



wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 03:50 pm GMT

PDB ID : 5LFB
EMDB ID : EMD-4046
Title : Structure of the bacterial sex F pilus (12.5 Angstrom rise)
Authors : Costa, T.R.D.; Ilangovan, I.; Ukleja, M.; Redzej, A.; Santini, J.M.; Smith, T.K.; Egelman, E.H.; Waksman, G.
Deposited on : 2016-06-30
Resolution : 5.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

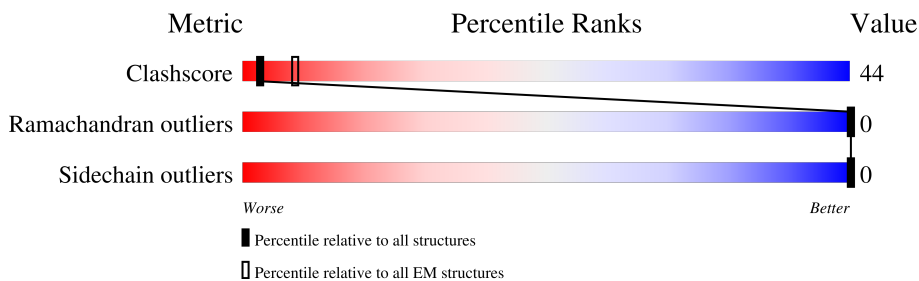
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

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 5.00 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 ≥ 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	1A	65	
1	1B	65	
1	1C	65	
1	1D	65	
1	1E	65	
1	1F	65	
1	1G	65	
1	1H	65	

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Mol	Chain	Length	Quality of chain	
1	1I	65	45%	54%
1	1J	65	40%	58%
1	1K	65	45%	54%
1	1L	65	38%	60%
1	1M	65	40%	58%
1	1N	65	46%	52%
1	1O	65	49%	49%
1	2A	65	48%	51%
1	2B	65	45%	54%
1	2C	65	34%	65%
1	2D	65	42%	57%
1	2E	65	40%	58%
1	2F	65	43%	55%
1	2G	65	40%	58%
1	2H	65	42%	57%
1	2I	65	43%	55%
1	2J	65	42%	57%
1	2K	65	43%	55%
1	2L	65	42%	57%
1	2M	65	46%	52%
1	2N	65	46%	52%
1	2O	65	51%	48%
1	3A	65	51%	48%
1	3B	65	46%	52%
1	3C	65	37%	62%

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Mol	Chain	Length	Quality of chain
1	3D	65	5% 43% 55%
1	3E	65	6% 40% 58%
1	3F	65	4% 40% 58%
1	3G	65	8% 40% 58%
1	3H	65	8% 40% 58%
1	3I	65	12% 45% 54%
1	3J	65	12% 40% 58%
1	3K	65	9% 42% 57%
1	3L	65	17% 42% 57%
1	3M	65	15% 45% 54%
1	3N	65	12% 46% 52%
1	3O	65	14% 49% 49%
1	4A	65	9% 48% 51%
1	4B	65	1% 43% 55%
1	4C	65	1% 37% 62%
1	4D	65	5% 45% 54%
1	4E	65	5% 40% 58%
1	4F	65	8% 42% 57%
1	4G	65	6% 40% 58%
1	4H	65	8% 45% 54%
1	4I	65	11% 43% 55%
1	4J	65	15% 38% 60%
1	4K	65	15% 42% 57%
1	4L	65	22% 42% 57%
1	4M	65	20% 46% 52%

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Mol	Chain	Length	Quality of chain	
1	4N	65	17%	45% 54%
1	4O	65	15%	51% 48%
1	5A	65	11%	48% 51%
1	5B	65	6%	42% 57%
1	5C	65	•	37% 62%
1	5D	65	•	43% 55%
1	5E	65	5%	43% 55%
1	5F	65	5%	43% 55%
1	5G	65	6%	42% 57%
1	5H	65	9%	43% 55%
1	5I	65	12%	43% 55%
1	5J	65	14%	42% 57%
1	5K	65	14%	46% 52%
1	5L	65	18%	43% 55%
1	5M	65	18%	48% 51%
1	5N	65	18%	48% 51%
1	5O	65	17%	46% 52%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 36600 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 Pilin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1A	65	476	314	74	83	5	0	0
1	1B	65	476	314	74	83	5	0	0
1	1C	65	476	314	74	83	5	0	0
1	1D	65	476	314	74	83	5	0	0
1	1E	65	476	314	74	83	5	0	0
1	1F	65	476	314	74	83	5	0	0
1	1G	65	476	314	74	83	5	0	0
1	1H	65	476	314	74	83	5	0	0
1	1I	65	476	314	74	83	5	0	0
1	1J	65	476	314	74	83	5	0	0
1	1K	65	476	314	74	83	5	0	0
1	1L	65	476	314	74	83	5	0	0
1	1M	65	476	314	74	83	5	0	0
1	1N	65	476	314	74	83	5	0	0
1	1O	65	476	314	74	83	5	0	0
1	2A	65	476	314	74	83	5	0	0
1	2B	65	476	314	74	83	5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	2C	65	476	314	74	83	5	0	0
1	2D	65	476	314	74	83	5	0	0
1	2E	65	476	314	74	83	5	0	0
1	2F	65	476	314	74	83	5	0	0
1	2G	65	476	314	74	83	5	0	0
1	2H	65	476	314	74	83	5	0	0
1	2I	65	476	314	74	83	5	0	0
1	2J	65	476	314	74	83	5	0	0
1	2K	65	476	314	74	83	5	0	0
1	2L	65	476	314	74	83	5	0	0
1	2M	65	476	314	74	83	5	0	0
1	2N	65	476	314	74	83	5	0	0
1	2O	65	476	314	74	83	5	0	0
1	3A	65	476	314	74	83	5	0	0
1	3B	65	476	314	74	83	5	0	0
1	3C	65	476	314	74	83	5	0	0
1	3D	65	476	314	74	83	5	0	0
1	3E	65	476	314	74	83	5	0	0
1	3F	65	476	314	74	83	5	0	0
1	3G	65	476	314	74	83	5	0	0
1	3H	65	476	314	74	83	5	0	0

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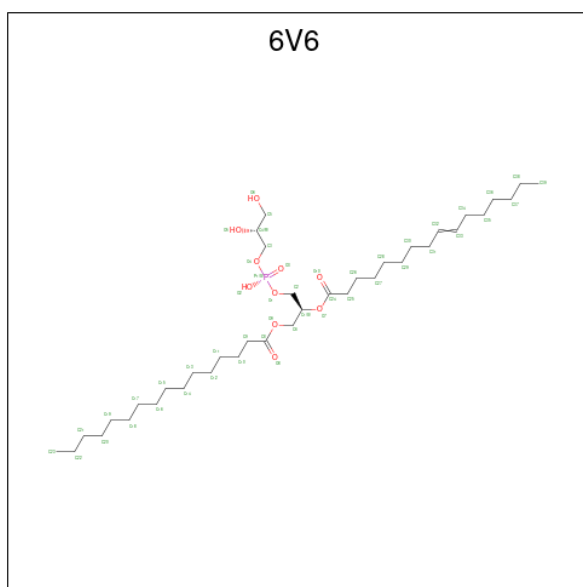
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	3I	65	476	314	74	83	5	0	0
1	3J	65	476	314	74	83	5	0	0
1	3K	65	476	314	74	83	5	0	0
1	3L	65	476	314	74	83	5	0	0
1	3M	65	476	314	74	83	5	0	0
1	3N	65	476	314	74	83	5	0	0
1	3O	65	476	314	74	83	5	0	0
1	4A	65	476	314	74	83	5	0	0
1	4B	65	476	314	74	83	5	0	0
1	4C	65	476	314	74	83	5	0	0
1	4D	65	476	314	74	83	5	0	0
1	4E	65	476	314	74	83	5	0	0
1	4F	65	476	314	74	83	5	0	0
1	4G	65	476	314	74	83	5	0	0
1	4H	65	476	314	74	83	5	0	0
1	4I	65	476	314	74	83	5	0	0
1	4J	65	476	314	74	83	5	0	0
1	4K	65	476	314	74	83	5	0	0
1	4L	65	476	314	74	83	5	0	0
1	4M	65	476	314	74	83	5	0	0
1	4N	65	476	314	74	83	5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	4O	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	5A	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	5B	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	5C	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	5D	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	5E	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	5F	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	5G	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	5H	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	5I	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	5J	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	5K	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	5L	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	5M	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	5N	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	5O	65	Total	C	N	O	S	0	0
			476	314	74	83	5		

- Molecule 2 is [(2 {S})-3-[(2 {R})-2,3-bis(oxidanyl)propoxy]-oxidanyl-phosphoryl]oxy-2-hexadec-9-enoyloxy-propyl] hexadecanoate (three-letter code: 6V6) (formula: C₃₈H₇₃O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
2	1A	1	12	5	6	1	0
2	1B	1	12	5	6	1	0
2	1C	1	12	5	6	1	0
2	1D	1	12	5	6	1	0
2	1E	1	12	5	6	1	0
2	1F	1	12	5	6	1	0
2	1G	1	12	5	6	1	0
2	1H	1	12	5	6	1	0
2	1I	1	12	5	6	1	0
2	1J	1	12	5	6	1	0
2	1K	1	12	5	6	1	0
2	1L	1	12	5	6	1	0
2	1M	1	12	5	6	1	0
2	1N	1	12	5	6	1	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
2	1O	1	12	5	6	1	0
2	2A	1	12	5	6	1	0
2	2B	1	12	5	6	1	0
2	2C	1	12	5	6	1	0
2	2D	1	12	5	6	1	0
2	2E	1	12	5	6	1	0
2	2F	1	12	5	6	1	0
2	2G	1	12	5	6	1	0
2	2H	1	12	5	6	1	0
2	2I	1	12	5	6	1	0
2	2J	1	12	5	6	1	0
2	2K	1	12	5	6	1	0
2	2L	1	12	5	6	1	0
2	2M	1	12	5	6	1	0
2	2N	1	12	5	6	1	0
2	2O	1	12	5	6	1	0
2	3A	1	12	5	6	1	0
2	3B	1	12	5	6	1	0
2	3C	1	12	5	6	1	0
2	3D	1	12	5	6	1	0
2	3E	1	12	5	6	1	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
2	3F	1	12	5	6	1	0
2	3G	1	12	5	6	1	0
2	3H	1	12	5	6	1	0
2	3I	1	12	5	6	1	0
2	3J	1	12	5	6	1	0
2	3K	1	12	5	6	1	0
2	3L	1	12	5	6	1	0
2	3M	1	12	5	6	1	0
2	3N	1	12	5	6	1	0
2	3O	1	12	5	6	1	0
2	4A	1	12	5	6	1	0
2	4B	1	12	5	6	1	0
2	4C	1	12	5	6	1	0
2	4D	1	12	5	6	1	0
2	4E	1	12	5	6	1	0
2	4F	1	12	5	6	1	0
2	4G	1	12	5	6	1	0
2	4H	1	12	5	6	1	0
2	4I	1	12	5	6	1	0
2	4J	1	12	5	6	1	0
2	4K	1	12	5	6	1	0

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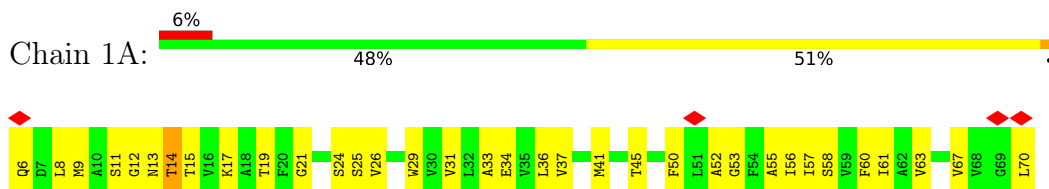
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
2	4L	1	Total 12	C 5	O 6	P 1	0
2	4M	1	Total 12	C 5	O 6	P 1	0
2	4N	1	Total 12	C 5	O 6	P 1	0
2	4O	1	Total 12	C 5	O 6	P 1	0
2	5A	1	Total 12	C 5	O 6	P 1	0
2	5B	1	Total 12	C 5	O 6	P 1	0
2	5C	1	Total 12	C 5	O 6	P 1	0
2	5D	1	Total 12	C 5	O 6	P 1	0
2	5E	1	Total 12	C 5	O 6	P 1	0
2	5F	1	Total 12	C 5	O 6	P 1	0
2	5G	1	Total 12	C 5	O 6	P 1	0
2	5H	1	Total 12	C 5	O 6	P 1	0
2	5I	1	Total 12	C 5	O 6	P 1	0
2	5J	1	Total 12	C 5	O 6	P 1	0
2	5K	1	Total 12	C 5	O 6	P 1	0
2	5L	1	Total 12	C 5	O 6	P 1	0
2	5M	1	Total 12	C 5	O 6	P 1	0
2	5N	1	Total 12	C 5	O 6	P 1	0
2	5O	1	Total 12	C 5	O 6	P 1	0

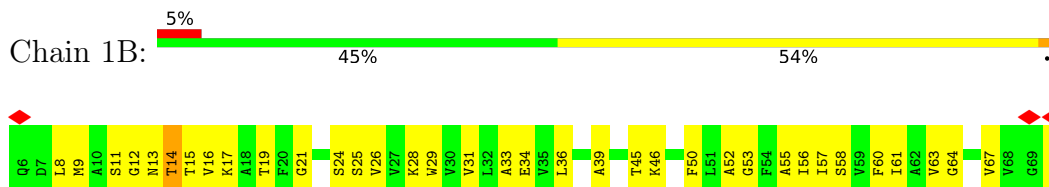
3 Residue-property plots [i](#)

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.

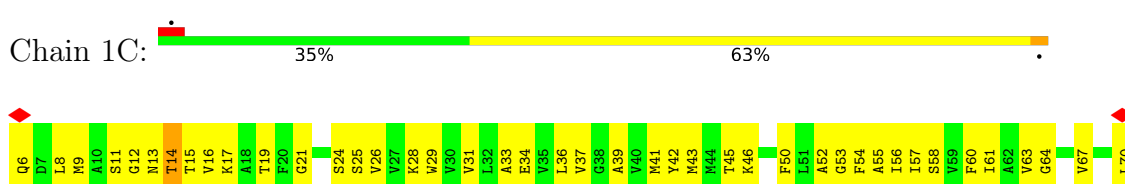
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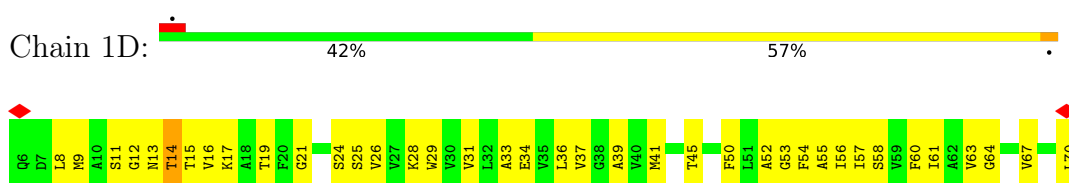
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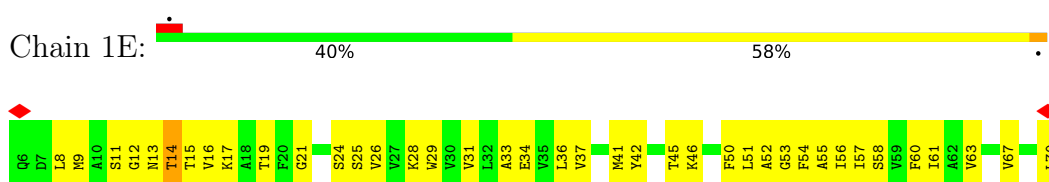
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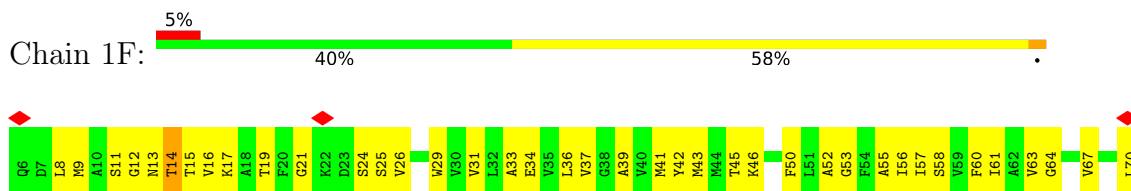
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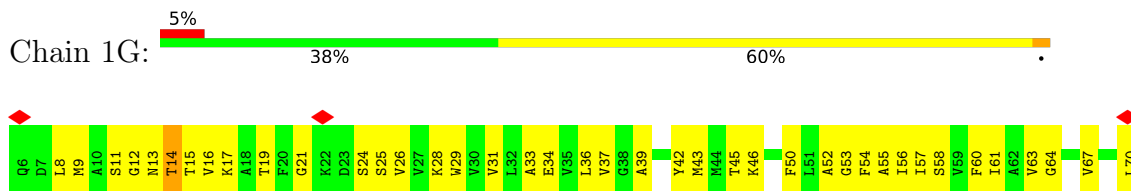
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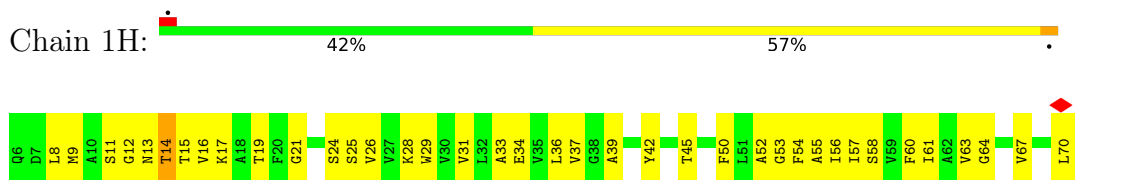
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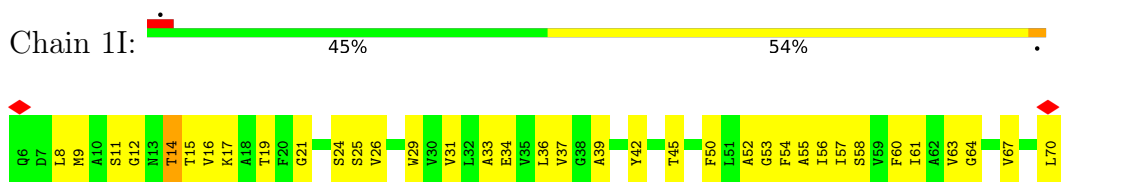
• Molecule 1: Pilin



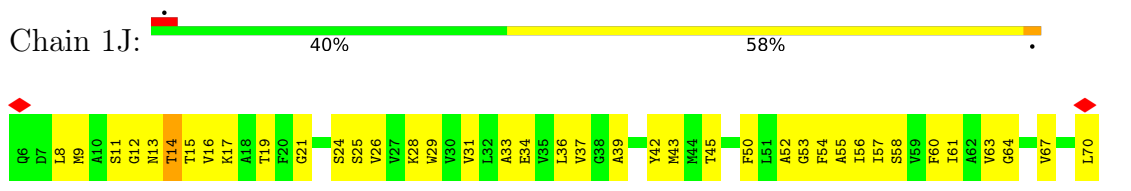
• Molecule 1: Pilin



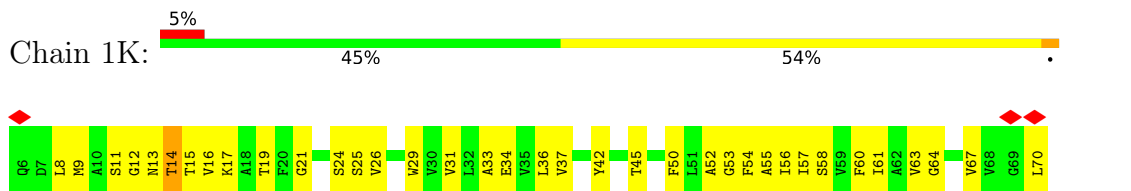
• Molecule 1: Pilin



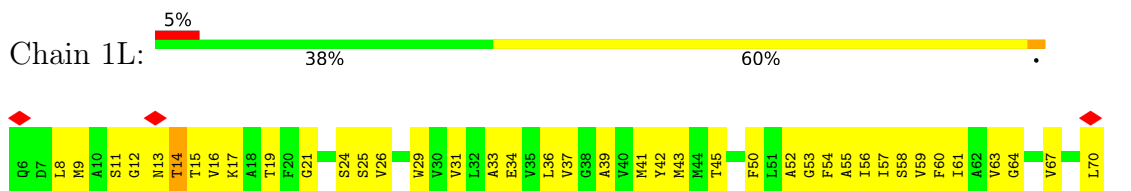
• Molecule 1: Pilin



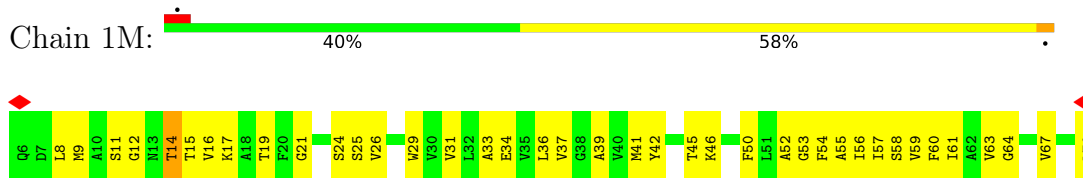
• Molecule 1: Pilin



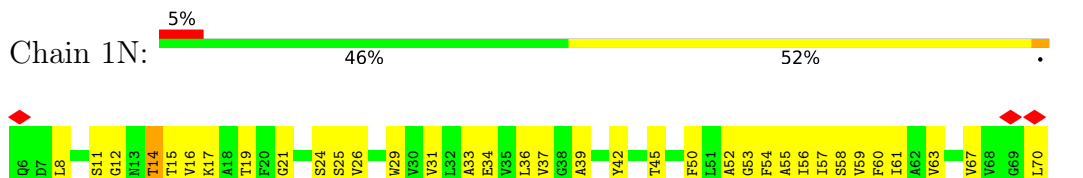
• Molecule 1: Pilin



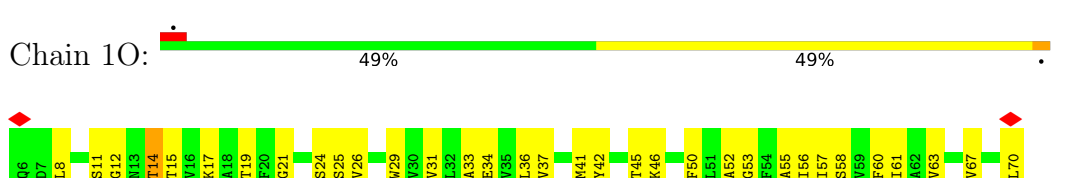
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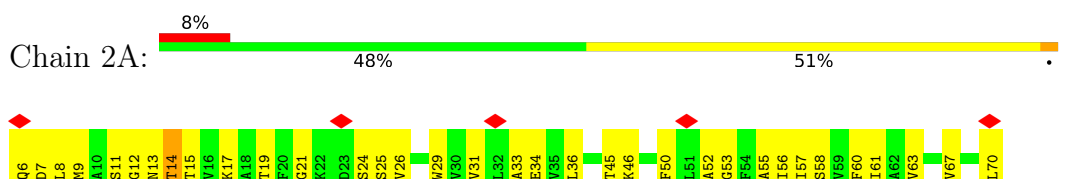
• Molecule 1: Pilin



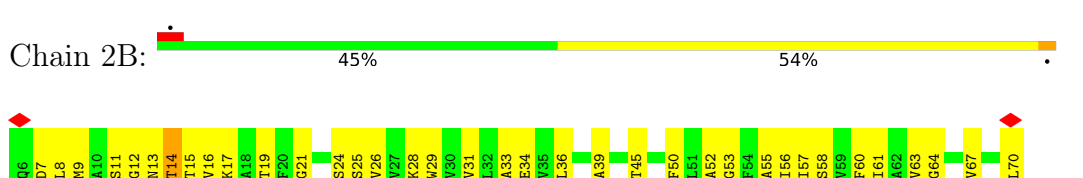
• Molecule 1: Pilin



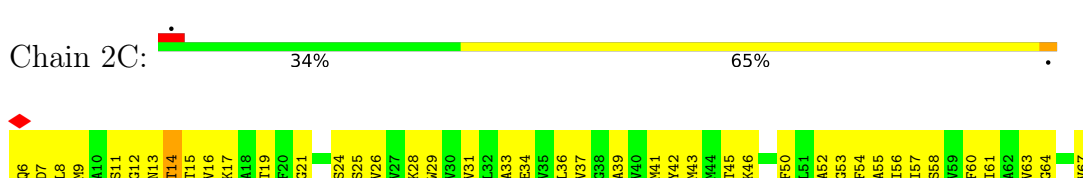
• Molecule 1: Pilin



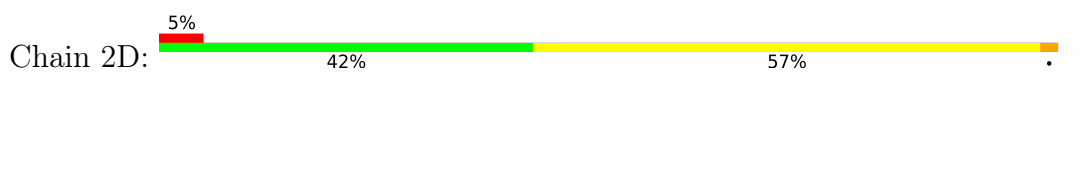
• Molecule 1: Pilin



• Molecule 1: Pilin



• Molecule 1: Pilin





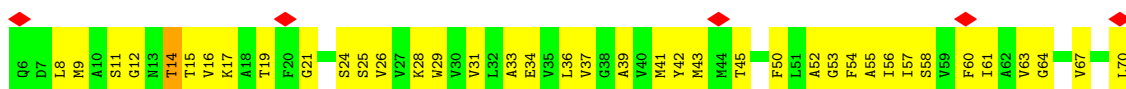
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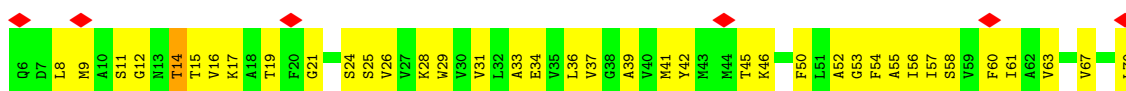
• Molecule 1: Pilin



• Molecule 1: Pilin



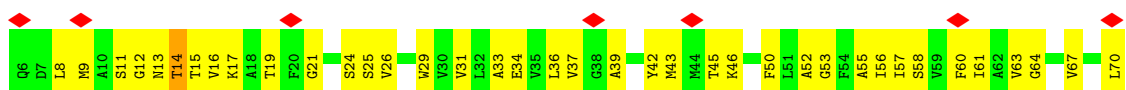
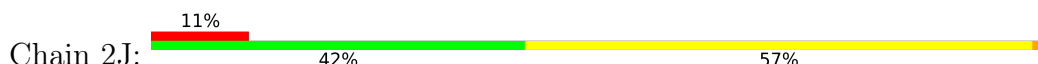
• Molecule 1: Pilin



