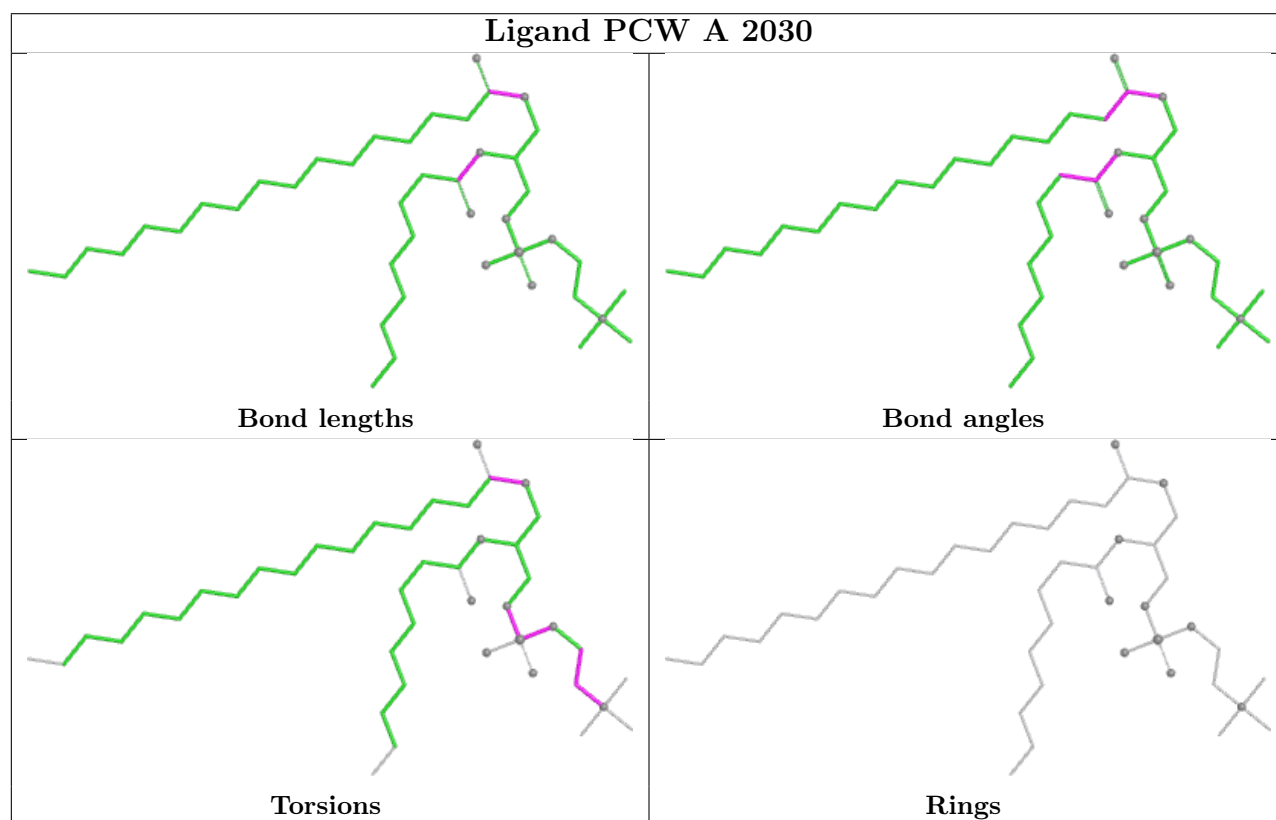
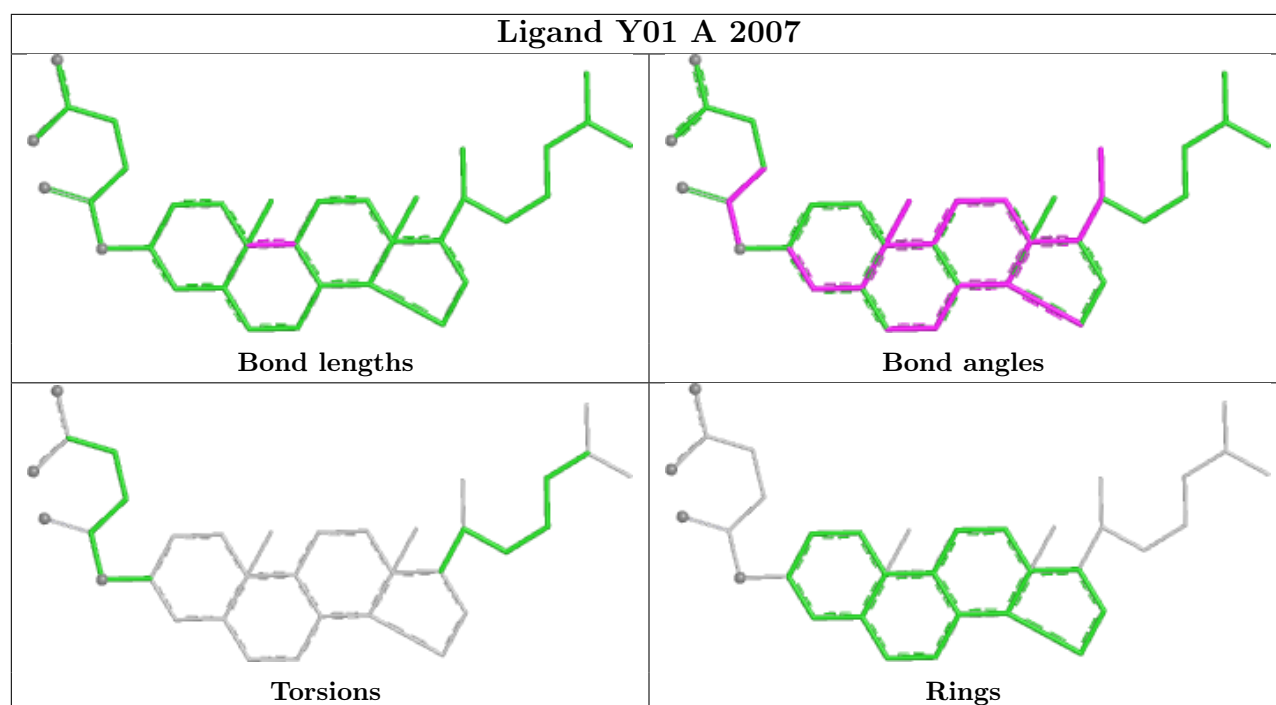


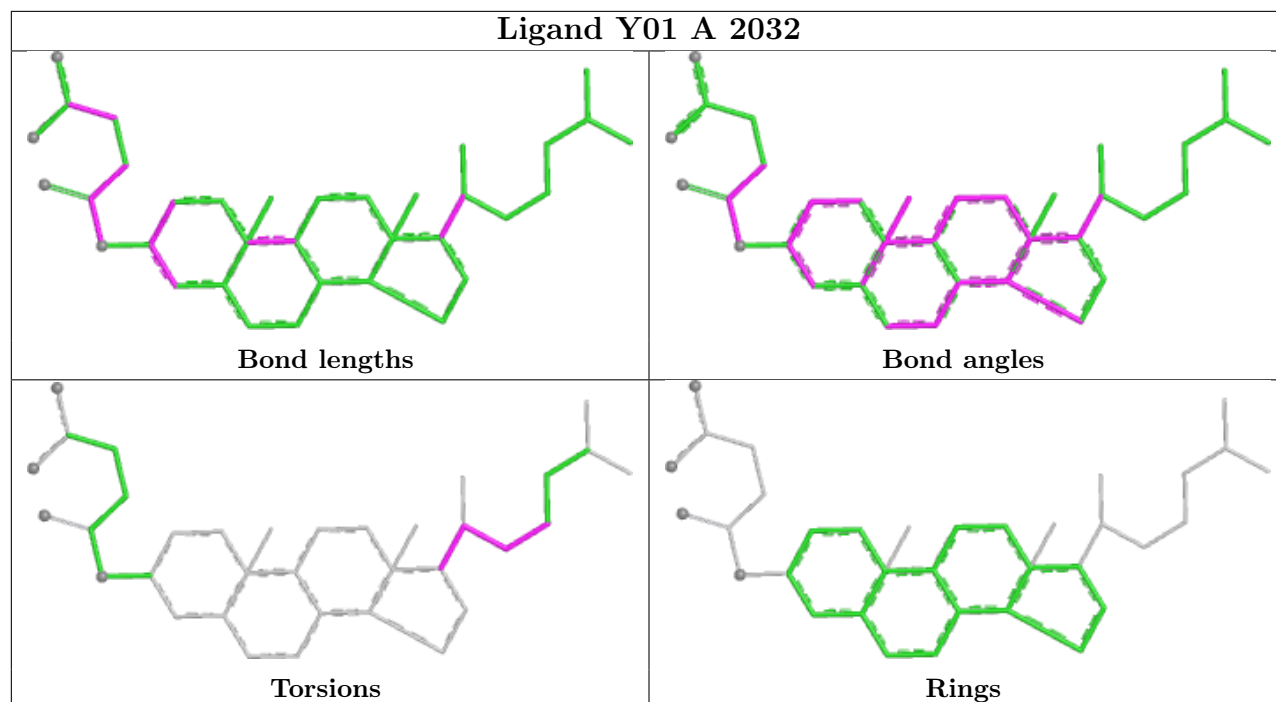
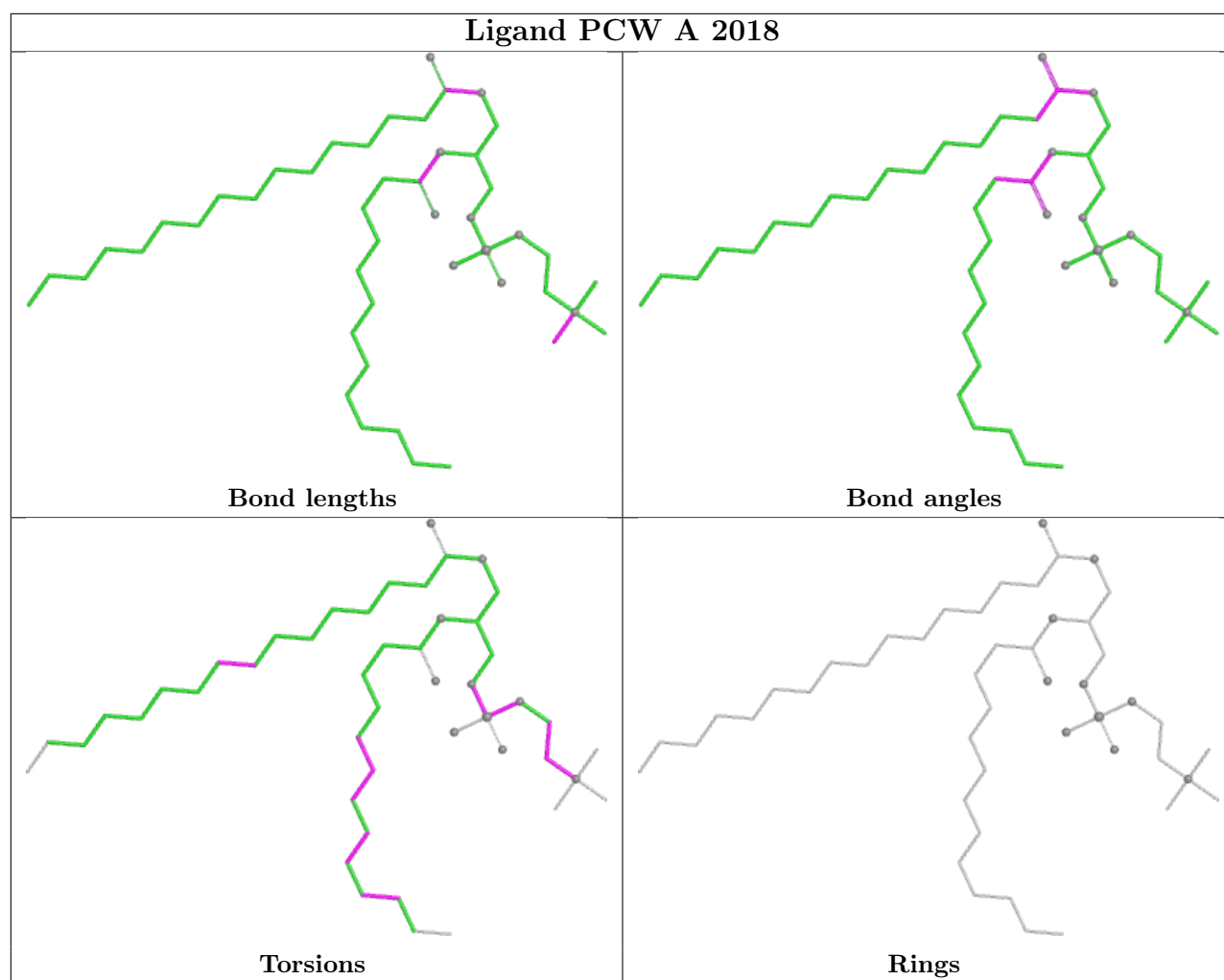