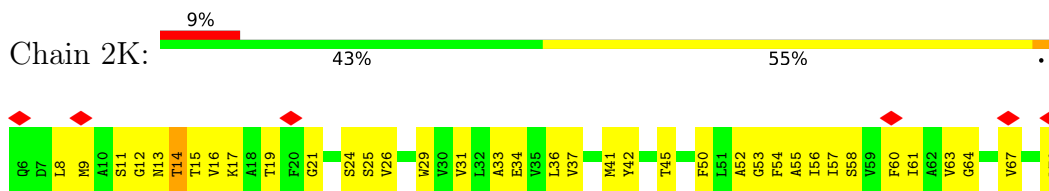
• Molecule 1: Pilin



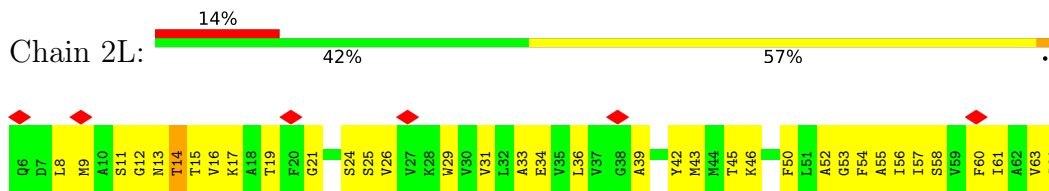
• Molecule 1: Pilin



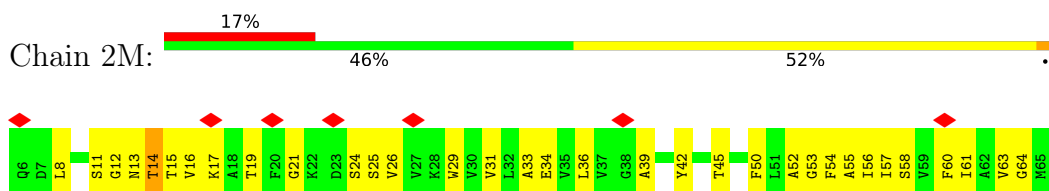
• Molecule 1: Pilin



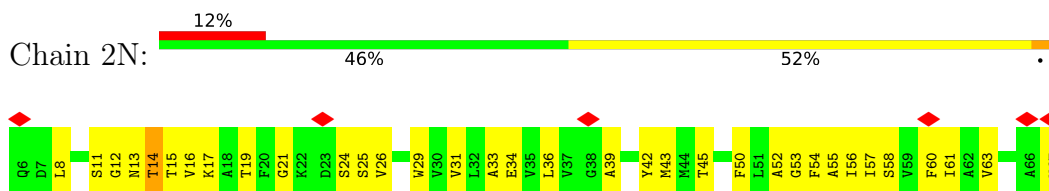
• Molecule 1: Pilin



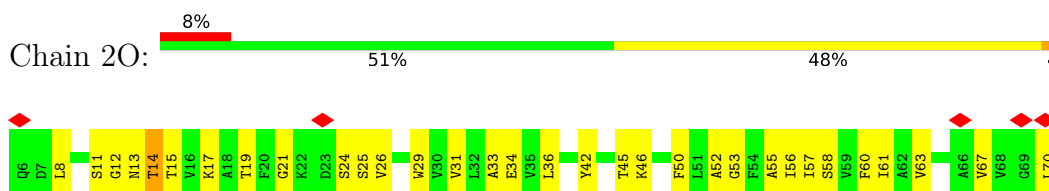
• Molecule 1: Pilin



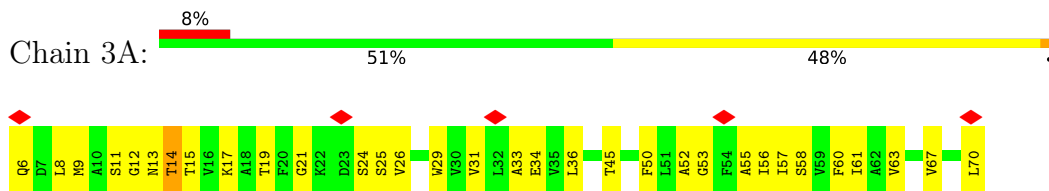
• Molecule 1: Pilin



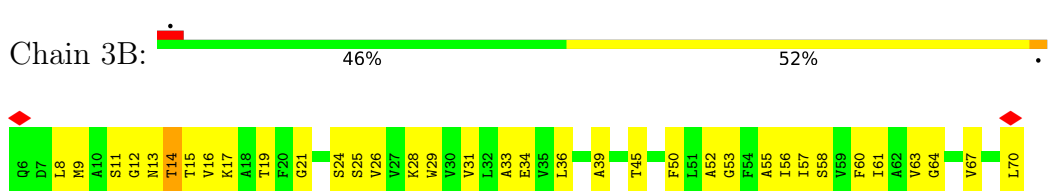
• Molecule 1: Pilin



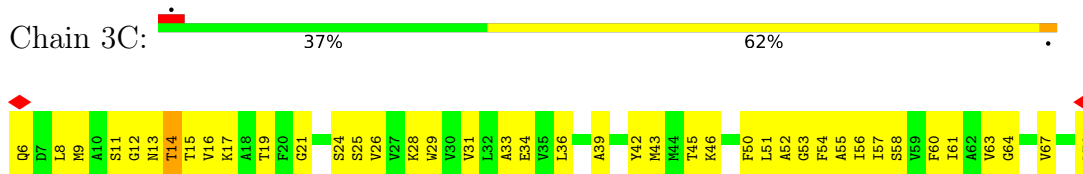
• Molecule 1: Pilin



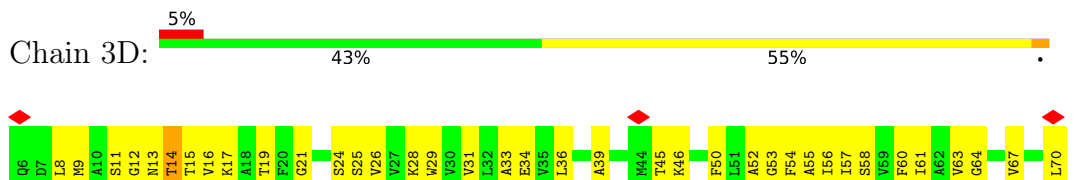
• Molecule 1: Pilin



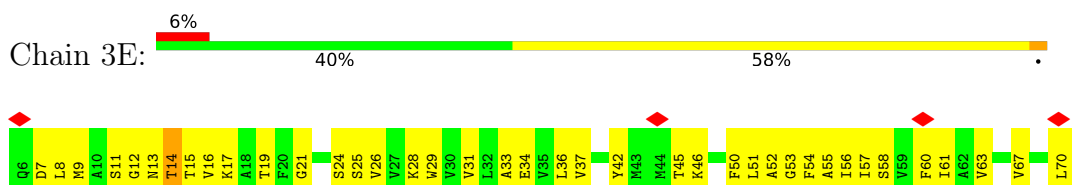
• Molecule 1: Pilin



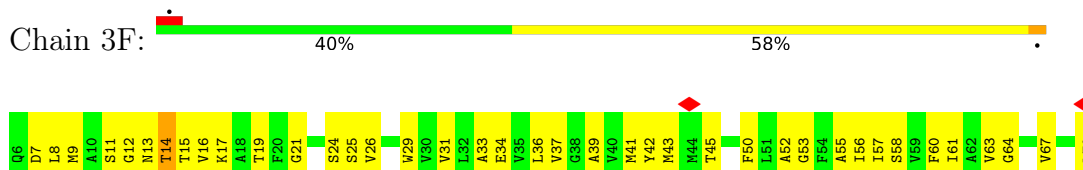
• Molecule 1: Pilin



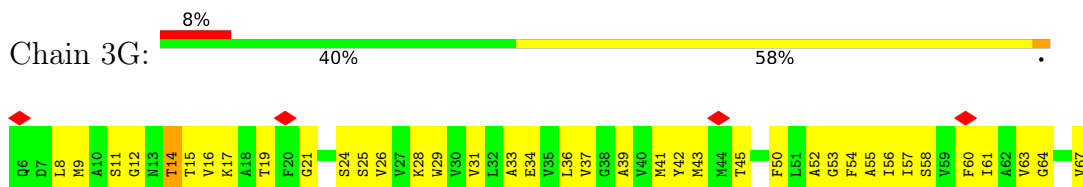
• Molecule 1: Pilin



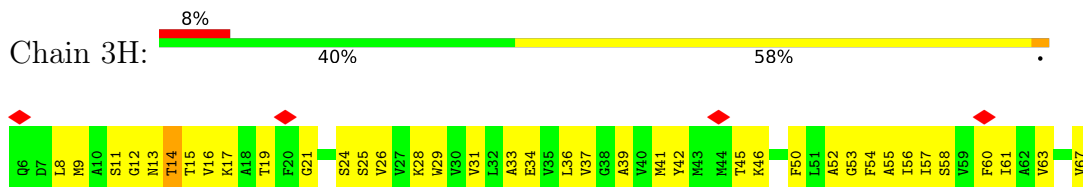
• Molecule 1: Pilin



• Molecule 1: Pilin



• Molecule 1: Pilin

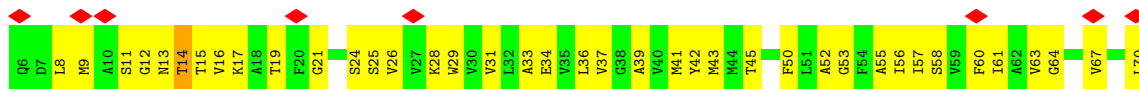


• Molecule 1: Pilin

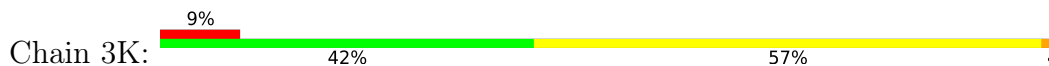




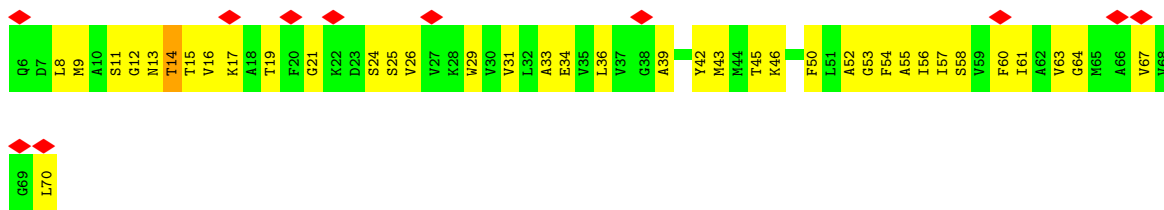
• Molecule 1: Pilin



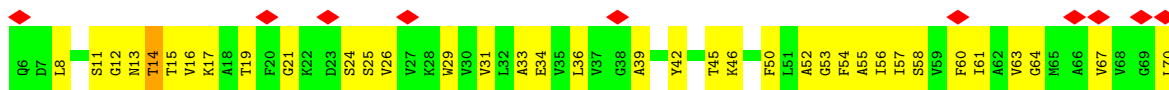
• Molecule 1: Pilin



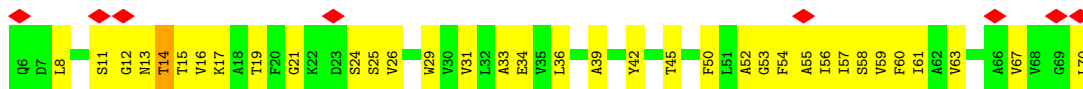
• Molecule 1: Pilin



• Molecule 1: Pilin

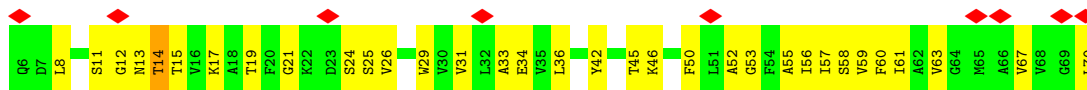


• Molecule 1: Pilin

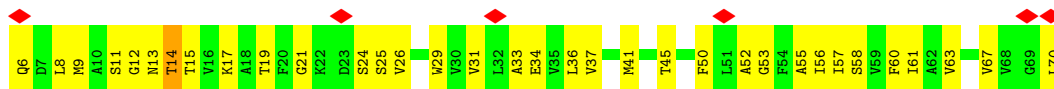


• Molecule 1: Pilin





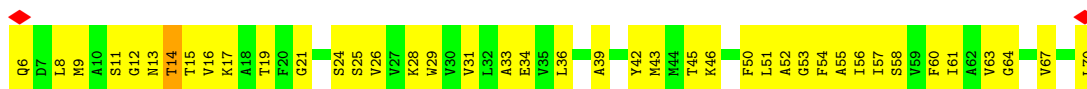
● Molecule 1: Pilin



● Molecule 1: Pilin



● Molecule 1: Pilin



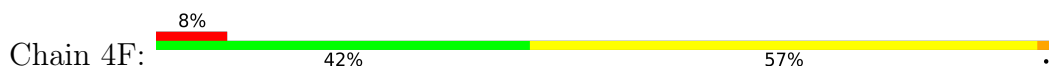
● Molecule 1: Pilin



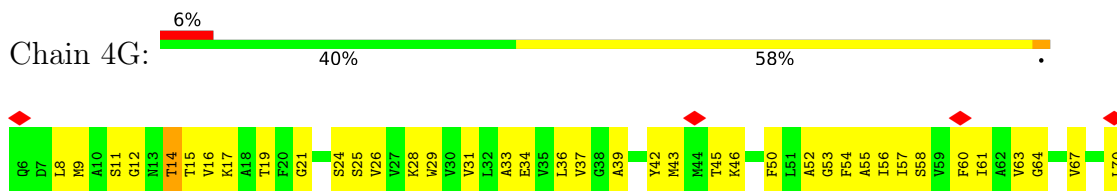
● Molecule 1: Pilin



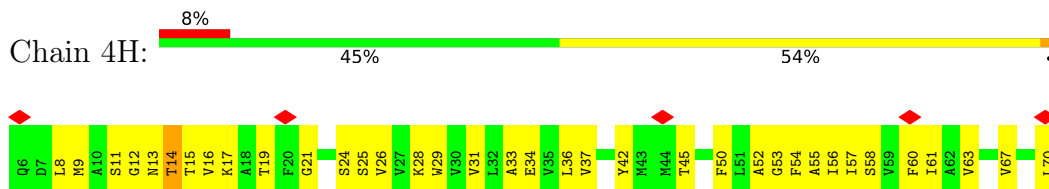
● Molecule 1: Pilin



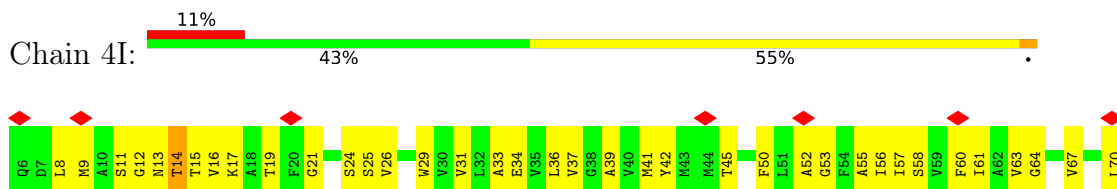
● Molecule 1: Pilin



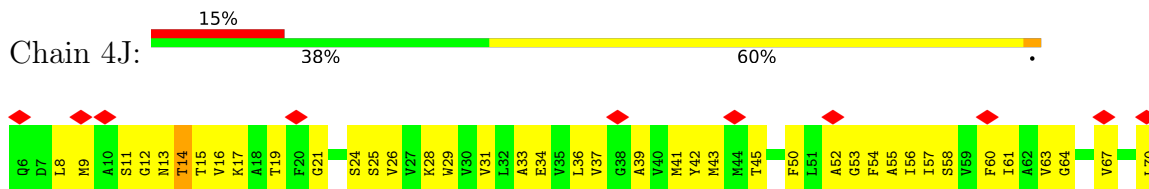
• Molecule 1: Pilin



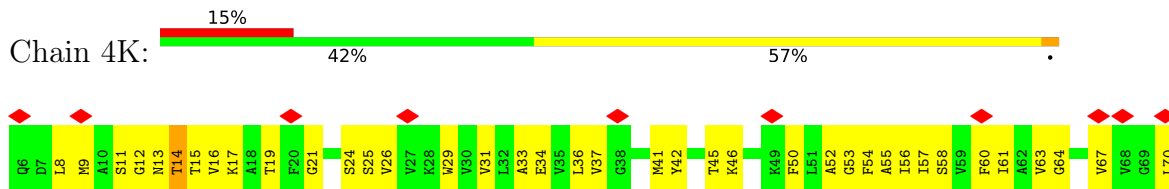
• Molecule 1: Pilin



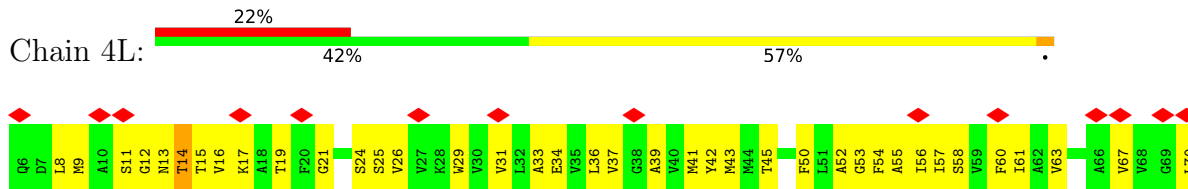
• Molecule 1: Pilin



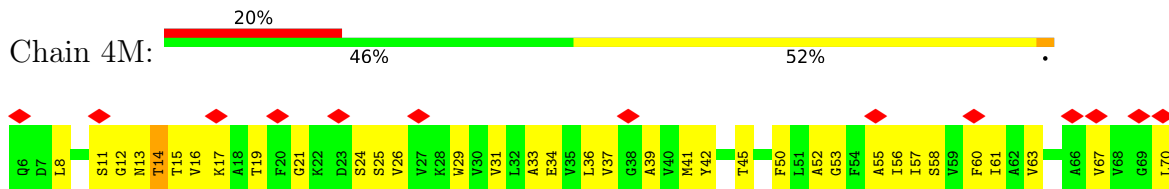
• Molecule 1: Pilin



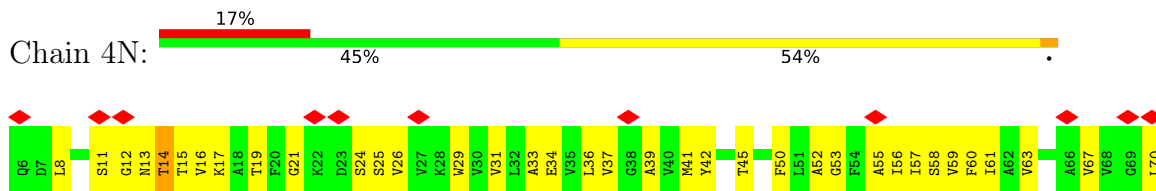
• Molecule 1: Pilin



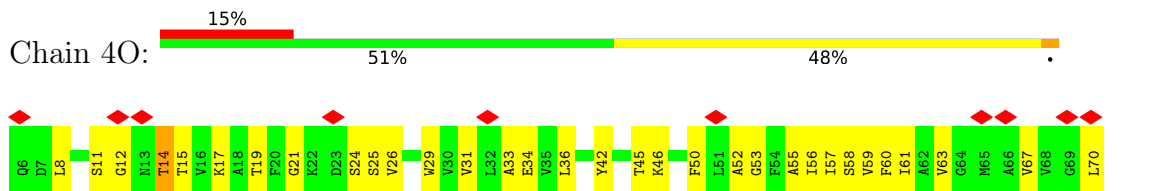
• Molecule 1: Pilin



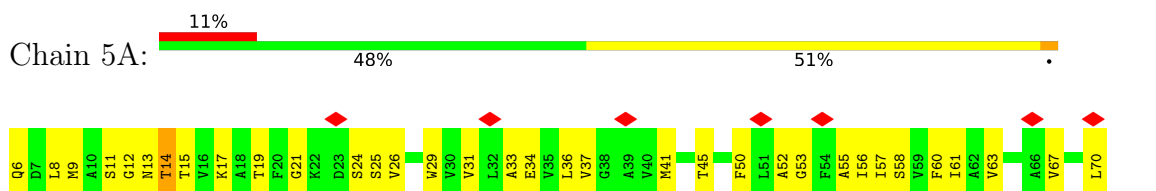
• Molecule 1: Pilin



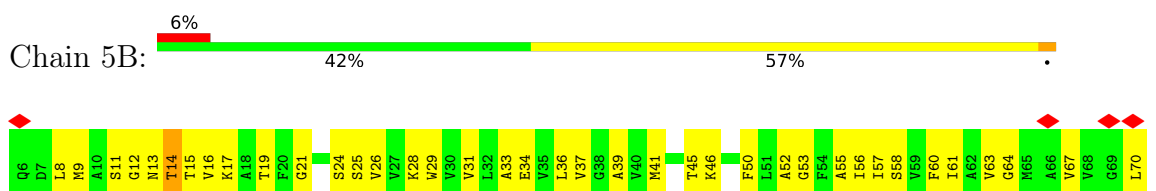
• Molecule 1: Pilin



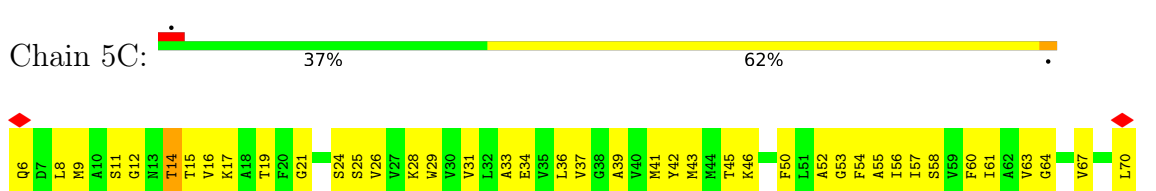
• Molecule 1: Pilin



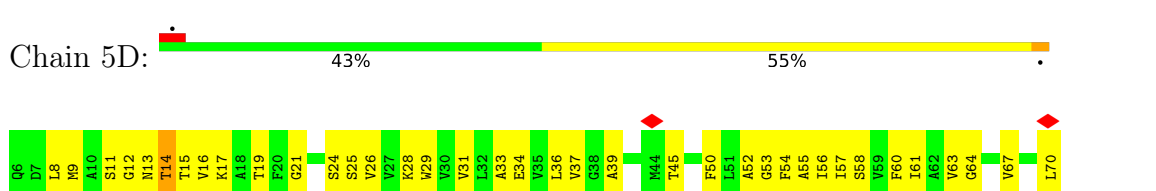
• Molecule 1: Pilin



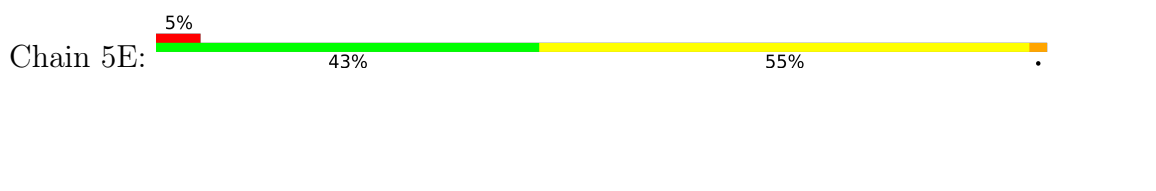
• Molecule 1: Pilin



• Molecule 1: Pilin



• Molecule 1: Pilin

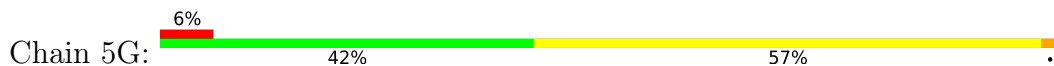




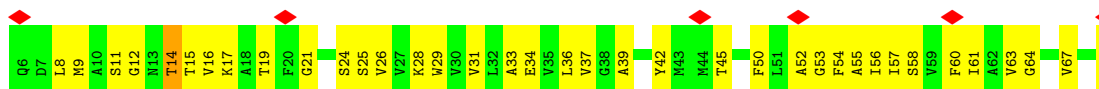
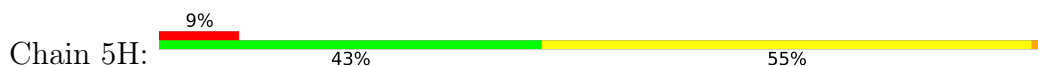
• Molecule 1: Pilin



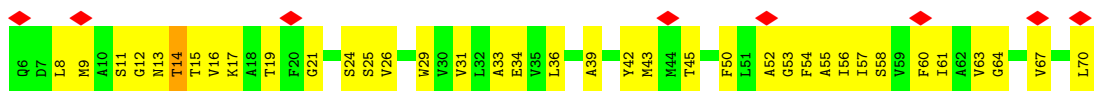
• Molecule 1: Pilin



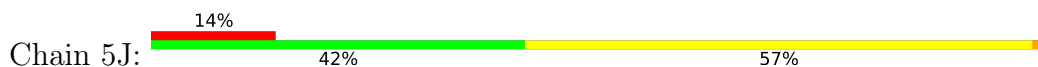
• Molecule 1: Pilin



• Molecule 1: Pilin



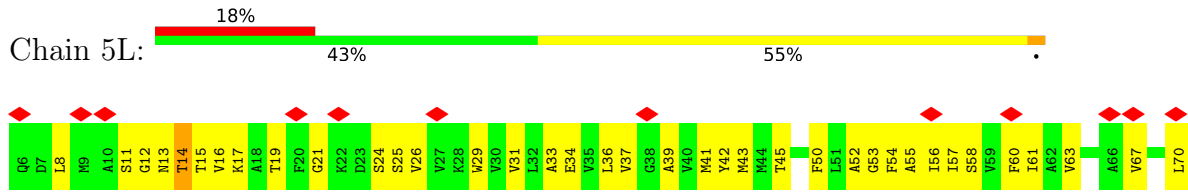
• Molecule 1: Pilin



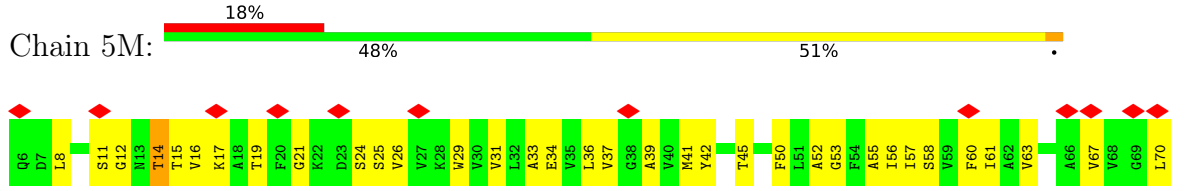
• Molecule 1: Pilin



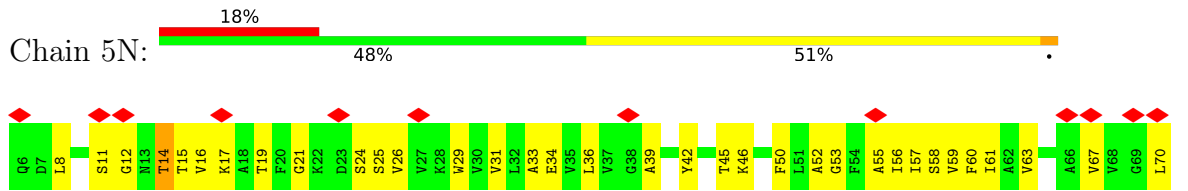
• Molecule 1: Pilin



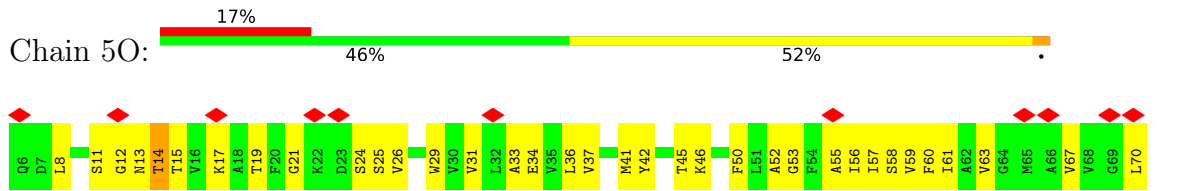
• Molecule 1: Pilin



• Molecule 1: Pilin



• Molecule 1: Pilin



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=28.1°, rise=12.5 Å, axial sym=C5	Depositor
Number of segments used	16426	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	1.67	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	145.206	Depositor
Minimum map value	-40.862	Depositor
Average map value	6.742	Depositor
Map value standard deviation	19.044	Depositor
Recommended contour level	44.0	Depositor
Map size (Å)	140.8, 140.8, 281.6	wwPDB
Map dimensions	128, 128, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 6V6

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	1A	0.51	0/482	0.63	0/651
1	1B	0.51	0/482	0.63	0/651
1	1C	0.51	0/482	0.63	0/651
1	1D	0.51	0/482	0.63	0/651
1	1E	0.51	0/482	0.63	0/651
1	1F	0.51	0/482	0.63	0/651
1	1G	0.51	0/482	0.63	0/651
1	1H	0.51	0/482	0.63	0/651
1	1I	0.51	0/482	0.63	0/651
1	1J	0.51	0/482	0.63	0/651
1	1K	0.51	0/482	0.63	0/651
1	1L	0.51	0/482	0.63	0/651
1	1M	0.51	0/482	0.63	0/651
1	1N	0.51	0/482	0.63	0/651
1	1O	0.51	0/482	0.63	0/651
1	2A	0.51	0/482	0.63	0/651
1	2B	0.51	0/482	0.63	0/651
1	2C	0.51	0/482	0.63	0/651
1	2D	0.51	0/482	0.63	0/651
1	2E	0.51	0/482	0.63	0/651
1	2F	0.51	0/482	0.63	0/651
1	2G	0.51	0/482	0.63	0/651
1	2H	0.51	0/482	0.63	0/651
1	2I	0.51	0/482	0.63	0/651
1	2J	0.51	0/482	0.63	0/651
1	2K	0.51	0/482	0.63	0/651
1	2L	0.51	0/482	0.63	0/651
1	2M	0.51	0/482	0.63	0/651
1	2N	0.51	0/482	0.63	0/651
1	2O	0.51	0/482	0.63	0/651
1	3A	0.51	0/482	0.63	0/651
1	3B	0.51	0/482	0.63	0/651

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	3C	0.51	0/482	0.63	0/651
1	3D	0.51	0/482	0.63	0/651
1	3E	0.51	0/482	0.63	0/651
1	3F	0.51	0/482	0.63	0/651
1	3G	0.51	0/482	0.63	0/651
1	3H	0.51	0/482	0.63	0/651
1	3I	0.51	0/482	0.63	0/651
1	3J	0.51	0/482	0.63	0/651
1	3K	0.51	0/482	0.63	0/651
1	3L	0.51	0/482	0.63	0/651
1	3M	0.51	0/482	0.63	0/651
1	3N	0.51	0/482	0.63	0/651
1	3O	0.51	0/482	0.63	0/651
1	4A	0.51	0/482	0.63	0/651
1	4B	0.51	0/482	0.63	0/651
1	4C	0.51	0/482	0.63	0/651
1	4D	0.51	0/482	0.63	0/651
1	4E	0.51	0/482	0.63	0/651
1	4F	0.51	0/482	0.63	0/651
1	4G	0.51	0/482	0.63	0/651
1	4H	0.51	0/482	0.63	0/651
1	4I	0.51	0/482	0.63	0/651
1	4J	0.51	0/482	0.63	0/651
1	4K	0.51	0/482	0.63	0/651
1	4L	0.51	0/482	0.63	0/651
1	4M	0.51	0/482	0.63	0/651
1	4N	0.51	0/482	0.63	0/651
1	4O	0.51	0/482	0.63	0/651
1	5A	0.51	0/482	0.63	0/651
1	5B	0.51	0/482	0.63	0/651
1	5C	0.51	0/482	0.63	0/651
1	5D	0.51	0/482	0.63	0/651
1	5E	0.51	0/482	0.63	0/651
1	5F	0.51	0/482	0.63	0/651
1	5G	0.51	0/482	0.63	0/651
1	5H	0.51	0/482	0.63	0/651
1	5I	0.51	0/482	0.63	0/651
1	5J	0.51	0/482	0.63	0/651
1	5K	0.51	0/482	0.63	0/651
1	5L	0.51	0/482	0.63	0/651
1	5M	0.51	0/482	0.63	0/651
1	5N	0.51	0/482	0.63	0/651
1	5O	0.51	0/482	0.63	0/651

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.51	0/36150	0.63	0/48825

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	1A	0	1
1	1B	0	1
1	1C	0	1
1	1D	0	1
1	1E	0	1
1	1F	0	1
1	1G	0	1
1	1H	0	1
1	1I	0	1
1	1J	0	1
1	1K	0	1
1	1L	0	1
1	1M	0	1
1	1N	0	1
1	1O	0	1
1	2A	0	1
1	2B	0	1
1	2C	0	1
1	2D	0	1
1	2E	0	1
1	2F	0	1
1	2G	0	1
1	2H	0	1
1	2I	0	1
1	2J	0	1
1	2K	0	1
1	2L	0	1
1	2M	0	1
1	2N	0	1
1	2O	0	1
1	3A	0	1
1	3B	0	1
1	3C	0	1
1	3D	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	3E	0	1
1	3F	0	1
1	3G	0	1
1	3H	0	1
1	3I	0	1
1	3J	0	1
1	3K	0	1
1	3L	0	1
1	3M	0	1
1	3N	0	1
1	3O	0	1
1	4A	0	1
1	4B	0	1
1	4C	0	1
1	4D	0	1
1	4E	0	1
1	4F	0	1
1	4G	0	1
1	4H	0	1
1	4I	0	1
1	4J	0	1
1	4K	0	1
1	4L	0	1
1	4M	0	1
1	4N	0	1
1	4O	0	1
1	5A	0	1
1	5B	0	1
1	5C	0	1
1	5D	0	1
1	5E	0	1
1	5F	0	1
1	5G	0	1
1	5H	0	1
1	5I	0	1
1	5J	0	1
1	5K	0	1
1	5L	0	1
1	5M	0	1
1	5N	0	1
1	5O	0	1
All	All	0	75

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 75 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1A	14	THR	Peptide
1	1B	14	THR	Peptide
1	1C	14	THR	Peptide
1	1D	14	THR	Peptide
1	1E	14	THR	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	1A	476	0	509	48	0
1	1B	476	0	509	60	0
1	1C	476	0	507	72	0
1	1D	476	0	509	70	0
1	1E	476	0	509	59	0
1	1F	476	0	509	70	0
1	1G	476	0	509	62	0
1	1H	476	0	509	63	0
1	1I	476	0	507	46	0
1	1J	476	0	507	56	0
1	1K	476	0	507	79	0
1	1L	476	0	509	83	0
1	1M	476	0	507	62	0
1	1N	476	0	509	44	0
1	1O	476	0	509	33	0
1	2A	476	0	509	46	0
1	2B	476	0	509	58	0
1	2C	476	0	509	79	0
1	2D	476	0	509	70	0
1	2E	476	0	509	66	0
1	2F	476	0	507	59	0
1	2G	476	0	507	62	0
1	2H	476	0	507	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2I	476	0	507	69	0
1	2J	476	0	507	64	0
1	2K	476	0	507	53	0
1	2L	476	0	509	70	0
1	2M	476	0	509	63	0
1	2N	476	0	509	58	0
1	2O	476	0	509	41	0
1	3A	476	0	509	42	0
1	3B	476	0	509	56	0
1	3C	476	0	509	75	0
1	3D	476	0	509	67	0
1	3E	476	0	509	68	0
1	3F	476	0	507	61	0
1	3G	476	0	507	62	0
1	3H	476	0	507	61	0
1	3I	476	0	507	58	0
1	3J	476	0	507	54	0
1	3K	476	0	507	60	0
1	3L	476	0	509	66	0
1	3M	476	0	509	53	0
1	3N	476	0	509	63	0
1	3O	476	0	509	48	0
1	4A	476	0	509	44	0
1	4B	476	0	509	57	0
1	4C	476	0	509	77	0
1	4D	476	0	509	64	0
1	4E	476	0	509	70	0
1	4F	476	0	507	63	0
1	4G	476	0	507	60	0
1	4H	476	0	507	59	0
1	4I	476	0	507	61	0
1	4J	476	0	507	53	0
1	4K	476	0	507	59	0
1	4L	476	0	509	64	0
1	4M	476	0	509	52	0
1	4N	476	0	509	62	0
1	4O	476	0	509	49	0
1	5A	476	0	509	47	0
1	5B	476	0	509	61	0
1	5C	476	0	508	67	0
1	5D	476	0	509	70	0
1	5E	476	0	507	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	5F	476	0	507	57	0
1	5G	476	0	507	60	0
1	5H	476	0	507	58	0
1	5I	476	0	509	69	0
1	5J	476	0	509	68	0
1	5K	476	0	509	58	0
1	5L	476	0	509	45	0
1	5M	476	0	509	45	0
1	5N	476	0	509	63	0
1	5O	476	0	509	48	0
2	1A	12	0	0	0	0
2	1B	12	0	0	0	0
2	1C	12	0	0	0	0
2	1D	12	0	0	1	0
2	1E	12	0	0	1	0
2	1F	12	0	0	1	0
2	1G	12	0	0	1	0
2	1H	12	0	0	1	0
2	1I	12	0	0	2	0
2	1J	12	0	0	0	0
2	1K	12	0	0	0	0
2	1L	12	0	0	0	0
2	1M	12	0	0	0	0
2	1N	12	0	0	0	0
2	1O	12	0	0	0	0
2	2A	12	0	0	0	0
2	2B	12	0	0	0	0
2	2C	12	0	0	0	0
2	2D	12	0	0	0	0
2	2E	12	0	0	0	0
2	2F	12	0	0	1	0
2	2G	12	0	0	1	0
2	2H	12	0	0	1	0
2	2I	12	0	0	2	0
2	2J	12	0	0	2	0
2	2K	12	0	0	2	0
2	2L	12	0	0	2	0
2	2M	12	0	0	2	0
2	2N	12	0	0	1	0
2	2O	12	0	0	1	0
2	3A	12	0	0	0	0
2	3B	12	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	3C	12	0	0	0	0
2	3D	12	0	0	0	0
2	3E	12	0	0	0	0
2	3F	12	0	0	1	0
2	3G	12	0	0	1	0
2	3H	12	0	0	2	0
2	3I	12	0	0	2	0
2	3J	12	0	0	4	0
2	3K	12	0	0	2	0
2	3L	12	0	0	2	0
2	3M	12	0	0	0	0
2	3N	12	0	0	0	0
2	3O	12	0	0	0	0
2	4A	12	0	0	0	0
2	4B	12	0	0	0	0
2	4C	12	0	0	0	0
2	4D	12	0	0	0	0
2	4E	12	0	0	0	0
2	4F	12	0	0	1	0
2	4G	12	0	0	1	0
2	4H	12	0	0	2	0
2	4I	12	0	0	2	0
2	4J	12	0	0	4	0
2	4K	12	0	0	2	0
2	4L	12	0	0	2	0
2	4M	12	0	0	0	0
2	4N	12	0	0	0	0
2	4O	12	0	0	0	0
2	5A	12	0	0	0	0
2	5B	12	0	0	0	0
2	5C	12	0	0	0	0
2	5D	12	0	0	0	0
2	5E	12	0	0	0	0
2	5F	12	0	0	1	0
2	5G	12	0	0	1	0
2	5H	12	0	0	2	0
2	5I	12	0	0	2	0
2	5J	12	0	0	4	0
2	5K	12	0	0	2	0
2	5L	12	0	0	2	0
2	5M	12	0	0	0	0
2	5N	12	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	5O	12	0	0	0	0
All	All	36600	0	38120	3319	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 44.

The worst 5 of 3319 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)
1:1G:9:MET:CE	1:2I:67:VAL:HG13	1.25	1.63
1:1L:13:ASN:HD21	1:2N:63:VAL:CB	1.12	1.62
1:1H:9:MET:HE2	1:2J:67:VAL:CG1	1.26	1.60
1:1J:9:MET:CE	1:2L:67:VAL:CG1	1.76	1.55
1:1H:9:MET:CE	1:2J:67:VAL:HG13	1.13	1.55

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	1A	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	1B	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	1C	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	1D	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	1E	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	1F	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	1G	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	1H	63/65 (97%)	51 (81%)	12 (19%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1I	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	1J	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	1K	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	1L	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	1M	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	1N	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	1O	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	2A	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	2B	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	2C	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	2D	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	2E	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	2F	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	2G	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	2H	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	2I	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	2J	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	2K	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	2L	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	2M	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	2N	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	2O	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	3A	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	3B	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	3C	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	3D	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	3E	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	3F	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	3G	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	3H	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	3I	63/65 (97%)	51 (81%)	12 (19%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	3J	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	3K	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	3L	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	3M	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	3N	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	3O	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	4A	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	4B	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	4C	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	4D	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	4E	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	4F	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	4G	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	4H	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	4I	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	4J	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	4K	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	4L	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	4M	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	4N	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	4O	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	5A	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	5B	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	5C	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	5D	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	5E	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	5F	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	5G	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	5H	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	5I	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	5J	63/65 (97%)	51 (81%)	12 (19%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	5K	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	5L	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	5M	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	5N	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	5O	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
All	All	4725/4875 (97%)	3825 (81%)	900 (19%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1A	51/51 (100%)	51 (100%)	0	100	100
1	1B	51/51 (100%)	51 (100%)	0	100	100
1	1C	51/51 (100%)	51 (100%)	0	100	100
1	1D	51/51 (100%)	51 (100%)	0	100	100
1	1E	51/51 (100%)	51 (100%)	0	100	100
1	1F	51/51 (100%)	51 (100%)	0	100	100
1	1G	51/51 (100%)	51 (100%)	0	100	100
1	1H	51/51 (100%)	51 (100%)	0	100	100
1	1I	51/51 (100%)	51 (100%)	0	100	100
1	1J	51/51 (100%)	51 (100%)	0	100	100
1	1K	51/51 (100%)	51 (100%)	0	100	100
1	1L	51/51 (100%)	51 (100%)	0	100	100
1	1M	51/51 (100%)	51 (100%)	0	100	100
1	1N	51/51 (100%)	51 (100%)	0	100	100
1	1O	51/51 (100%)	51 (100%)	0	100	100
1	2A	51/51 (100%)	51 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2B	51/51 (100%)	51 (100%)	0	100	100
1	2C	51/51 (100%)	51 (100%)	0	100	100
1	2D	51/51 (100%)	51 (100%)	0	100	100
1	2E	51/51 (100%)	51 (100%)	0	100	100
1	2F	51/51 (100%)	51 (100%)	0	100	100
1	2G	51/51 (100%)	51 (100%)	0	100	100
1	2H	51/51 (100%)	51 (100%)	0	100	100
1	2I	51/51 (100%)	51 (100%)	0	100	100
1	2J	51/51 (100%)	51 (100%)	0	100	100
1	2K	51/51 (100%)	51 (100%)	0	100	100
1	2L	51/51 (100%)	51 (100%)	0	100	100
1	2M	51/51 (100%)	51 (100%)	0	100	100
1	2N	51/51 (100%)	51 (100%)	0	100	100
1	2O	51/51 (100%)	51 (100%)	0	100	100
1	3A	51/51 (100%)	51 (100%)	0	100	100
1	3B	51/51 (100%)	51 (100%)	0	100	100
1	3C	51/51 (100%)	51 (100%)	0	100	100
1	3D	51/51 (100%)	51 (100%)	0	100	100
1	3E	51/51 (100%)	51 (100%)	0	100	100
1	3F	51/51 (100%)	51 (100%)	0	100	100
1	3G	51/51 (100%)	51 (100%)	0	100	100
1	3H	51/51 (100%)	51 (100%)	0	100	100
1	3I	51/51 (100%)	51 (100%)	0	100	100
1	3J	51/51 (100%)	51 (100%)	0	100	100
1	3K	51/51 (100%)	51 (100%)	0	100	100
1	3L	51/51 (100%)	51 (100%)	0	100	100
1	3M	51/51 (100%)	51 (100%)	0	100	100
1	3N	51/51 (100%)	51 (100%)	0	100	100
1	3O	51/51 (100%)	51 (100%)	0	100	100
1	4A	51/51 (100%)	51 (100%)	0	100	100
1	4B	51/51 (100%)	51 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	4C	51/51 (100%)	51 (100%)	0	100	100
1	4D	51/51 (100%)	51 (100%)	0	100	100
1	4E	51/51 (100%)	51 (100%)	0	100	100
1	4F	51/51 (100%)	51 (100%)	0	100	100
1	4G	51/51 (100%)	51 (100%)	0	100	100
1	4H	51/51 (100%)	51 (100%)	0	100	100
1	4I	51/51 (100%)	51 (100%)	0	100	100
1	4J	51/51 (100%)	51 (100%)	0	100	100
1	4K	51/51 (100%)	51 (100%)	0	100	100
1	4L	51/51 (100%)	51 (100%)	0	100	100
1	4M	51/51 (100%)	51 (100%)	0	100	100
1	4N	51/51 (100%)	51 (100%)	0	100	100
1	4O	51/51 (100%)	51 (100%)	0	100	100
1	5A	51/51 (100%)	51 (100%)	0	100	100
1	5B	51/51 (100%)	51 (100%)	0	100	100
1	5C	51/51 (100%)	51 (100%)	0	100	100
1	5D	51/51 (100%)	51 (100%)	0	100	100
1	5E	51/51 (100%)	51 (100%)	0	100	100
1	5F	51/51 (100%)	51 (100%)	0	100	100
1	5G	51/51 (100%)	51 (100%)	0	100	100
1	5H	51/51 (100%)	51 (100%)	0	100	100
1	5I	51/51 (100%)	51 (100%)	0	100	100
1	5J	51/51 (100%)	51 (100%)	0	100	100
1	5K	51/51 (100%)	51 (100%)	0	100	100
1	5L	51/51 (100%)	51 (100%)	0	100	100
1	5M	51/51 (100%)	51 (100%)	0	100	100
1	5N	51/51 (100%)	51 (100%)	0	100	100
1	5O	51/51 (100%)	51 (100%)	0	100	100
All	All	3825/3825 (100%)	3825 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36

such sidechains are listed below:

Mol	Chain	Res	Type
1	4M	13	ASN
1	5L	13	ASN
1	5A	13	ASN
1	5I	13	ASN
1	2E	13	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](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

75 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	$\# Z > 2$
2	6V6	1H	101	-	11,11,48	0.51	0	12,14,54	0.55	0
2	6V6	3J	101	-	11,11,48	0.51	0	12,14,54	0.55	0
2	6V6	2G	101	-	11,11,48	0.50	0	12,14,54	0.55	0
2	6V6	2J	101	-	11,11,48	0.52	0	12,14,54	0.55	0
2	6V6	4C	101	-	11,11,48	0.51	0	12,14,54	0.56	0
2	6V6	4G	101	-	11,11,48	0.50	0	12,14,54	0.55	0
2	6V6	5K	101	-	11,11,48	0.52	0	12,14,54	0.55	0
2	6V6	3I	101	-	11,11,48	0.51	0	12,14,54	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	6V6	1J	101	-	11,11,48	0.51	0	12,14,54	0.55	0
2	6V6	3N	101	-	11,11,48	0.51	0	12,14,54	0.55	0
2	6V6	5D	101	-	11,11,48	0.51	0	12,14,54	0.54	0
2	6V6	4F	101	-	11,11,48	0.51	0	12,14,54	0.56	0
2	6V6	2I	101	-	11,11,48	0.51	0	12,14,54	0.55	0
2	6V6	4H	101	-	11,11,48	0.51	0	12,14,54	0.55	0
2	6V6	4L	101	-	11,11,48	0.52	0	12,14,54	0.55	0
2	6V6	2K	101	-	11,11,48	0.52	0	12,14,54	0.55	0
2	6V6	2C	101	-	11,11,48	0.51	0	12,14,54	0.56	0
2	6V6	2N	101	-	11,11,48	0.51	0	12,14,54	0.55	0
2	6V6	5G	101	-	11,11,48	0.51	0	12,14,54	0.55	0
2	6V6	3G	101	-	11,11,48	0.51	0	12,14,54	0.55	0
2	6V6	5N	101	-	11,11,48	0.51	0	12,14,54	0.55	0
2	6V6	5O	101	-	11,11,48	0.53	0	12,14,54	0.55	0
2	6V6	1K	101	-	11,11,48	0.51	0	12,14,54	0.55	0
2	6V6	3C	101	-	11,11,48	0.51	0	12,14,54	0.56	0
2	6V6	4J	101	-	11,11,48	0.51	0	12,14,54	0.55	0
2	6V6	1A	101	-	11,11,48	0.51	0	12,14,54	0.55	0
2	6V6	1O	101	-	11,11,48	0.52	0	12,14,54	0.54	0
2	6V6	3A	101	-	11,11,48	0.51	0	12,14,54	0.55	0
2	6V6	4N	101	-	11,11,48	0.51	0	12,14,54	0.55	0
2	6V6	1N	101	-	11,11,48	0.51	0	12,14,54	0.55	0
2	6V6	1I	101	-	11,11,48	0.51	0	12,14,54	0.55	0
2	6V6	2A	101	-	11,11,48	0.51	0	12,14,54	0.55	0
2	6V6	2F	101	-	11,11,48	0.52	0	12,14,54	0.56	0
2	6V6	4O	101	-	11,11,48	0.53	0	12,14,54	0.55	0
2	6V6	1E	101	-	11,11,48	0.51	0	12,14,54	0.56	0
2	6V6	5F	101	-	11,11,48	0.51	0	12,14,54	0.56	0
2	6V6	5L	101	-	11,11,48	0.51	0	12,14,54	0.55	0
2	6V6	2E	101	-	11,11,48	0.51	0	12,14,54	0.56	0
2	6V6	2H	101	-	11,11,48	0.51	0	12,14,54	0.55	0
2	6V6	1L	101	-	11,11,48	0.51	0	12,14,54	0.55	0
2	6V6	3H	101	-	11,11,48	0.51	0	12,14,54	0.55	0
2	6V6	3K	101	-	11,11,48	0.52	0	12,14,54	0.55	0
2	6V6	2O	101	-	11,11,48	0.52	0	12,14,54	0.54	0
2	6V6	5H	101	-	11,11,48	0.51	0	12,14,54	0.55	0
2	6V6	1F	101	-	11,11,48	0.51	0	12,14,54	0.56	0
2	6V6	1G	101	-	11,11,48	0.51	0	12,14,54	0.55	0
2	6V6	5A	101	-	11,11,48	0.51	0	12,14,54	0.55	0
2	6V6	3M	101	-	11,11,48	0.51	0	12,14,54	0.55	0
2	6V6	3O	101	-	11,11,48	0.53	0	12,14,54	0.54	0
2	6V6	4E	101	-	11,11,48	0.51	0	12,14,54	0.55	0
2	6V6	2L	101	-	11,11,48	0.52	0	12,14,54	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	6V6	4B	101	-	11,11,48	0.50	0	12,14,54	0.54	0
2	6V6	2D	101	-	11,11,48	0.52	0	12,14,54	0.54	0
2	6V6	2B	101	-	11,11,48	0.51	0	12,14,54	0.55	0
2	6V6	3F	101	-	11,11,48	0.52	0	12,14,54	0.56	0
2	6V6	4A	101	-	11,11,48	0.52	0	12,14,54	0.55	0
2	6V6	1B	101	-	11,11,48	0.50	0	12,14,54	0.54	0
2	6V6	2M	101	-	11,11,48	0.51	0	12,14,54	0.55	0
2	6V6	3B	101	-	11,11,48	0.50	0	12,14,54	0.55	0
2	6V6	5J	101	-	11,11,48	0.51	0	12,14,54	0.55	0
2	6V6	1M	101	-	11,11,48	0.51	0	12,14,54	0.55	0
2	6V6	4K	101	-	11,11,48	0.51	0	12,14,54	0.55	0
2	6V6	5I	101	-	11,11,48	0.51	0	12,14,54	0.55	0
2	6V6	1C	101	-	11,11,48	0.51	0	12,14,54	0.56	0
2	6V6	1D	101	-	11,11,48	0.52	0	12,14,54	0.54	0
2	6V6	3D	101	-	11,11,48	0.52	0	12,14,54	0.54	0
2	6V6	4M	101	-	11,11,48	0.51	0	12,14,54	0.55	0
2	6V6	4D	101	-	11,11,48	0.52	0	12,14,54	0.54	0
2	6V6	5B	101	-	11,11,48	0.50	0	12,14,54	0.54	0
2	6V6	4I	101	-	11,11,48	0.51	0	12,14,54	0.56	0
2	6V6	5C	101	-	11,11,48	0.52	0	12,14,54	0.56	0
2	6V6	3L	101	-	11,11,48	0.51	0	12,14,54	0.55	0
2	6V6	5M	101	-	11,11,48	0.51	0	12,14,54	0.55	0
2	6V6	5E	101	-	11,11,48	0.51	0	12,14,54	0.56	0
2	6V6	3E	101	-	11,11,48	0.51	0	12,14,54	0.56	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	6V6	1H	101	-	-	1/12/12/53	-
2	6V6	3J	101	-	-	1/12/12/53	-
2	6V6	2G	101	-	-	1/12/12/53	-
2	6V6	2J	101	-	-	1/12/12/53	-
2	6V6	4C	101	-	-	1/12/12/53	-
2	6V6	4G	101	-	-	1/12/12/53	-
2	6V6	5K	101	-	-	1/12/12/53	-
2	6V6	3I	101	-	-	1/12/12/53	-
2	6V6	1J	101	-	-	1/12/12/53	-
2	6V6	3N	101	-	-	1/12/12/53	-
2	6V6	5D	101	-	-	1/12/12/53	-
2	6V6	4F	101	-	-	1/12/12/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	6V6	2I	101	-	-	1/12/12/53	-
2	6V6	4H	101	-	-	1/12/12/53	-
2	6V6	4L	101	-	-	1/12/12/53	-
2	6V6	2K	101	-	-	1/12/12/53	-
2	6V6	2C	101	-	-	1/12/12/53	-
2	6V6	2N	101	-	-	1/12/12/53	-
2	6V6	5G	101	-	-	1/12/12/53	-
2	6V6	3G	101	-	-	1/12/12/53	-
2	6V6	5N	101	-	-	1/12/12/53	-
2	6V6	5O	101	-	-	7/12/12/53	-
2	6V6	1K	101	-	-	1/12/12/53	-
2	6V6	3C	101	-	-	1/12/12/53	-
2	6V6	4J	101	-	-	1/12/12/53	-
2	6V6	1A	101	-	-	1/12/12/53	-
2	6V6	1O	101	-	-	7/12/12/53	-
2	6V6	3A	101	-	-	1/12/12/53	-
2	6V6	4N	101	-	-	1/12/12/53	-
2	6V6	1N	101	-	-	1/12/12/53	-
2	6V6	1I	101	-	-	1/12/12/53	-
2	6V6	2A	101	-	-	1/12/12/53	-
2	6V6	2F	101	-	-	1/12/12/53	-
2	6V6	4O	101	-	-	7/12/12/53	-
2	6V6	1E	101	-	-	1/12/12/53	-
2	6V6	5F	101	-	-	1/12/12/53	-
2	6V6	5L	101	-	-	1/12/12/53	-
2	6V6	2E	101	-	-	1/12/12/53	-
2	6V6	2H	101	-	-	1/12/12/53	-
2	6V6	1L	101	-	-	1/12/12/53	-
2	6V6	3H	101	-	-	1/12/12/53	-
2	6V6	3K	101	-	-	1/12/12/53	-
2	6V6	2O	101	-	-	7/12/12/53	-
2	6V6	5H	101	-	-	1/12/12/53	-
2	6V6	1F	101	-	-	1/12/12/53	-
2	6V6	1G	101	-	-	1/12/12/53	-
2	6V6	5A	101	-	-	1/12/12/53	-
2	6V6	3M	101	-	-	1/12/12/53	-
2	6V6	3O	101	-	-	7/12/12/53	-
2	6V6	4E	101	-	-	1/12/12/53	-
2	6V6	2L	101	-	-	1/12/12/53	-
2	6V6	4B	101	-	-	1/12/12/53	-
2	6V6	2D	101	-	-	1/12/12/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	6V6	2B	101	-	-	1/12/12/53	-
2	6V6	3F	101	-	-	1/12/12/53	-
2	6V6	4A	101	-	-	1/12/12/53	-
2	6V6	1B	101	-	-	1/12/12/53	-
2	6V6	2M	101	-	-	1/12/12/53	-
2	6V6	3B	101	-	-	1/12/12/53	-
2	6V6	5J	101	-	-	1/12/12/53	-
2	6V6	1M	101	-	-	1/12/12/53	-
2	6V6	4K	101	-	-	1/12/12/53	-
2	6V6	5I	101	-	-	1/12/12/53	-
2	6V6	1C	101	-	-	1/12/12/53	-
2	6V6	1D	101	-	-	1/12/12/53	-
2	6V6	3D	101	-	-	1/12/12/53	-
2	6V6	4M	101	-	-	1/12/12/53	-
2	6V6	4D	101	-	-	1/12/12/53	-
2	6V6	5B	101	-	-	1/12/12/53	-
2	6V6	4I	101	-	-	1/12/12/53	-
2	6V6	5C	101	-	-	1/12/12/53	-
2	6V6	3L	101	-	-	1/12/12/53	-
2	6V6	5M	101	-	-	1/12/12/53	-
2	6V6	5E	101	-	-	1/12/12/53	-
2	6V6	3E	101	-	-	1/12/12/53	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 105 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	1O	101	6V6	C3-O4-P1-O2
2	2O	101	6V6	C3-O4-P1-O2
2	3O	101	6V6	C3-O4-P1-O2
2	4O	101	6V6	C3-O4-P1-O2
2	5O	101	6V6	C3-O4-P1-O2

There are no ring outliers.