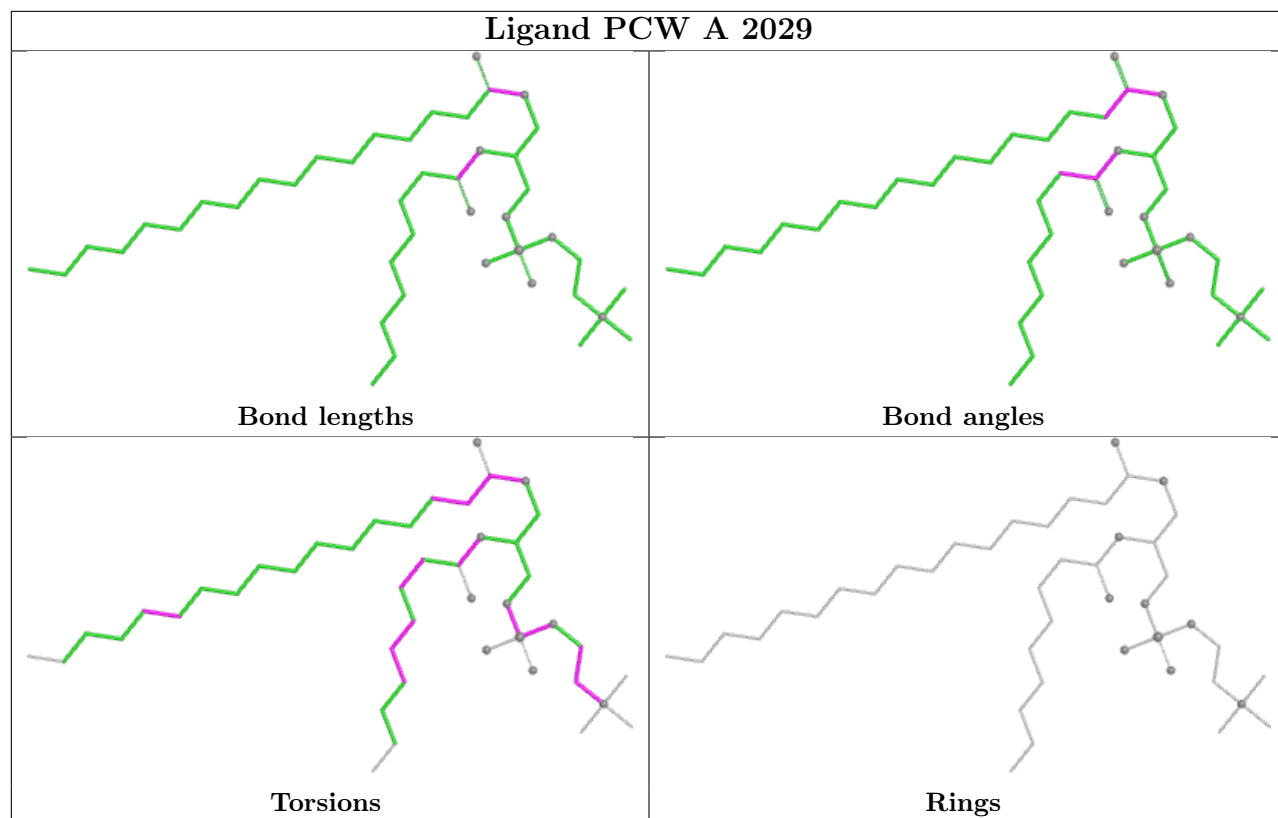


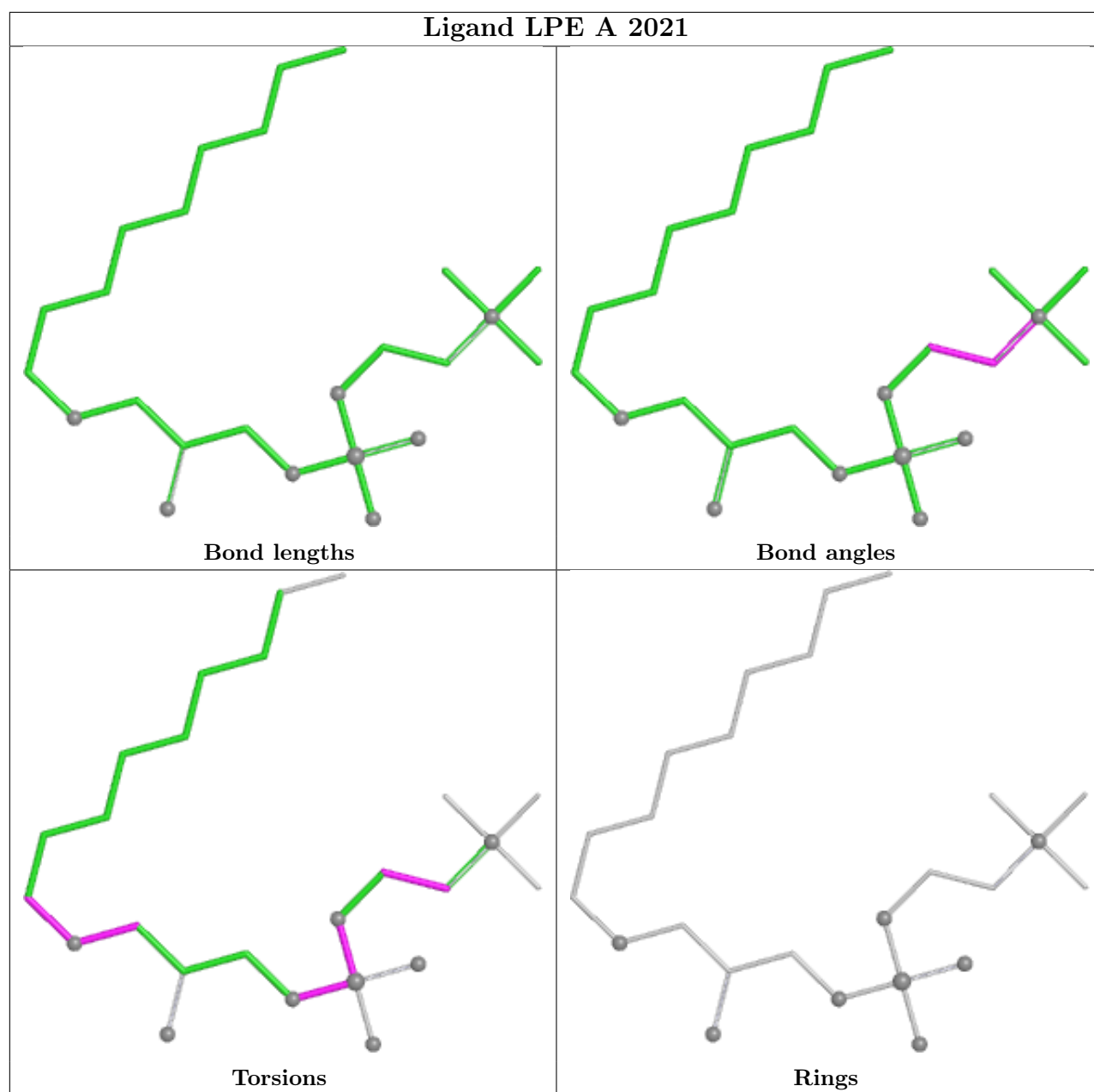




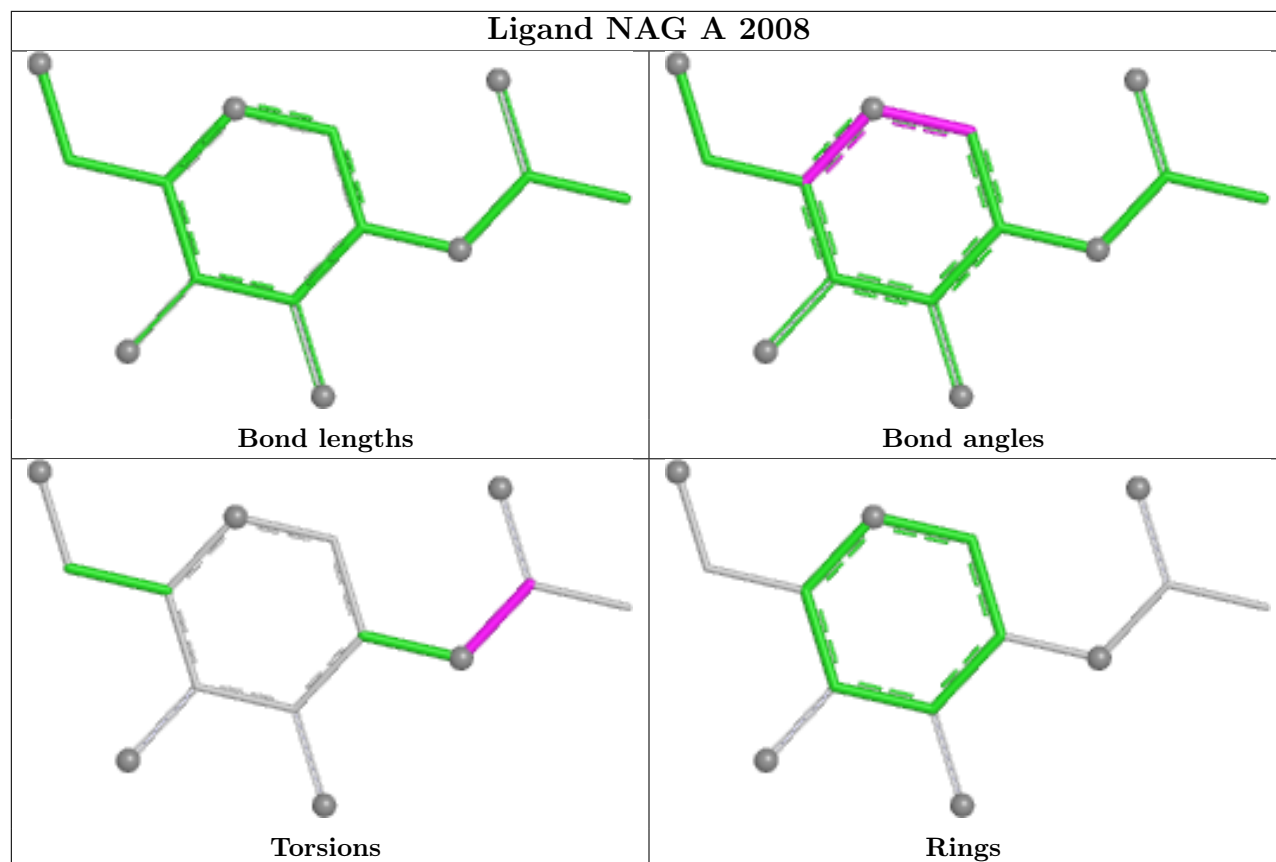




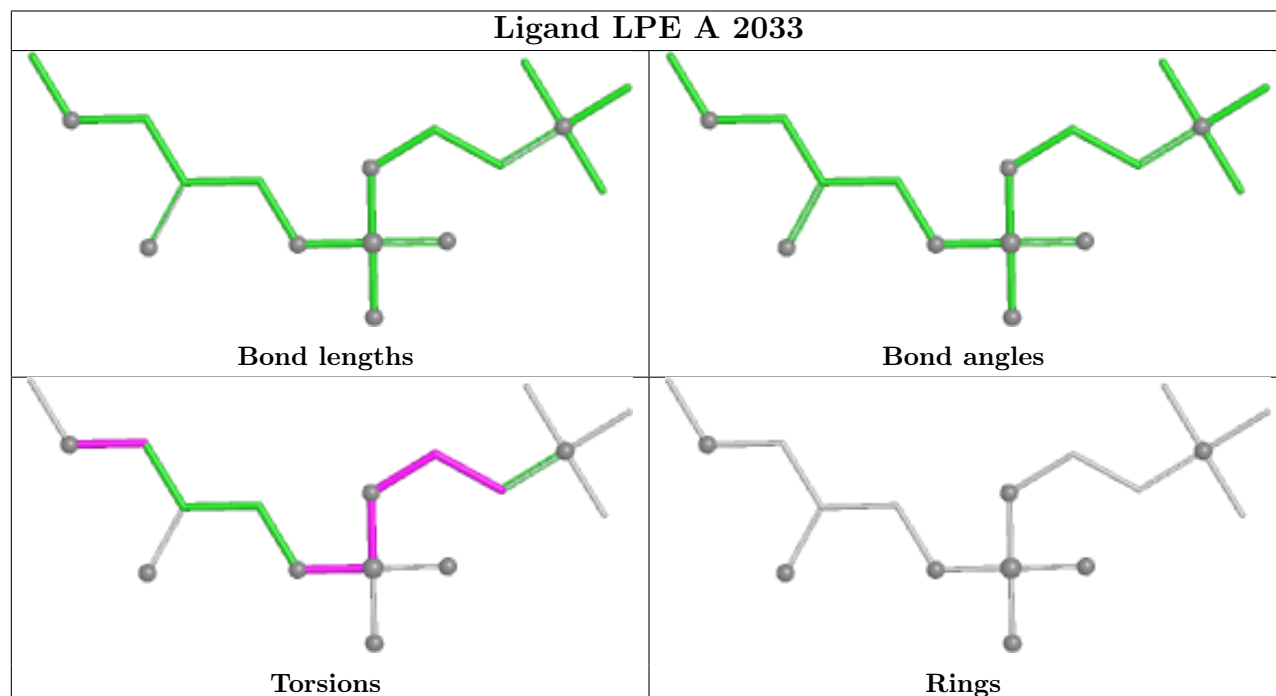


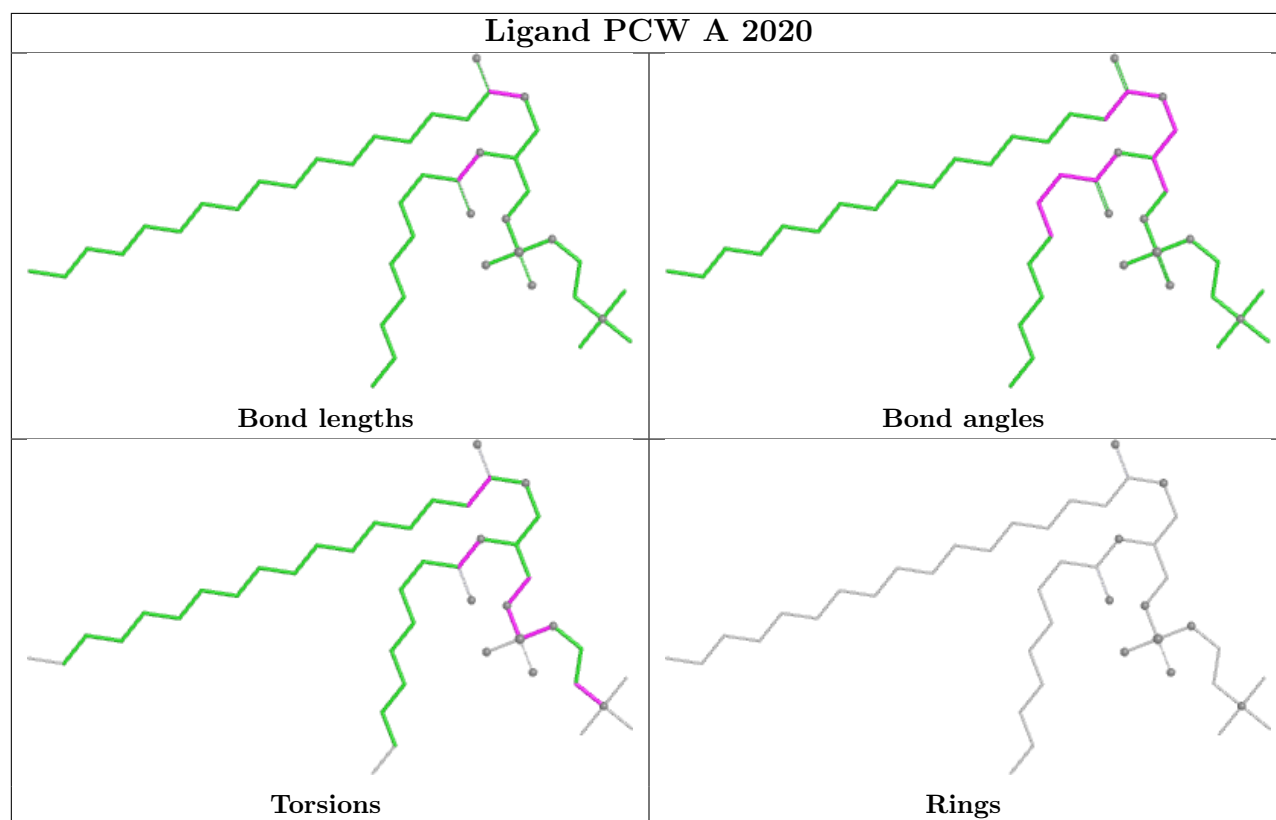
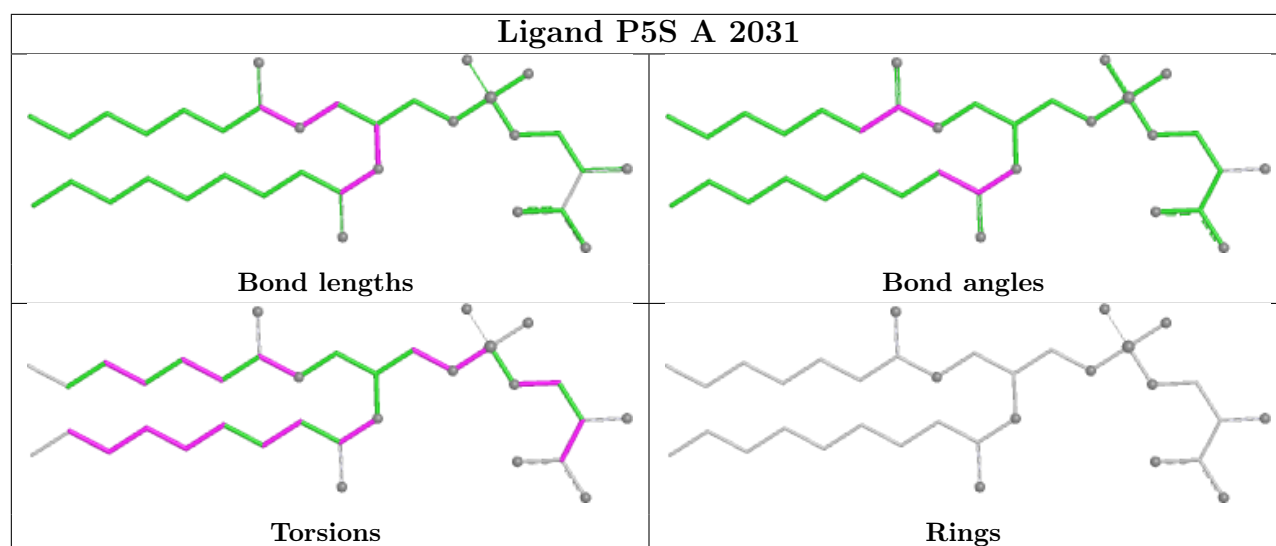