37 monomers are involved in 64 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	1H	101	6V6	1	0
2	3J	101	6V6	4	0

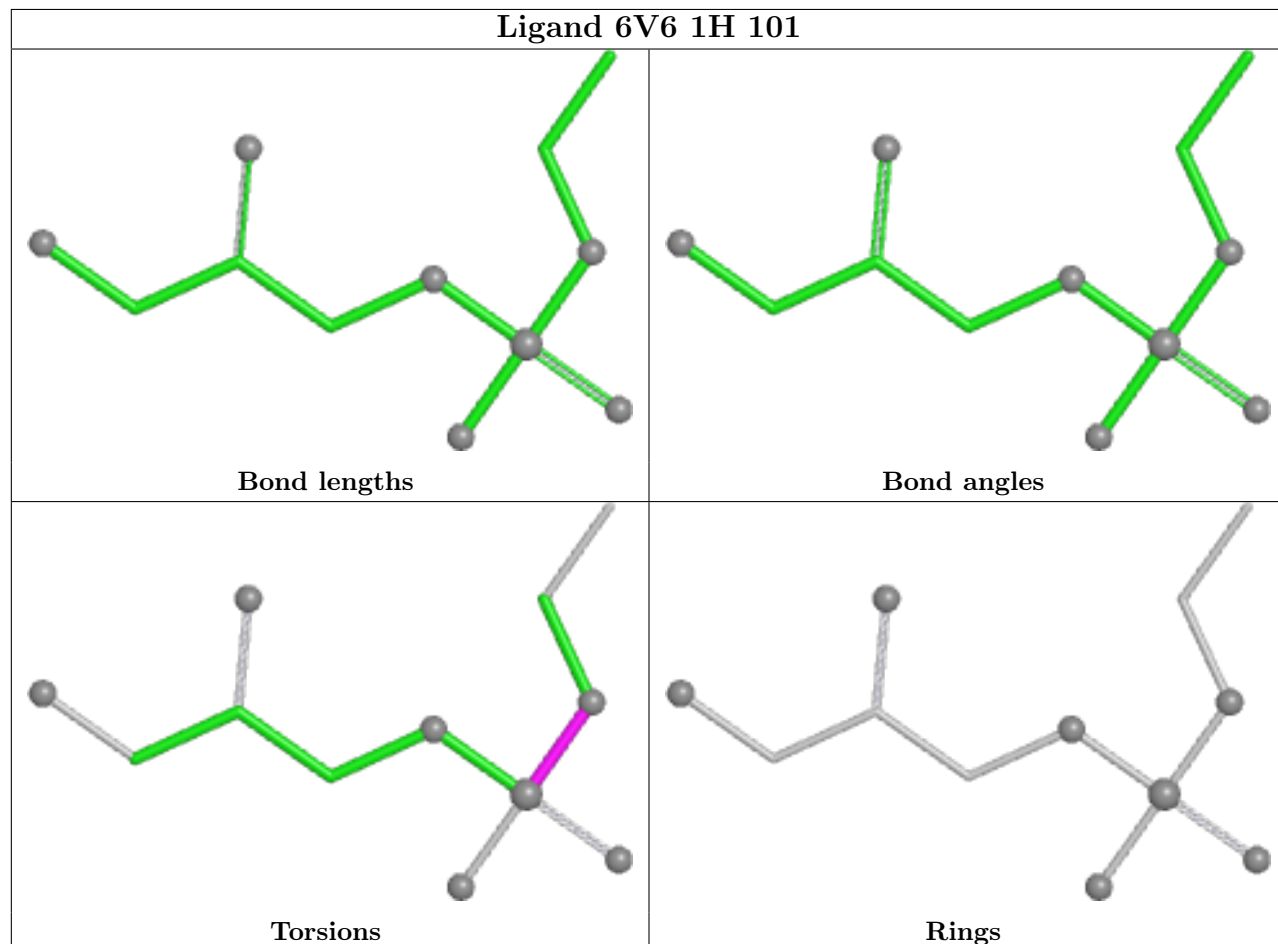
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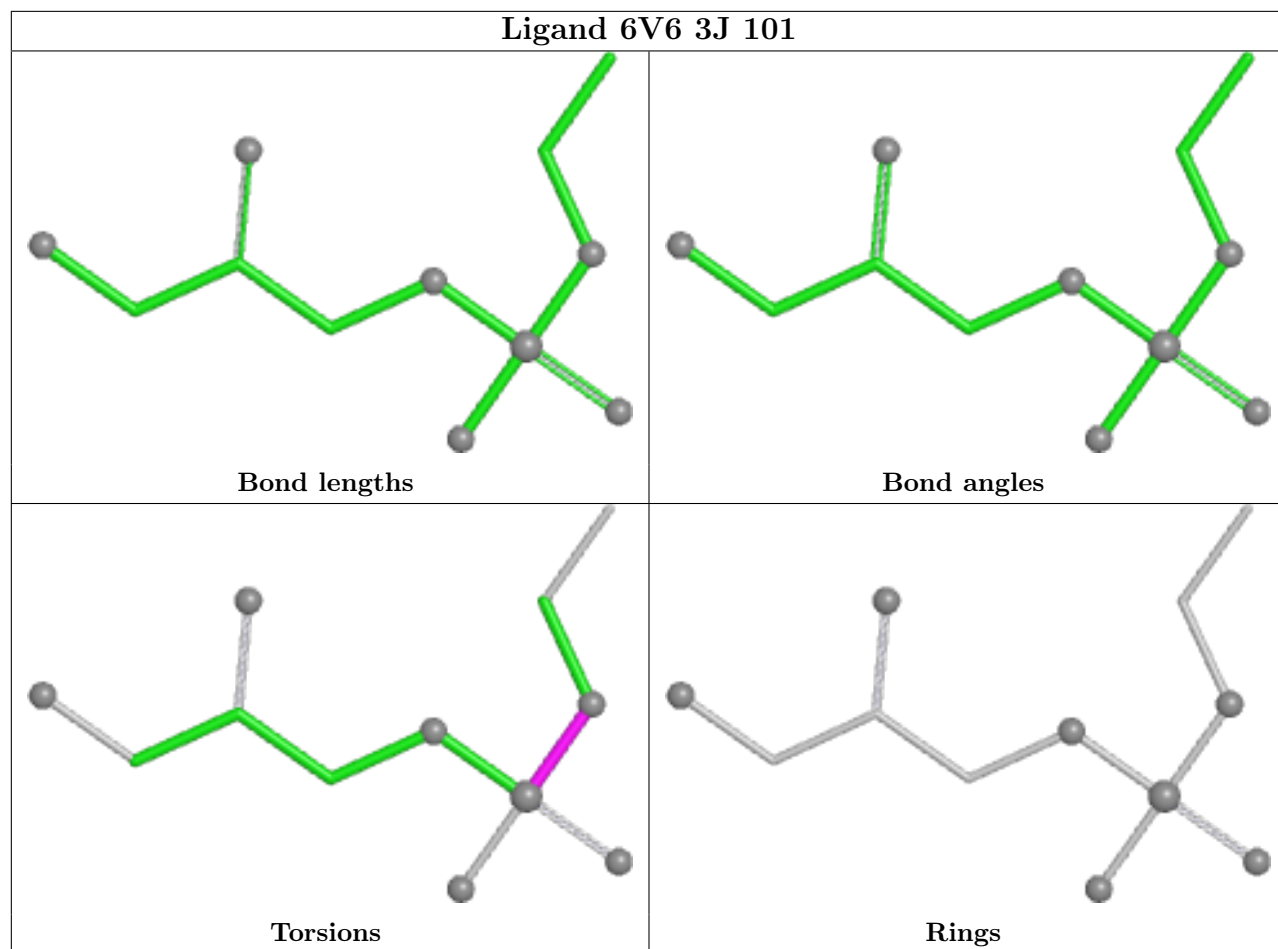
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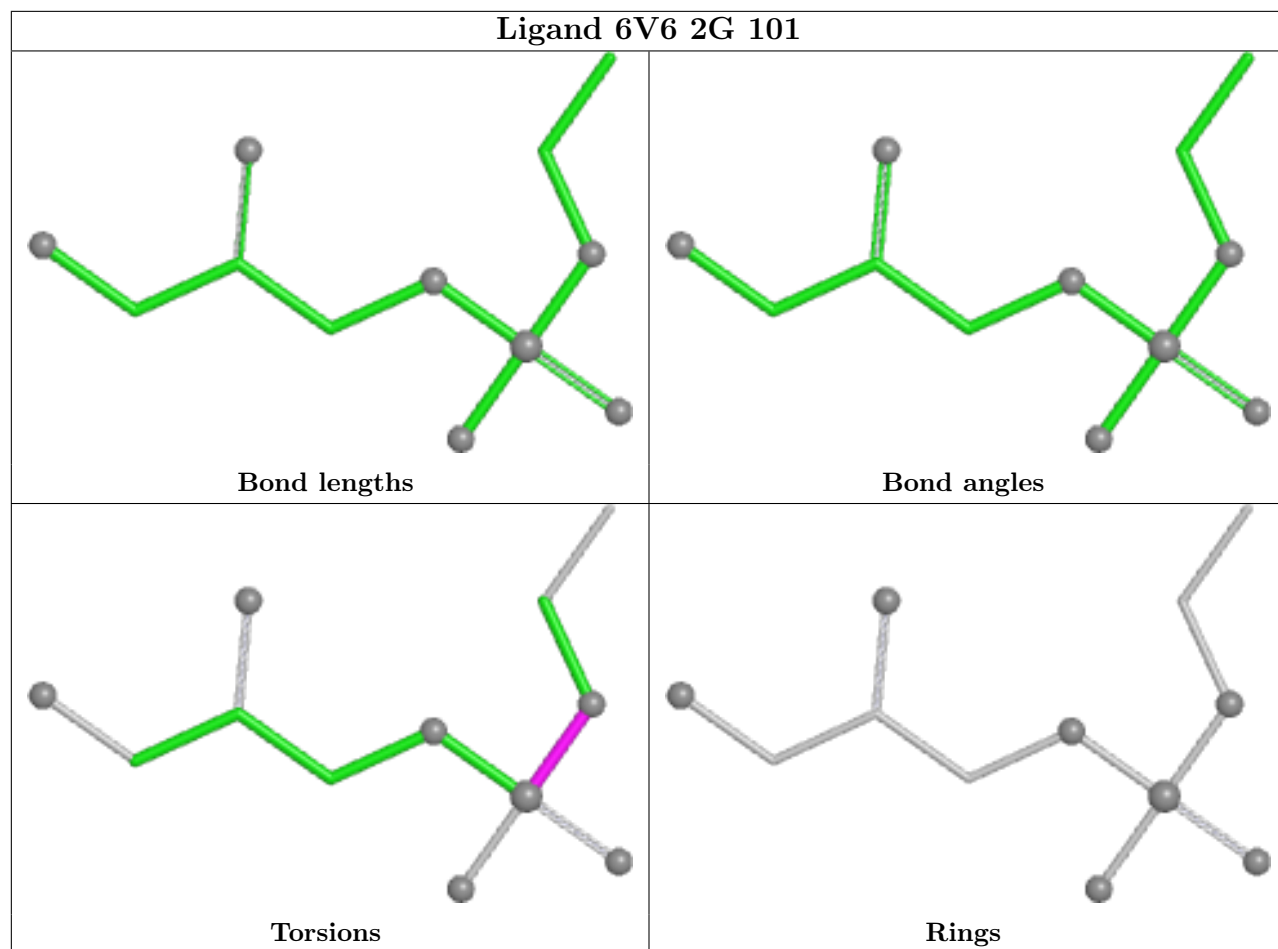
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	2G	101	6V6	1	0
2	2J	101	6V6	2	0
2	4G	101	6V6	1	0
2	5K	101	6V6	2	0
2	3I	101	6V6	2	0
2	4F	101	6V6	1	0
2	2I	101	6V6	2	0
2	4H	101	6V6	2	0
2	4L	101	6V6	2	0
2	2K	101	6V6	2	0
2	2N	101	6V6	1	0
2	5G	101	6V6	1	0
2	3G	101	6V6	1	0
2	4J	101	6V6	4	0
2	1I	101	6V6	2	0
2	2F	101	6V6	1	0
2	1E	101	6V6	1	0
2	5F	101	6V6	1	0
2	5L	101	6V6	2	0
2	2H	101	6V6	1	0
2	3H	101	6V6	2	0
2	3K	101	6V6	2	0
2	2O	101	6V6	1	0
2	5H	101	6V6	2	0
2	1F	101	6V6	1	0
2	1G	101	6V6	1	0
2	2L	101	6V6	2	0
2	3F	101	6V6	1	0
2	2M	101	6V6	2	0
2	5J	101	6V6	4	0
2	4K	101	6V6	2	0
2	5I	101	6V6	2	0
2	1D	101	6V6	1	0
2	4I	101	6V6	2	0
2	3L	101	6V6	2	0

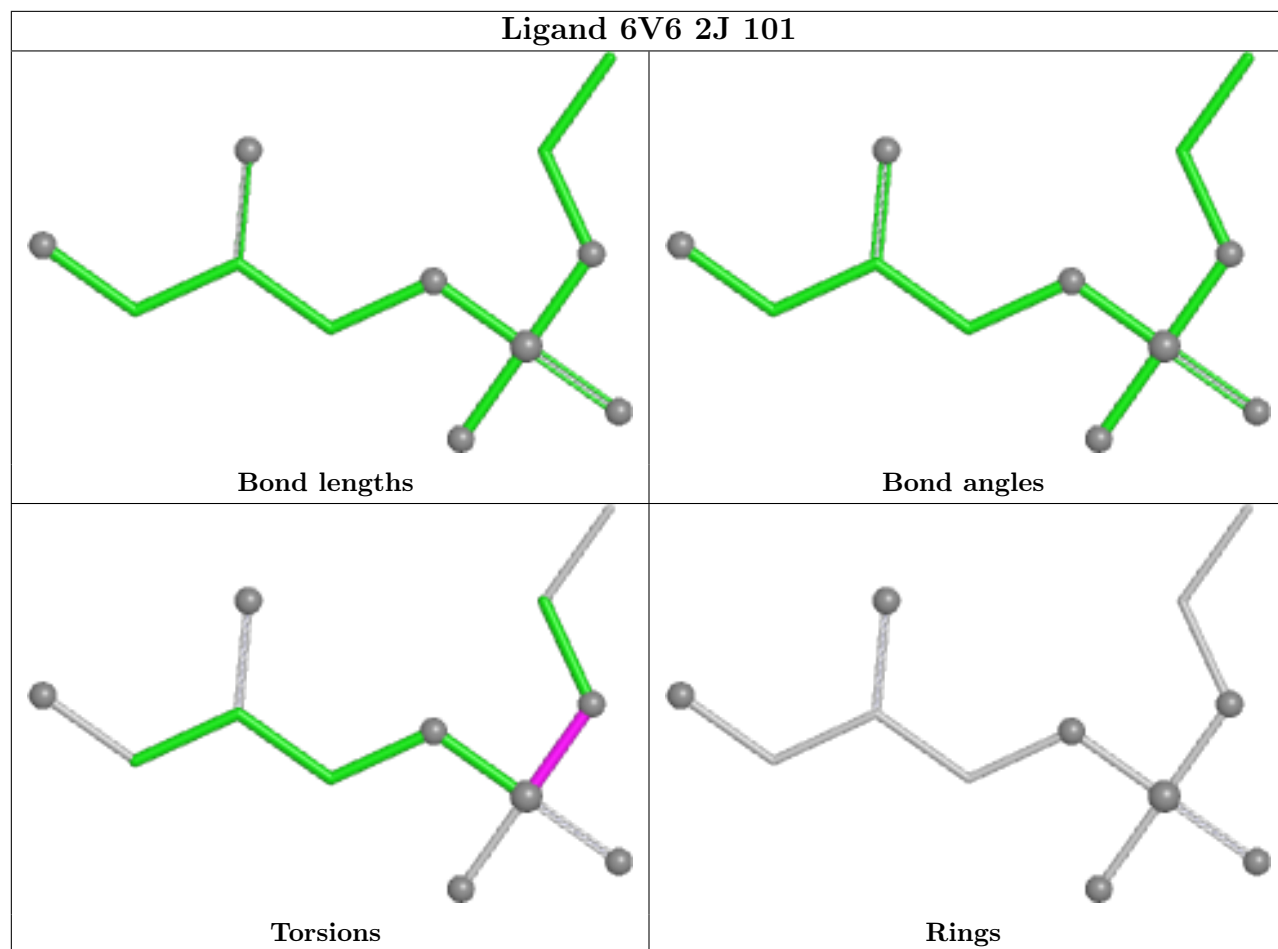
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

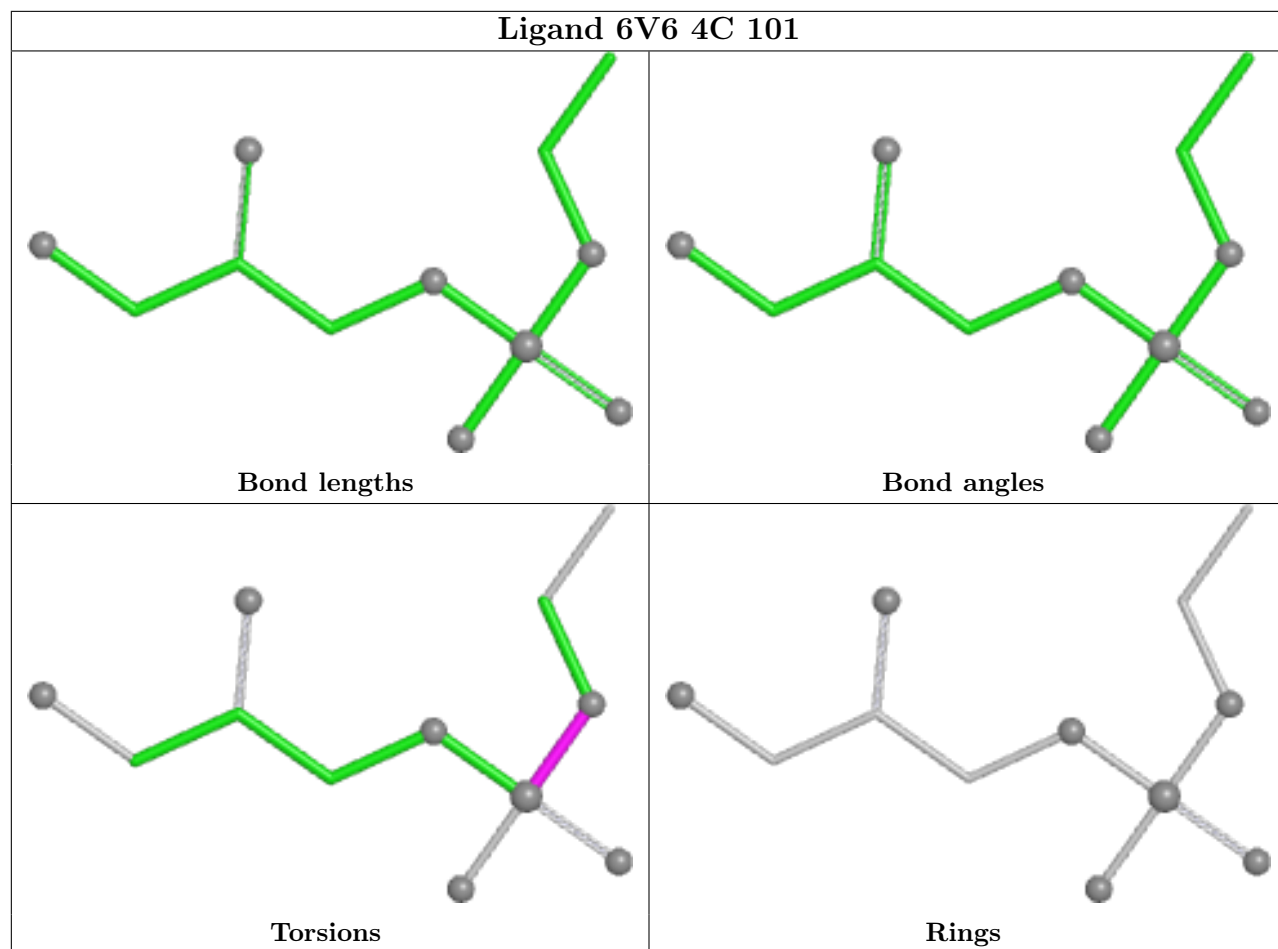
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