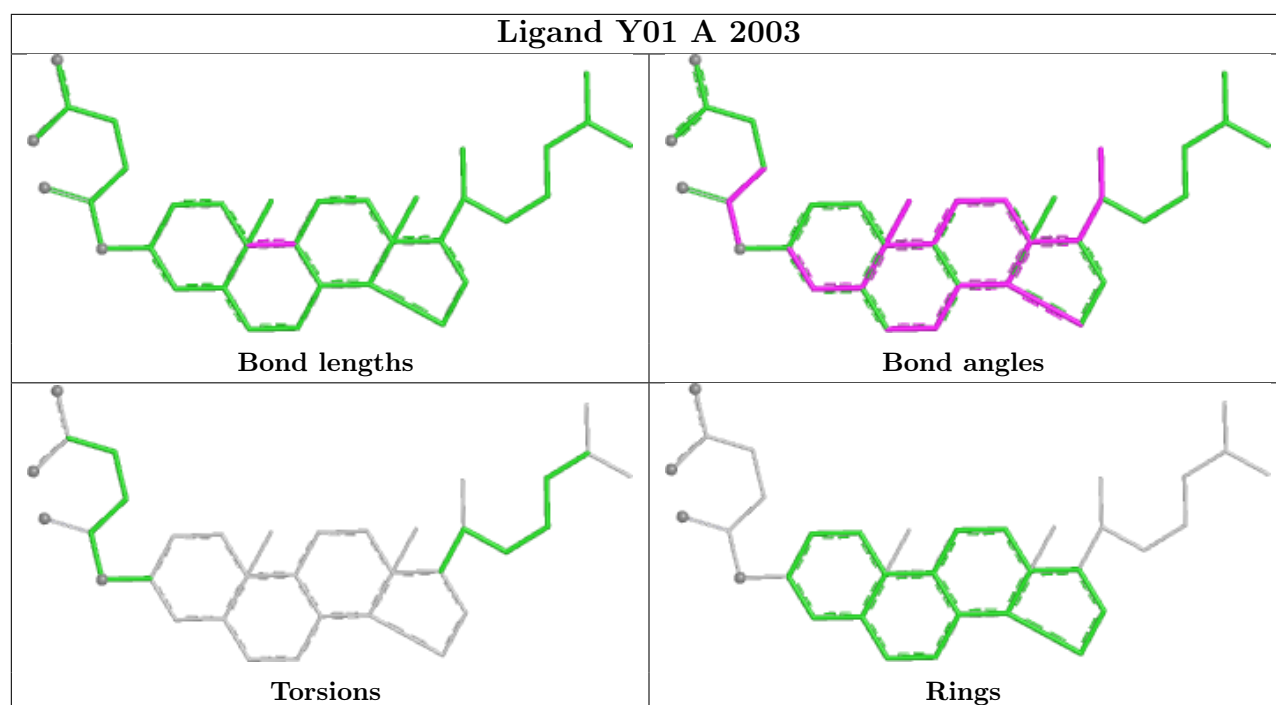
Ligand NAG A 2008

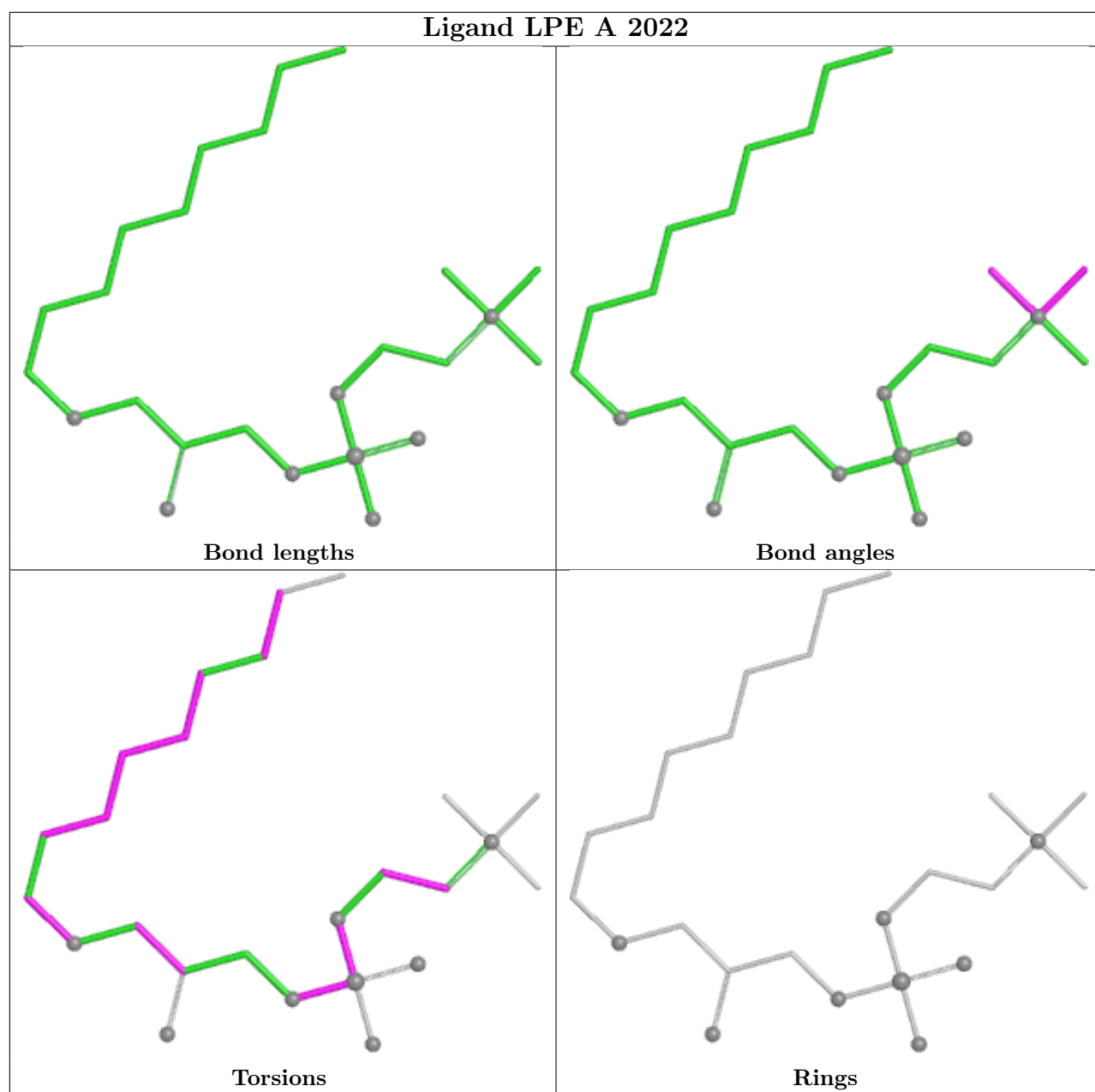


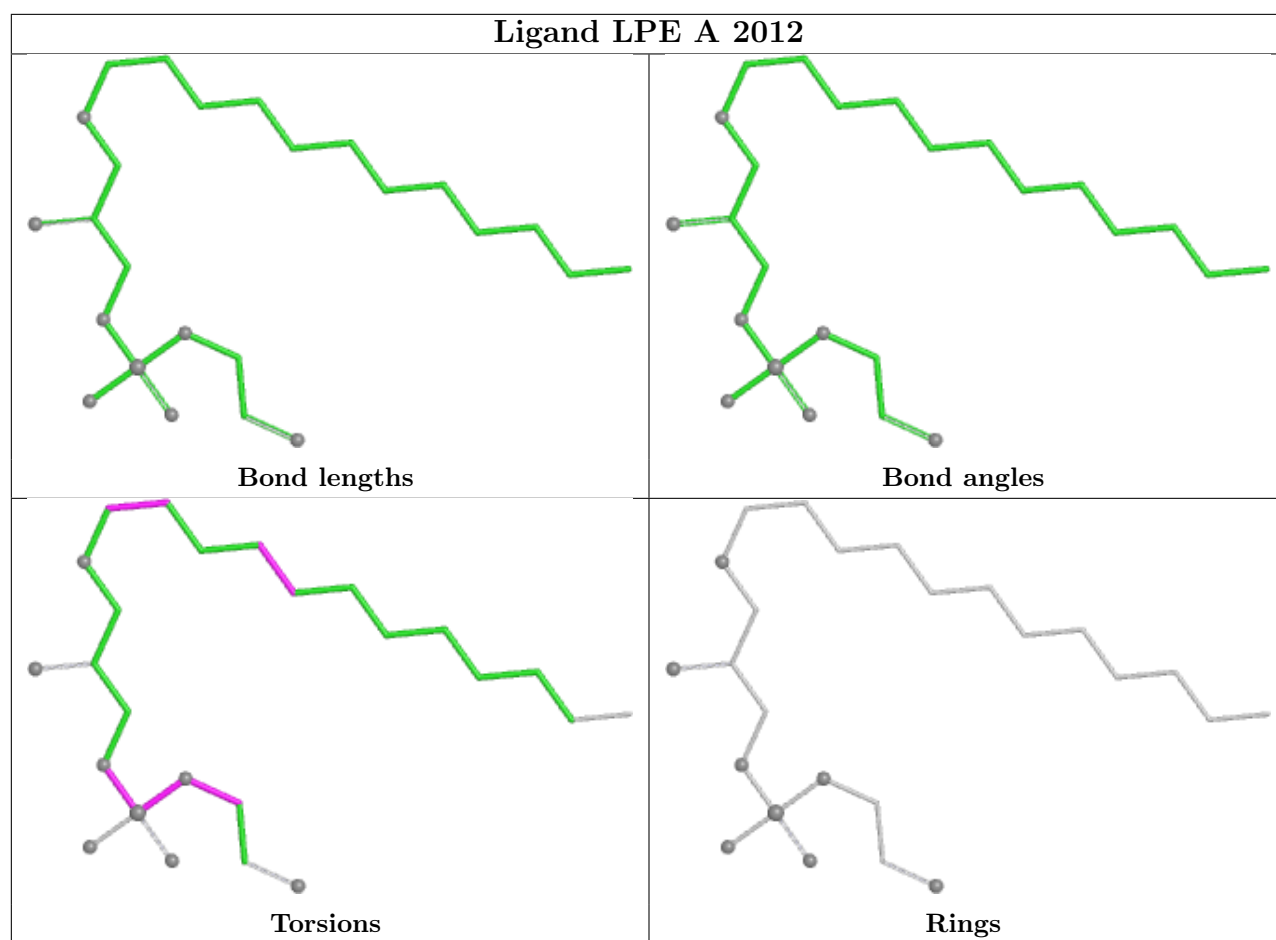
Ligand LPE A 2033

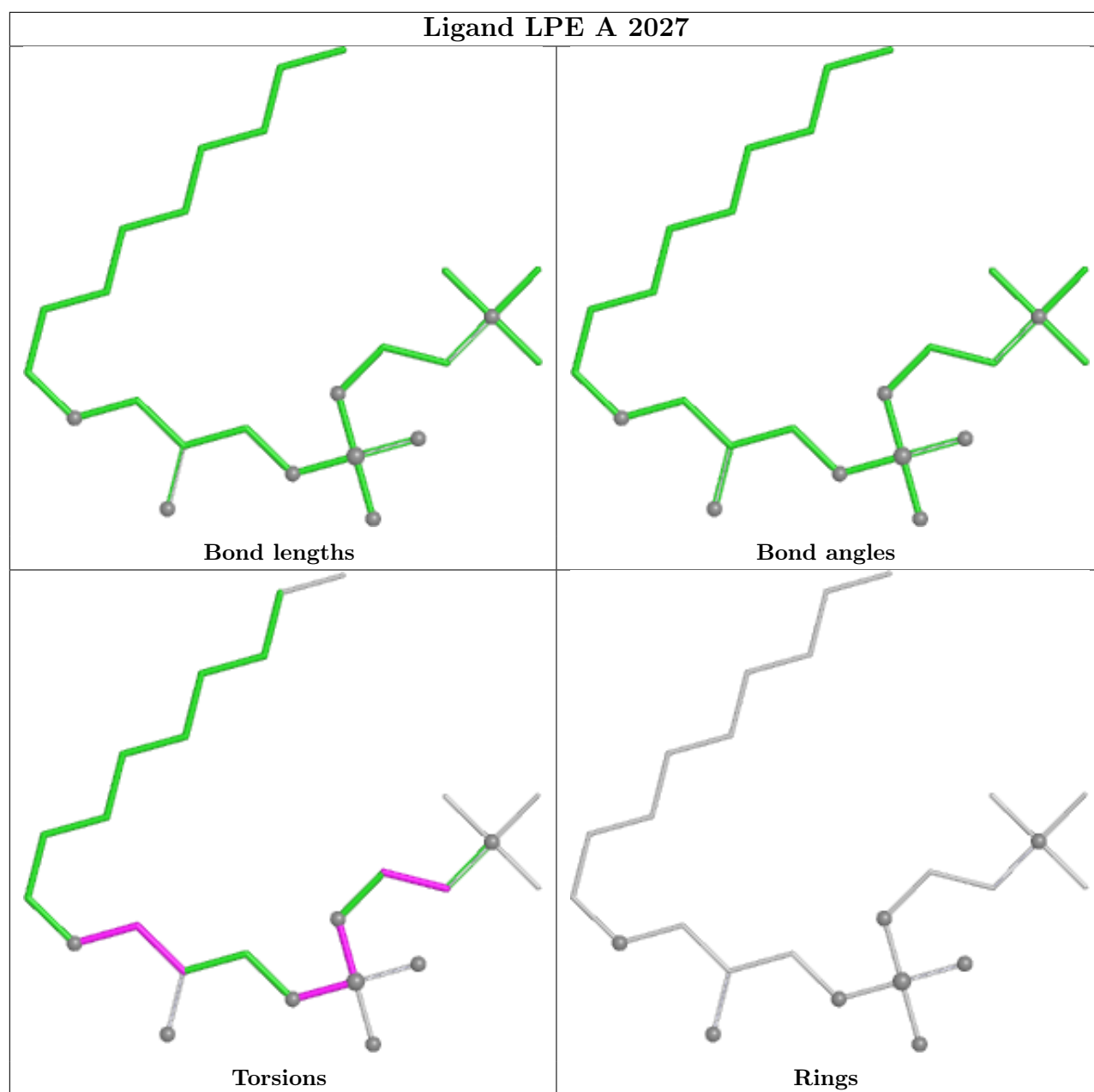


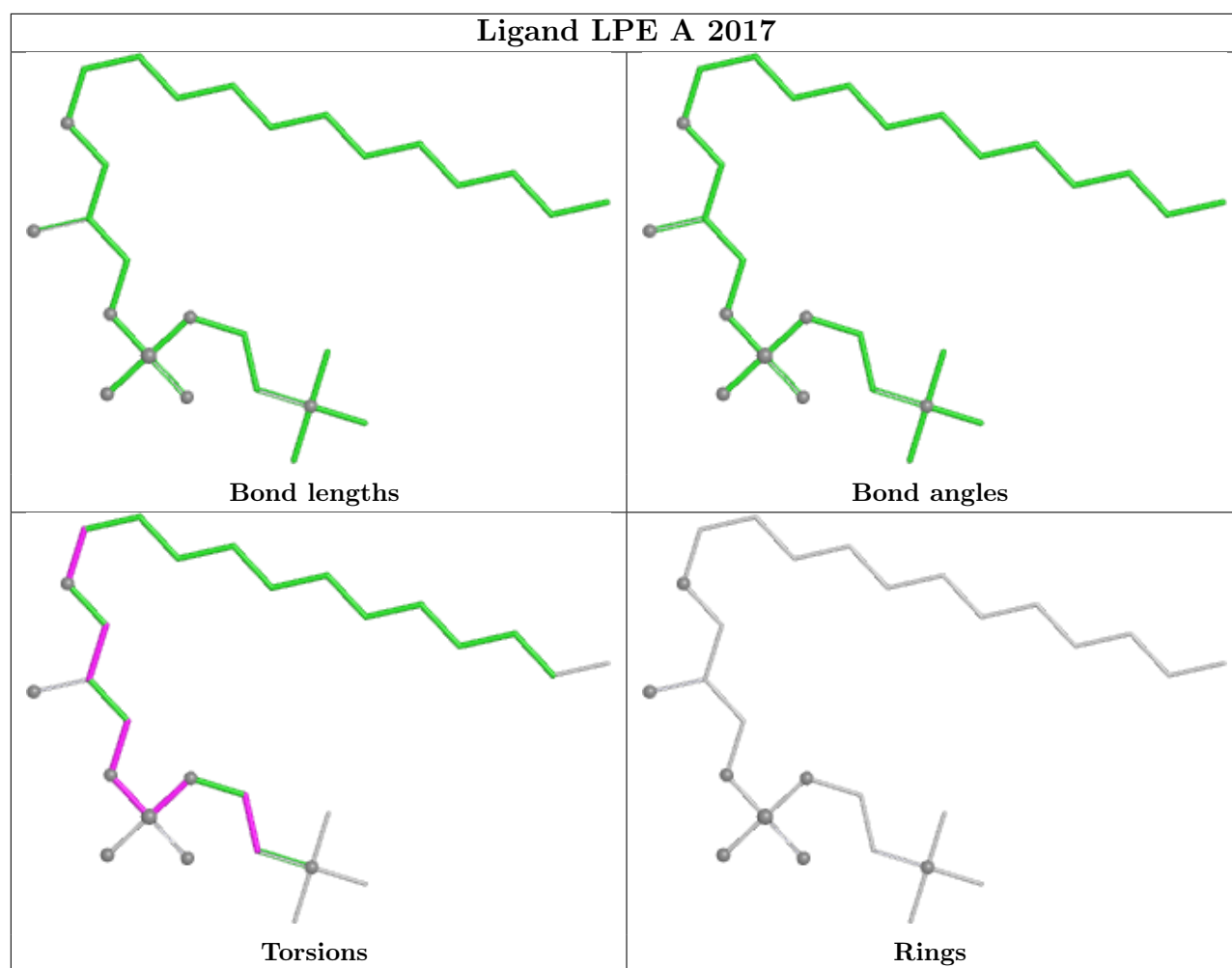


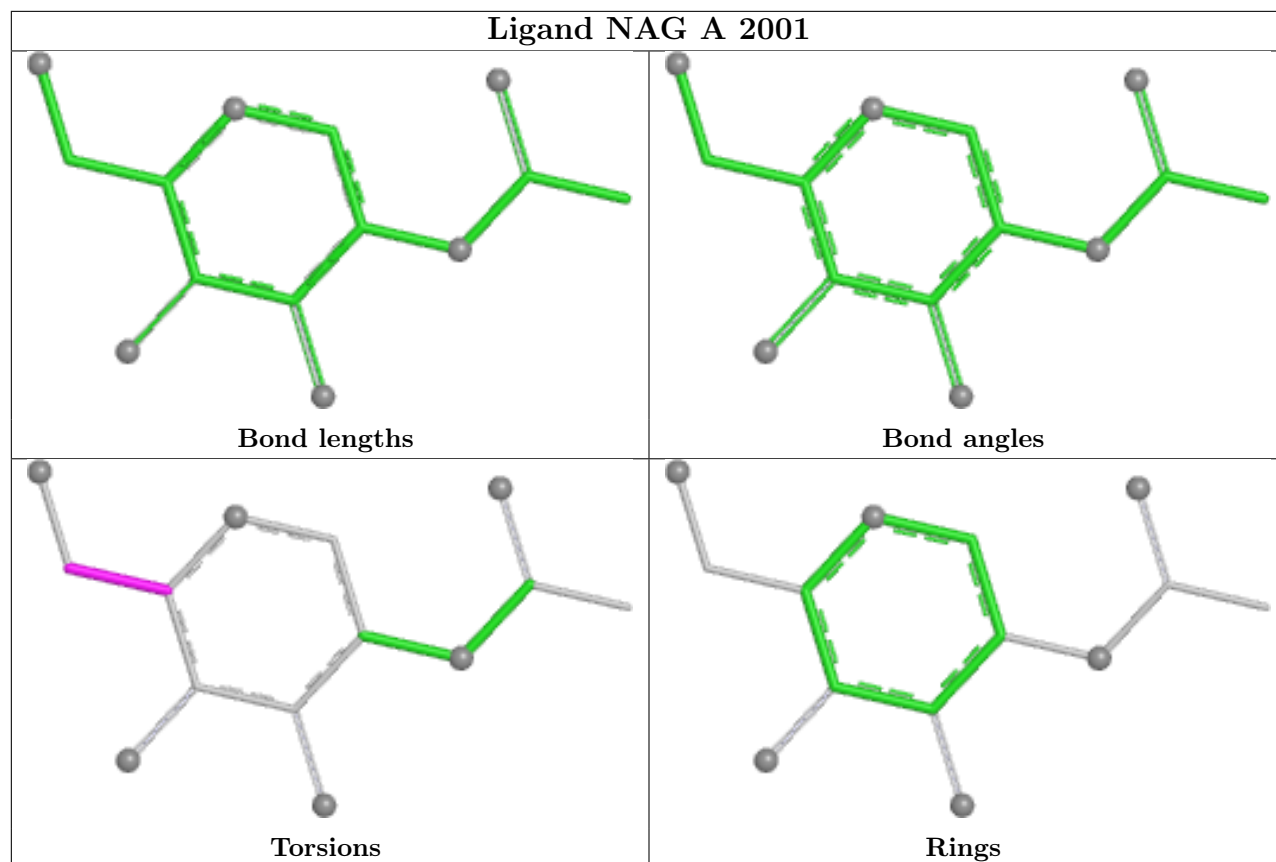


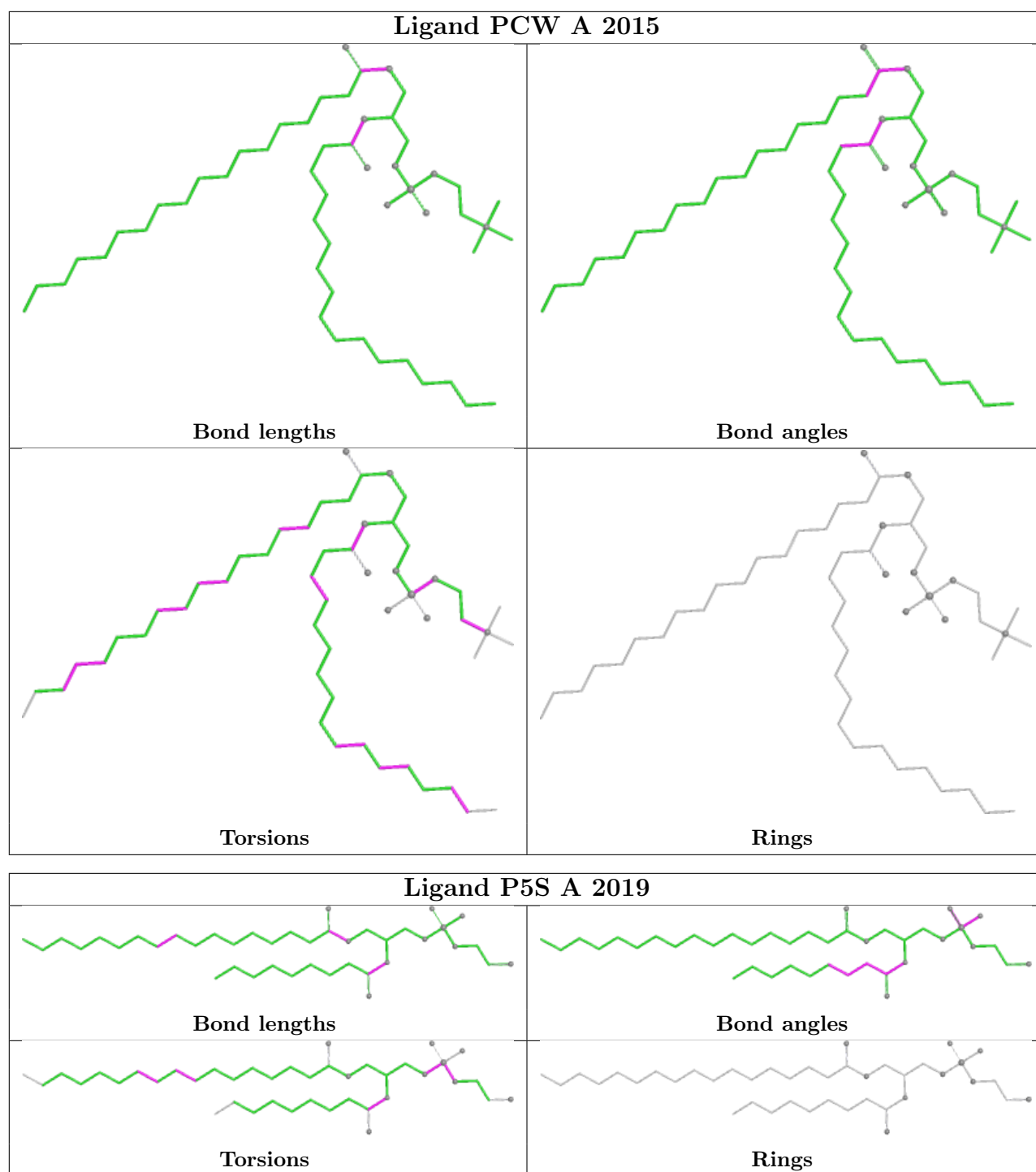


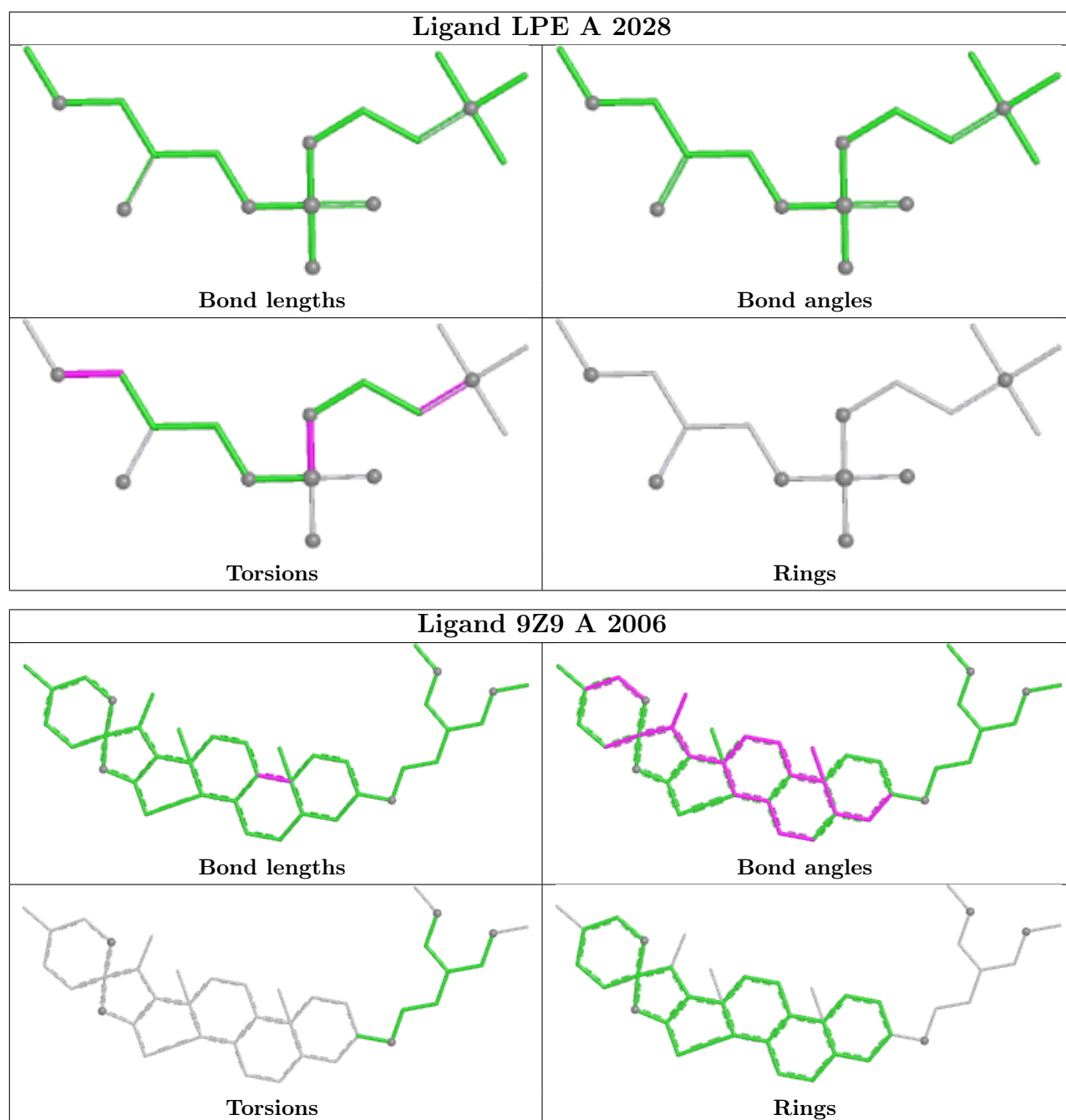


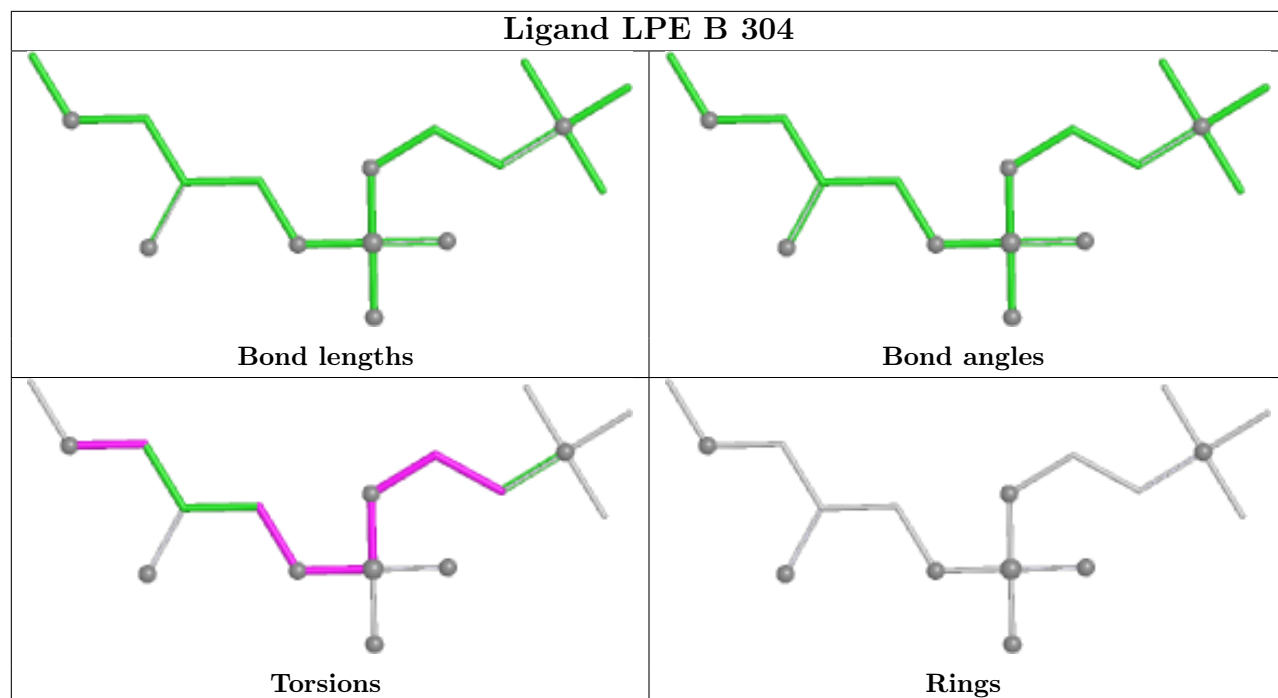


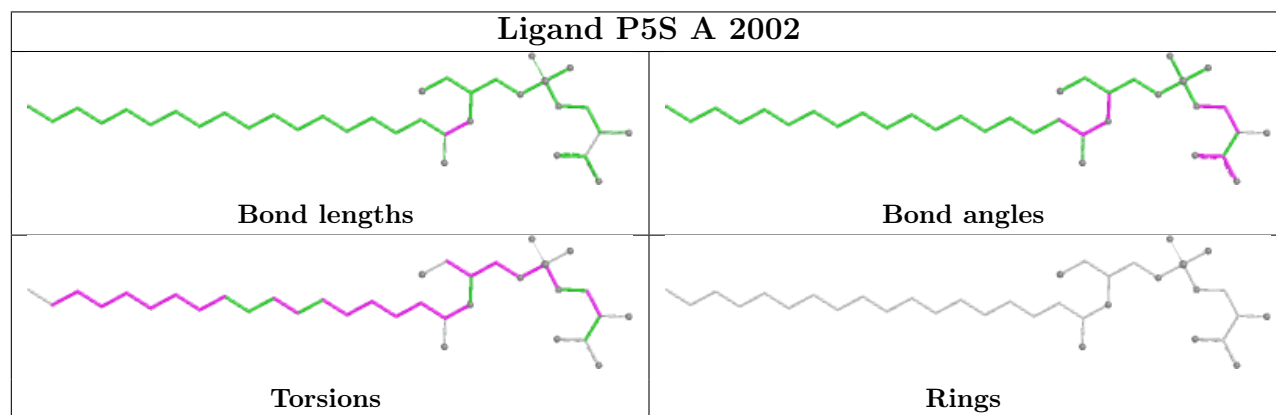
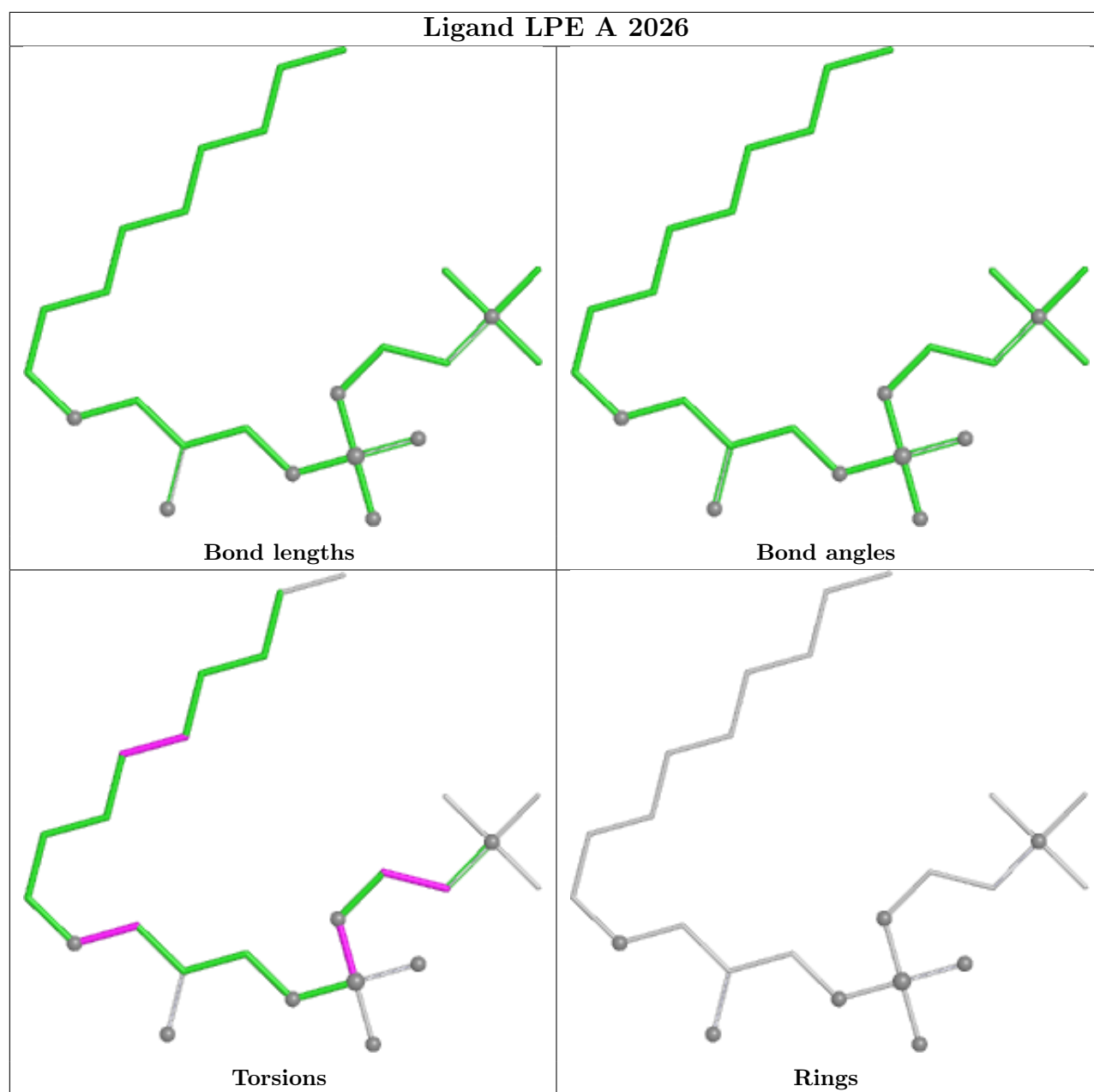












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

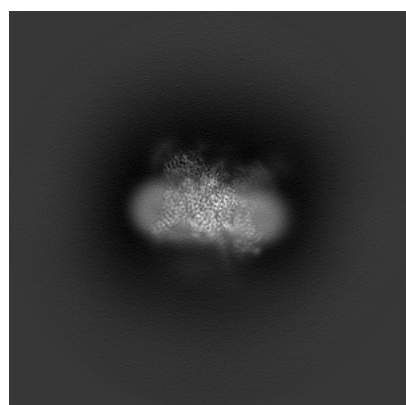
6 Map visualisation [i](#)

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.

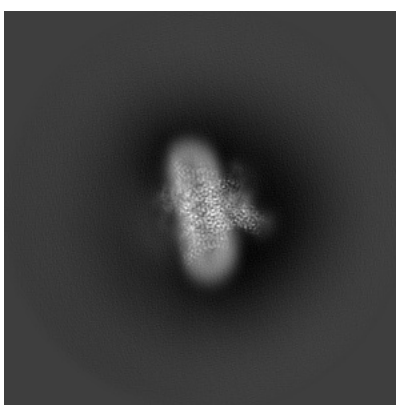
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

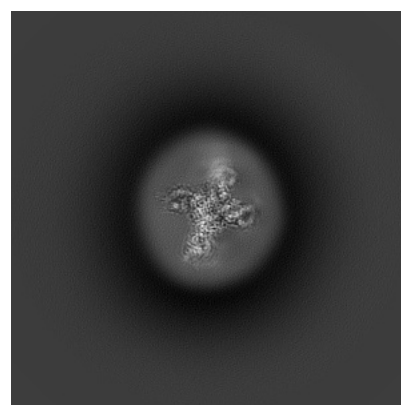