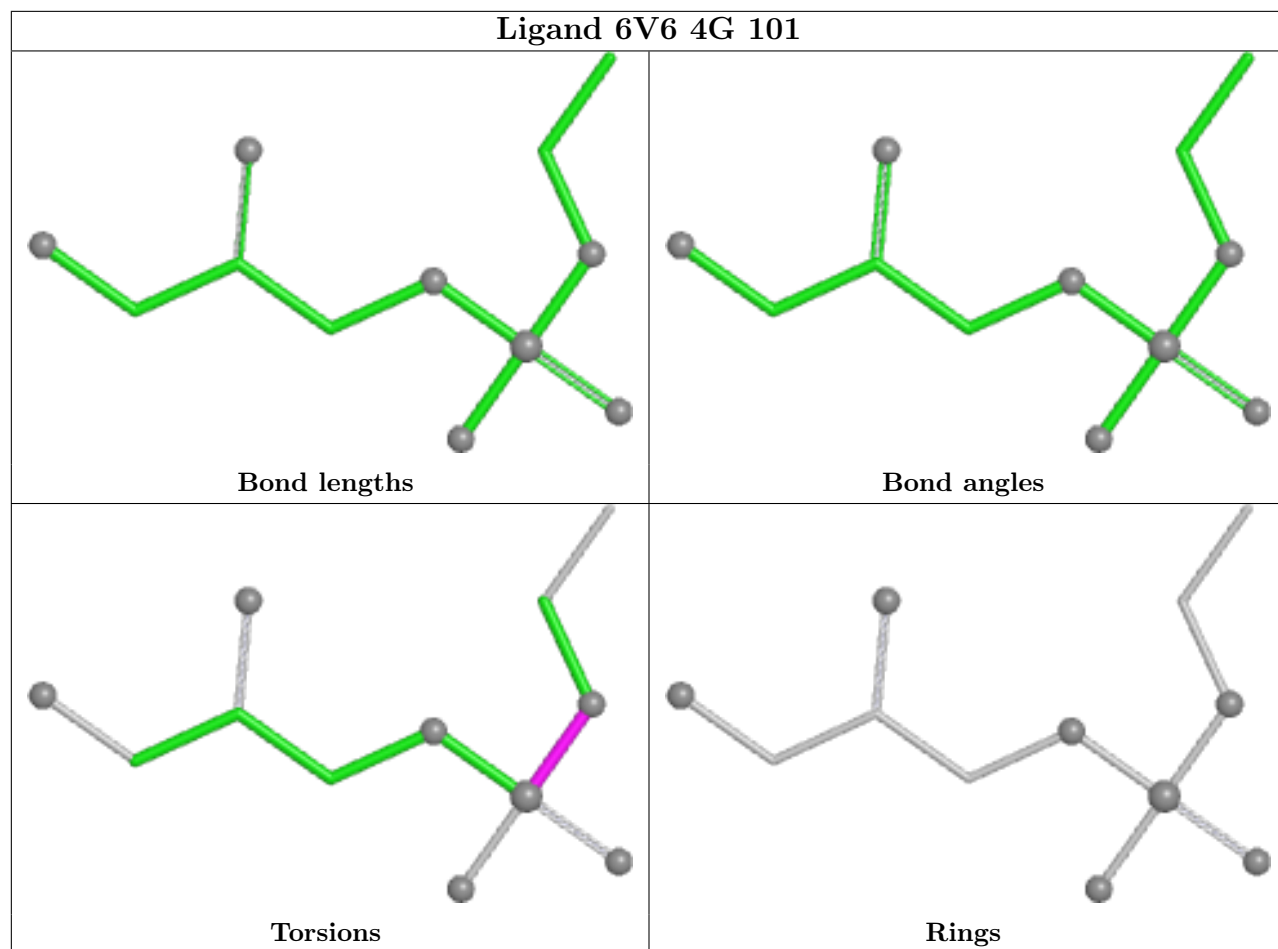


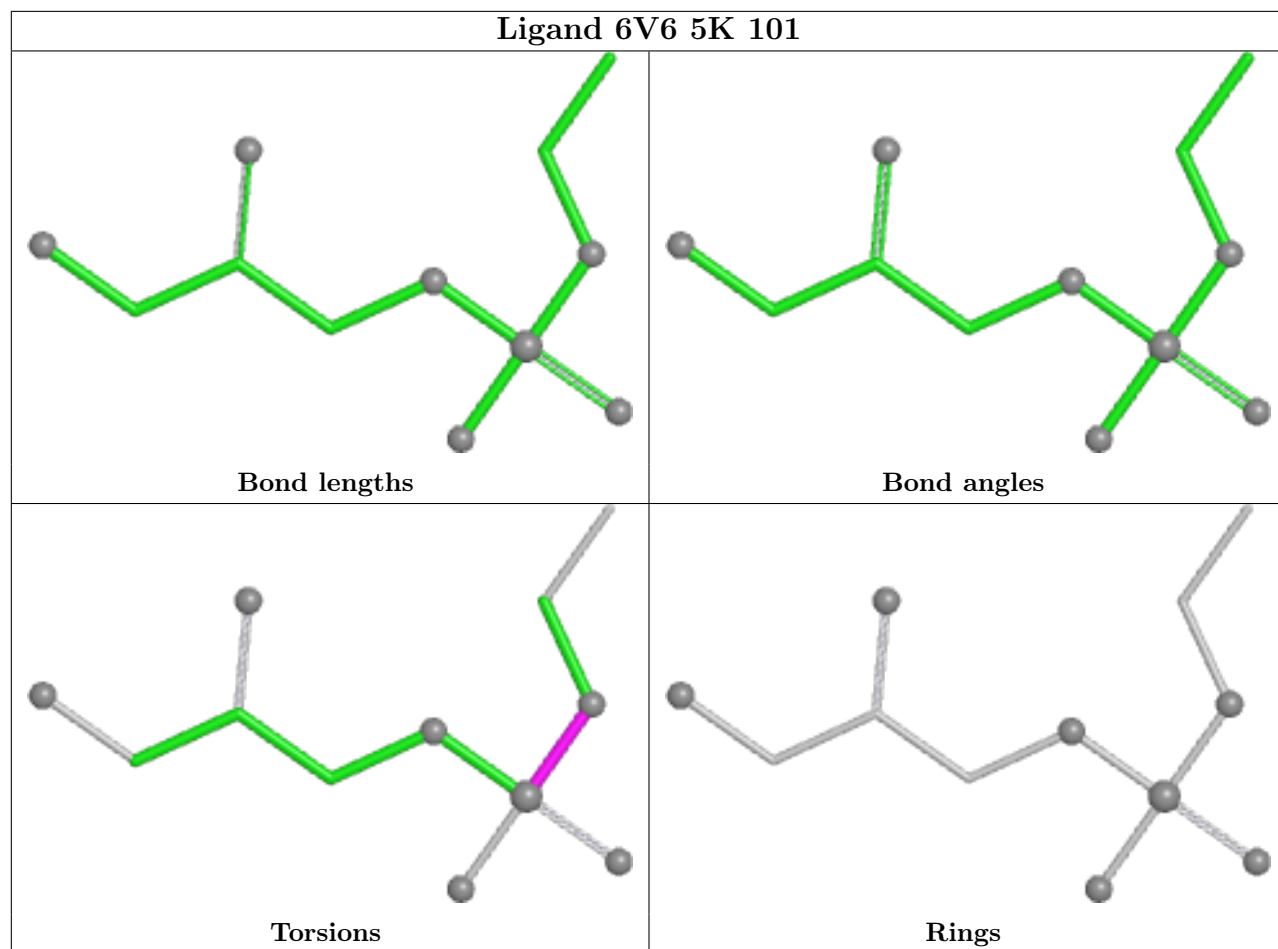


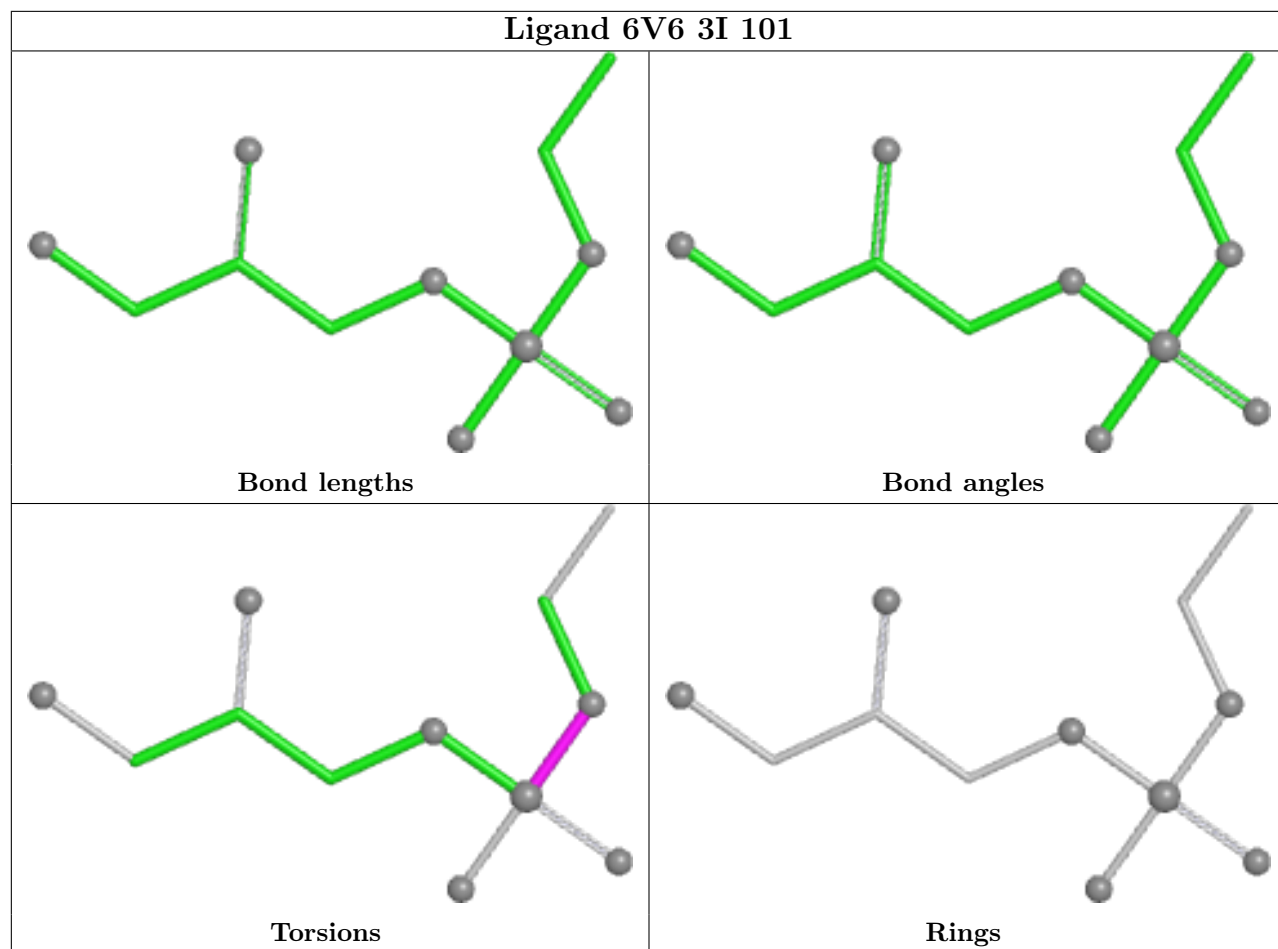


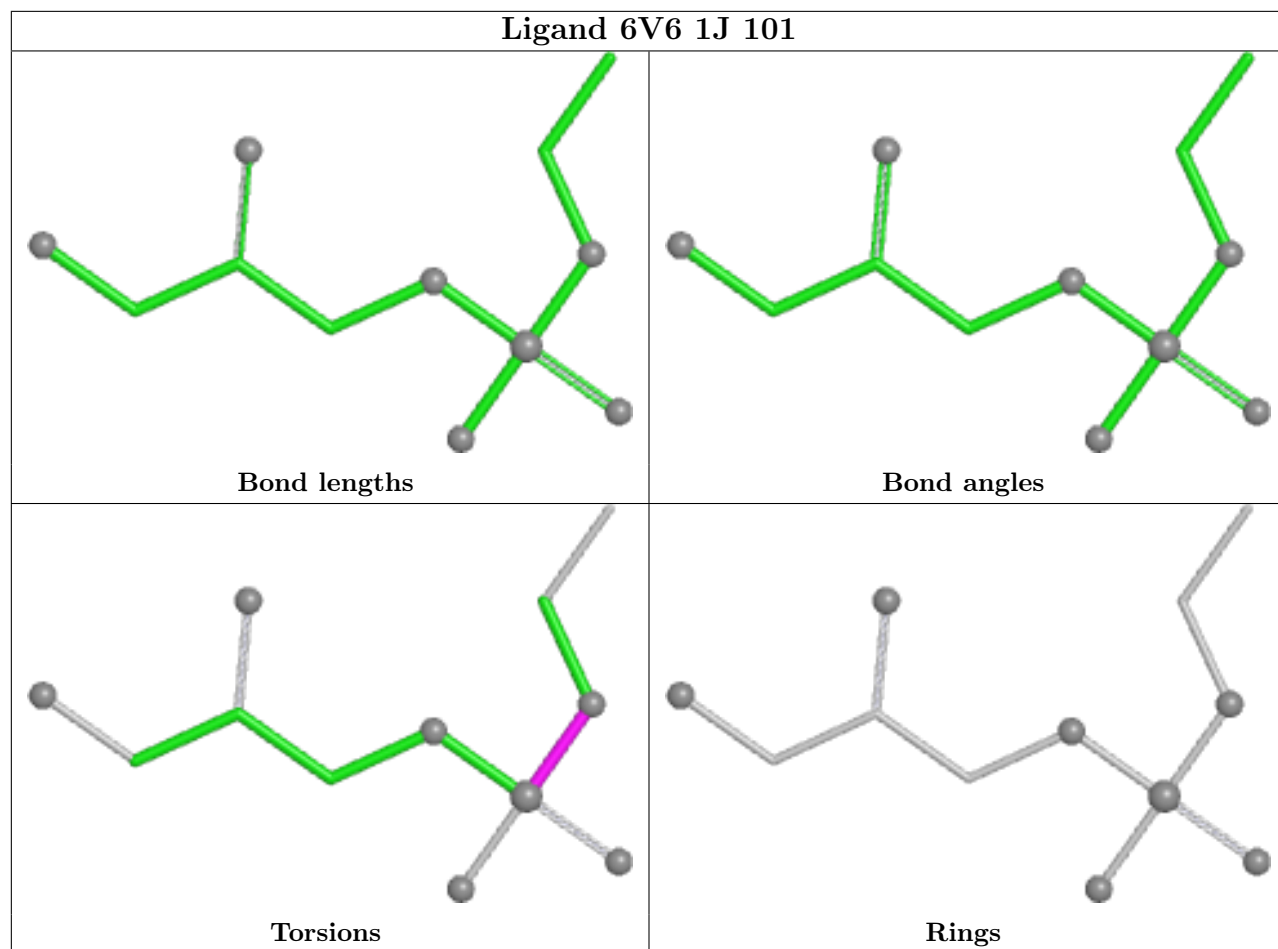


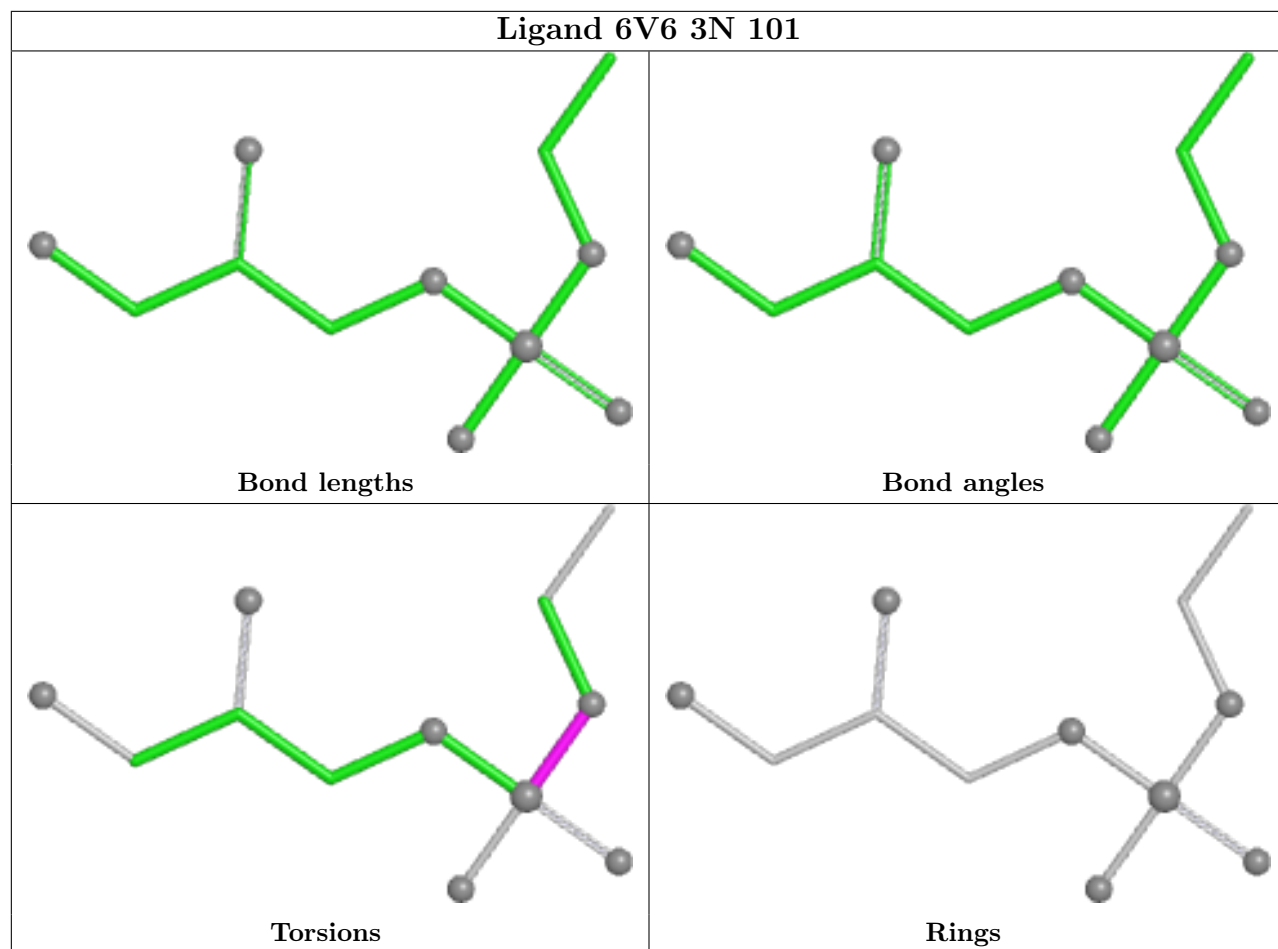


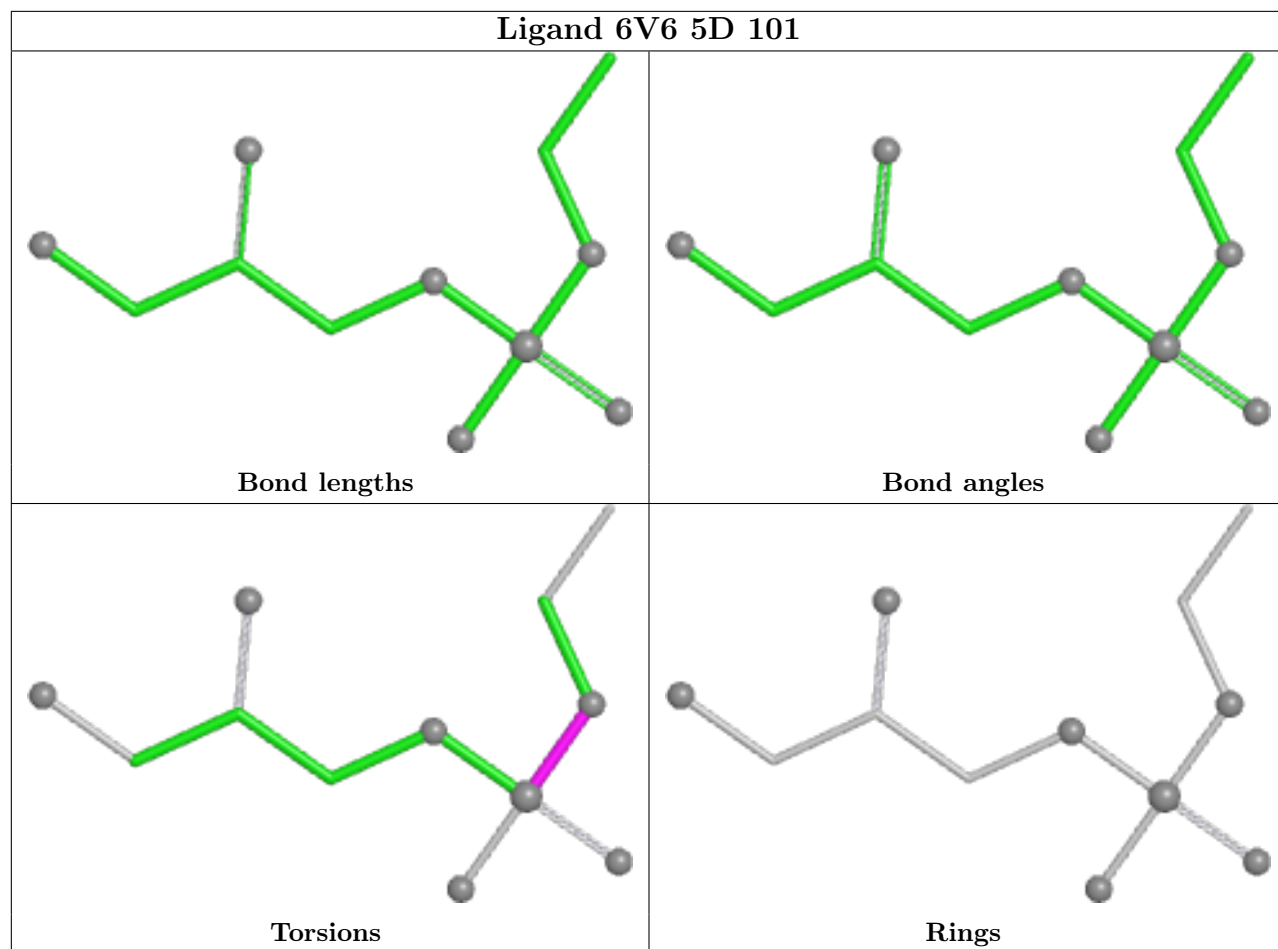


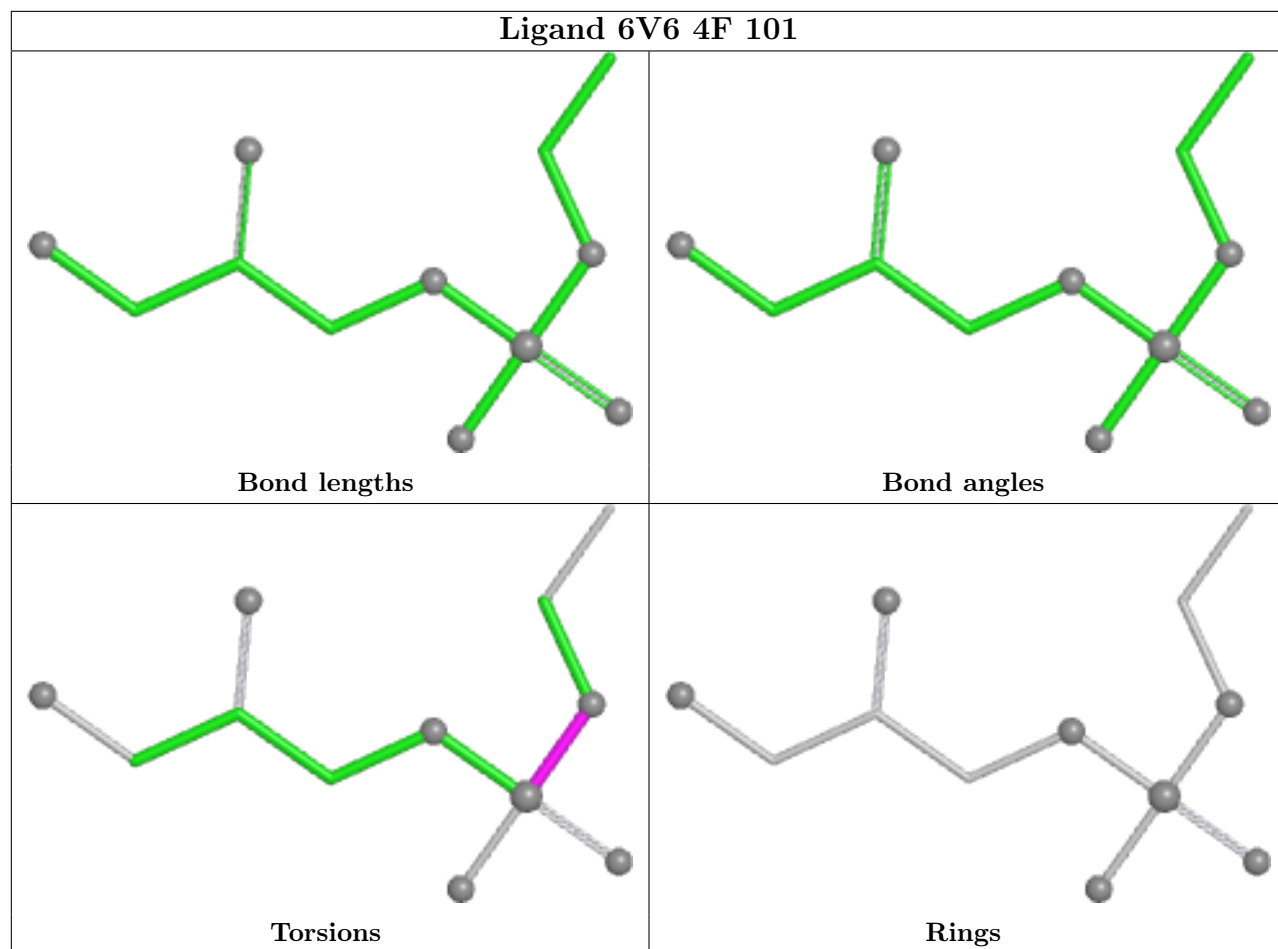


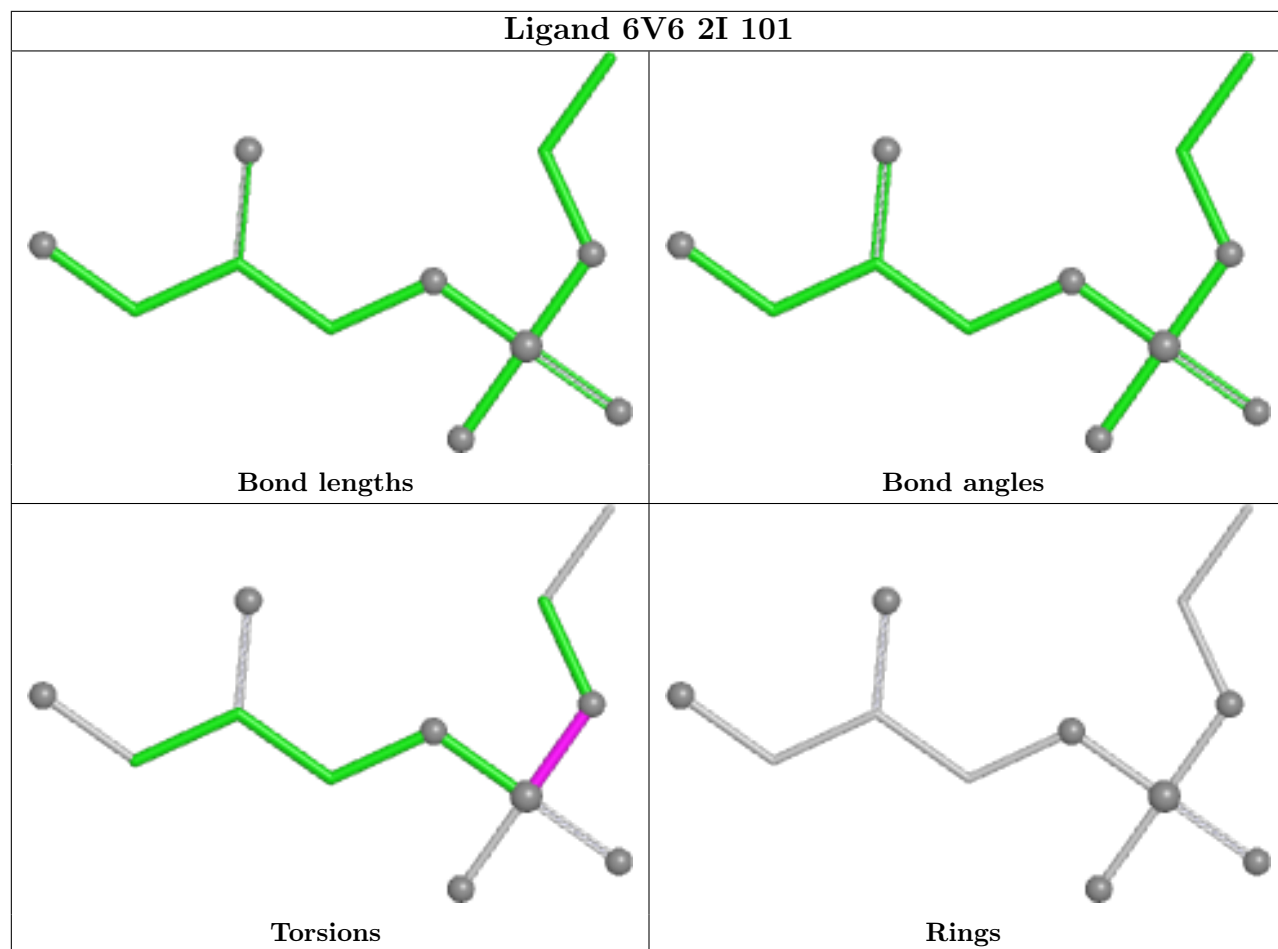


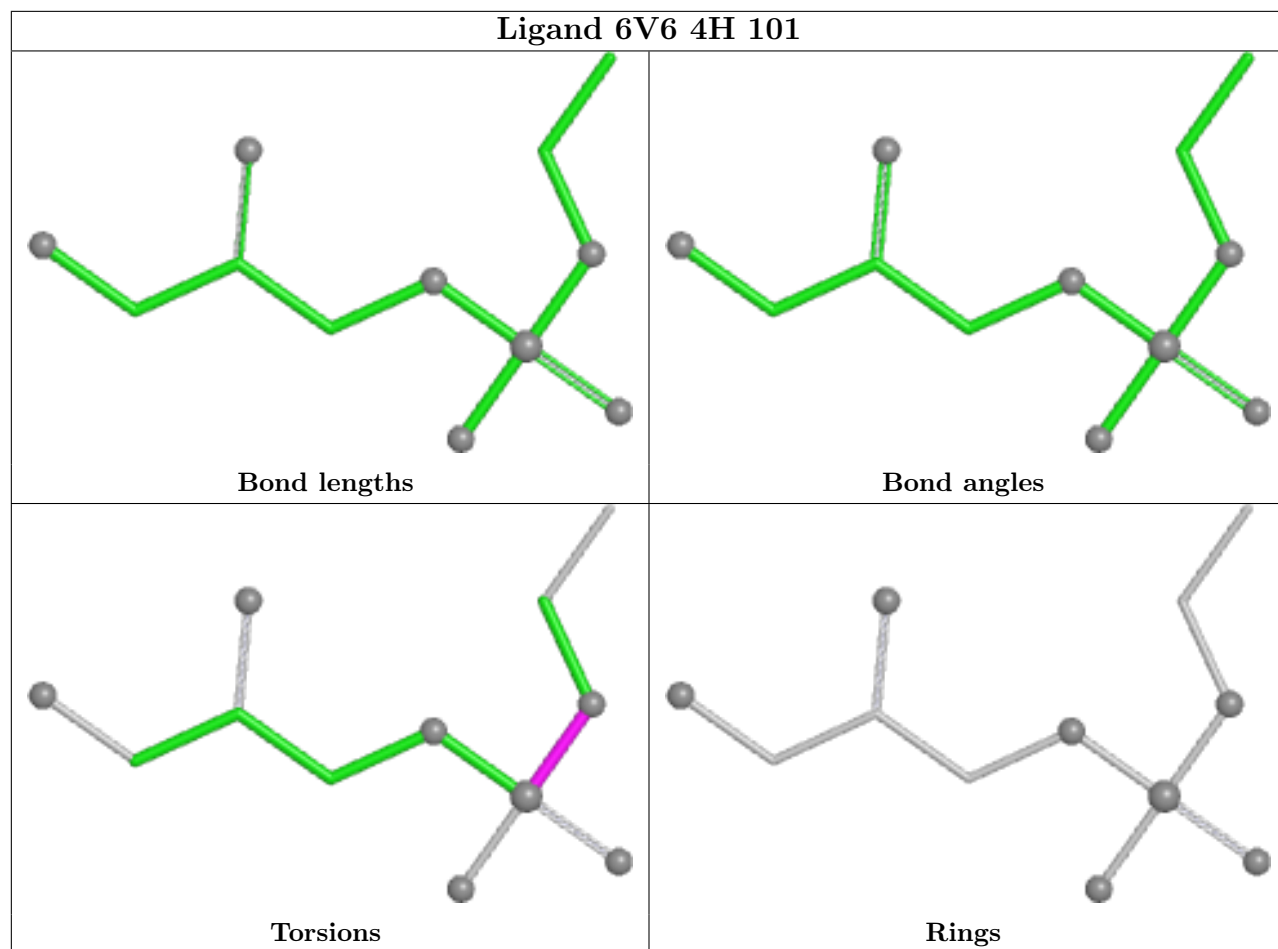


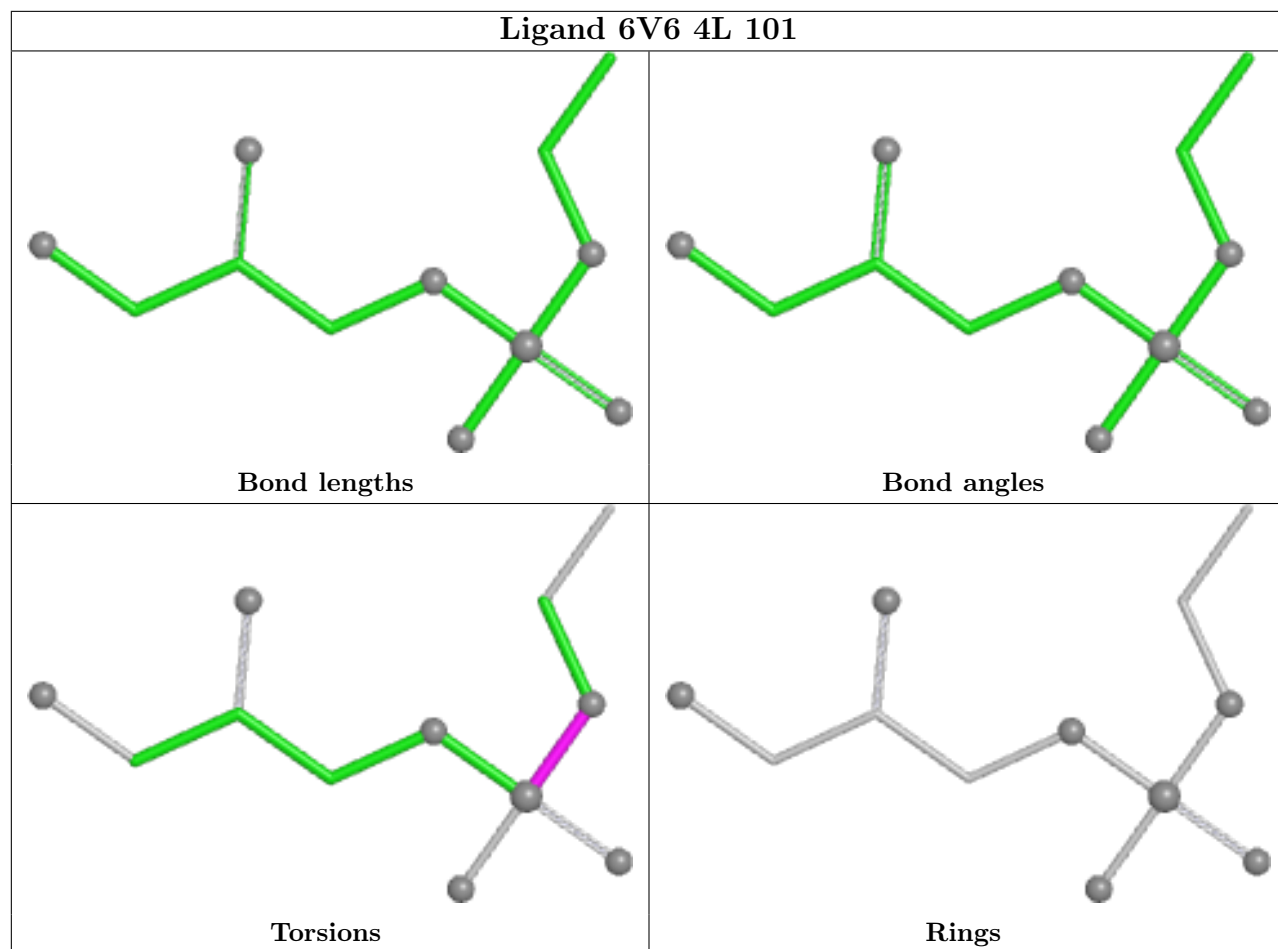


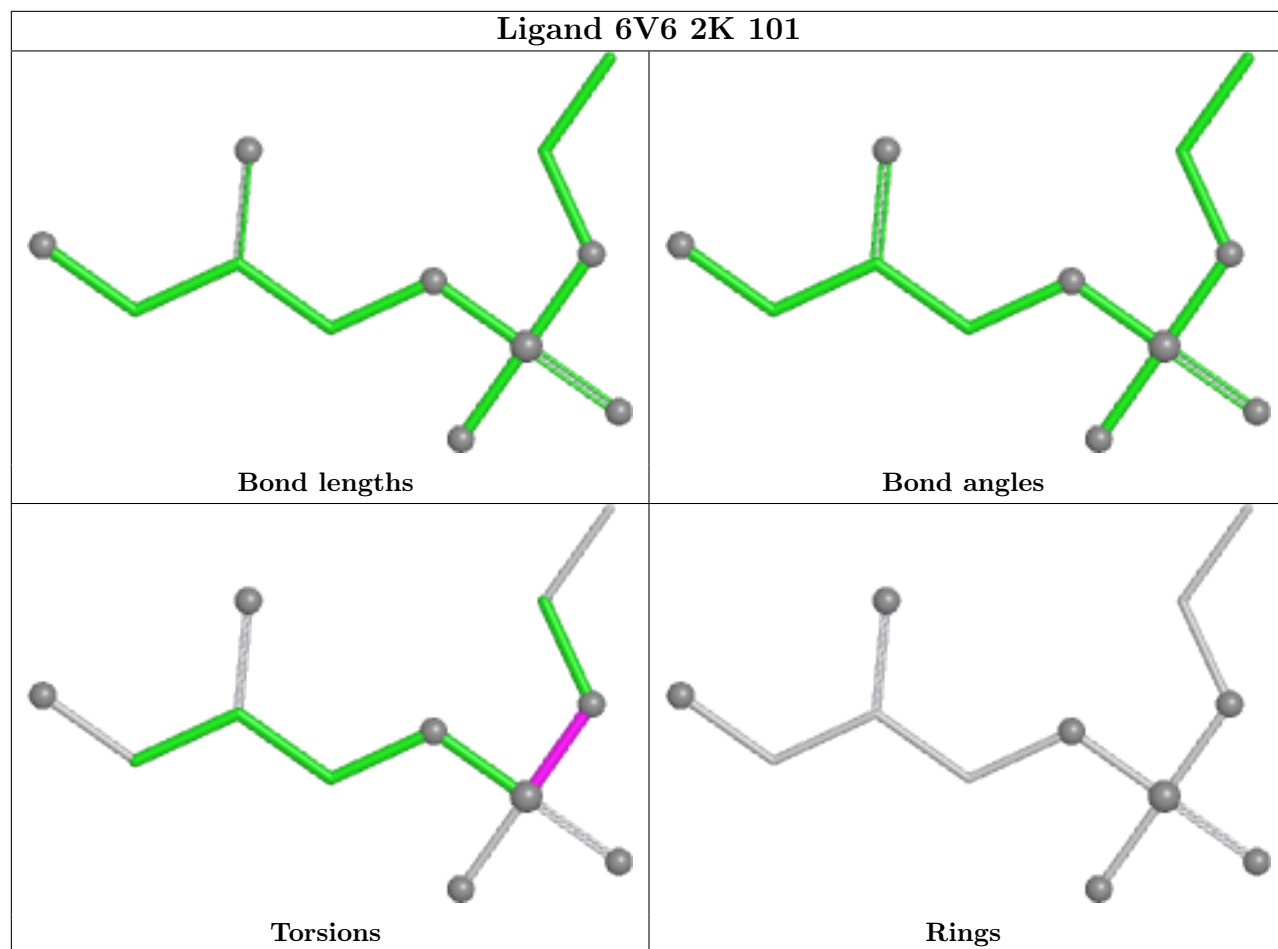


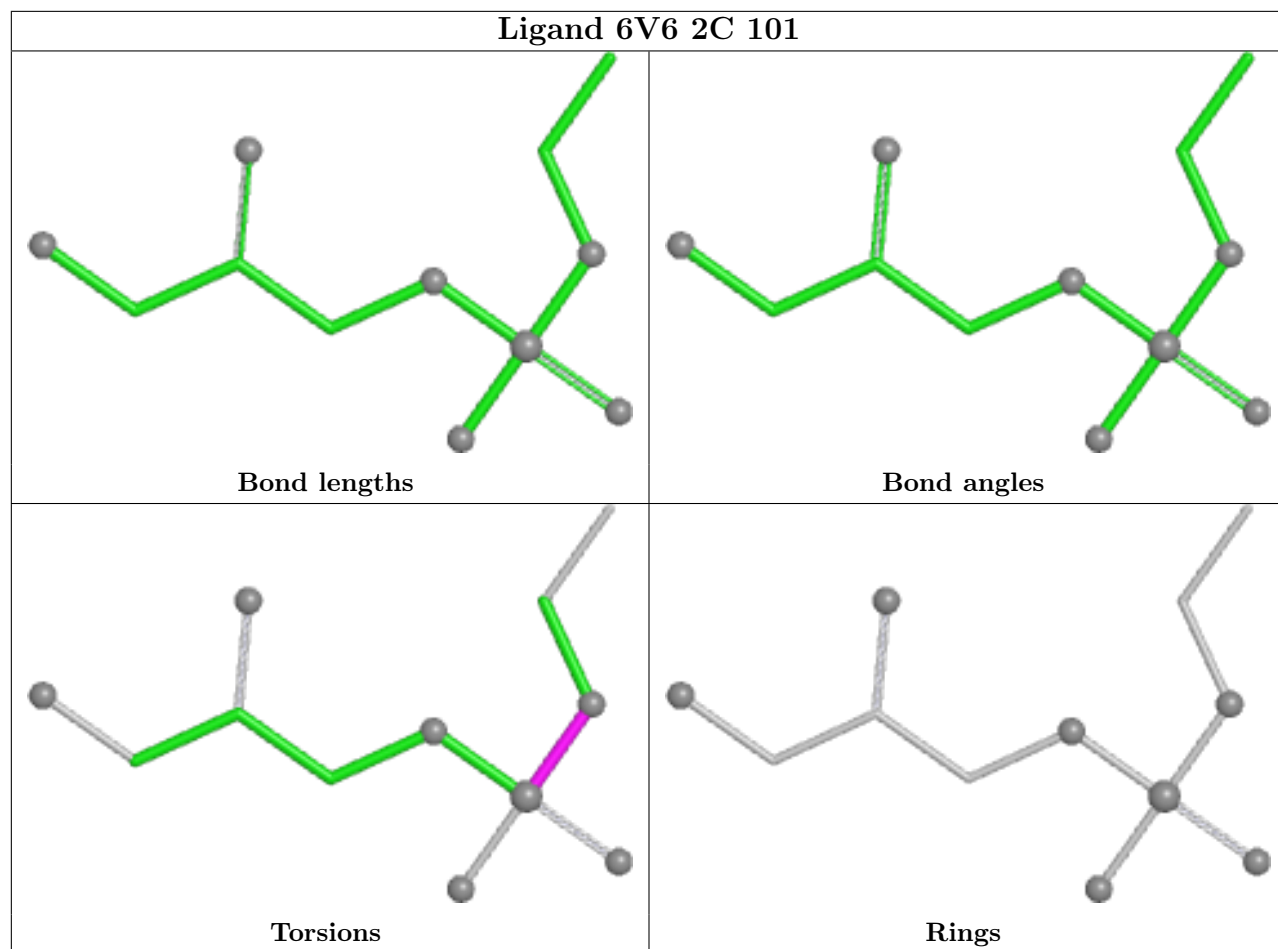


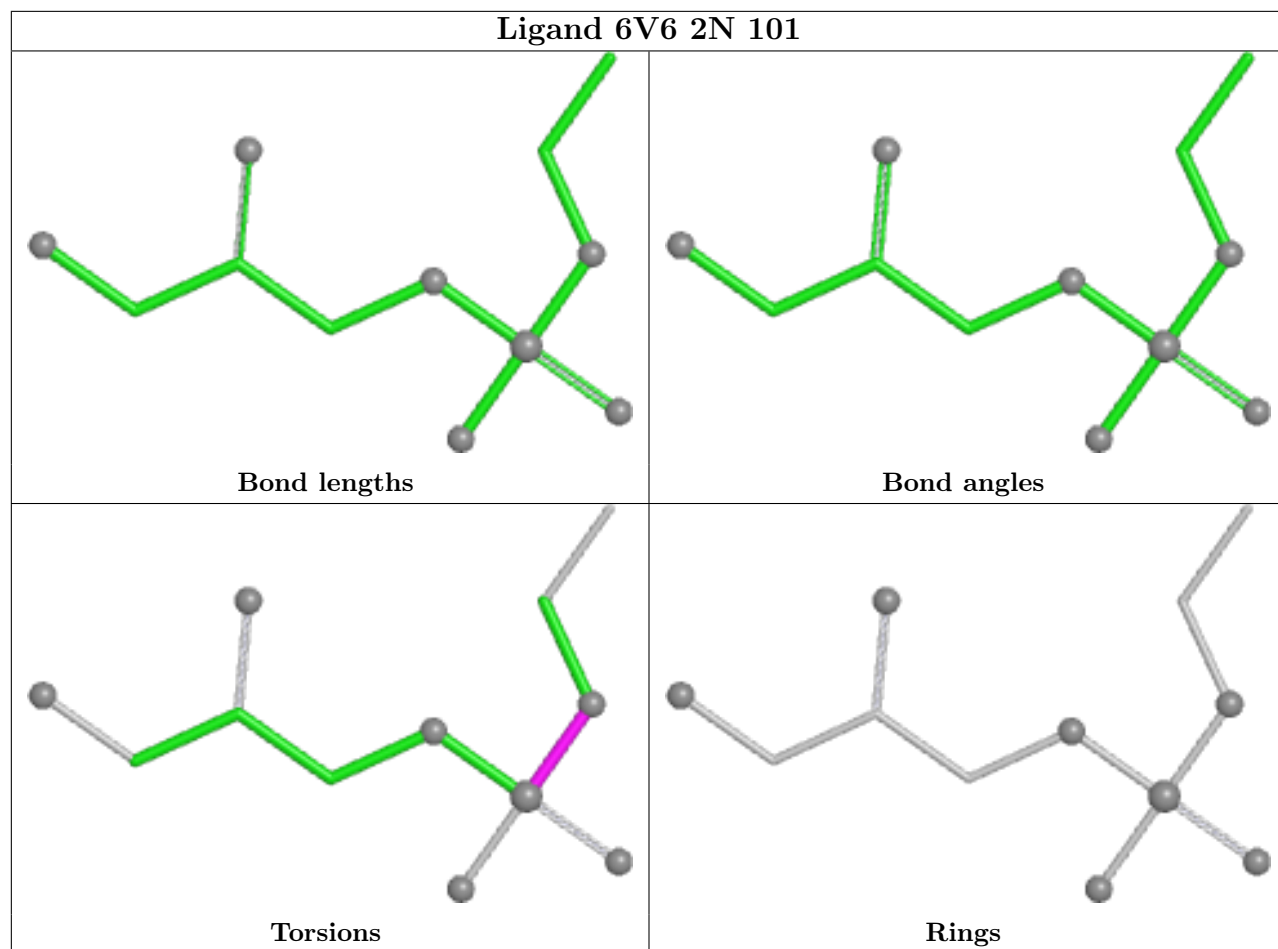