6.1.1 Primary map



X



Y

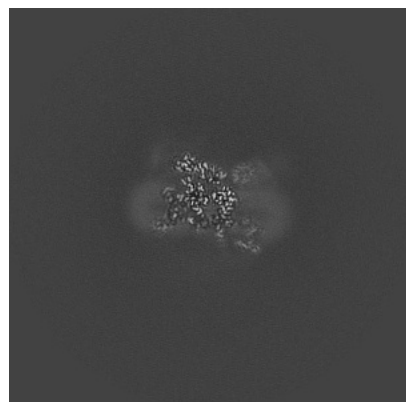


Z

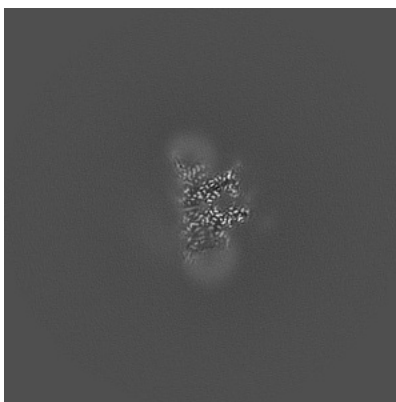
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

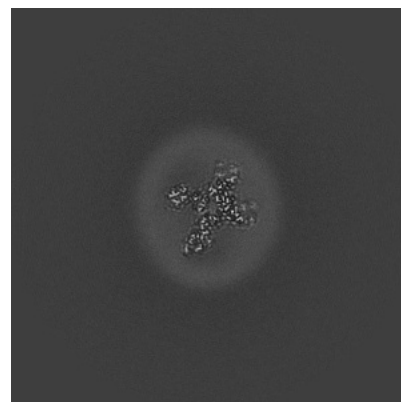
6.2.1 Primary map



X Index: 192



Y Index: 192

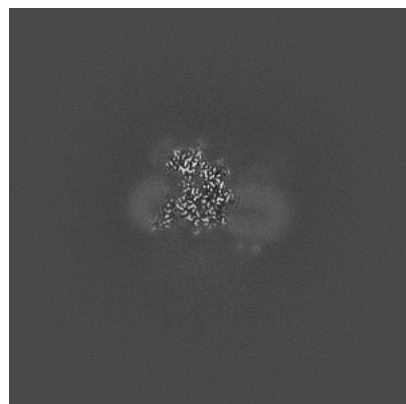


Z Index: 192

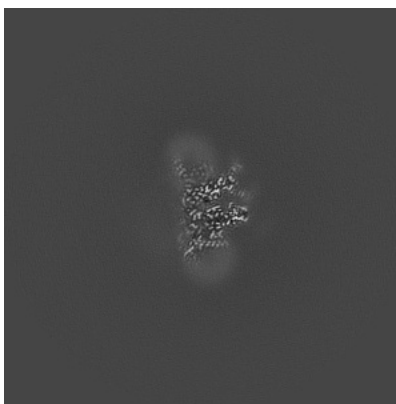
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

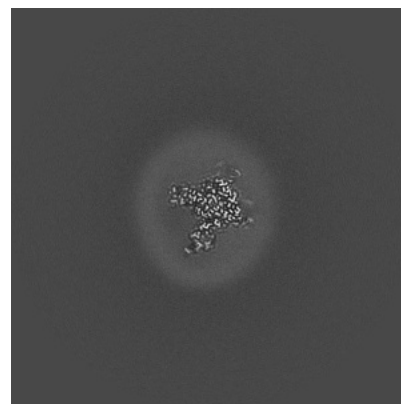
6.3.1 Primary map



X Index: 183



Y Index: 196

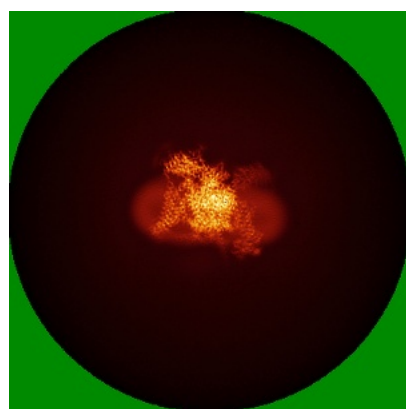


Z Index: 198

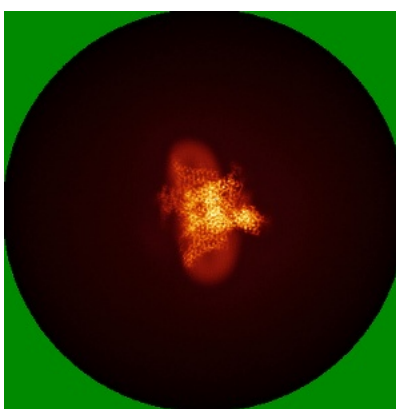
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X



Y

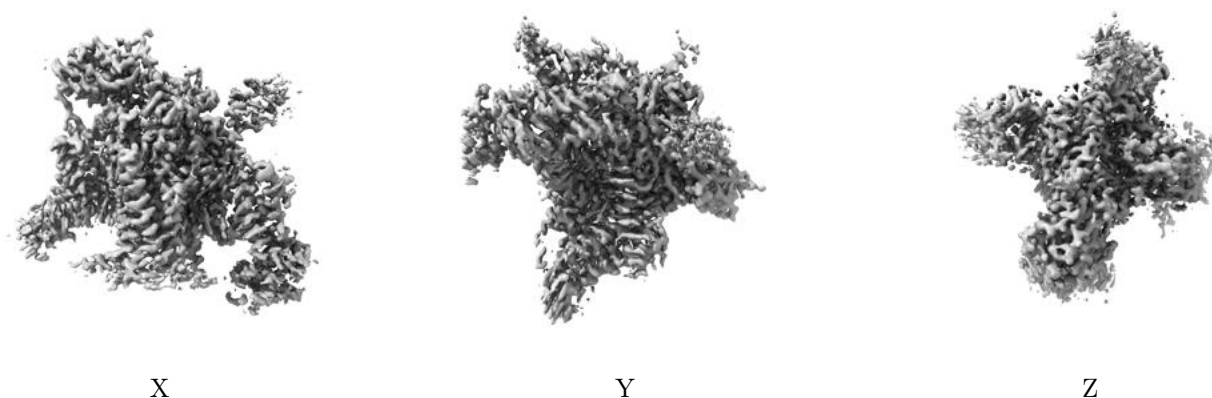


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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.

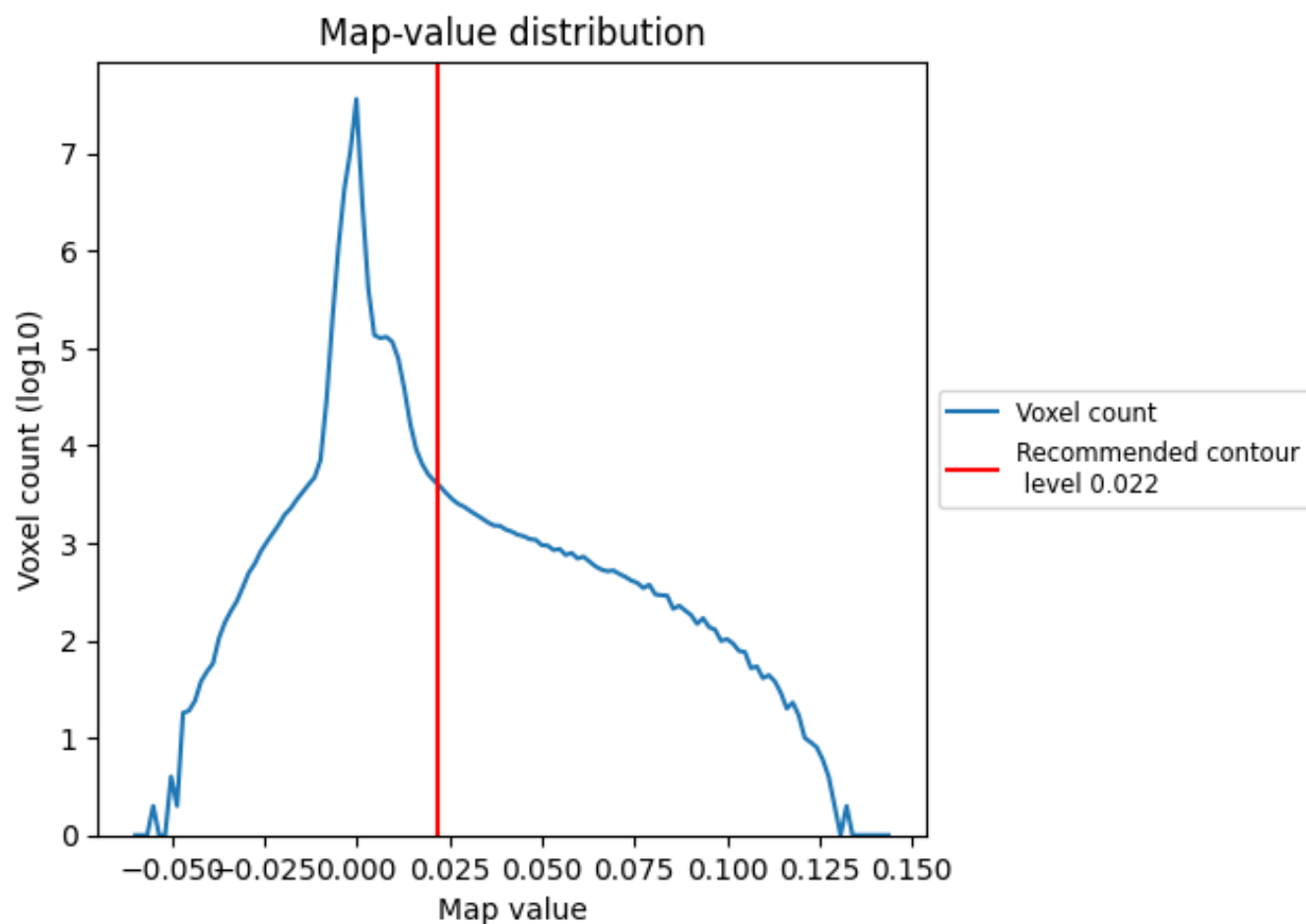
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

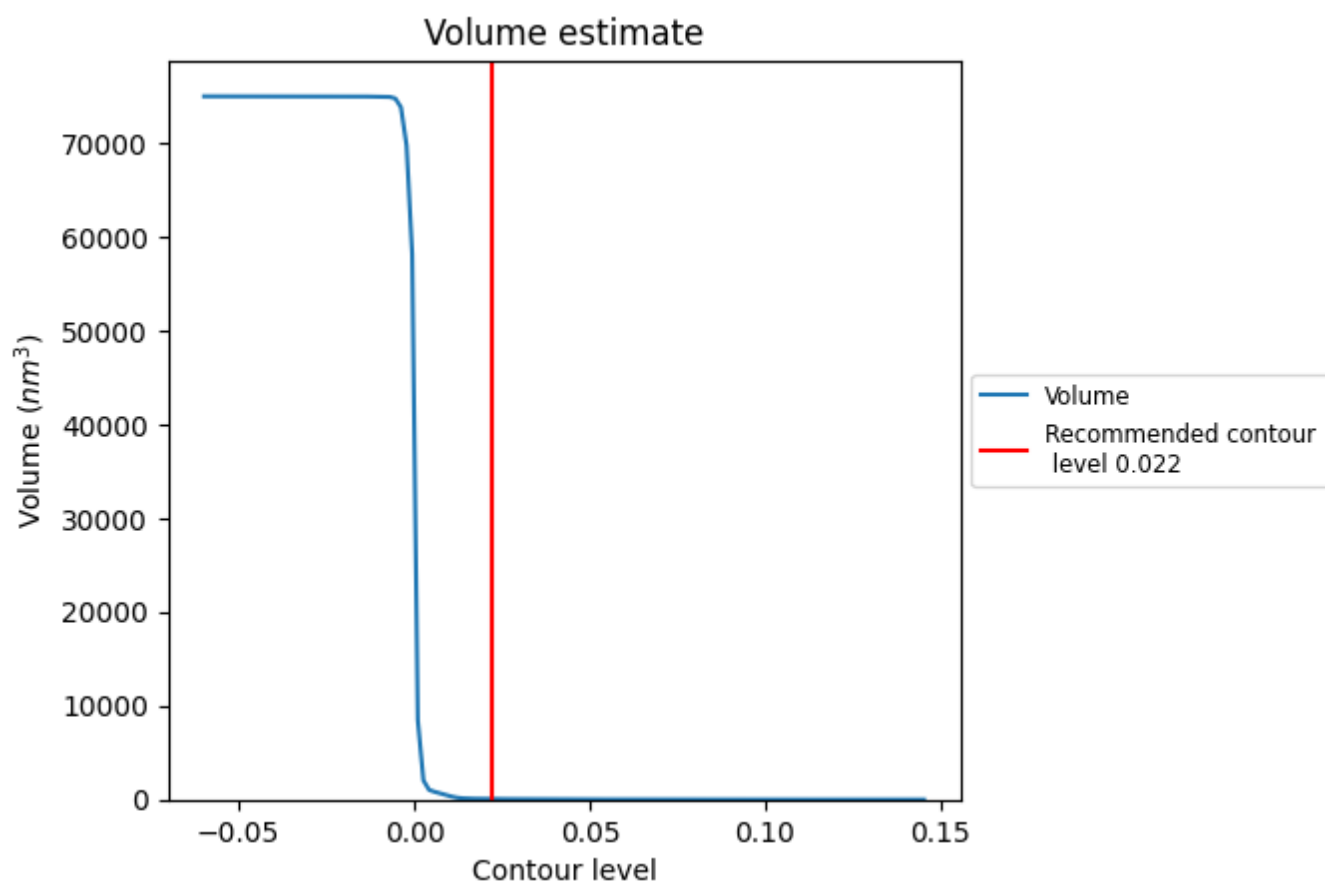
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