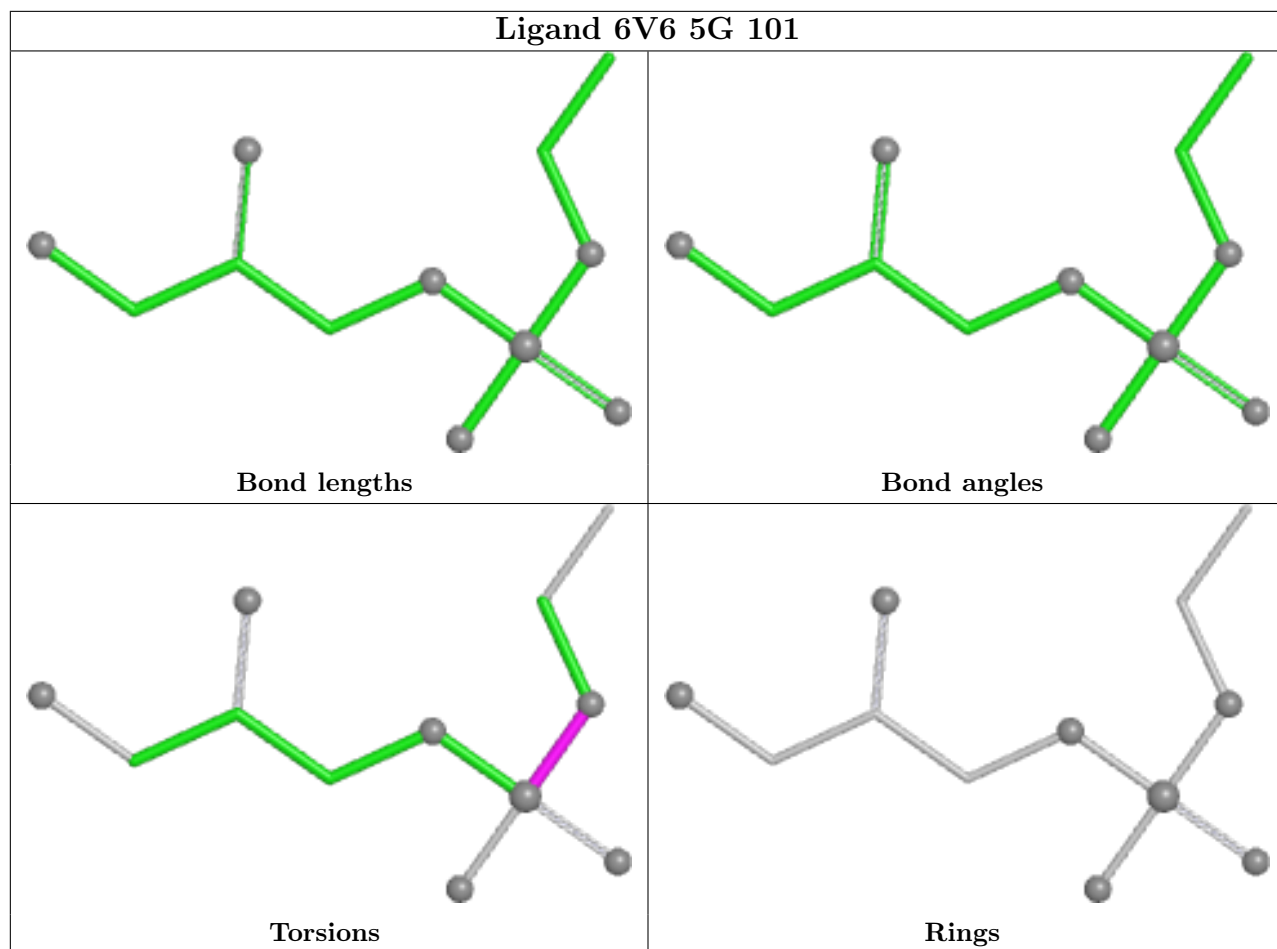


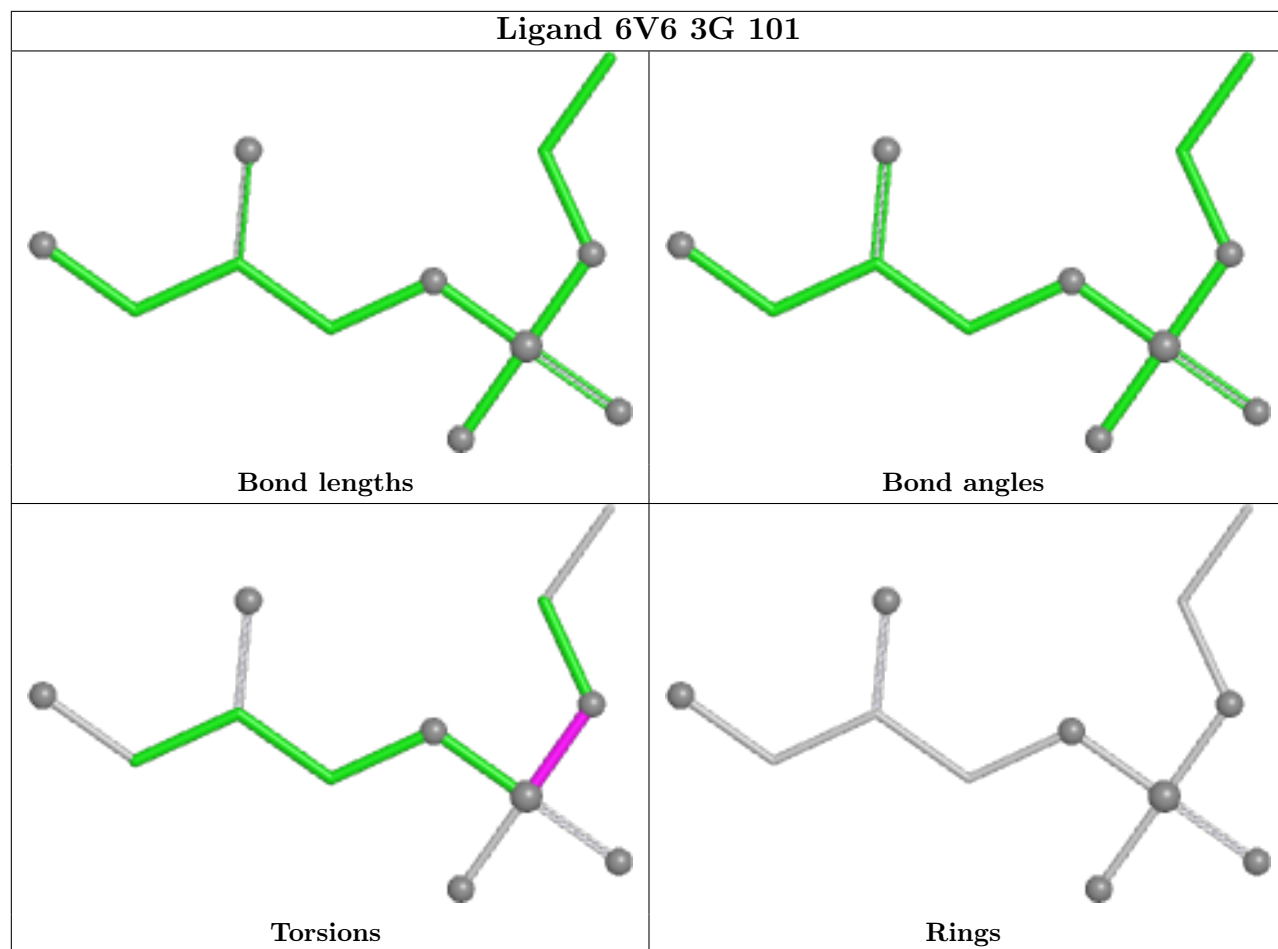


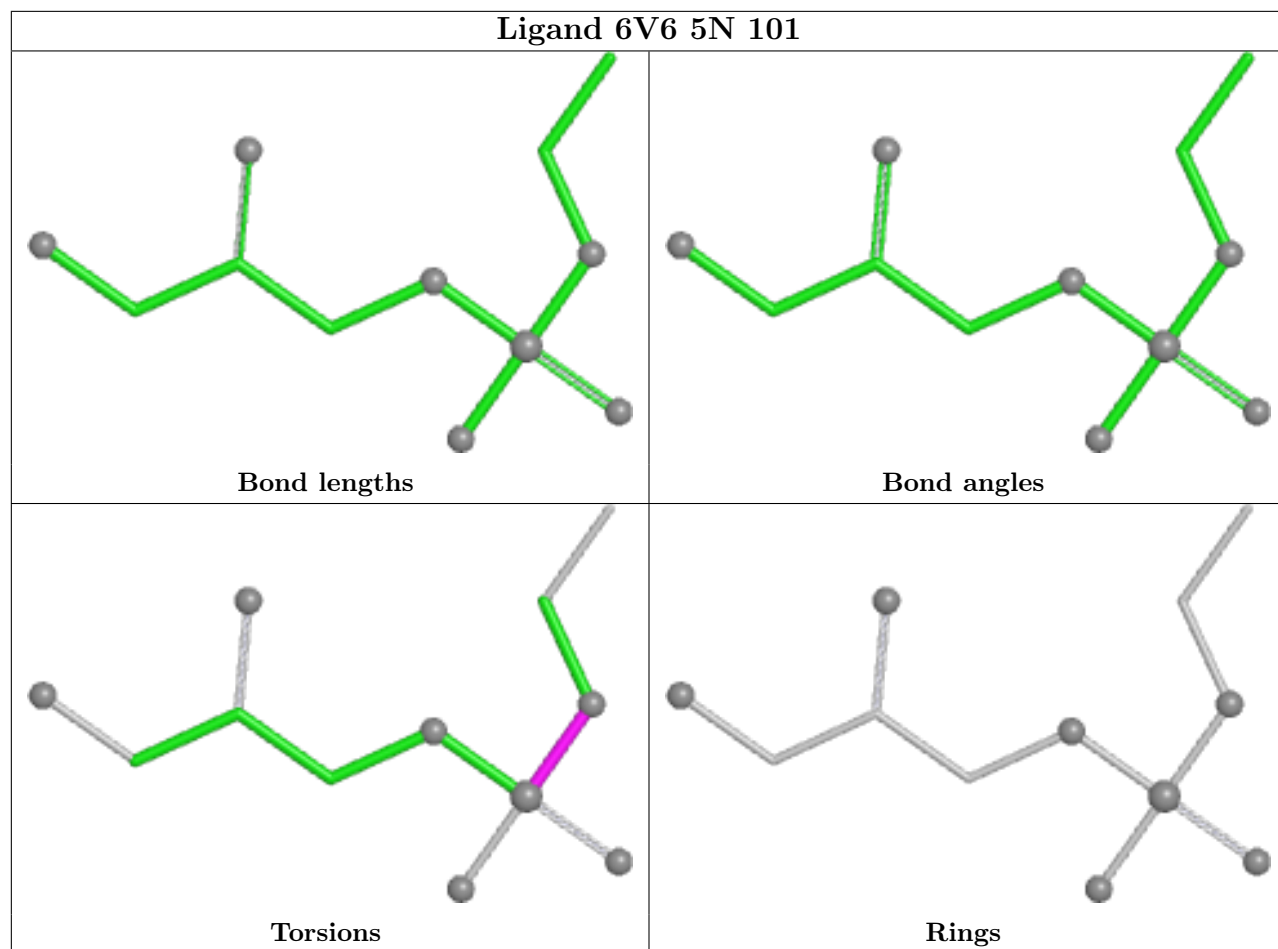


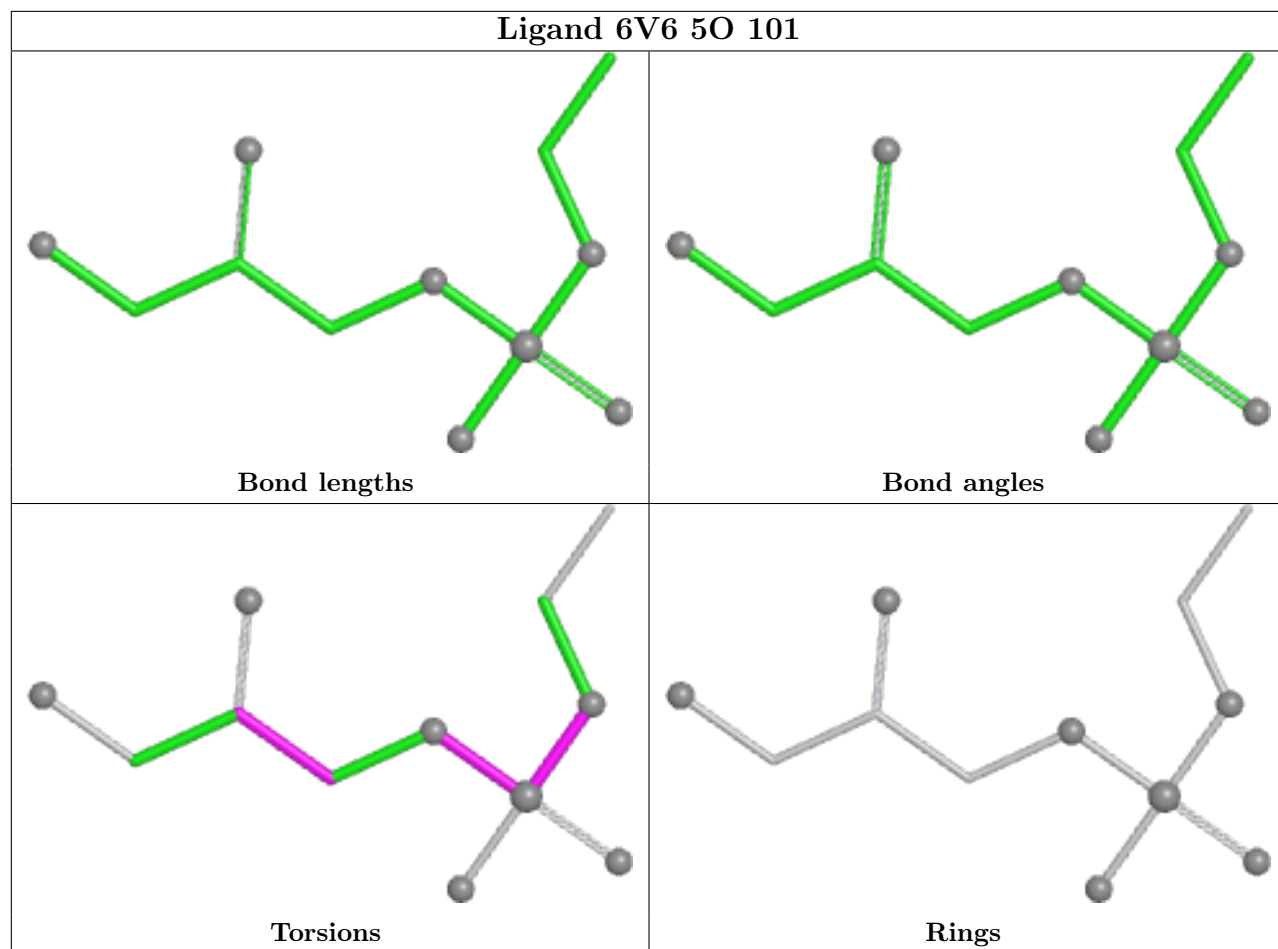


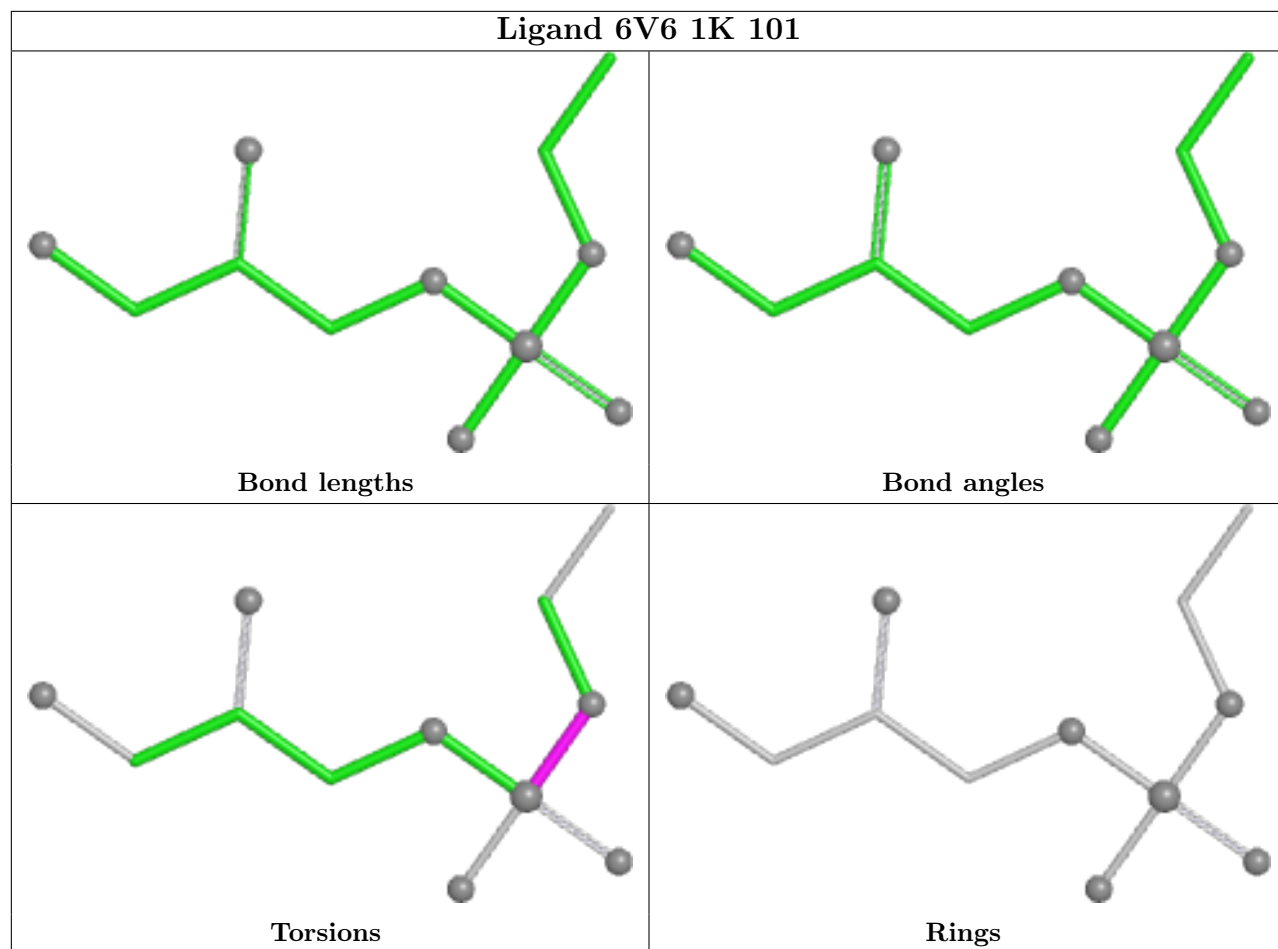


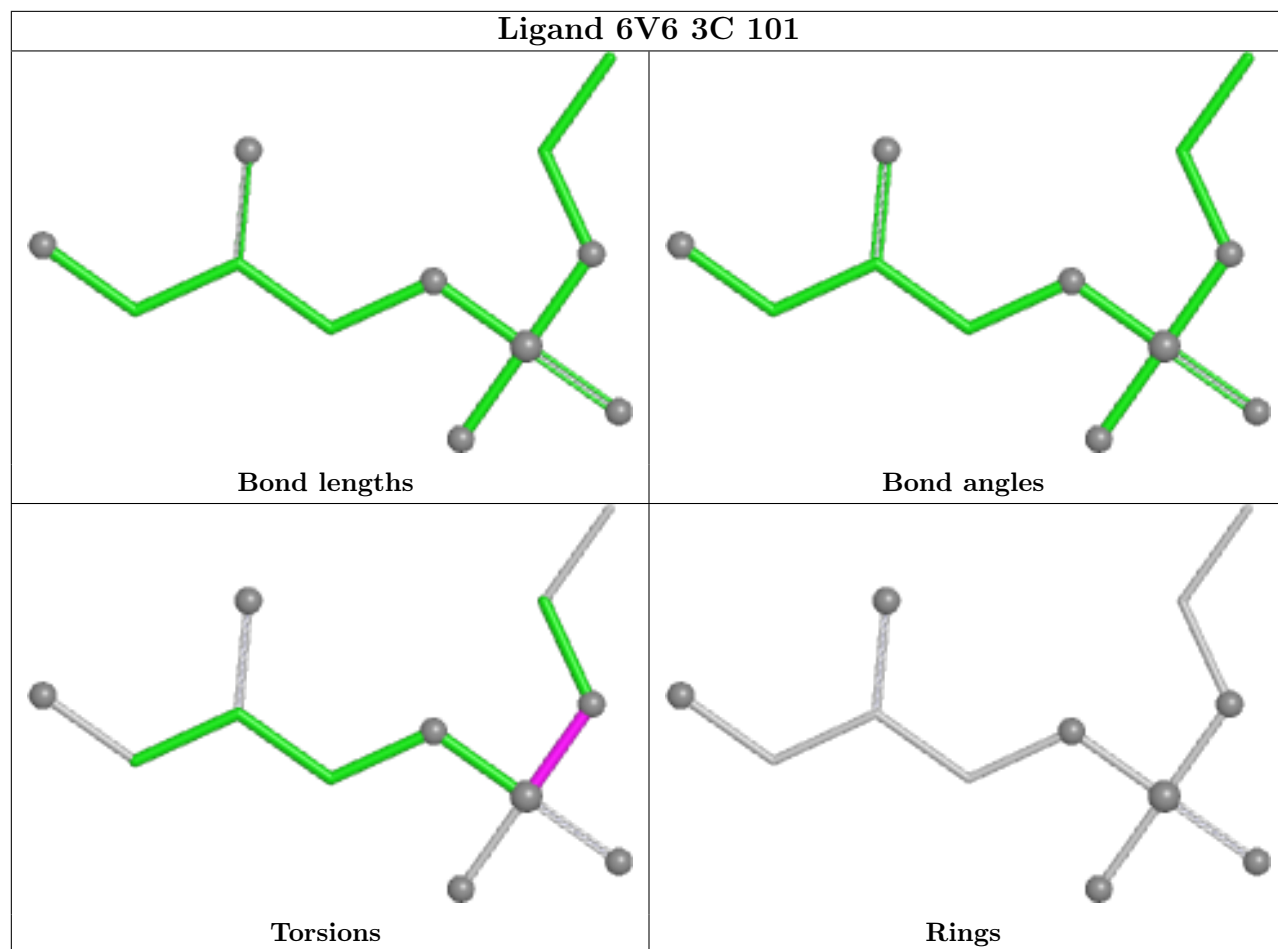


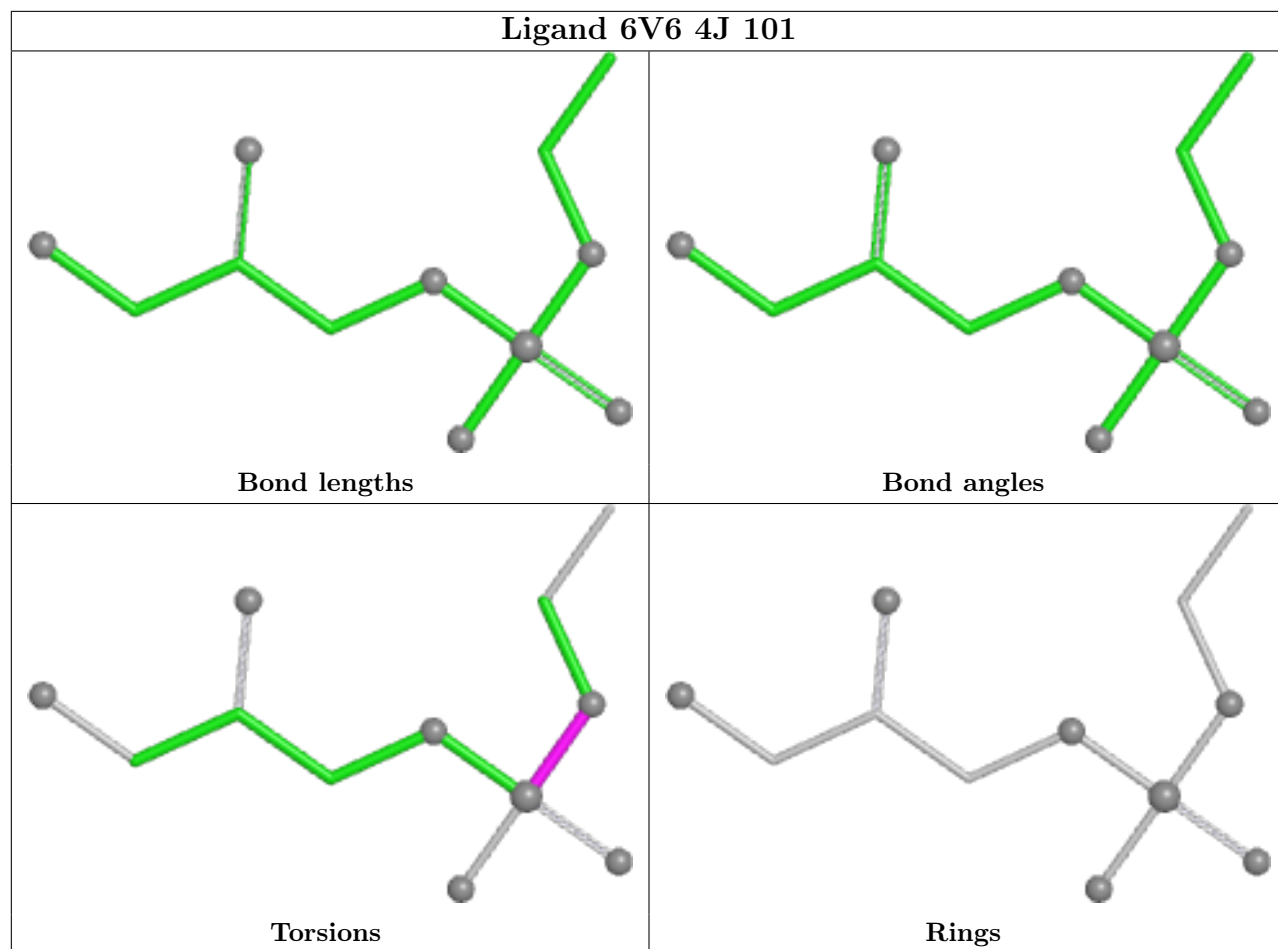


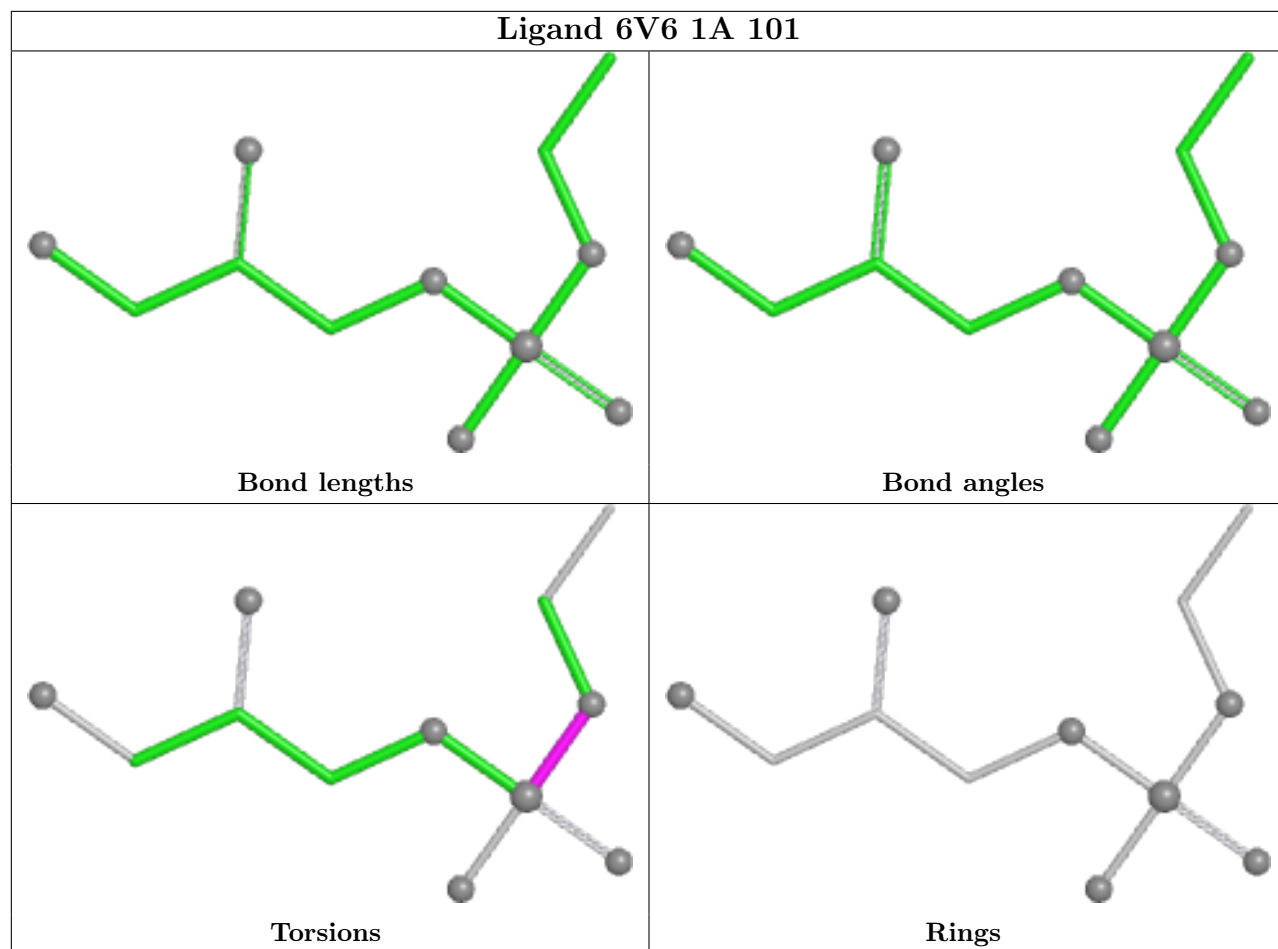


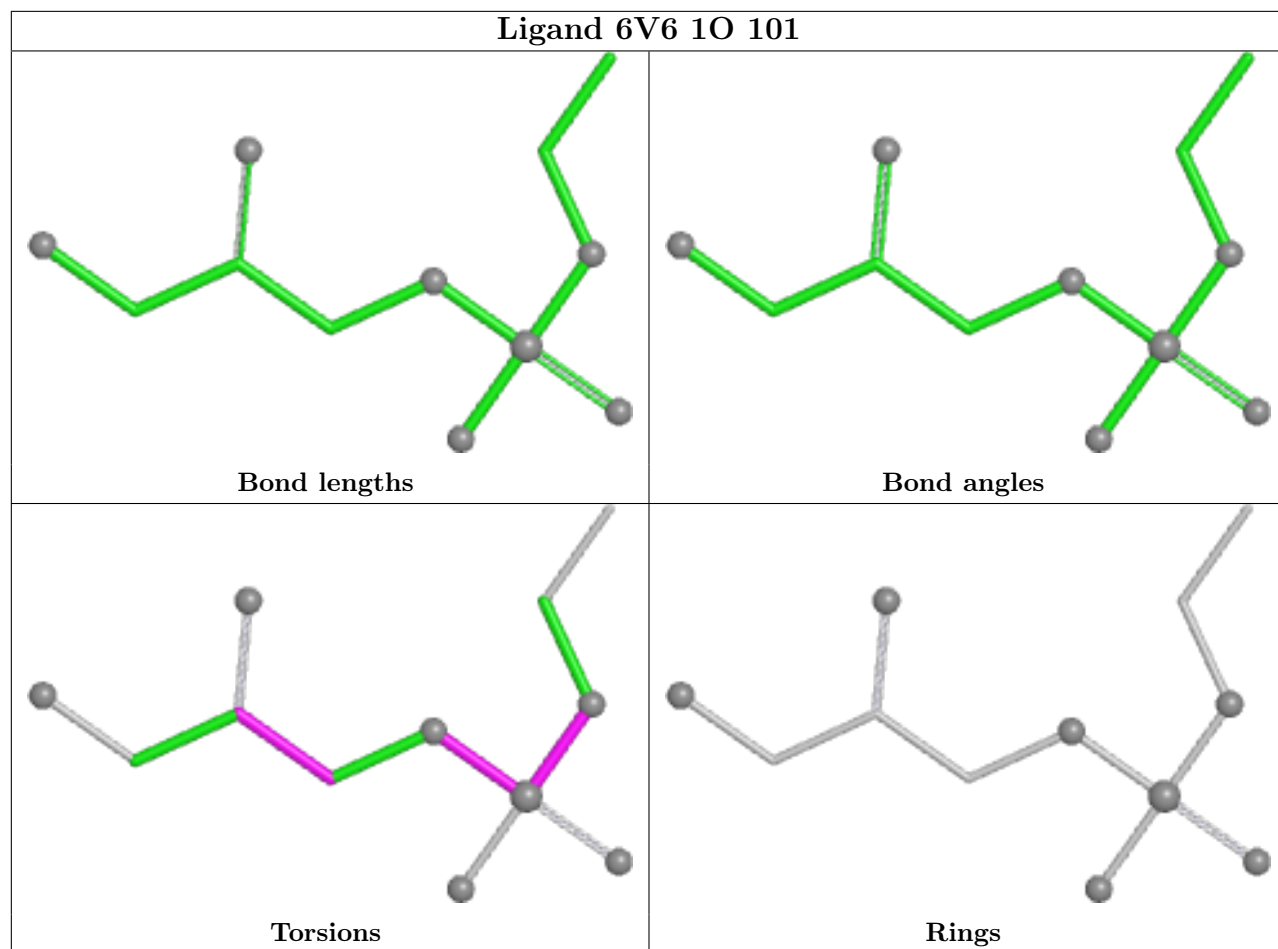


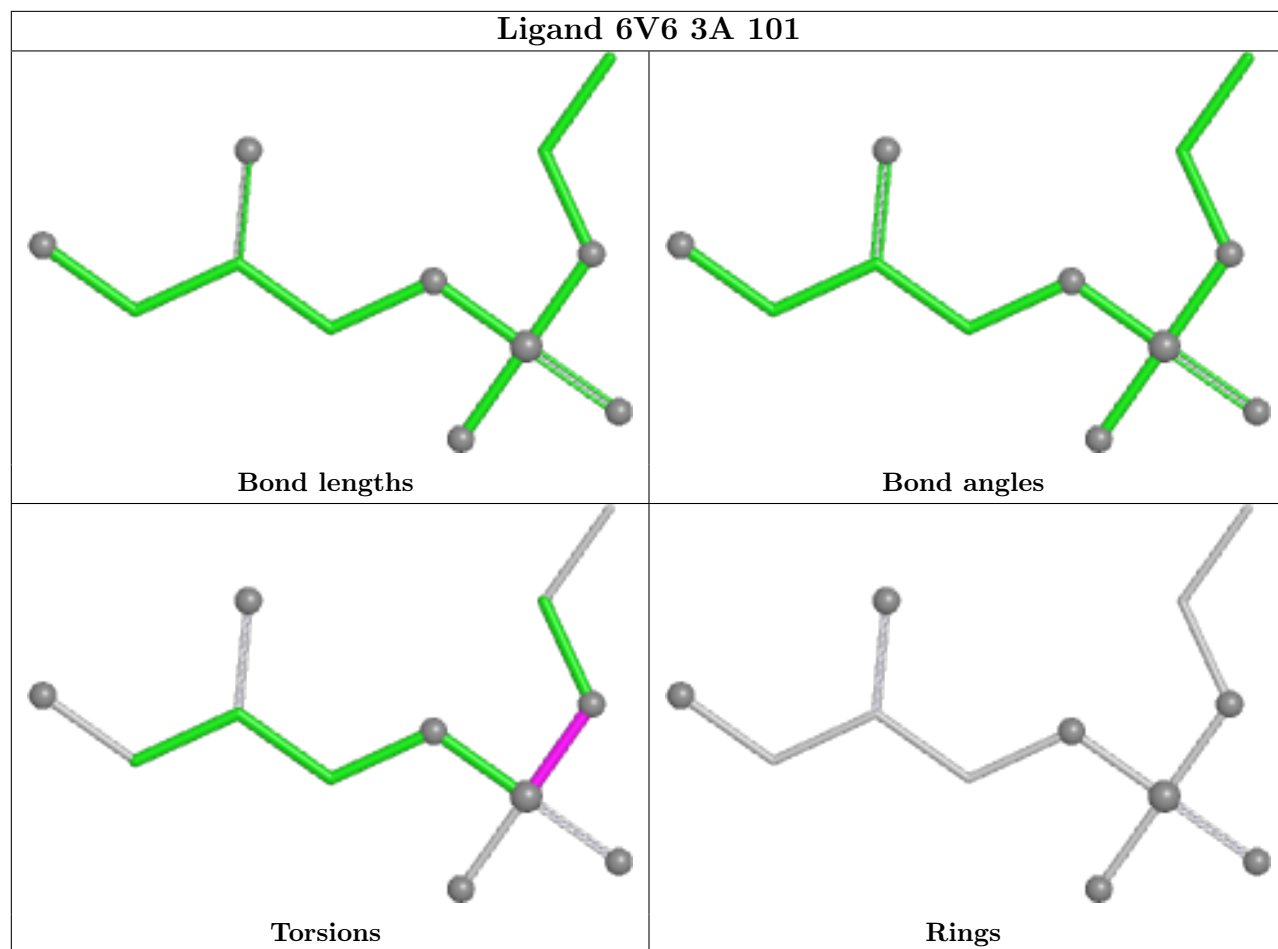


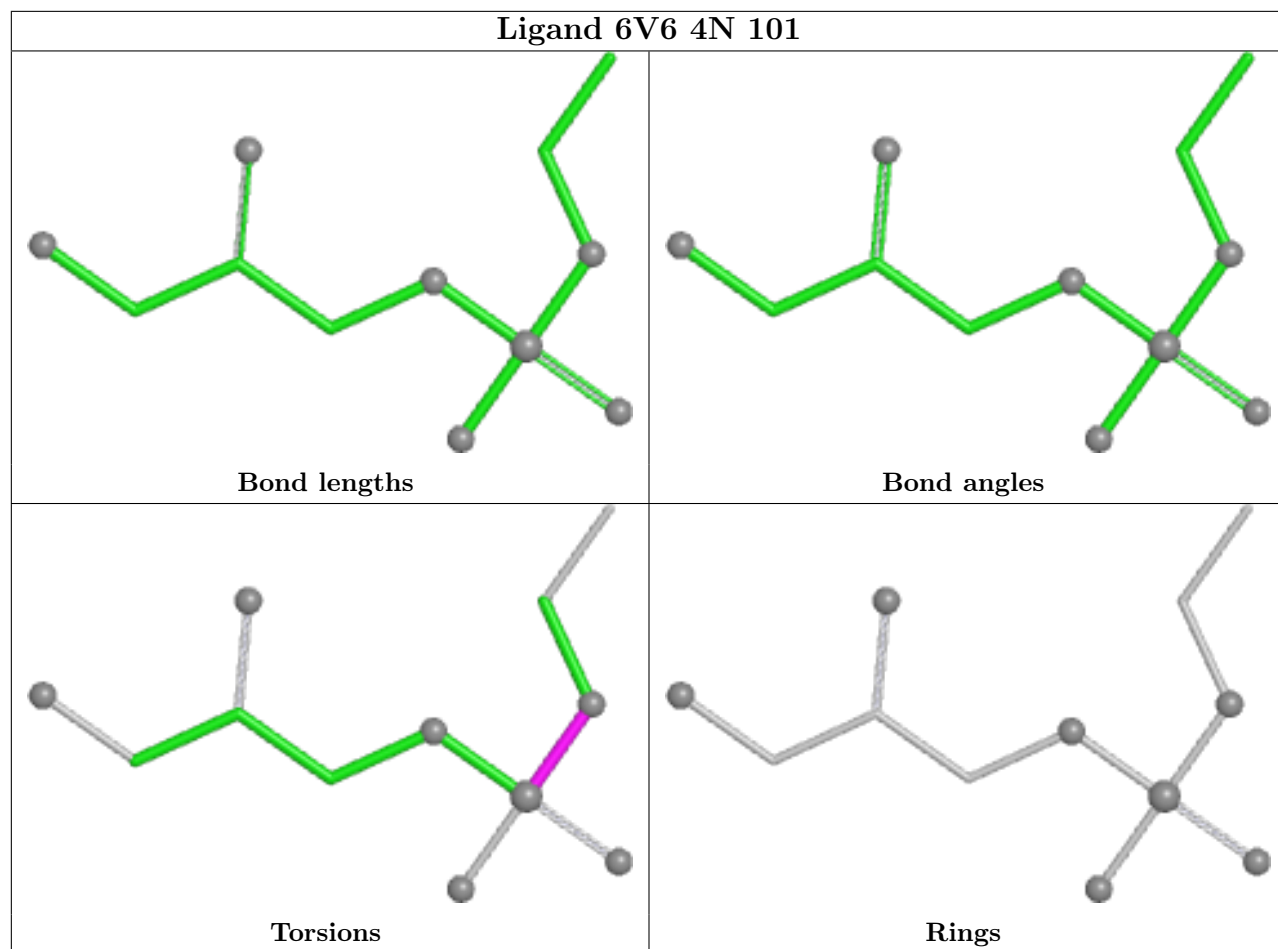


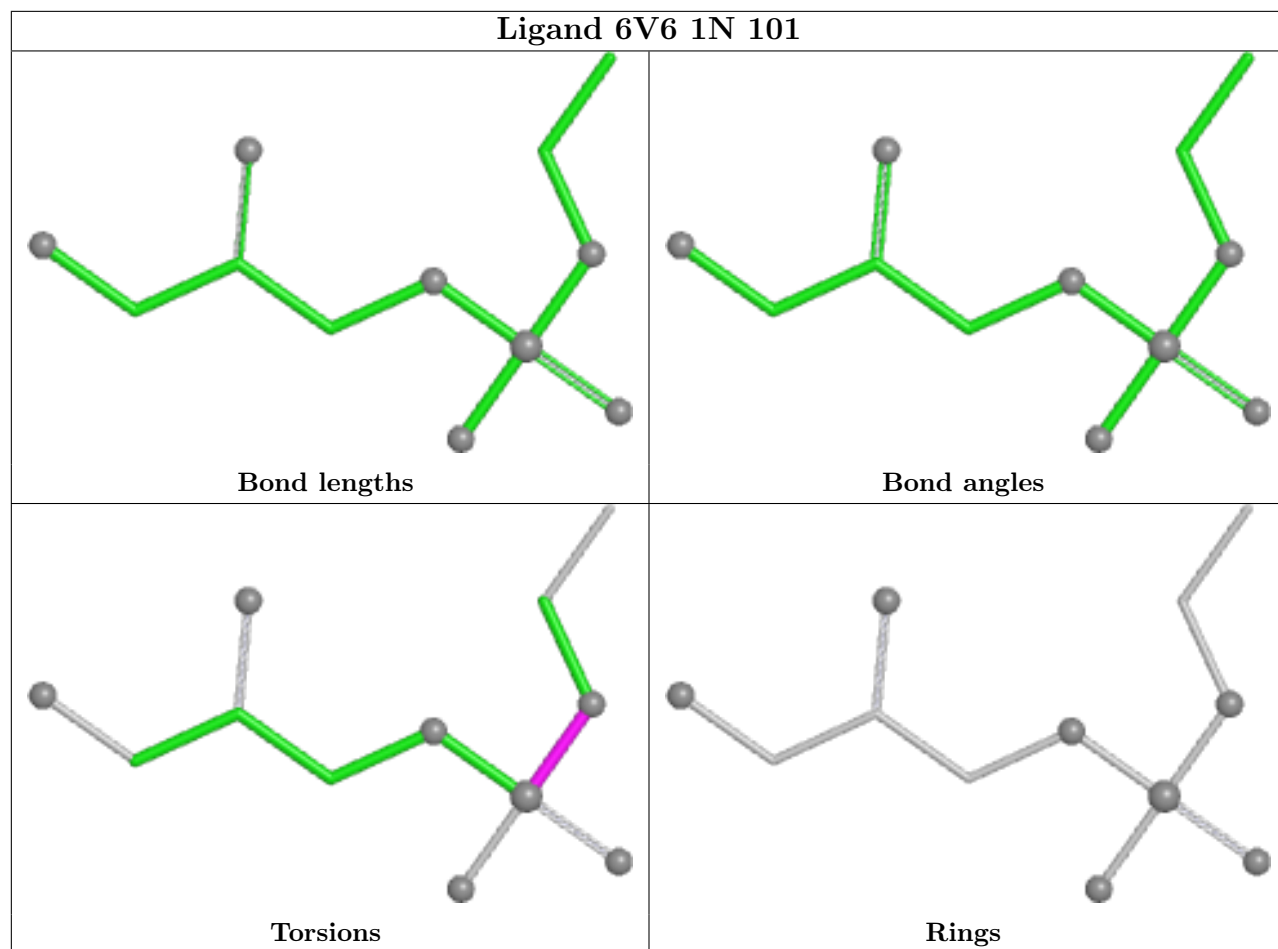