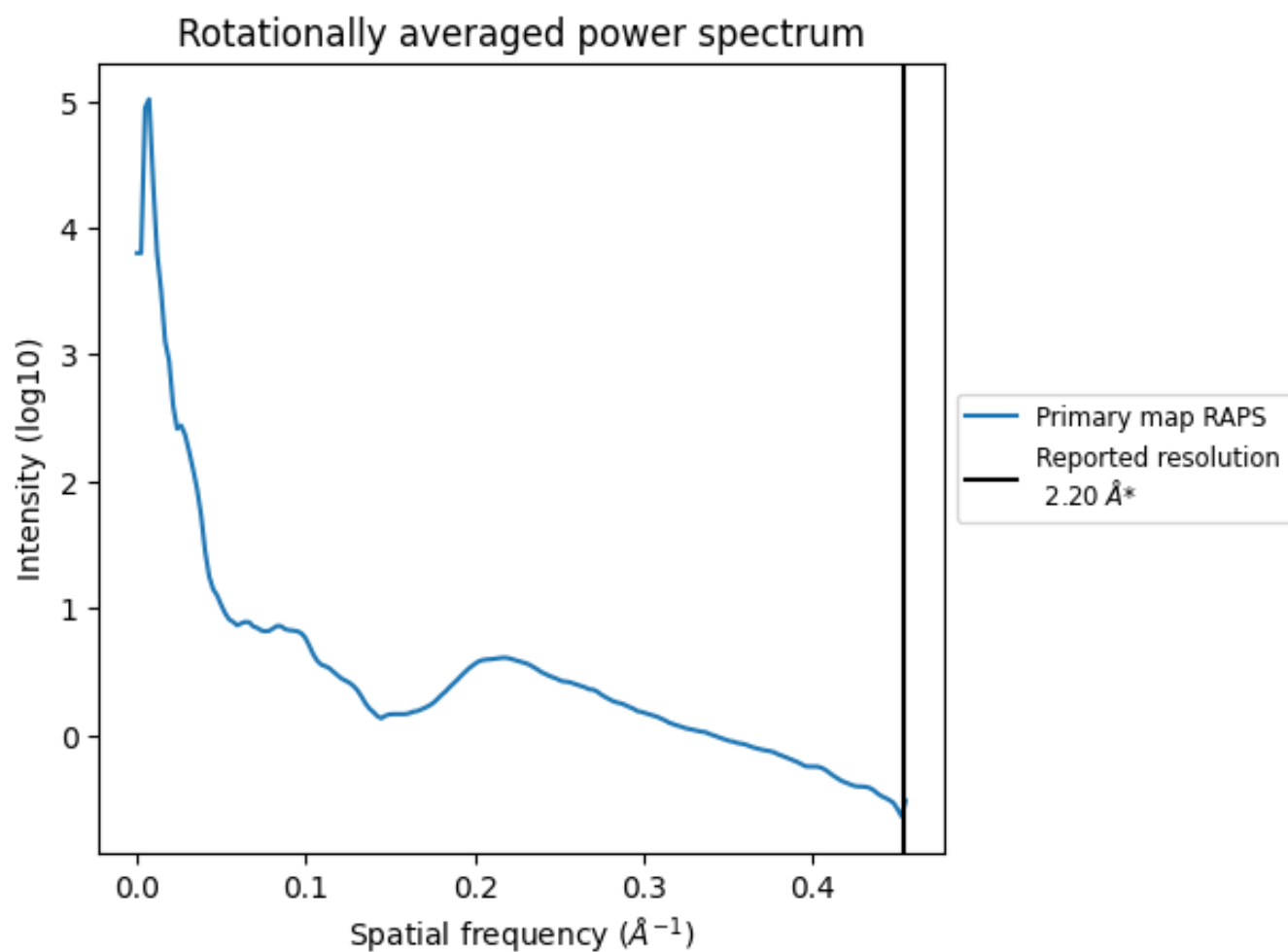
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 65 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.455 Å⁻¹

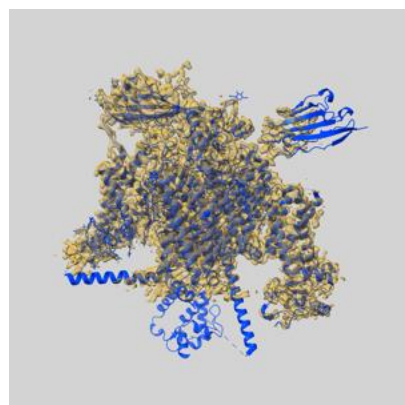
8 Fourier-Shell correlation ⓘ

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

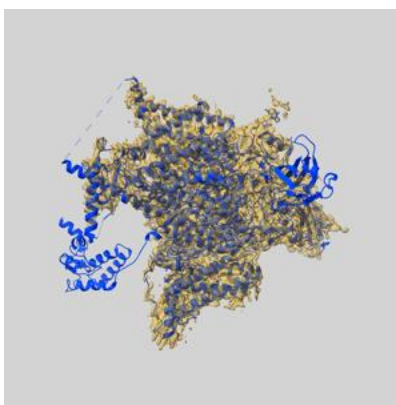
9 Map-model fit [i](#)

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 [12](#).

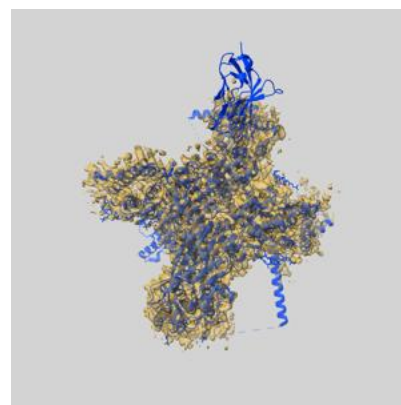
9.1 Map-model overlay [i](#)



X



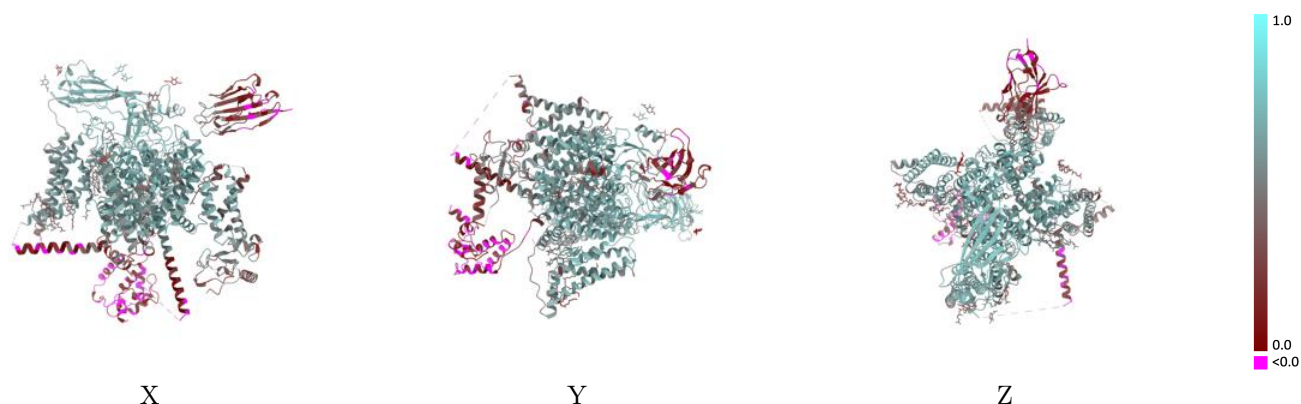
Y



Z

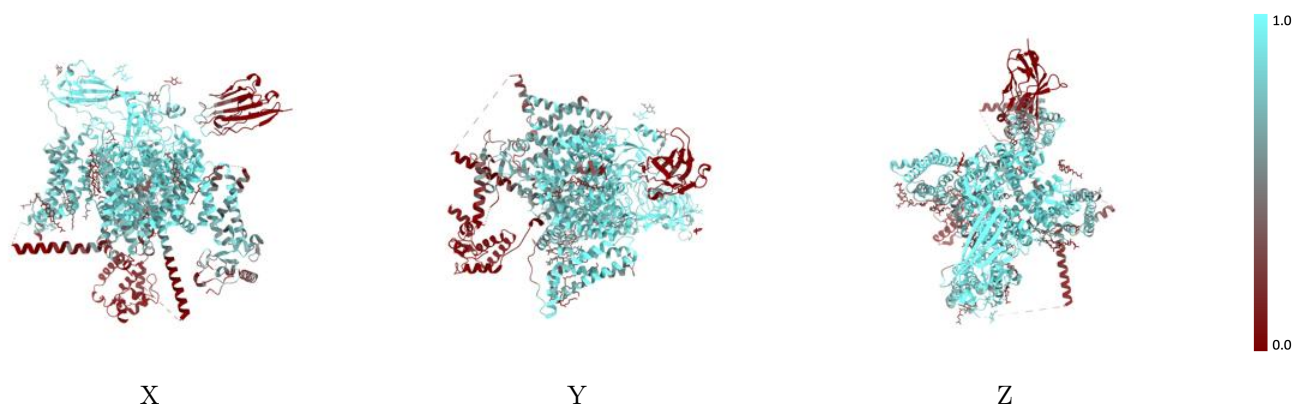
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



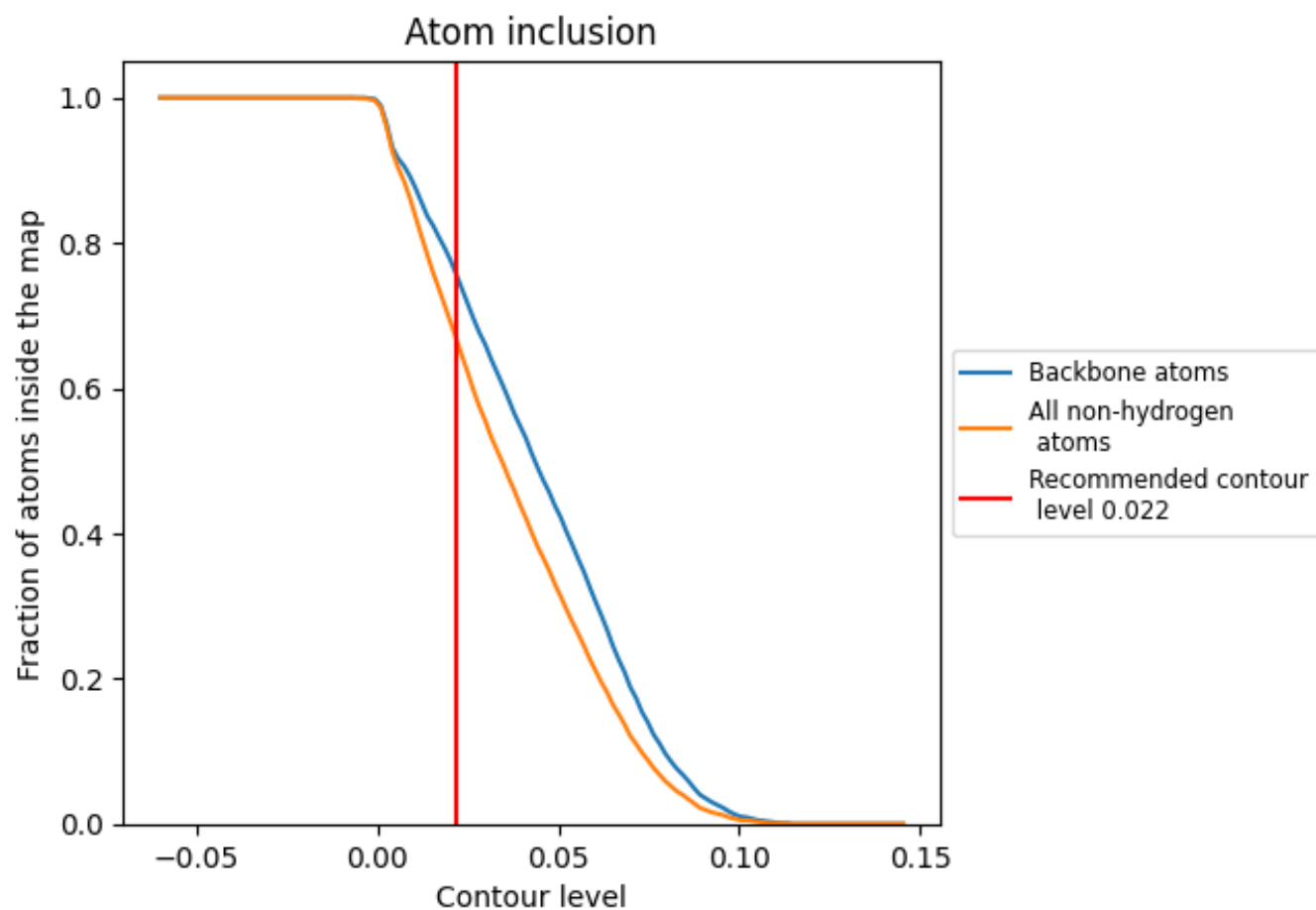
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	0.6840	0.5180
B	0.8590	0.6100
C	0.1440	0.2110
D	0.5000	0.4100
E	0.7140	0.4790
F	0.9290	0.6380

1.0

0.0

<0.0