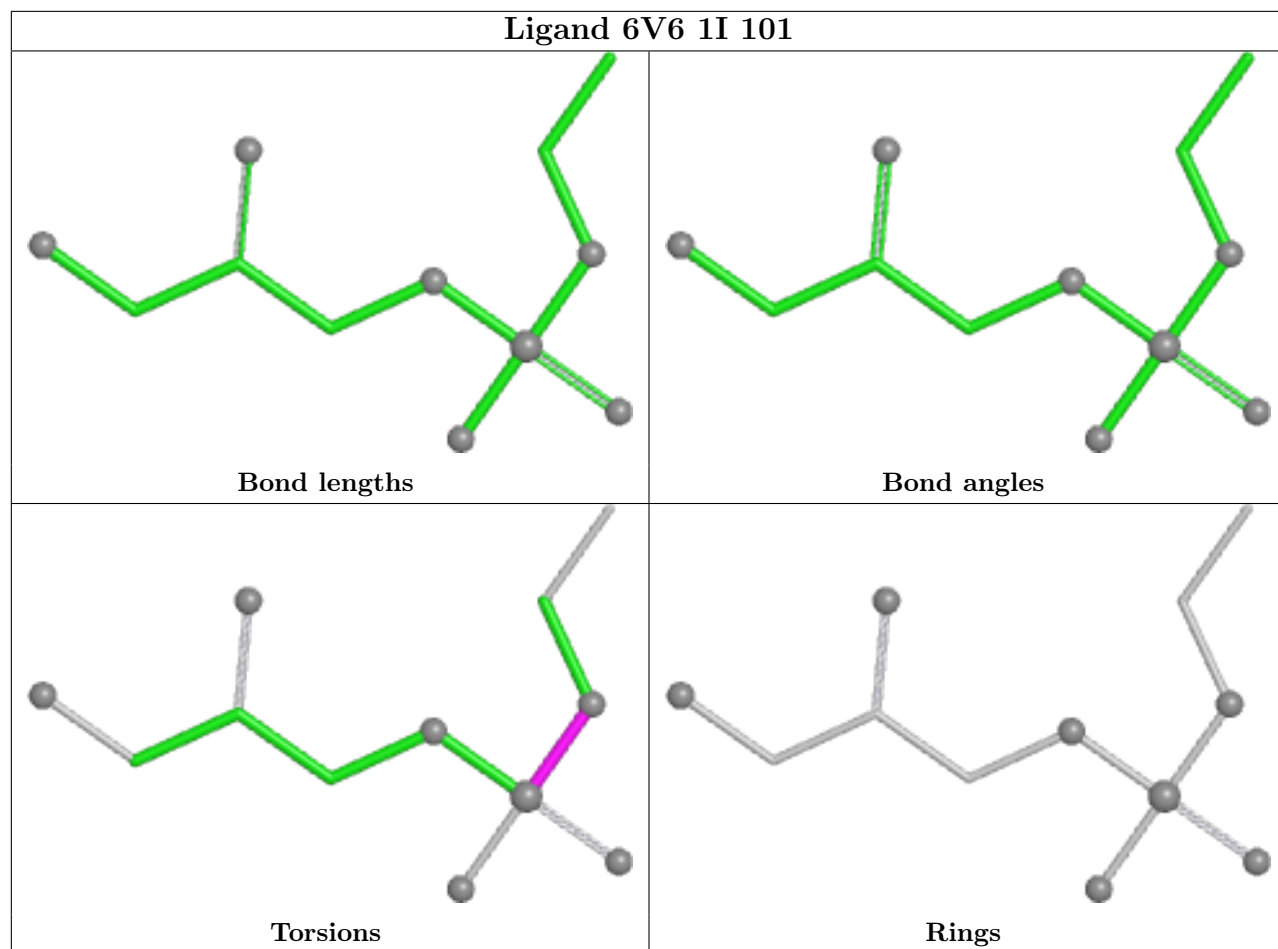


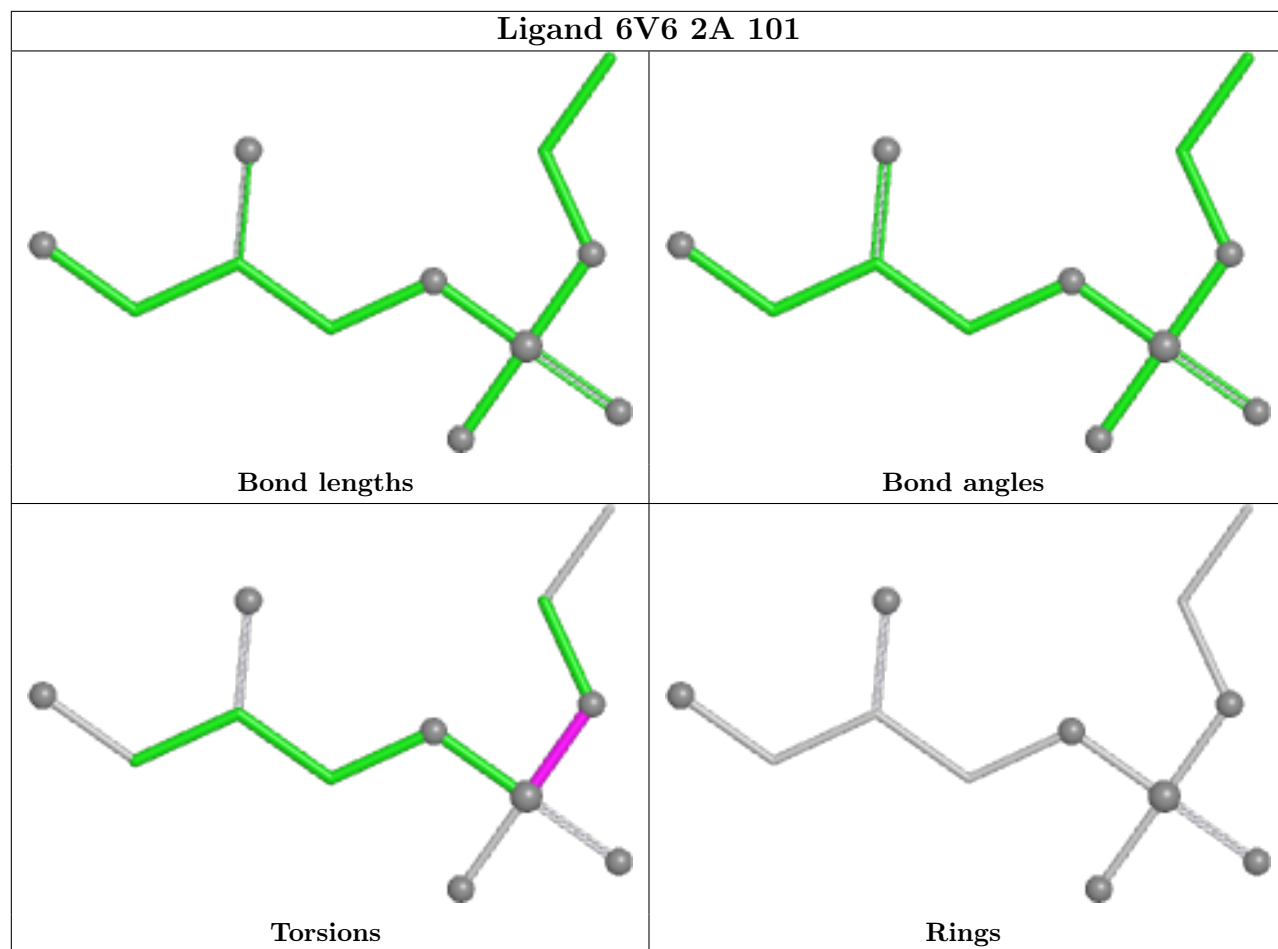


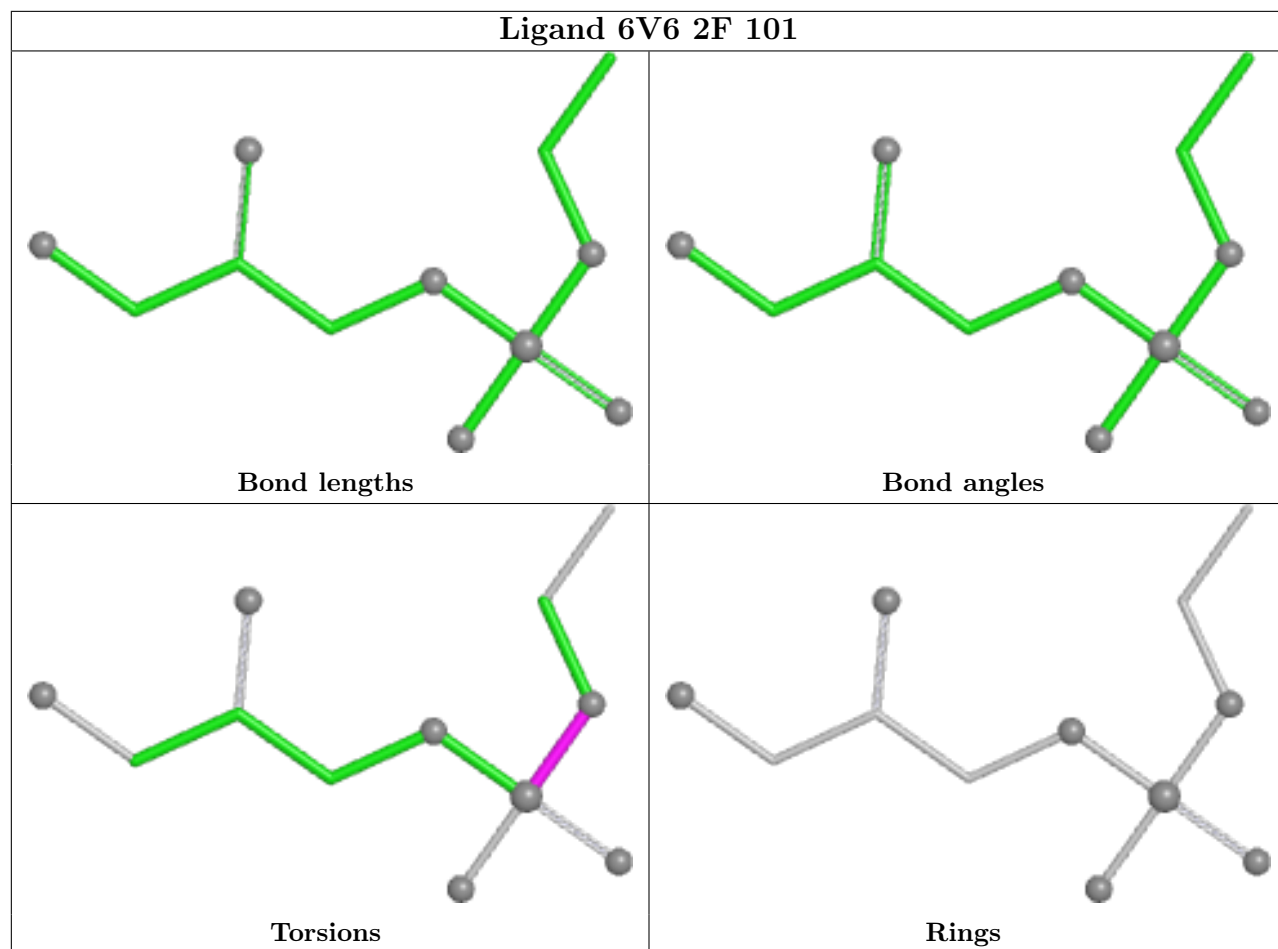


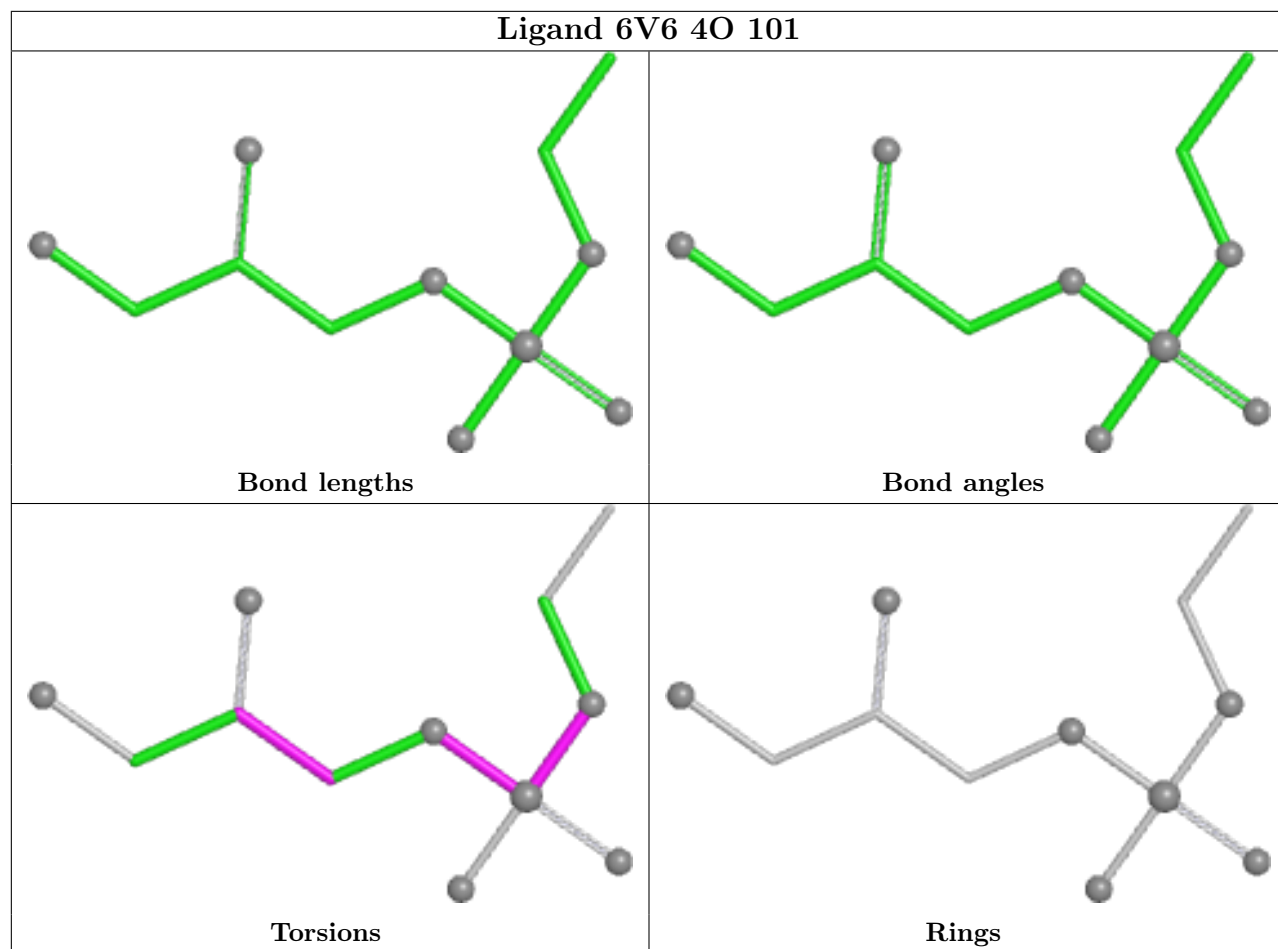


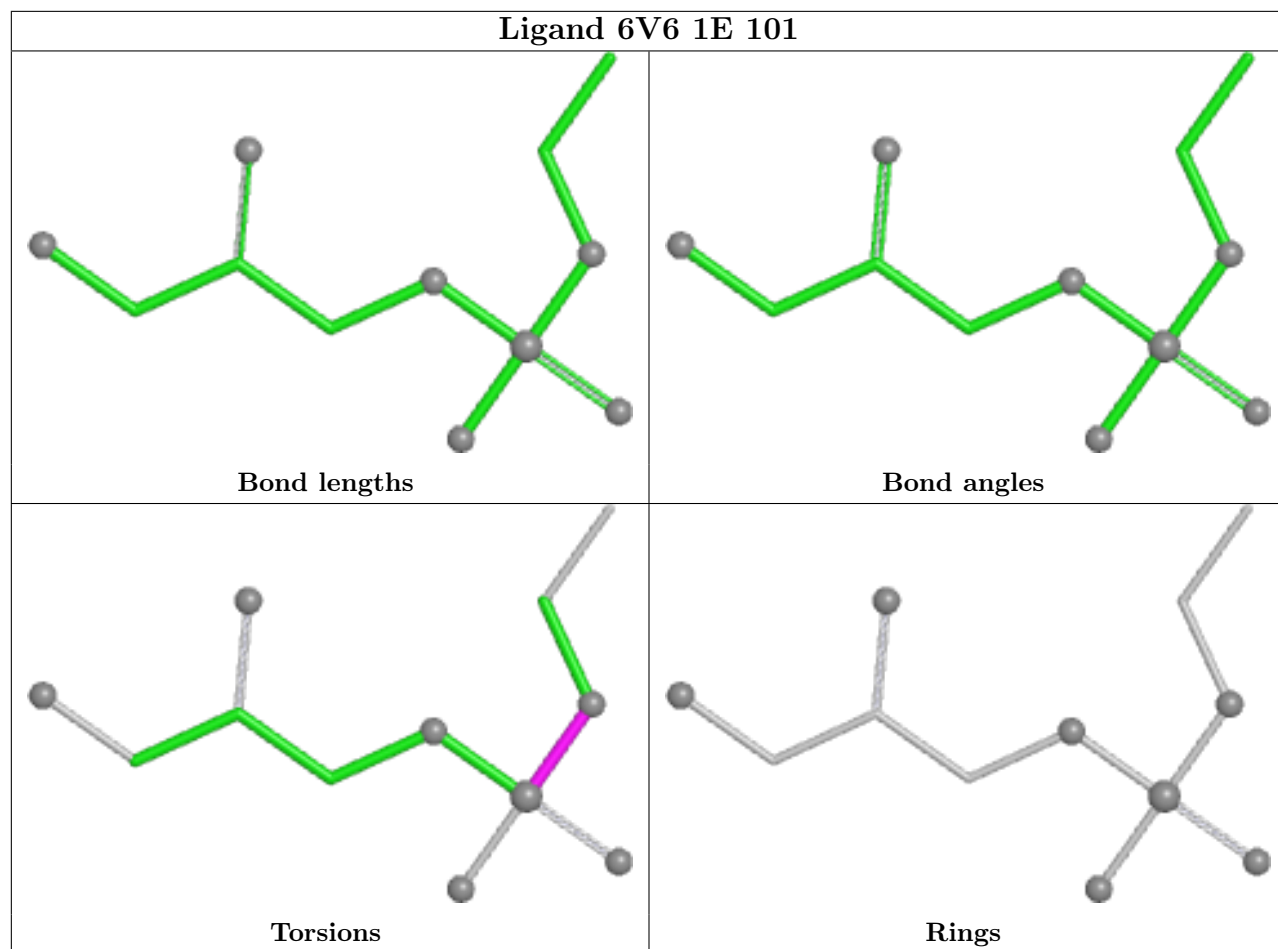


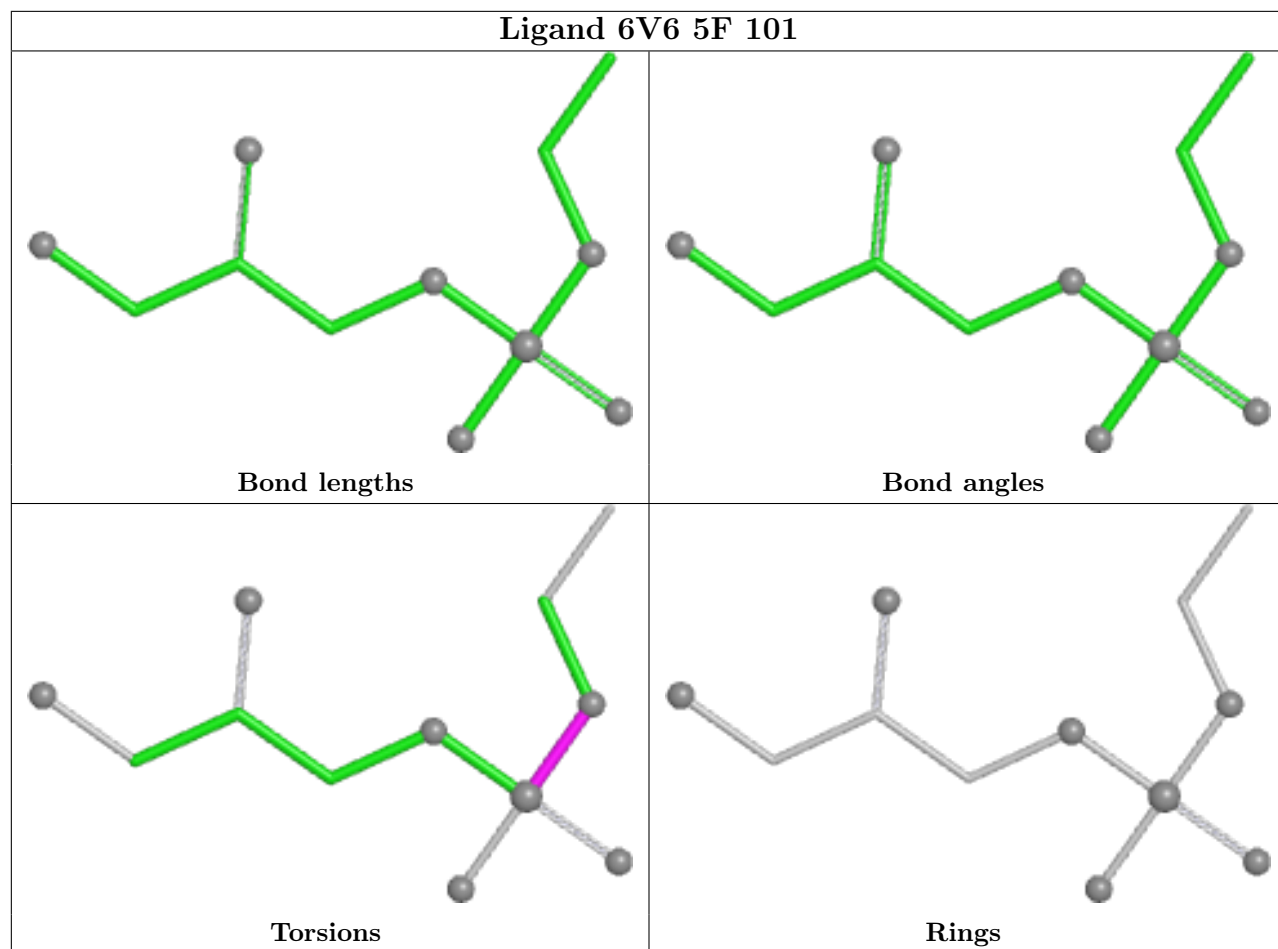


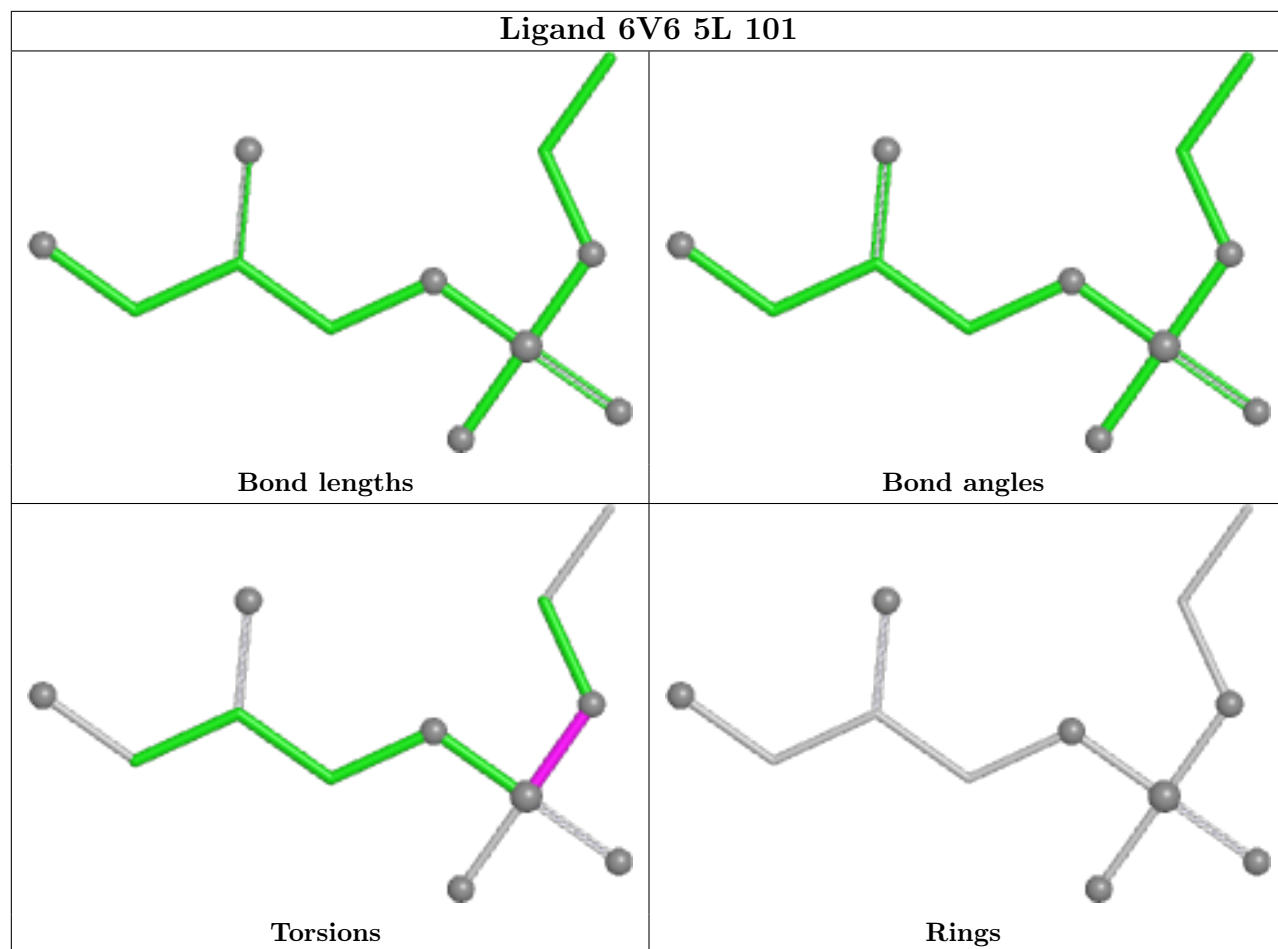


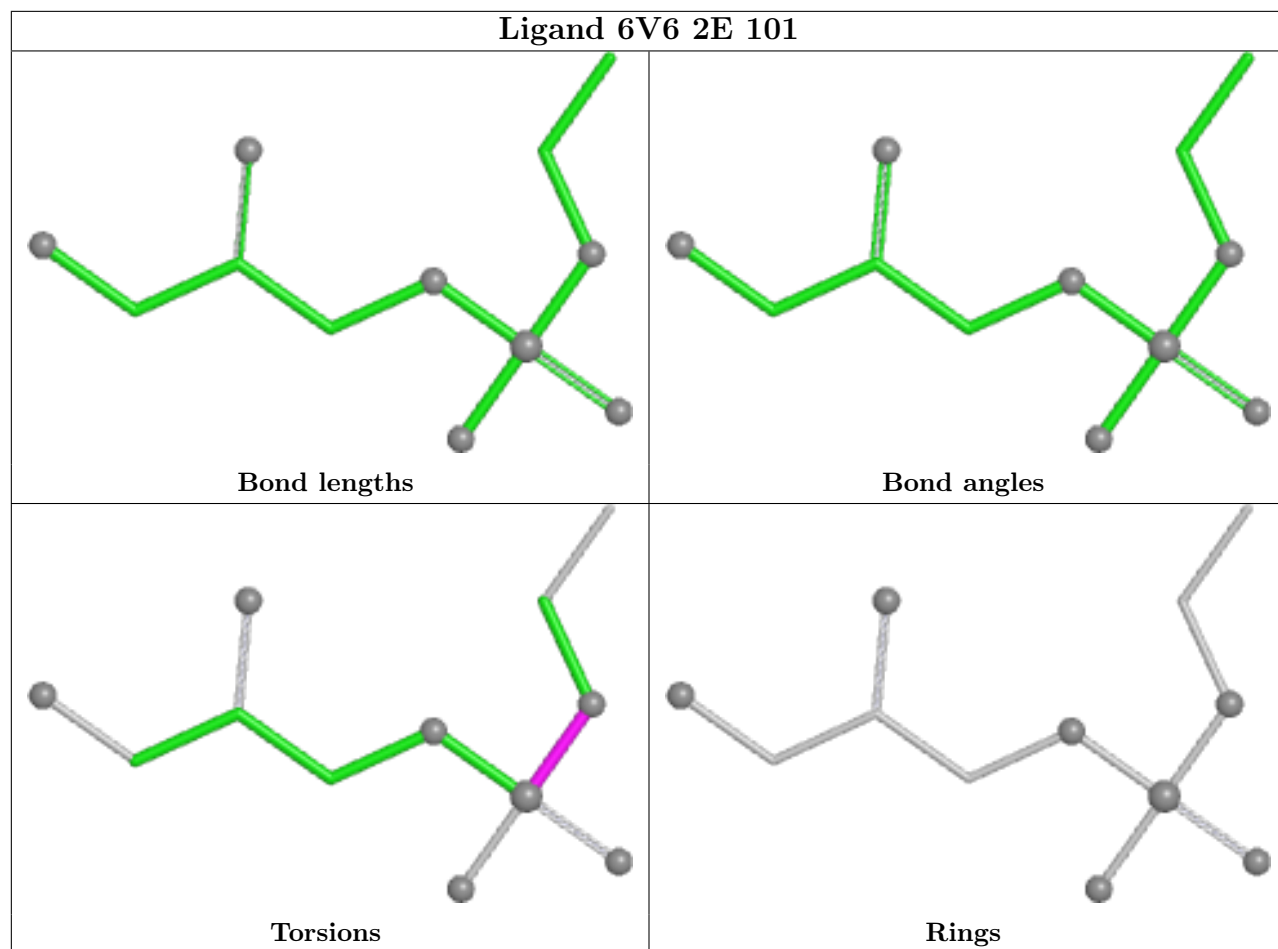


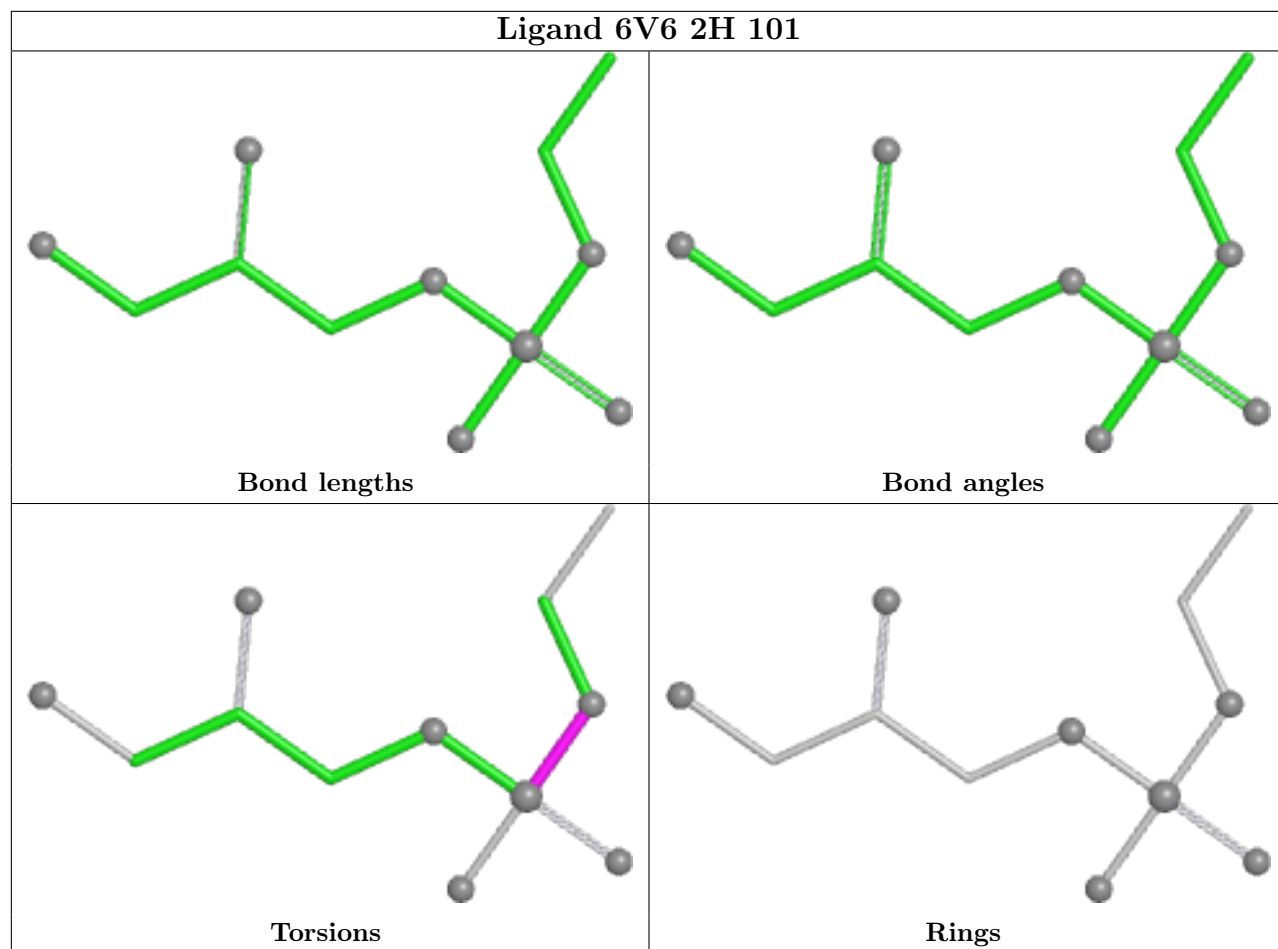


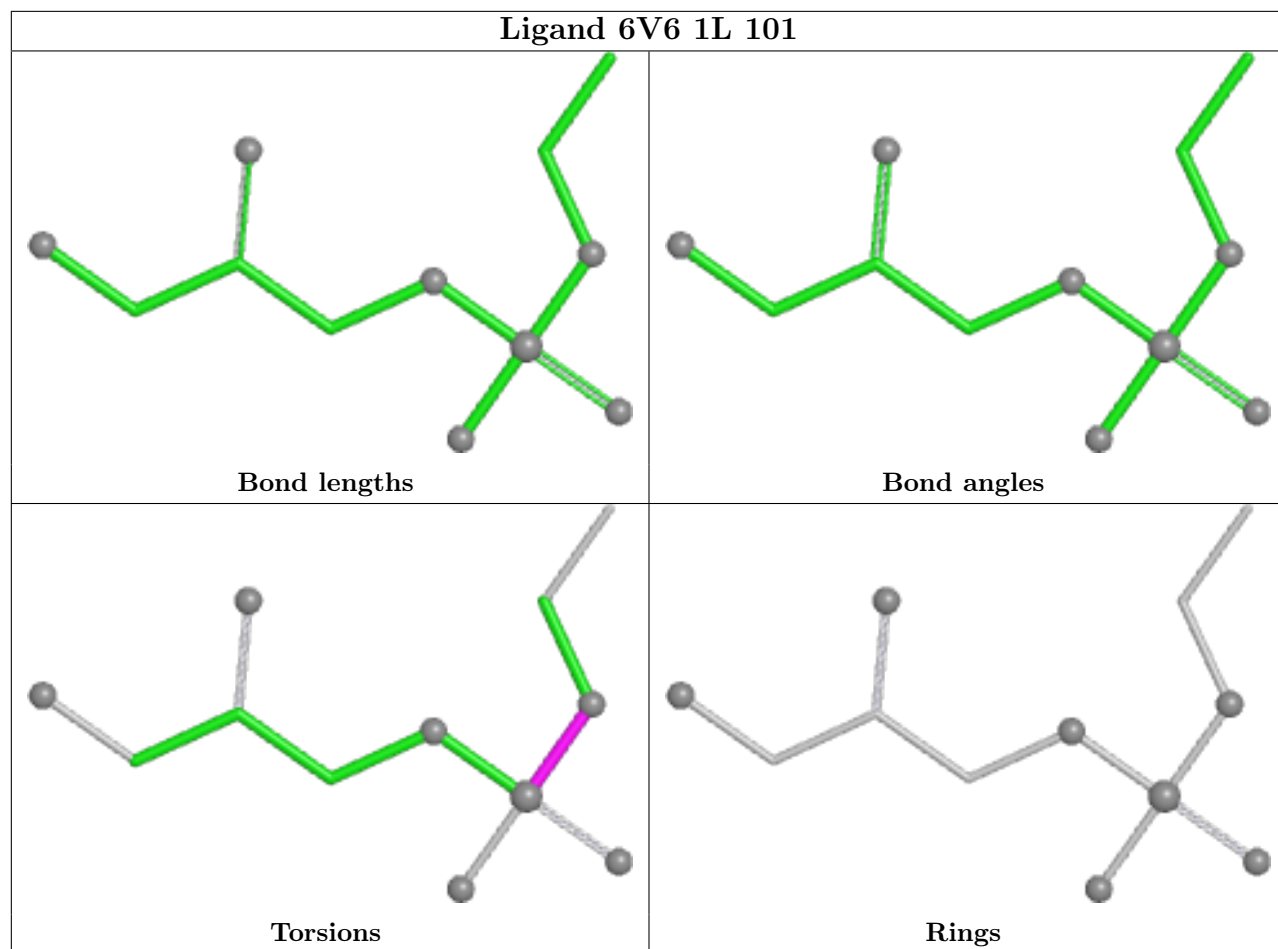


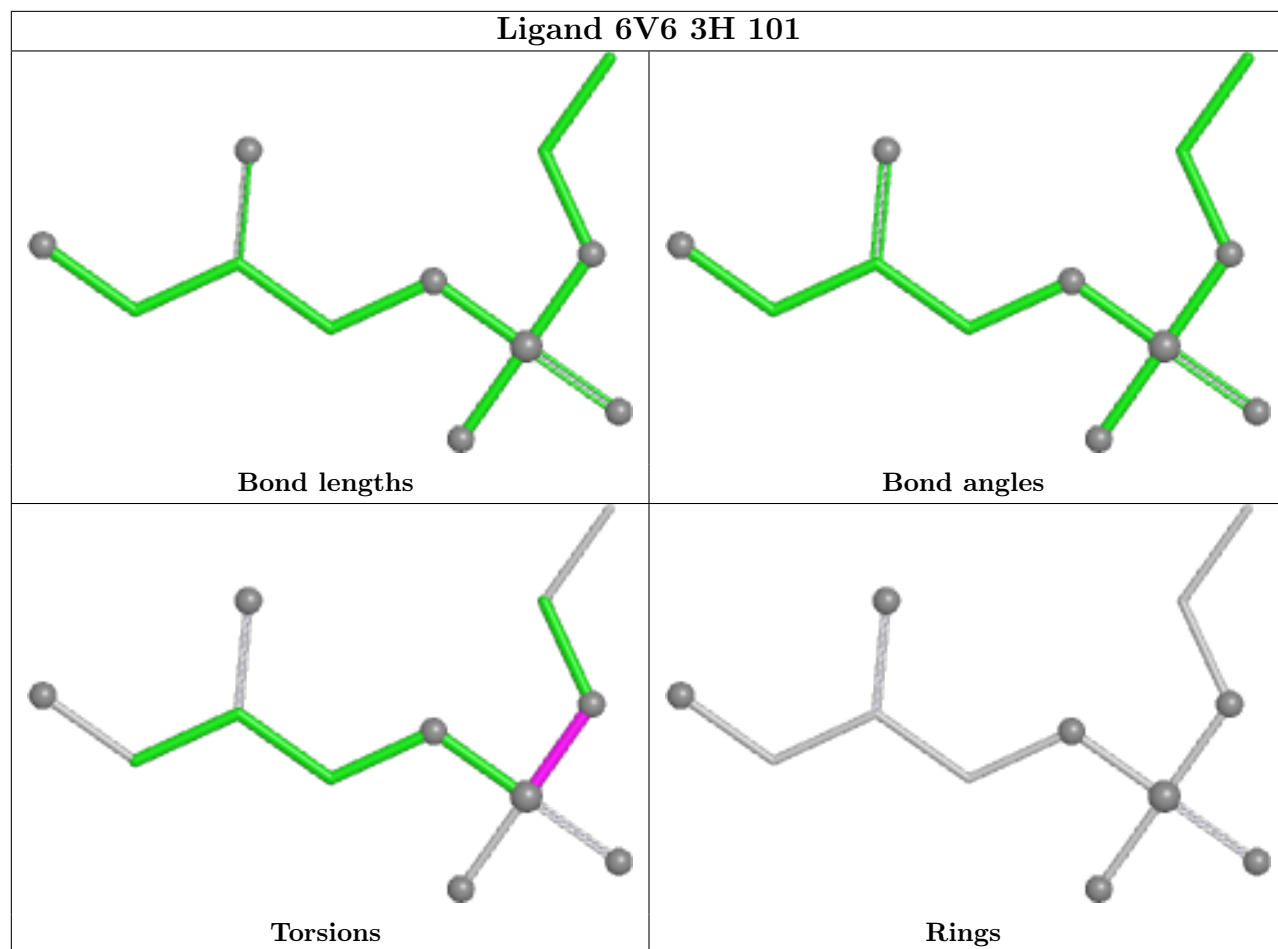


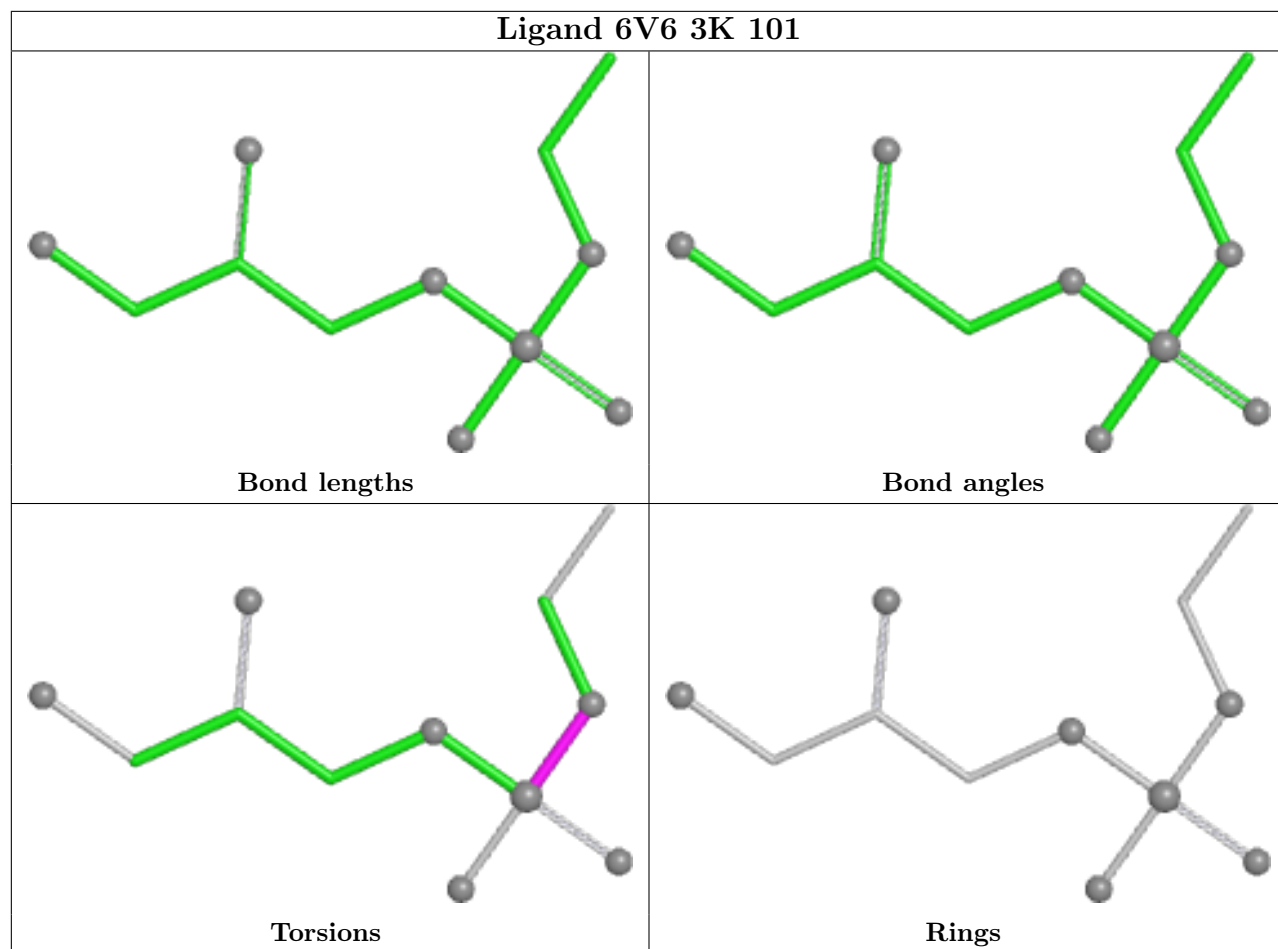


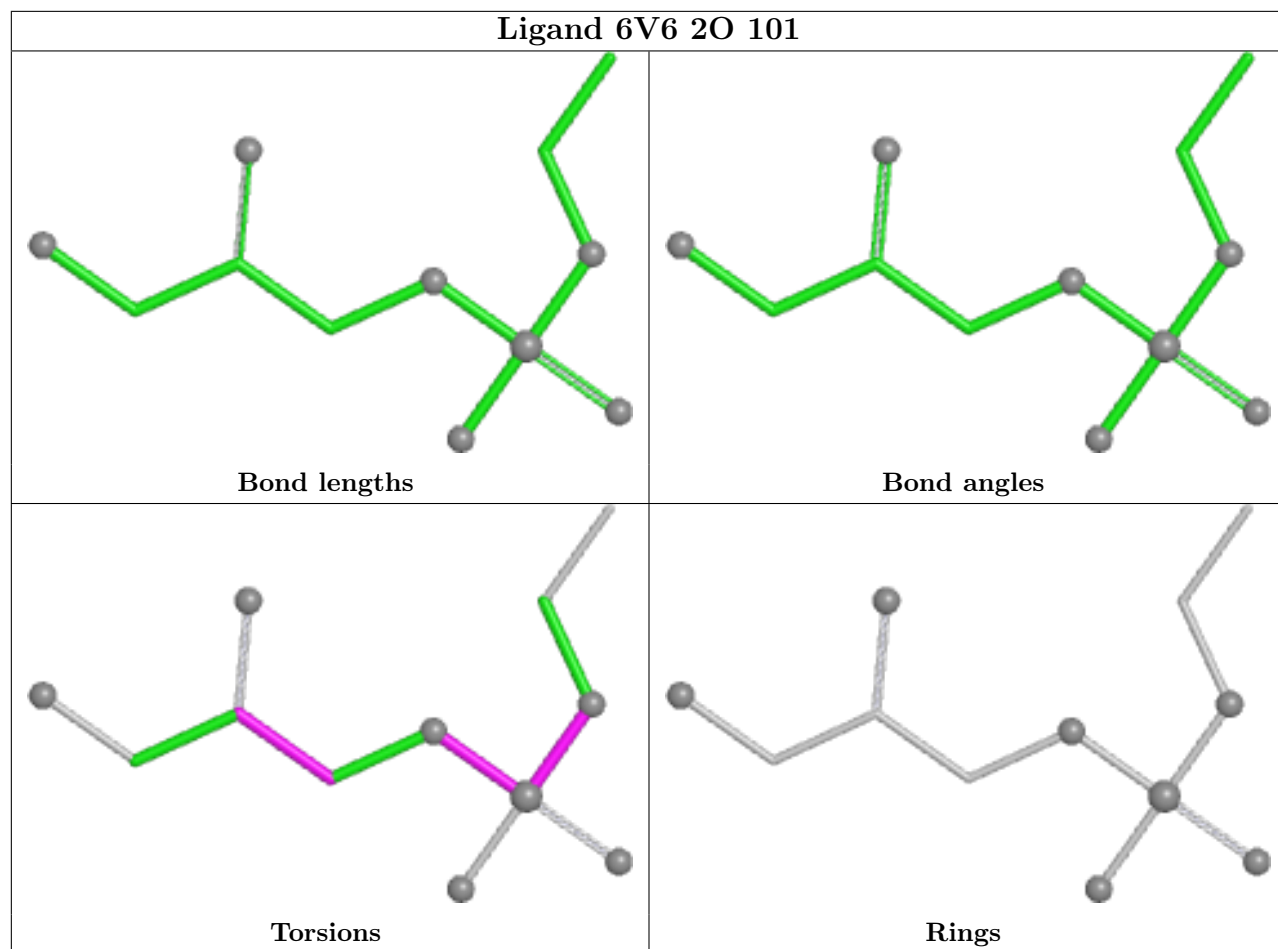


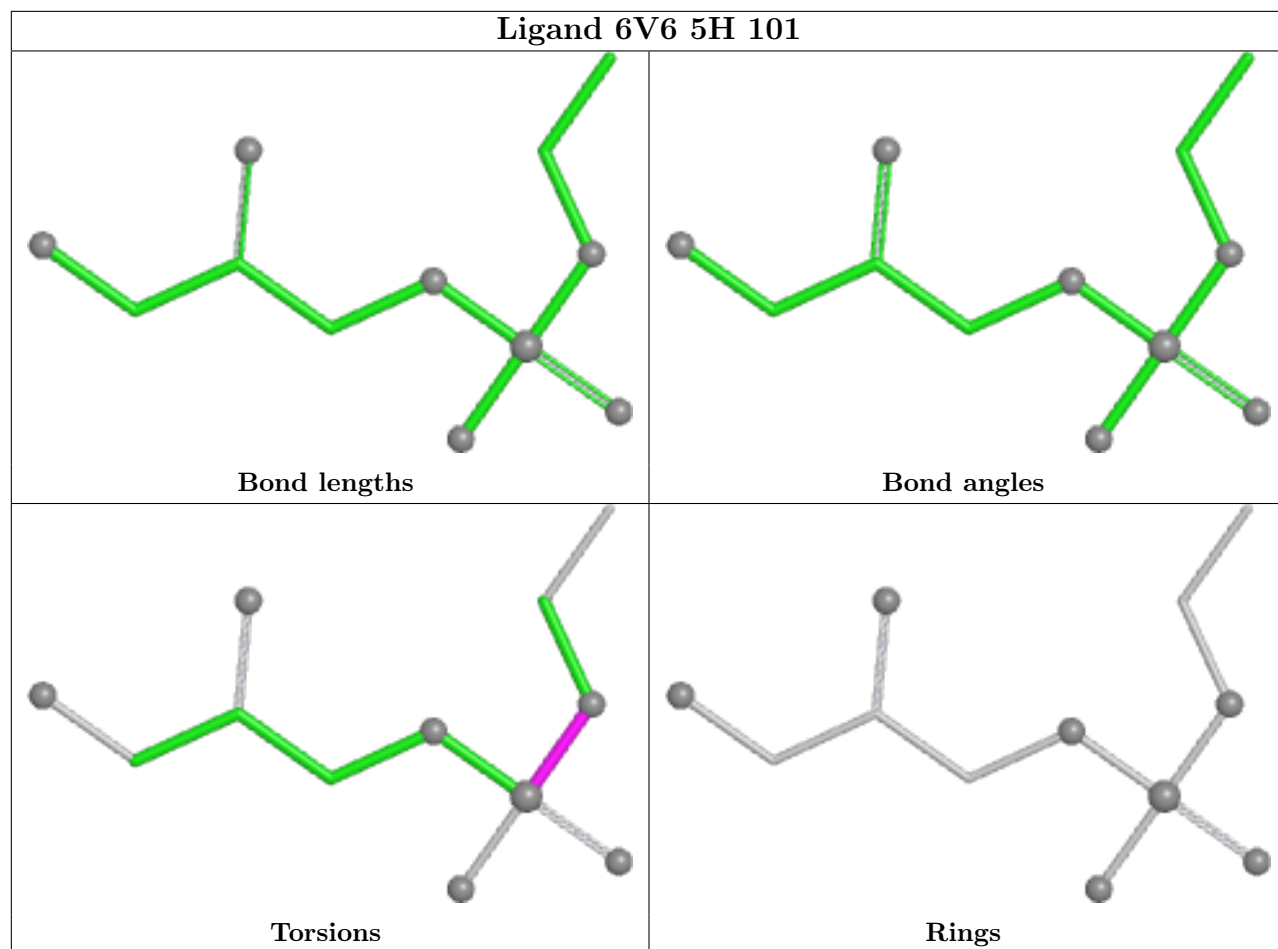


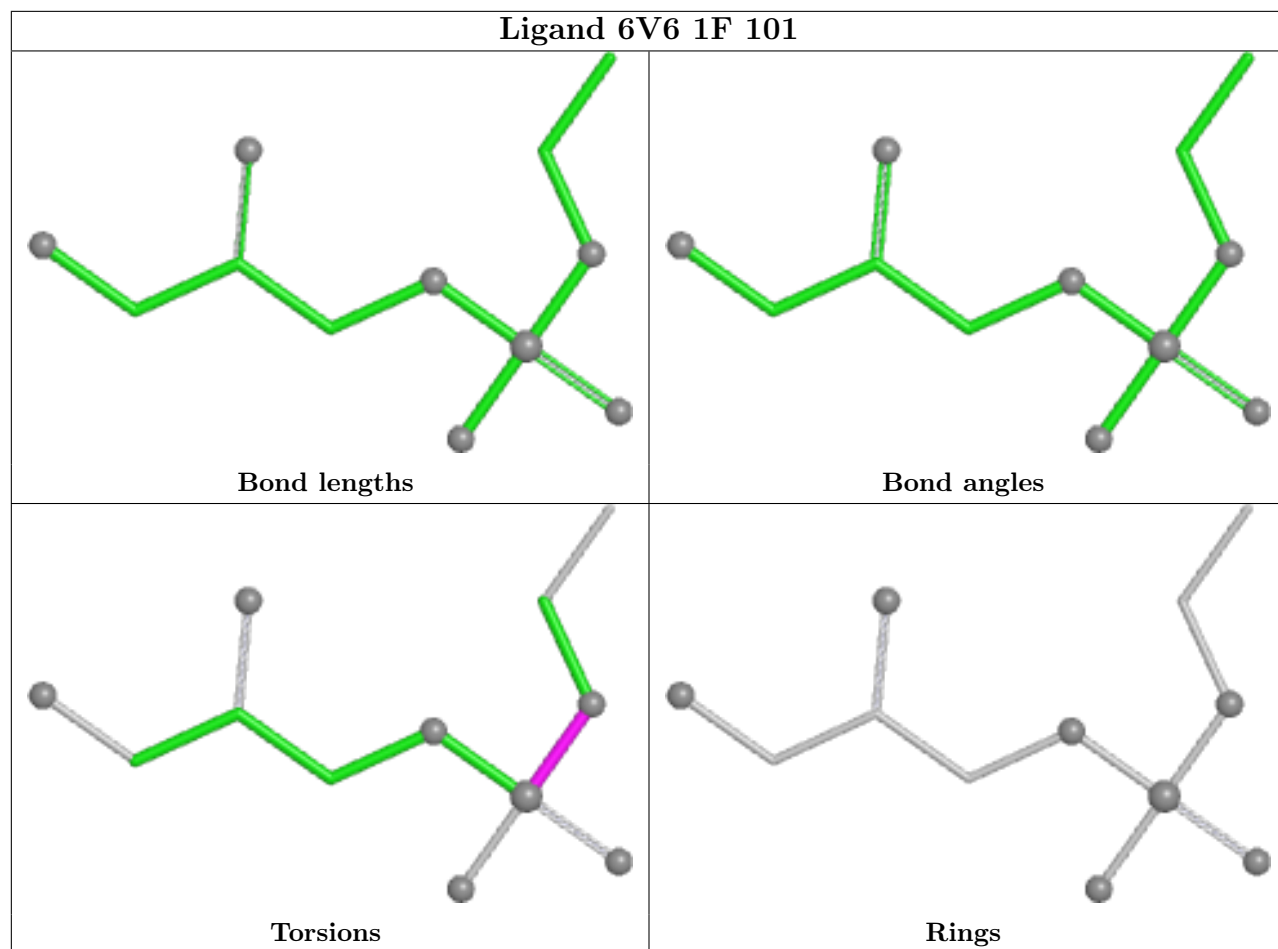


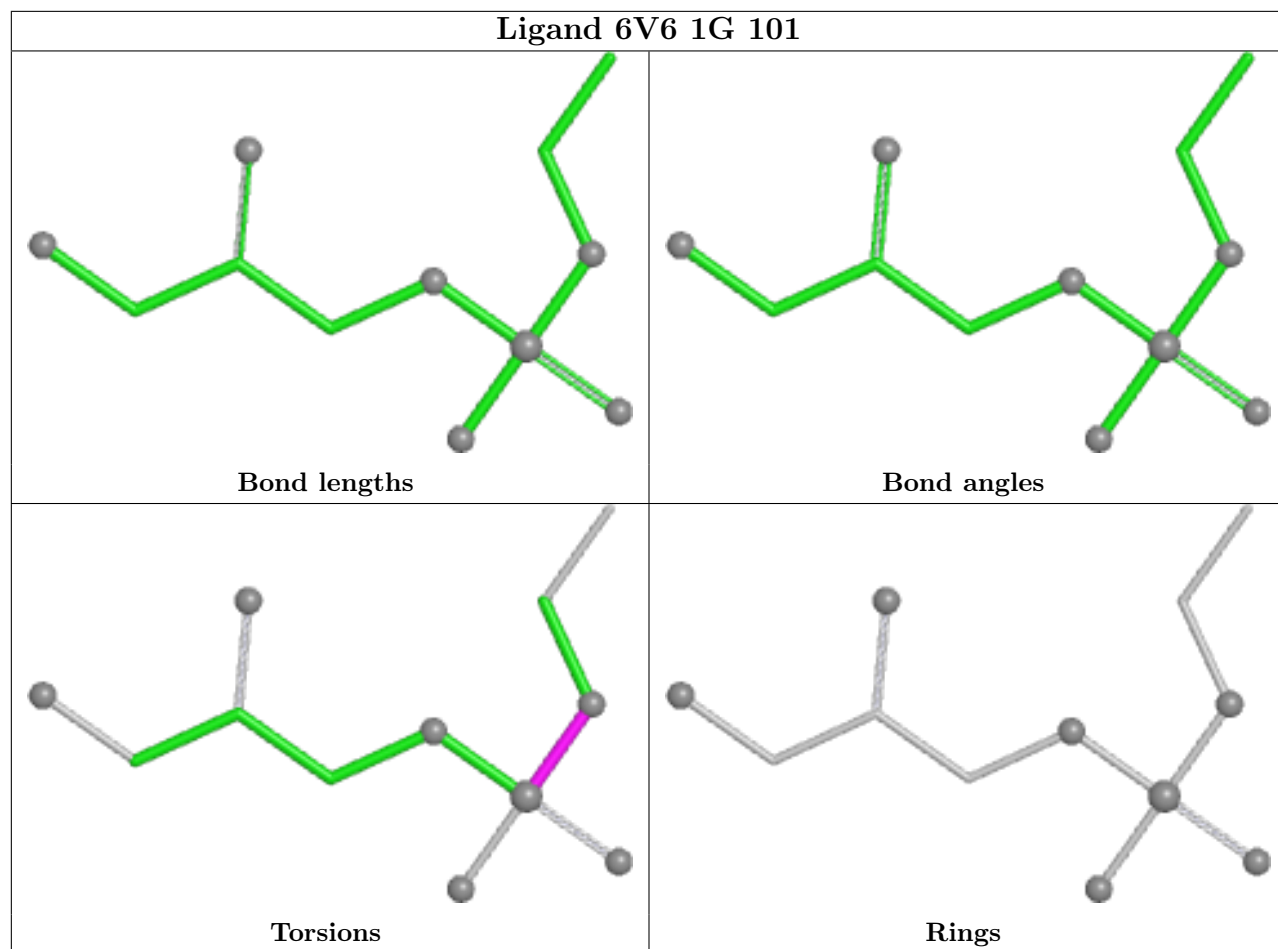


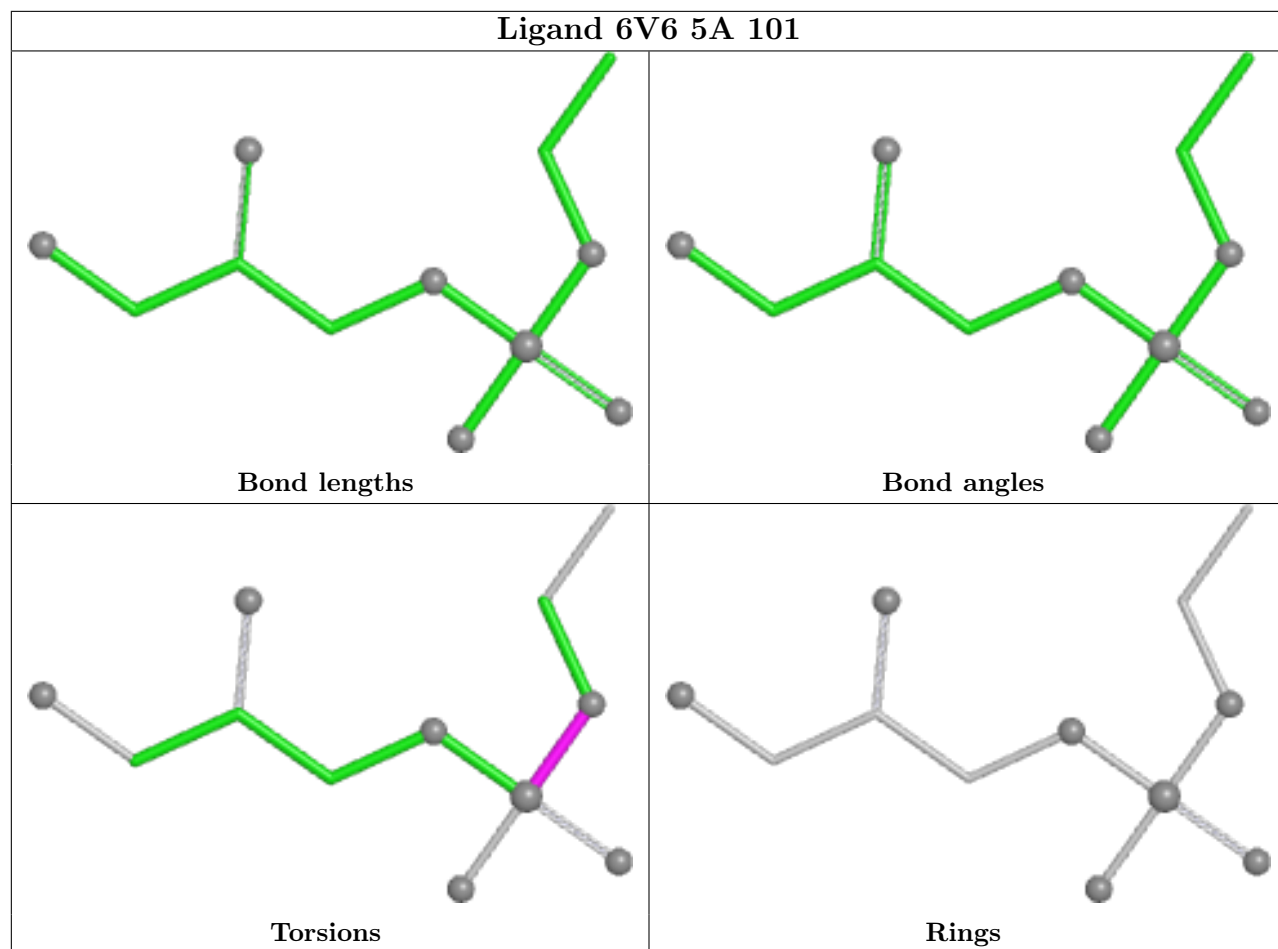


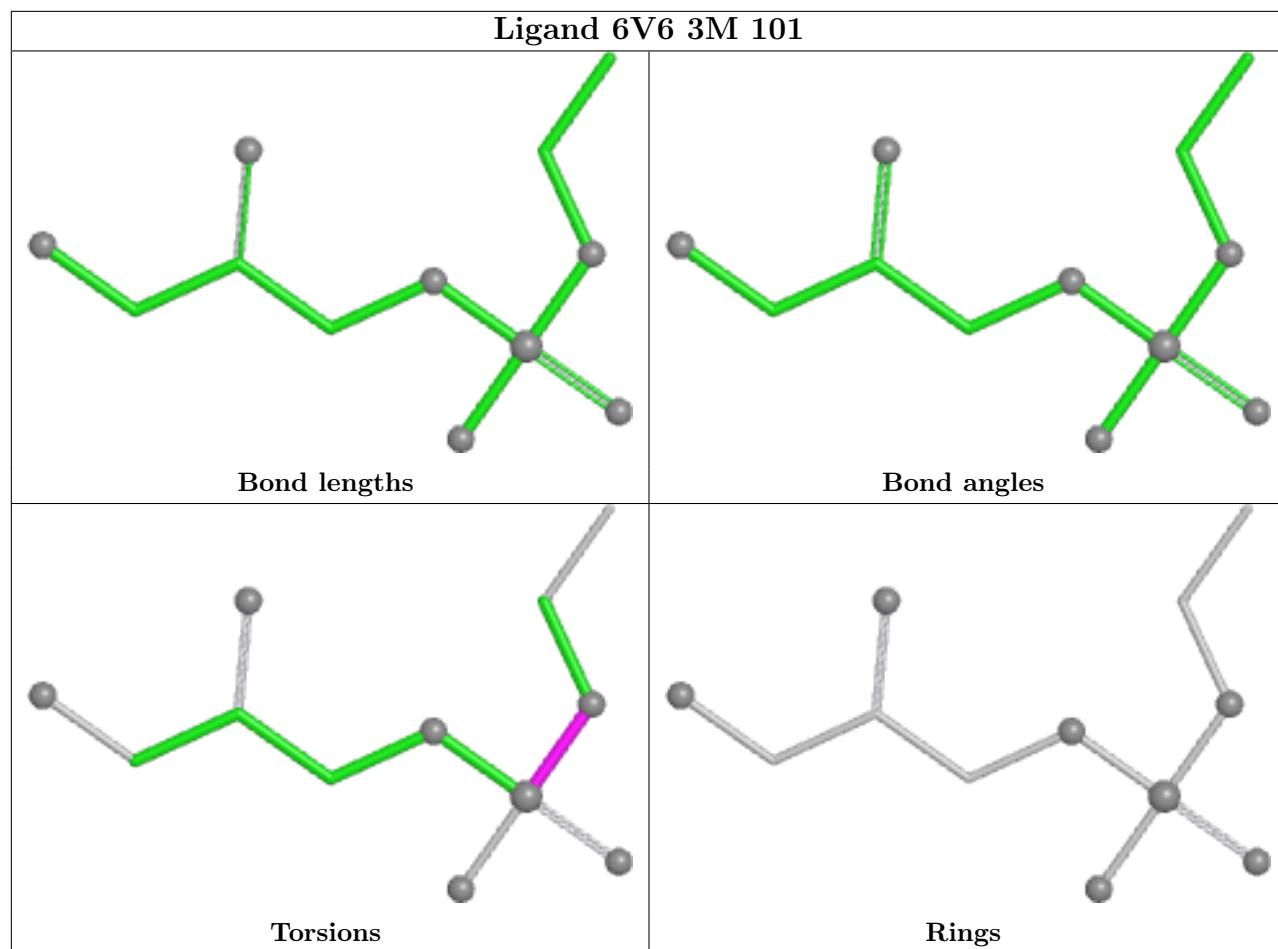


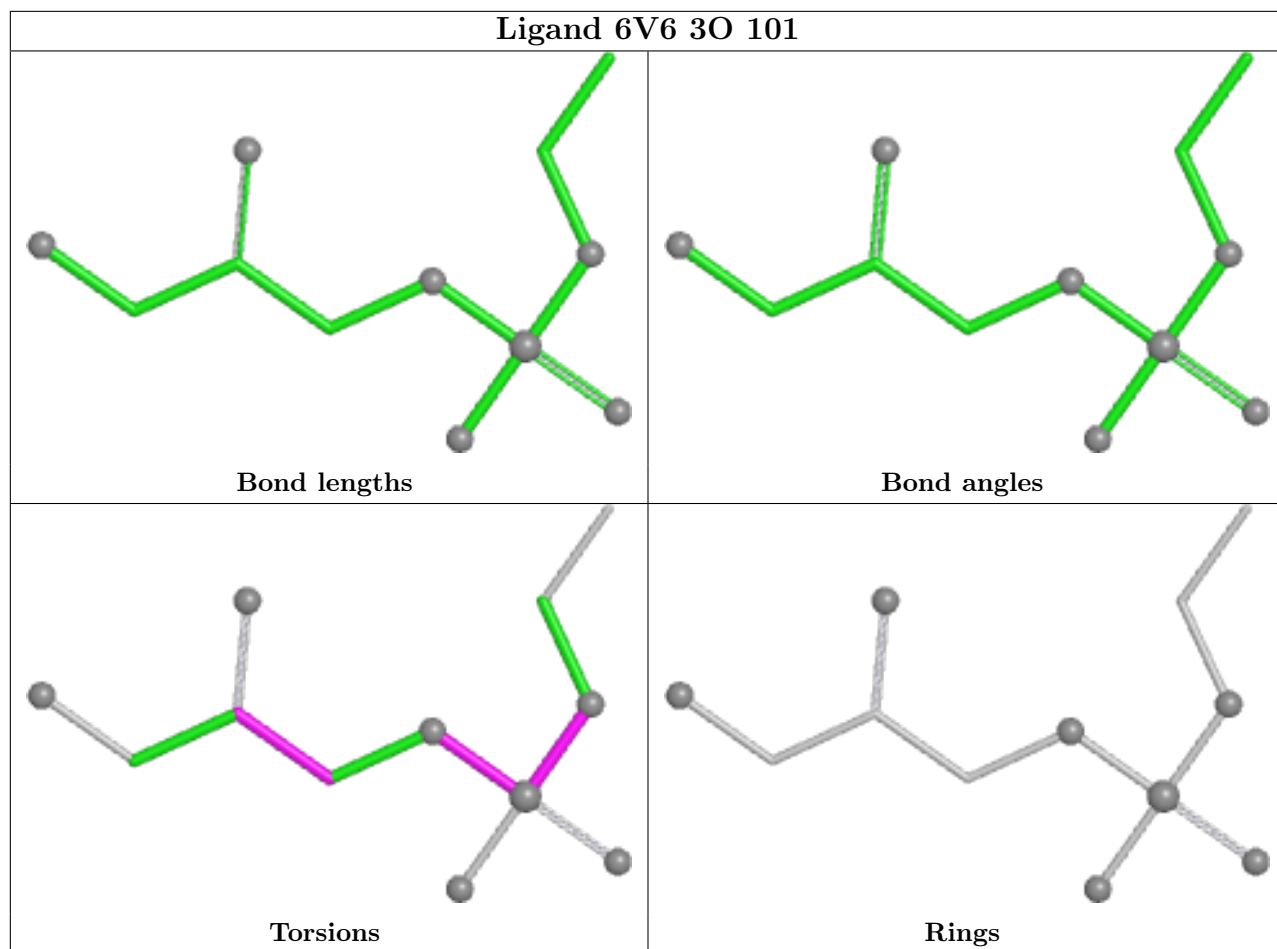


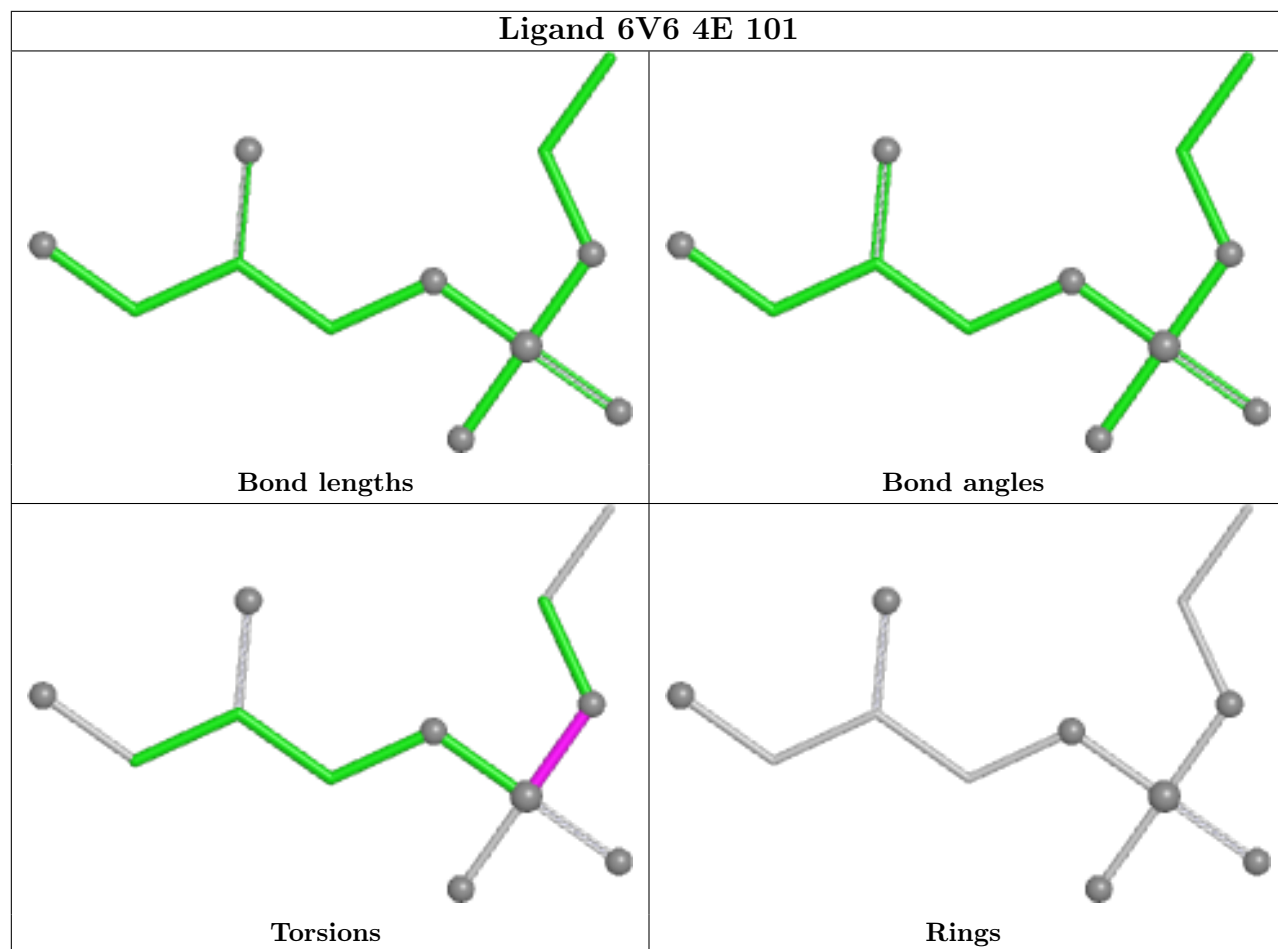


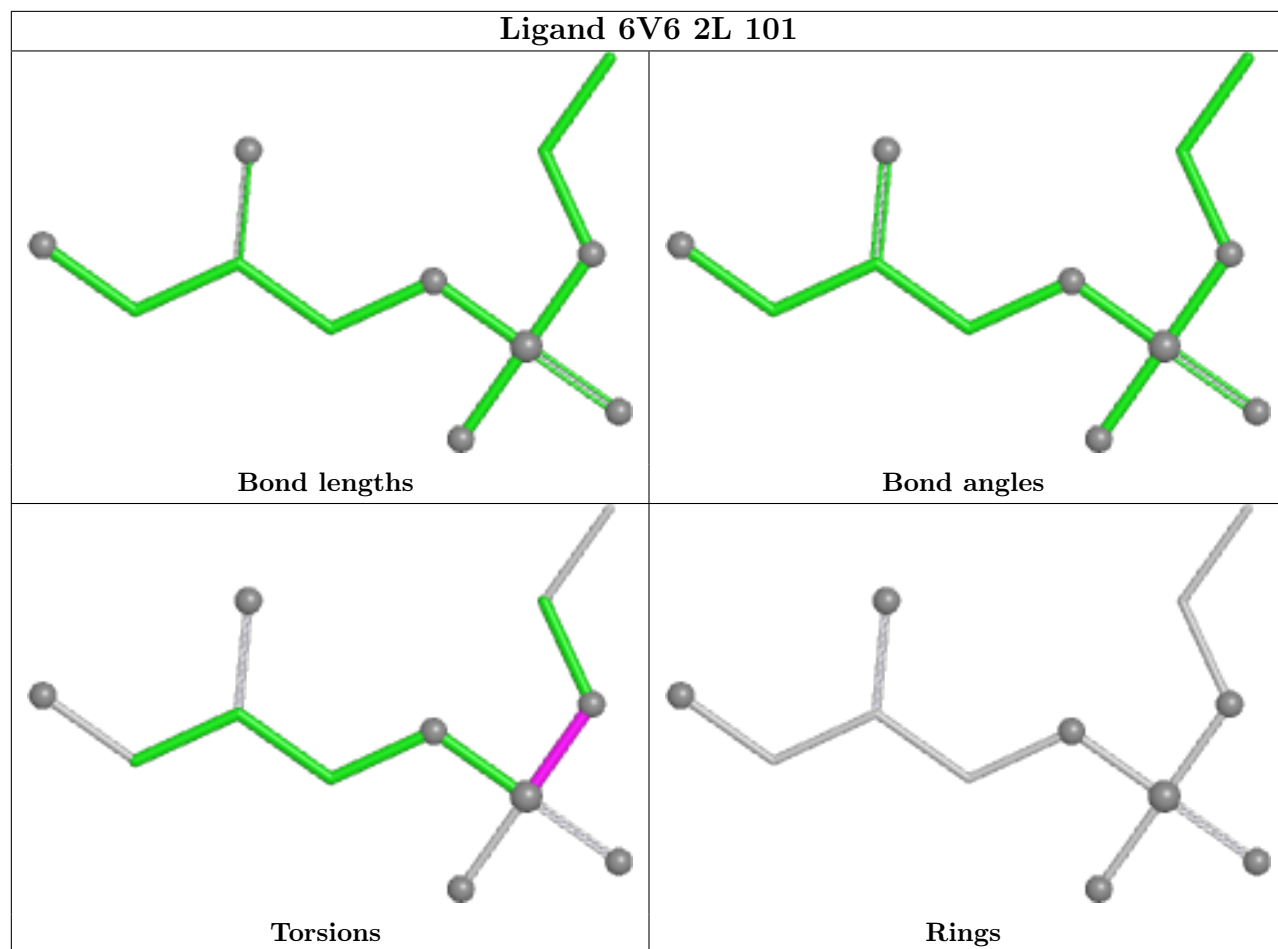


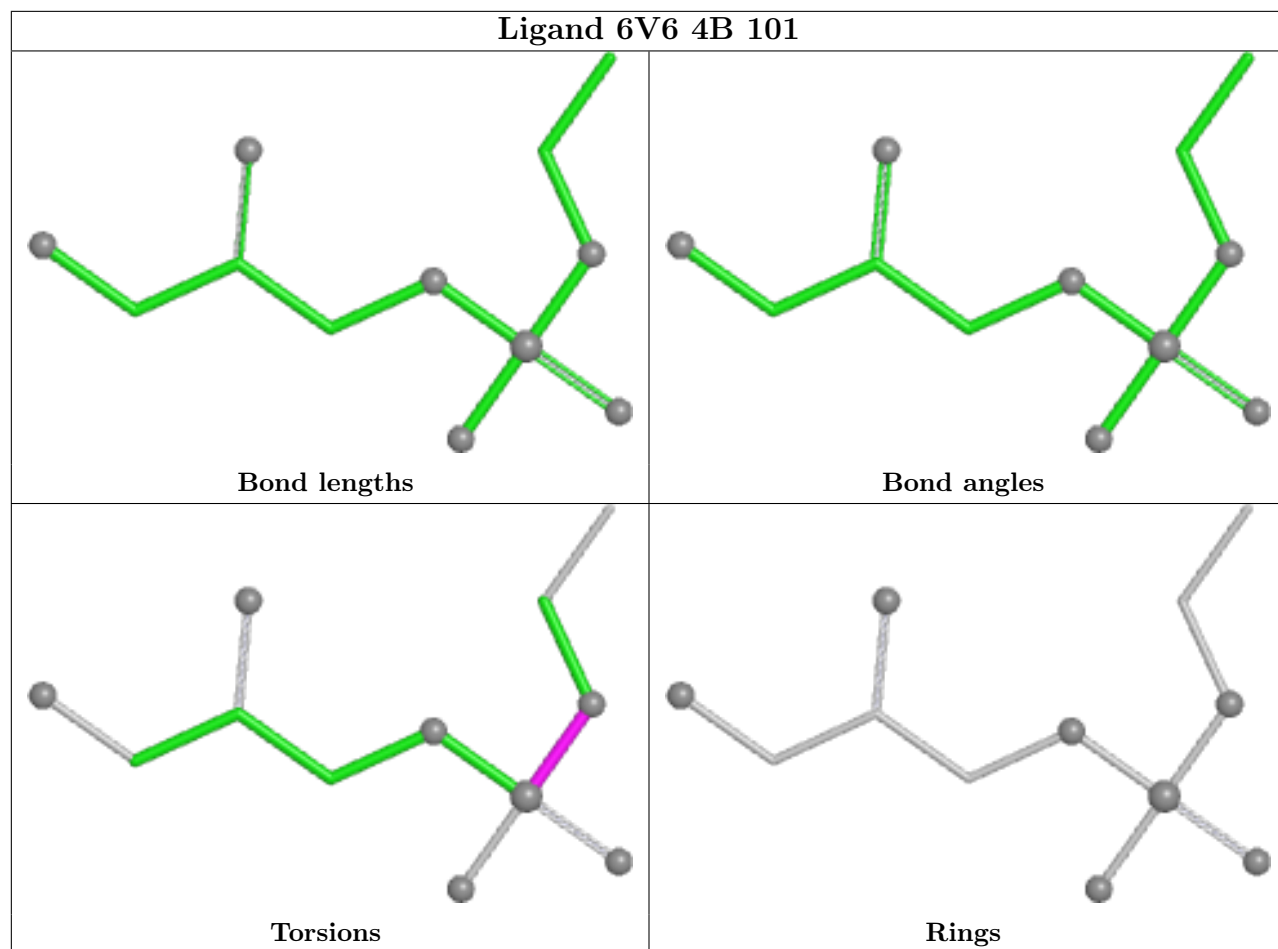


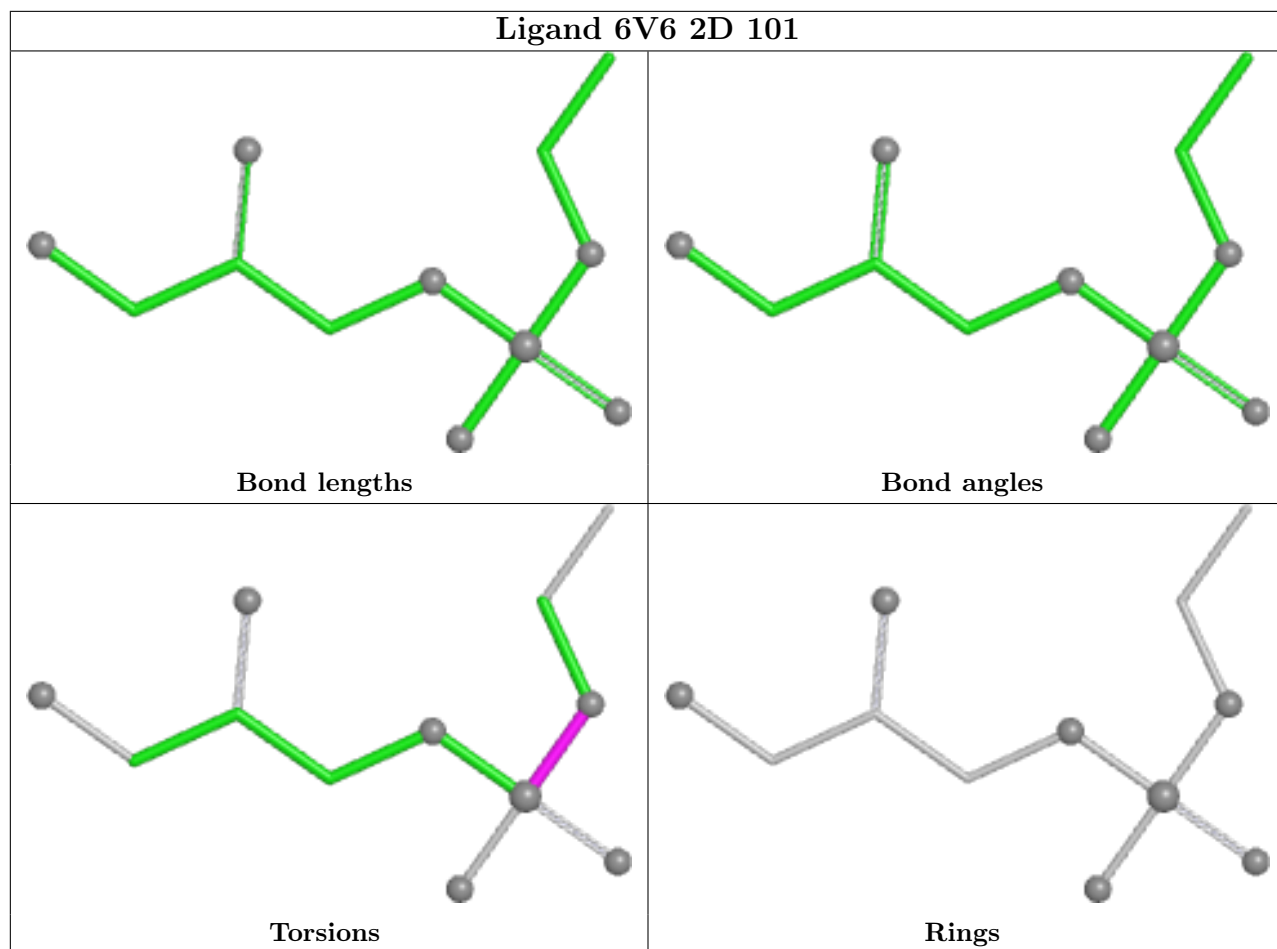


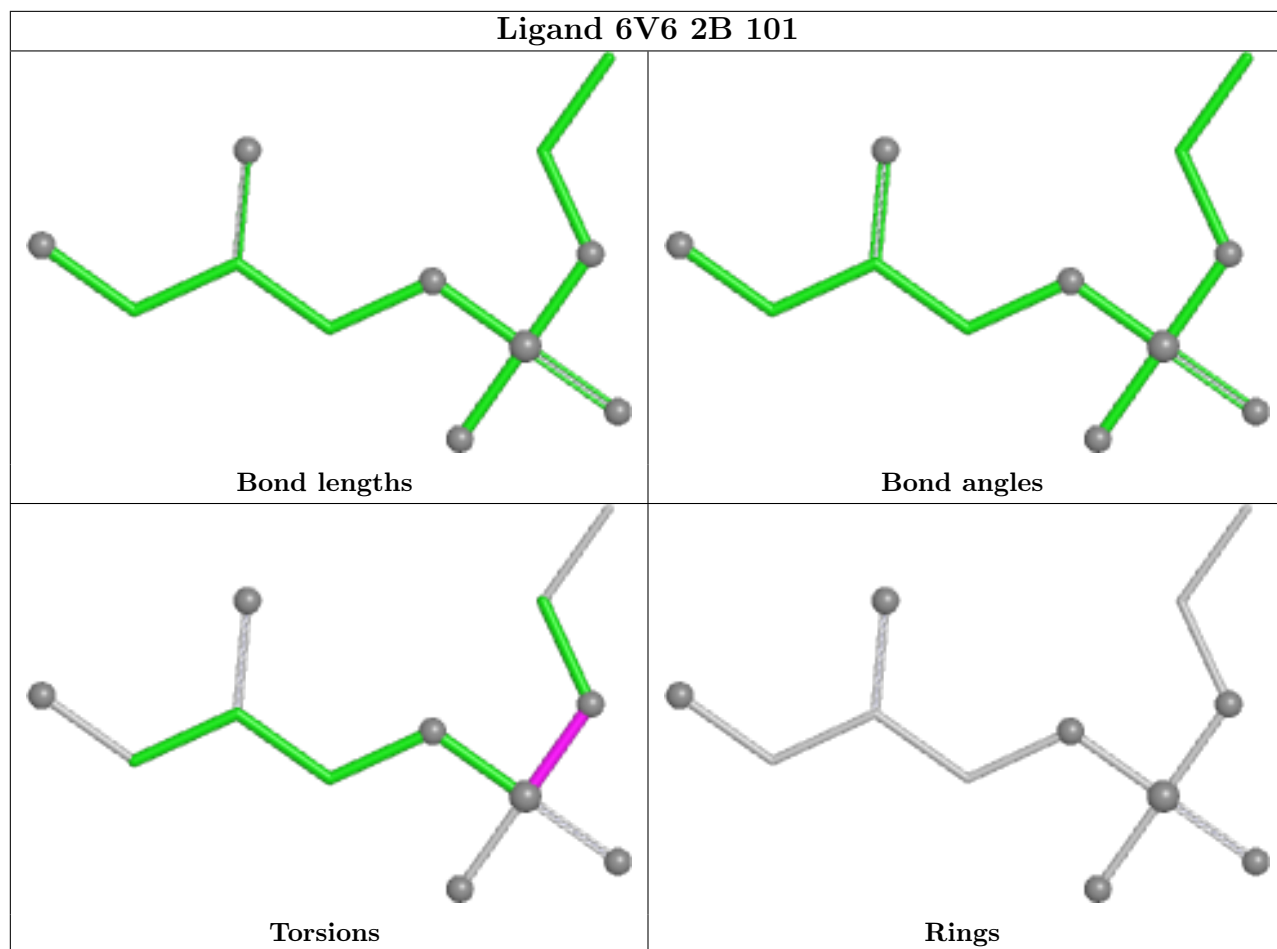


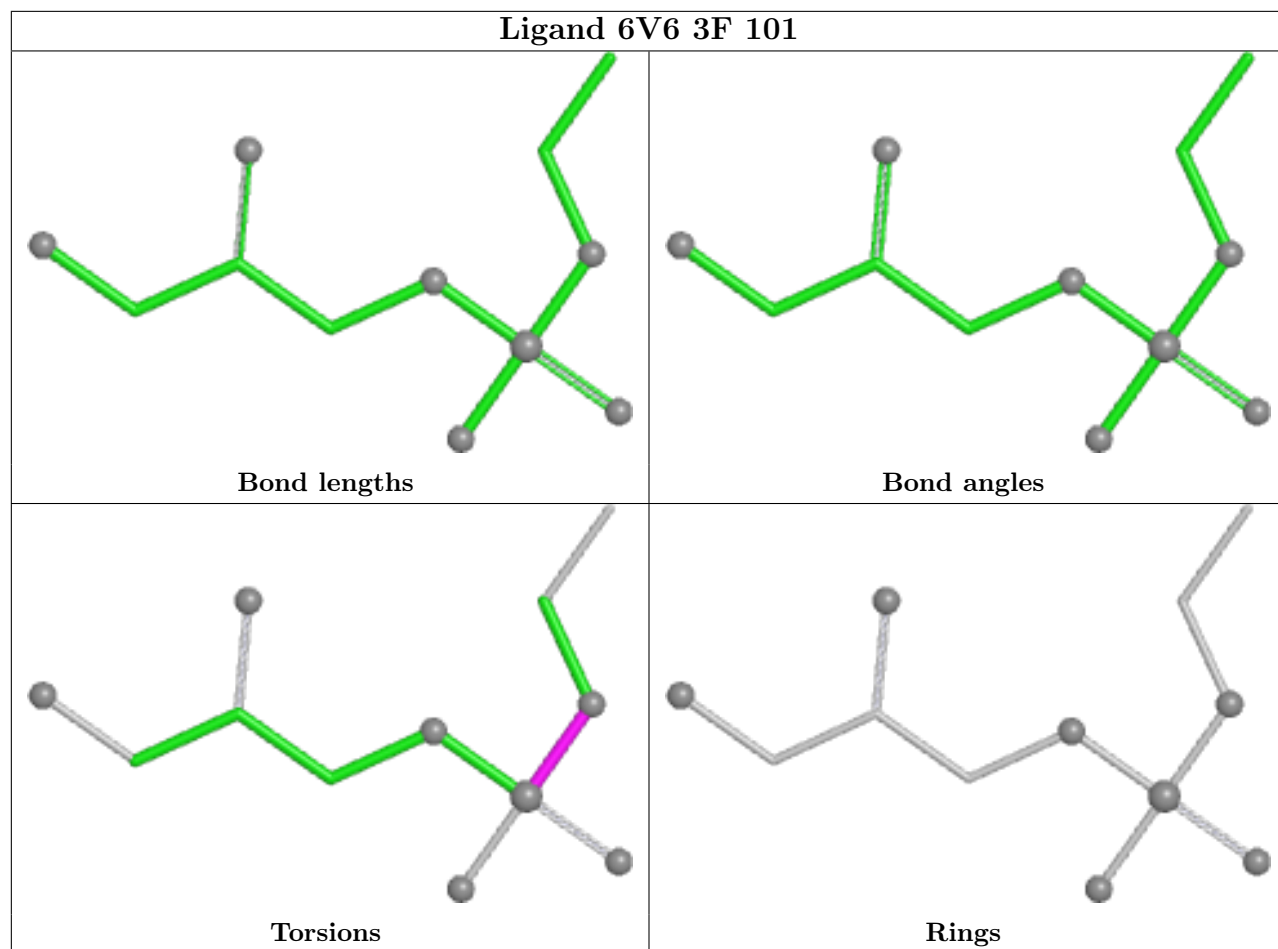


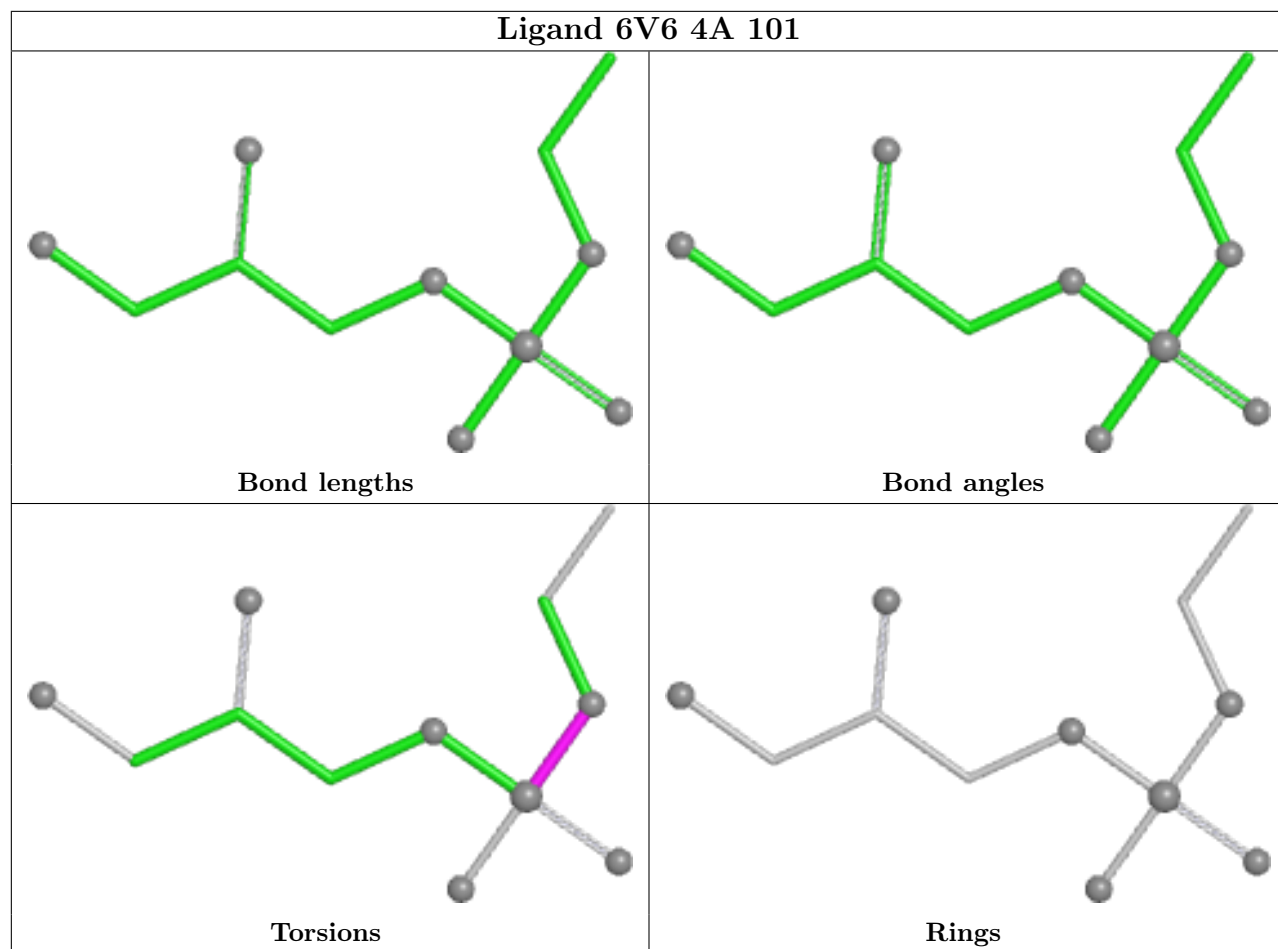


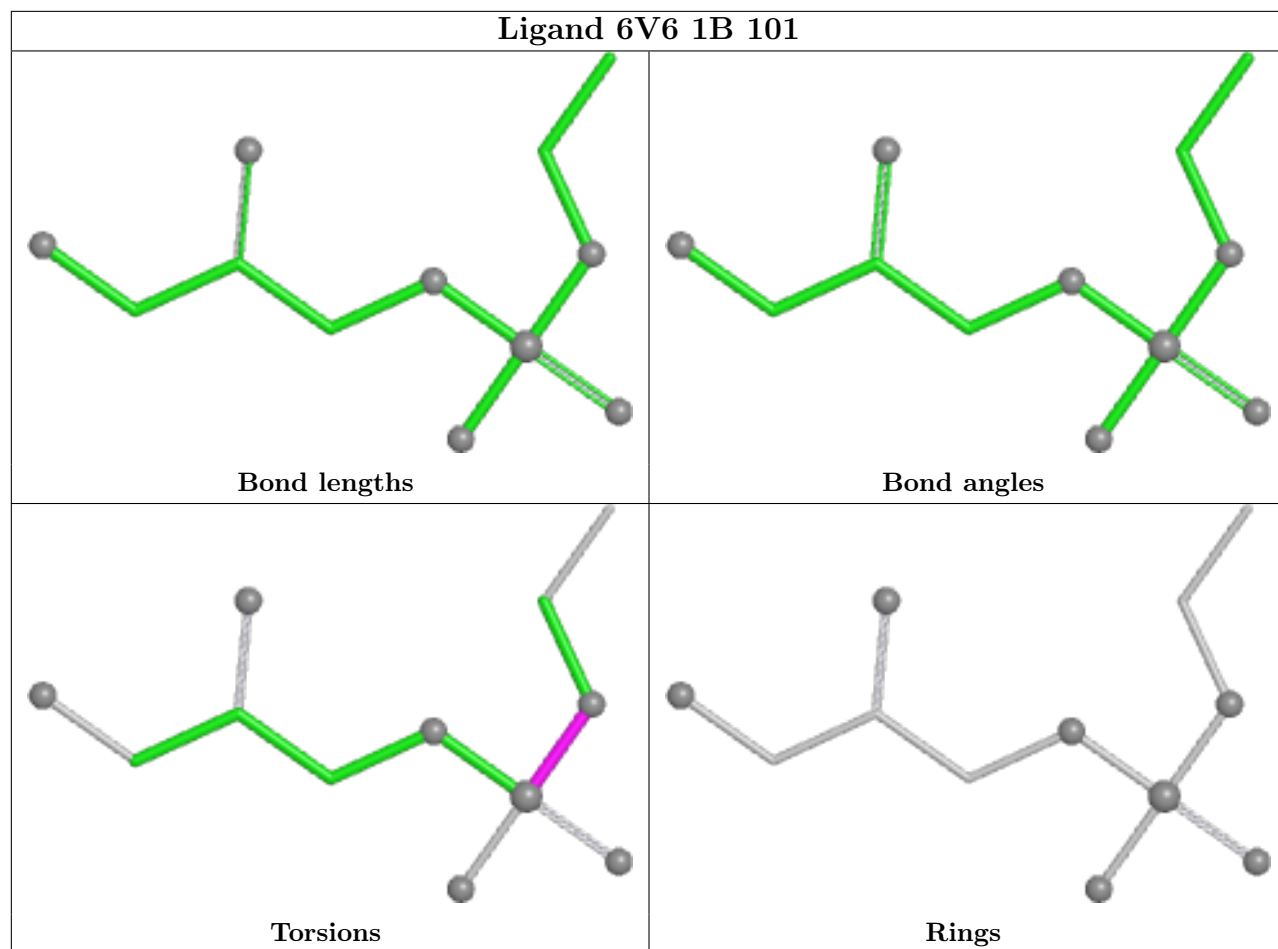


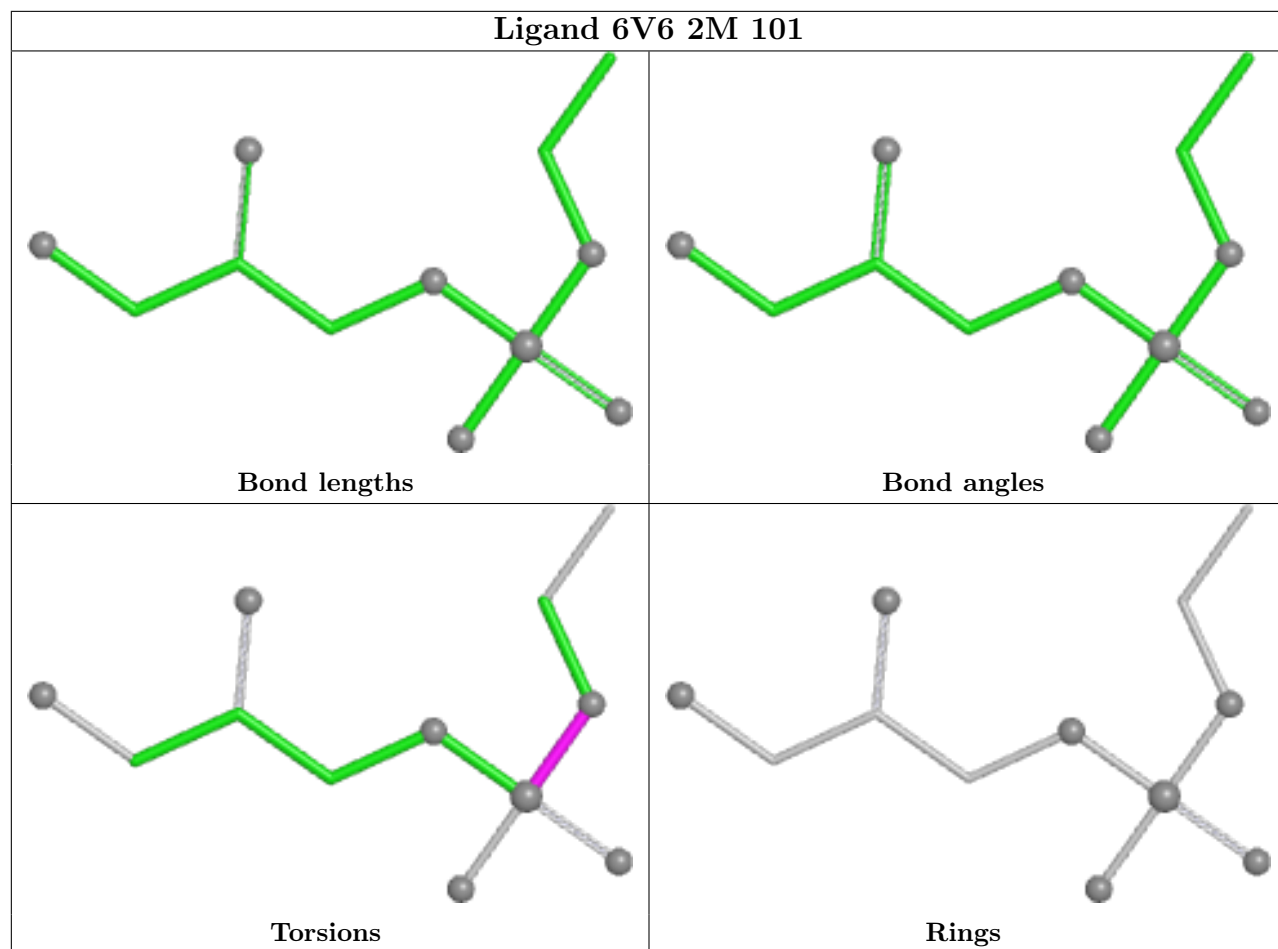


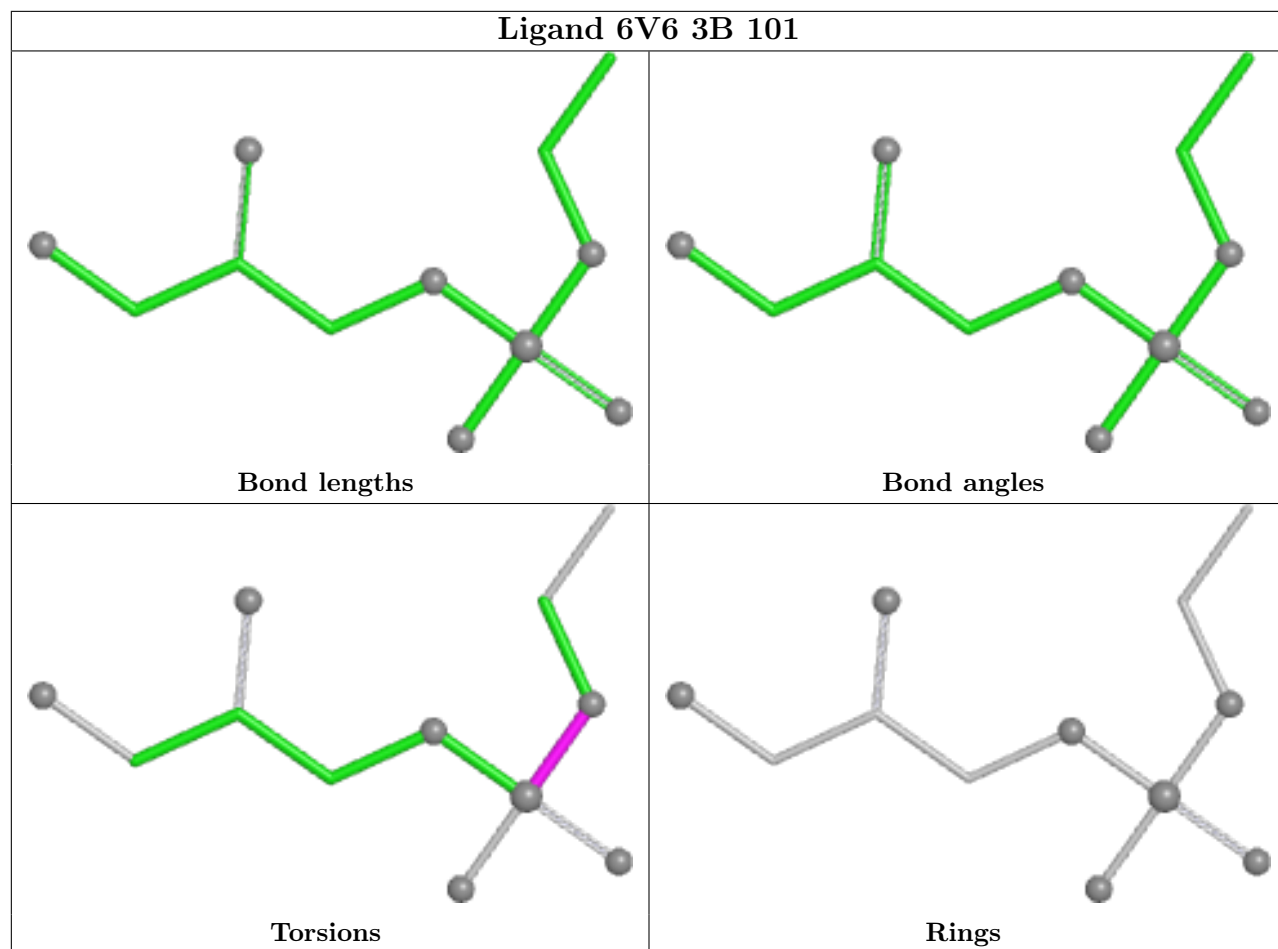


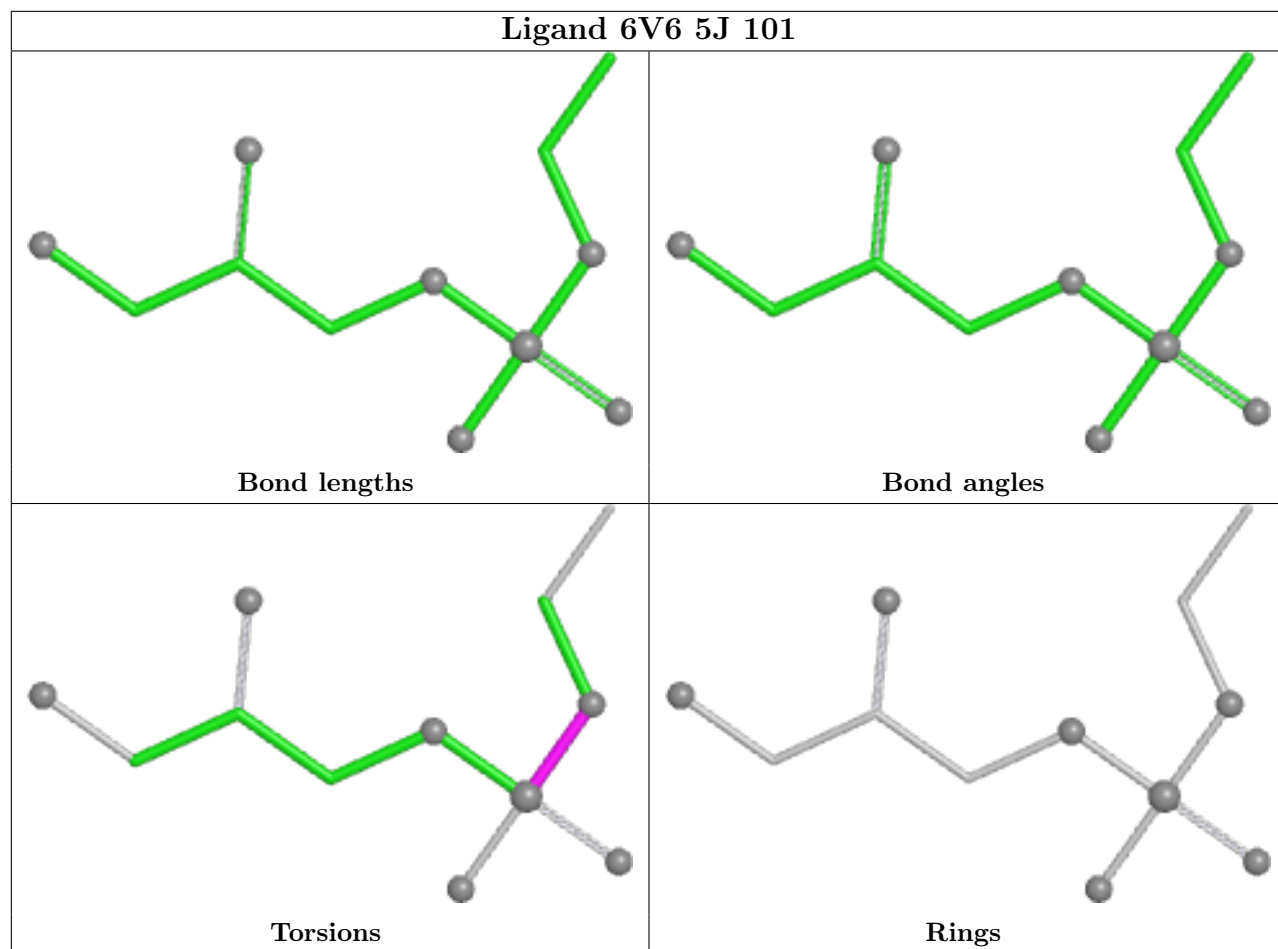


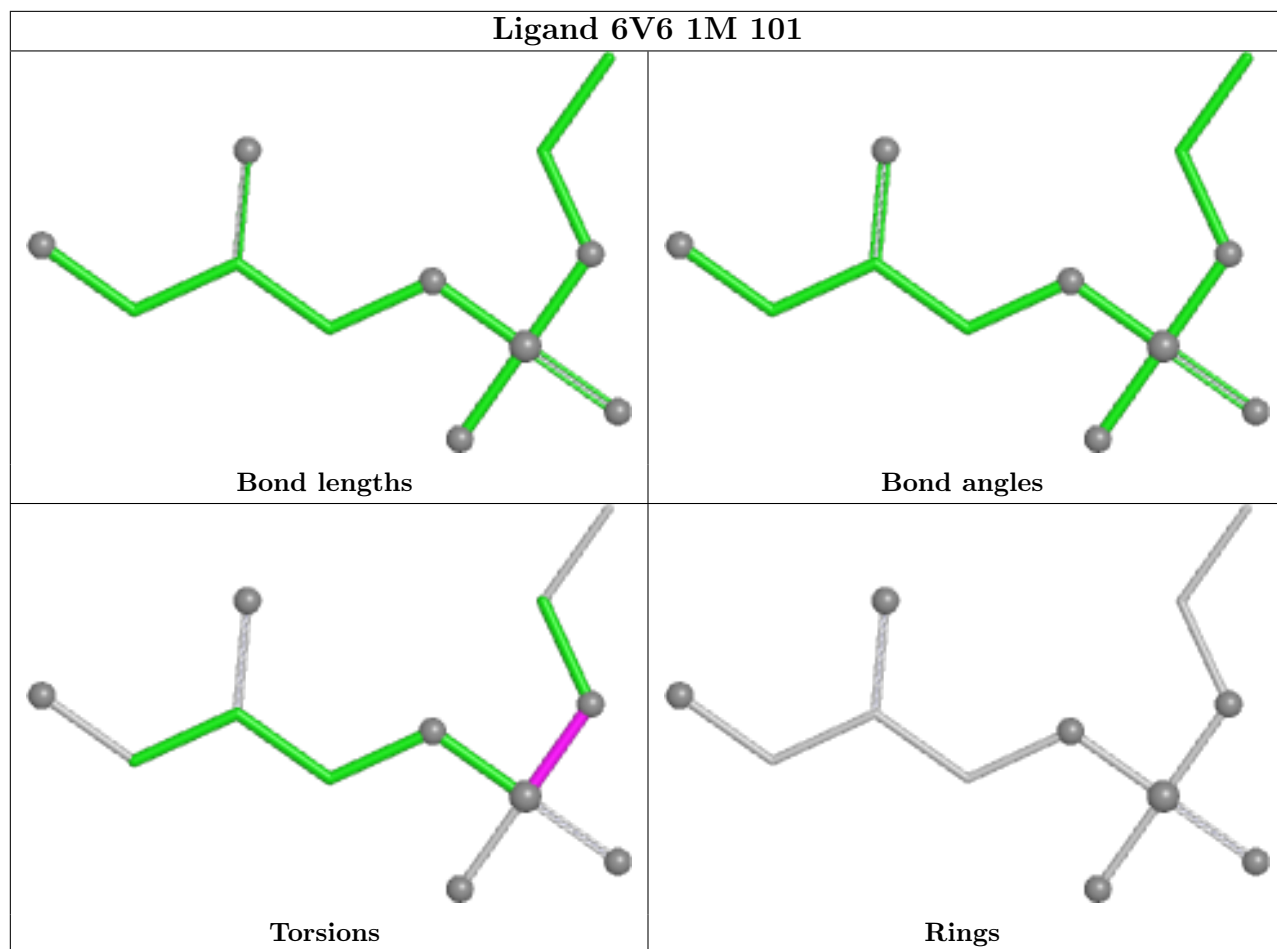


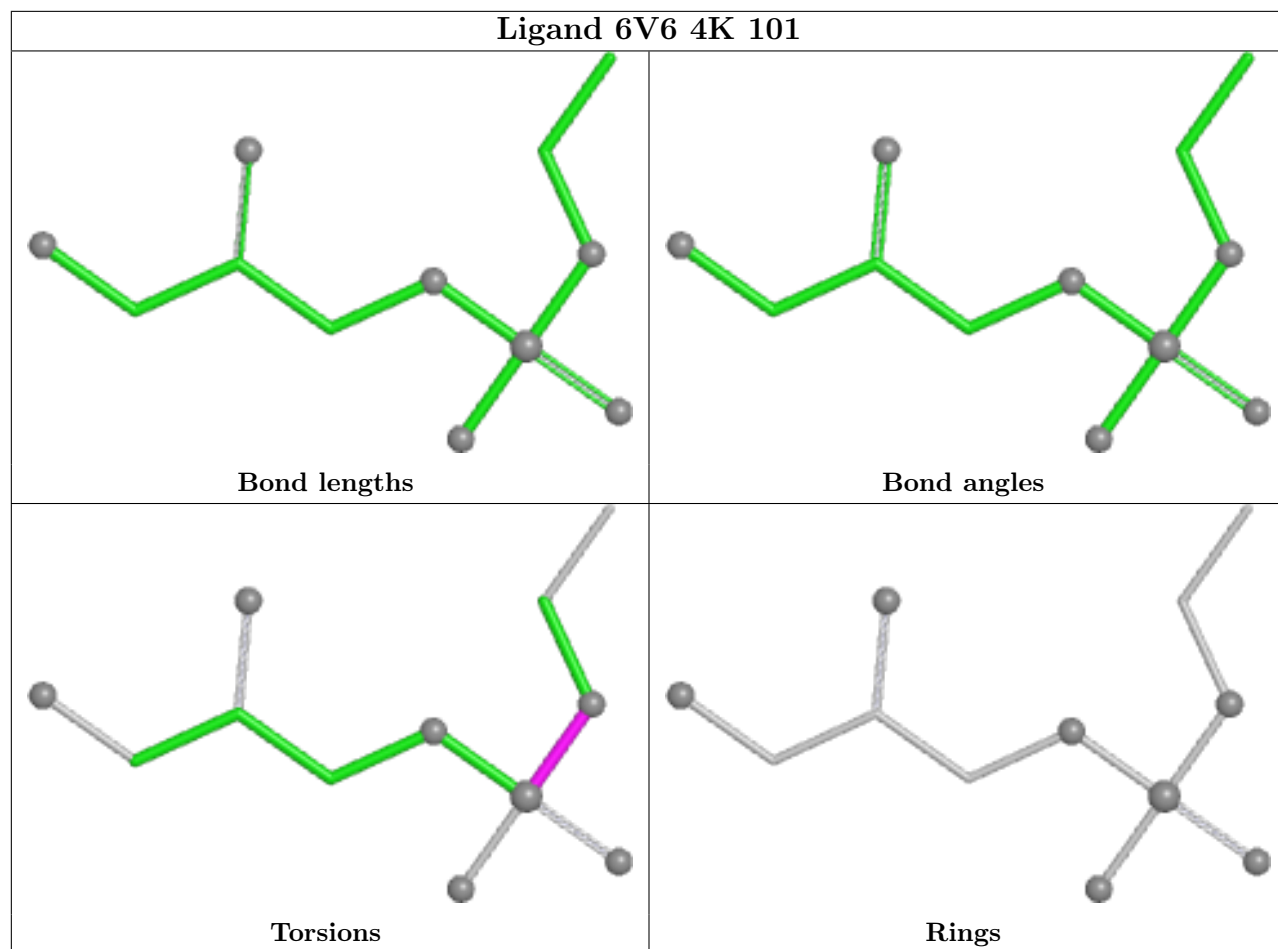


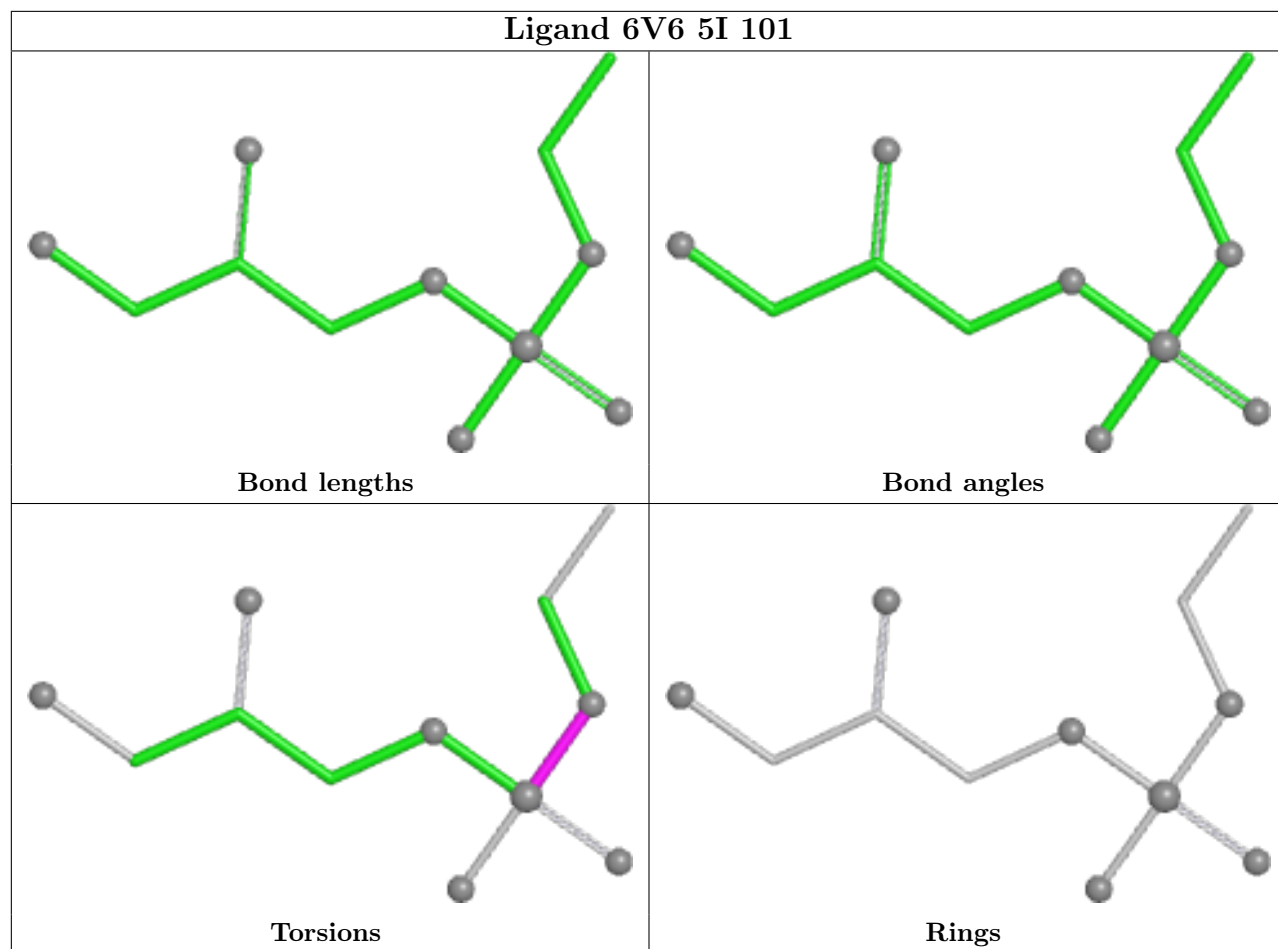


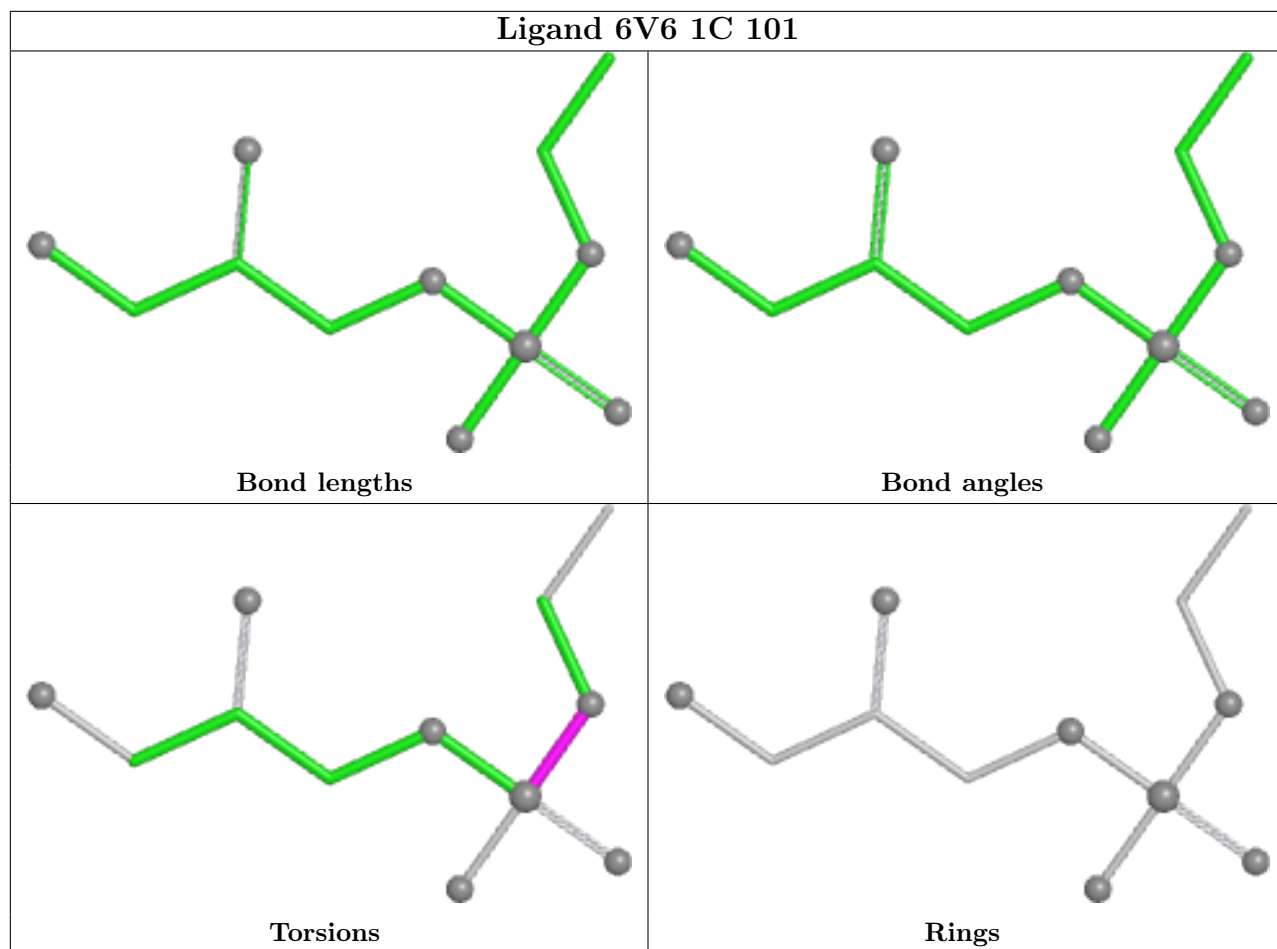


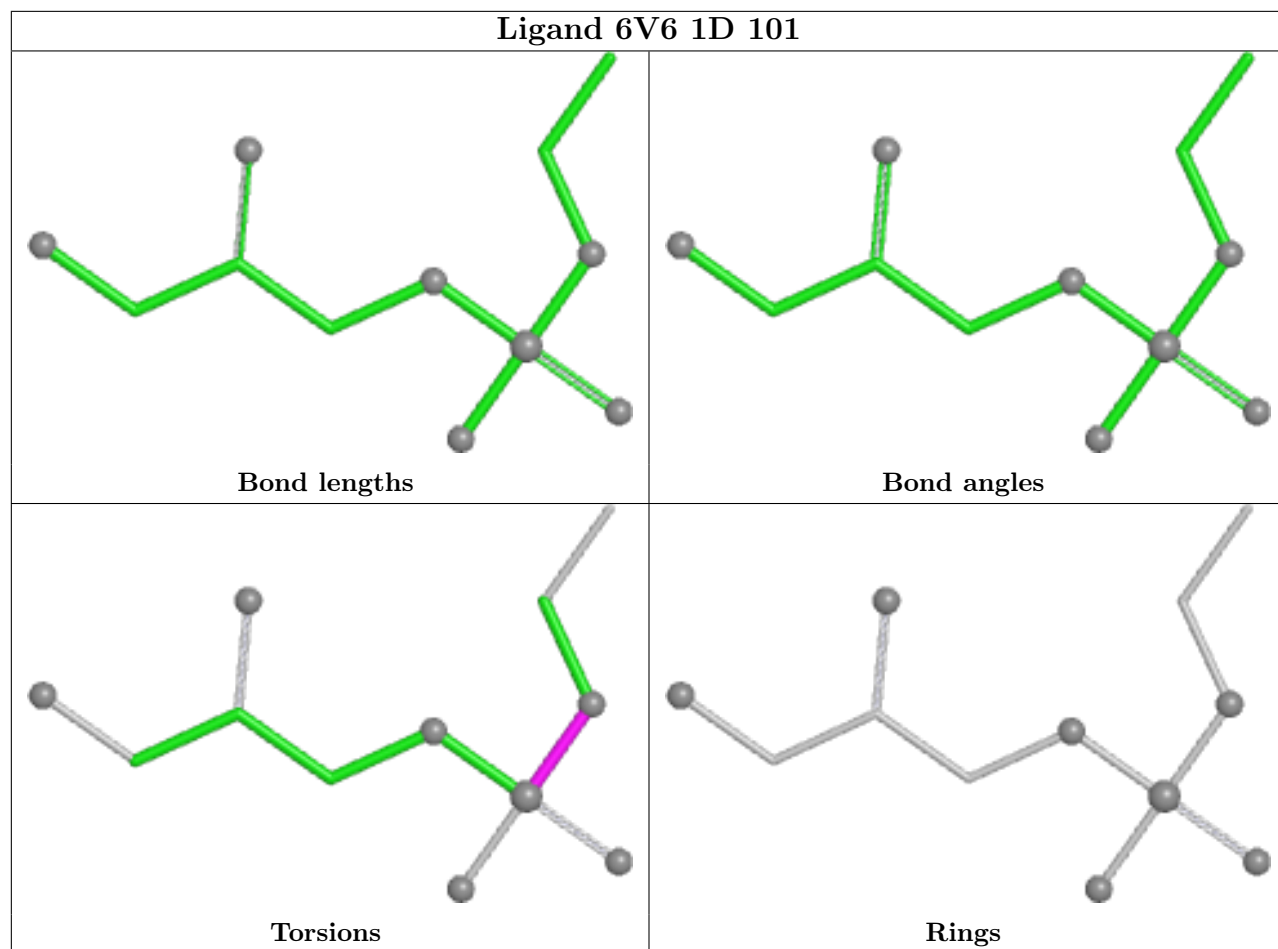


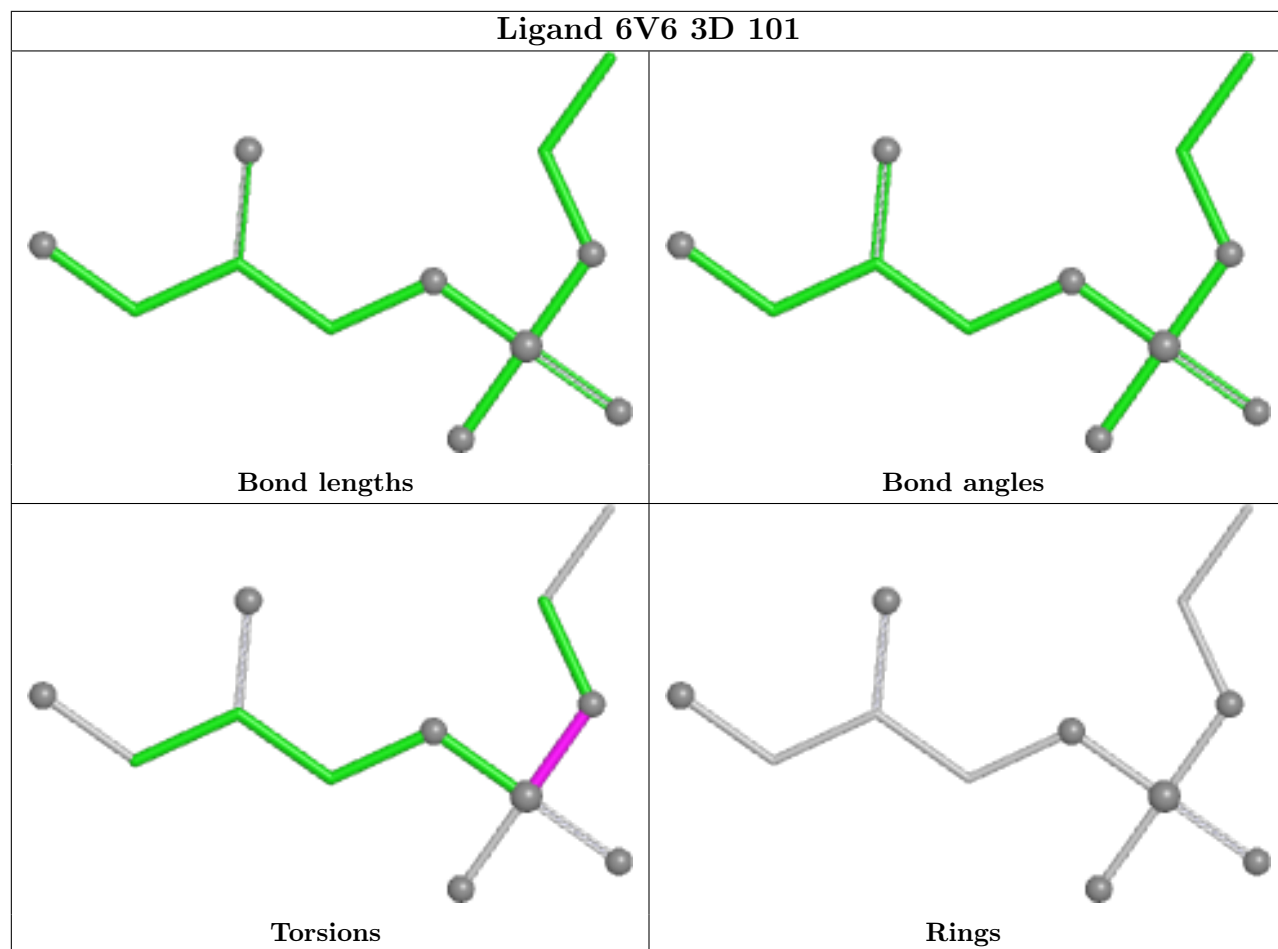


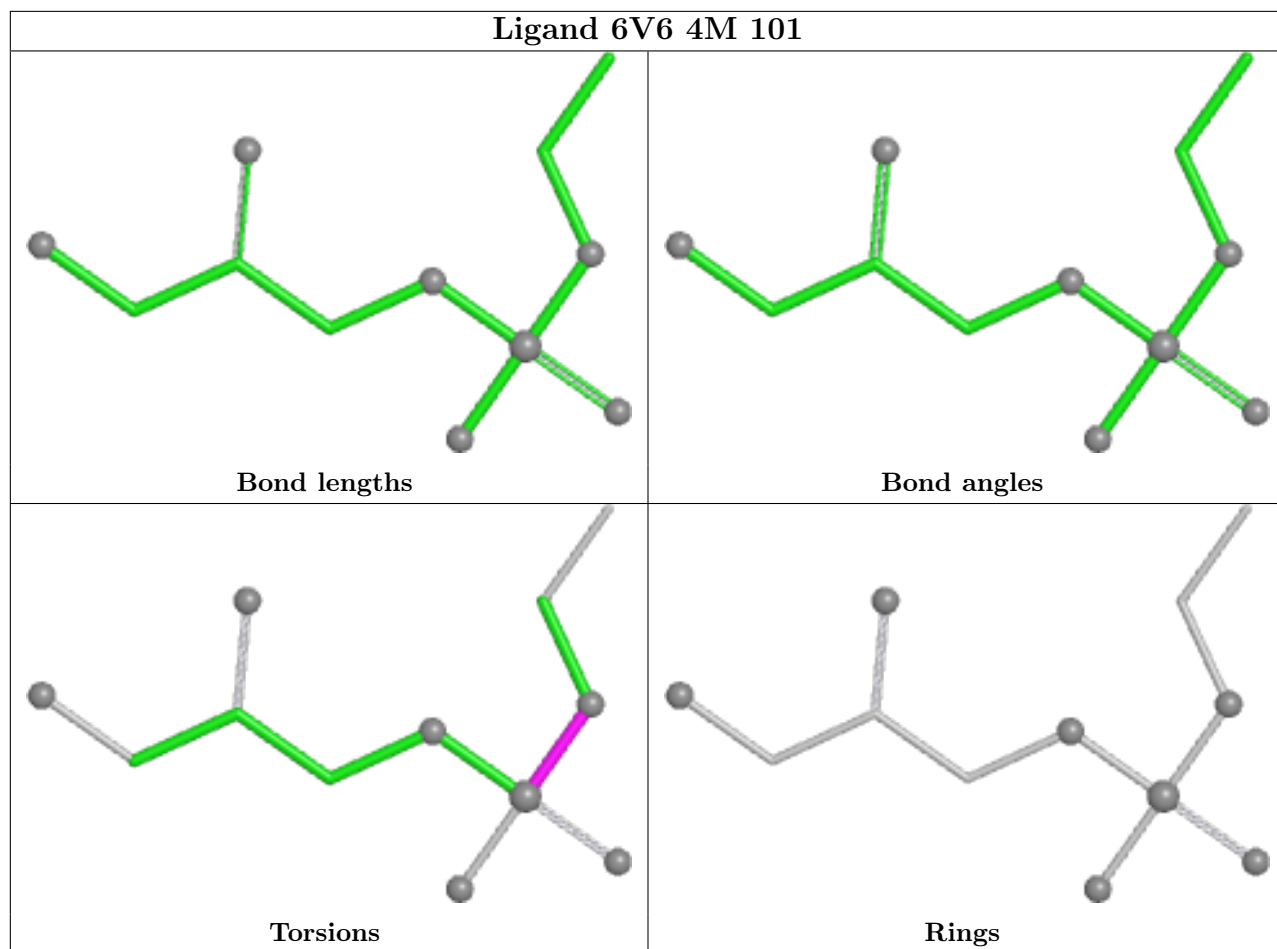


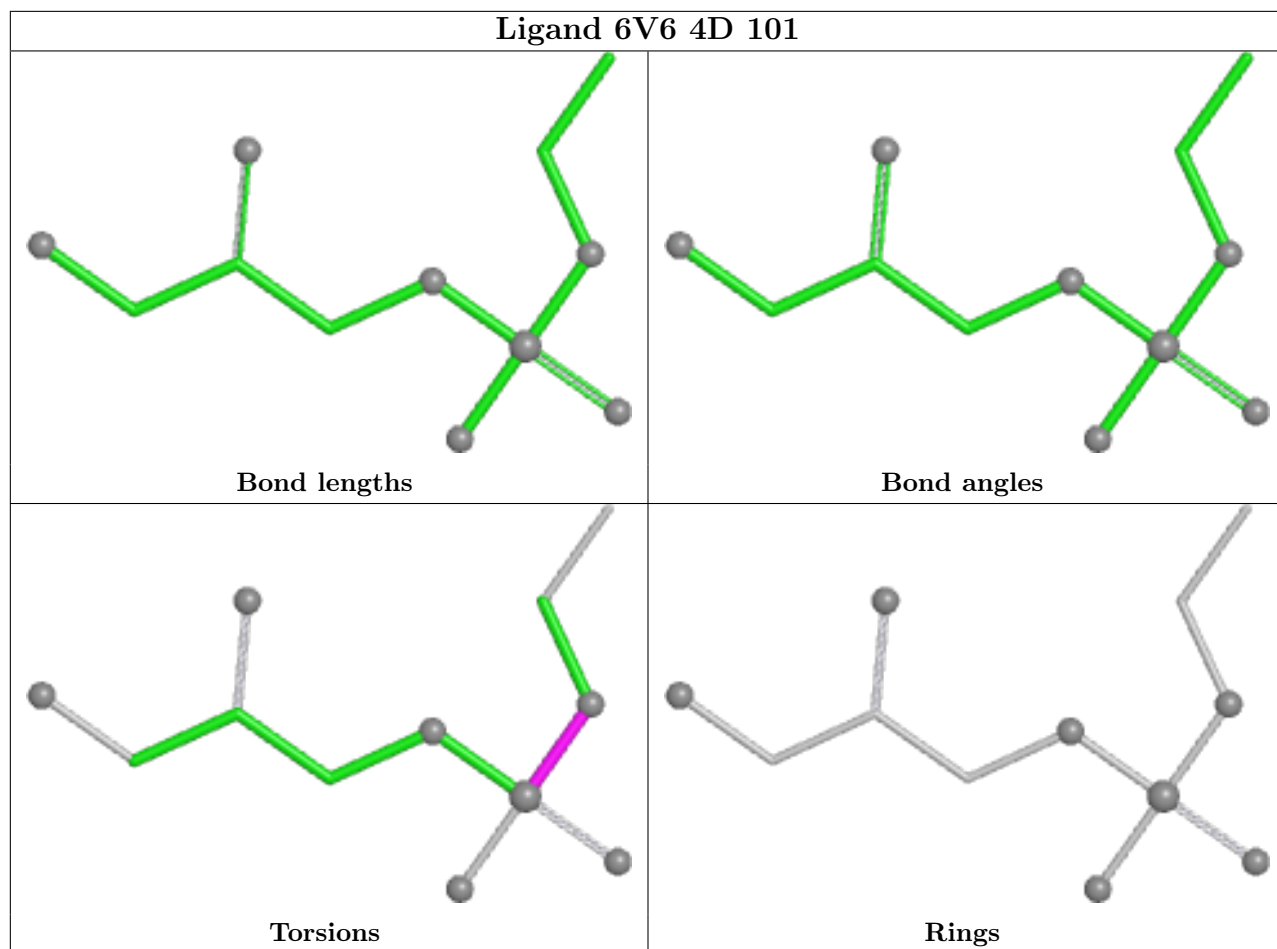


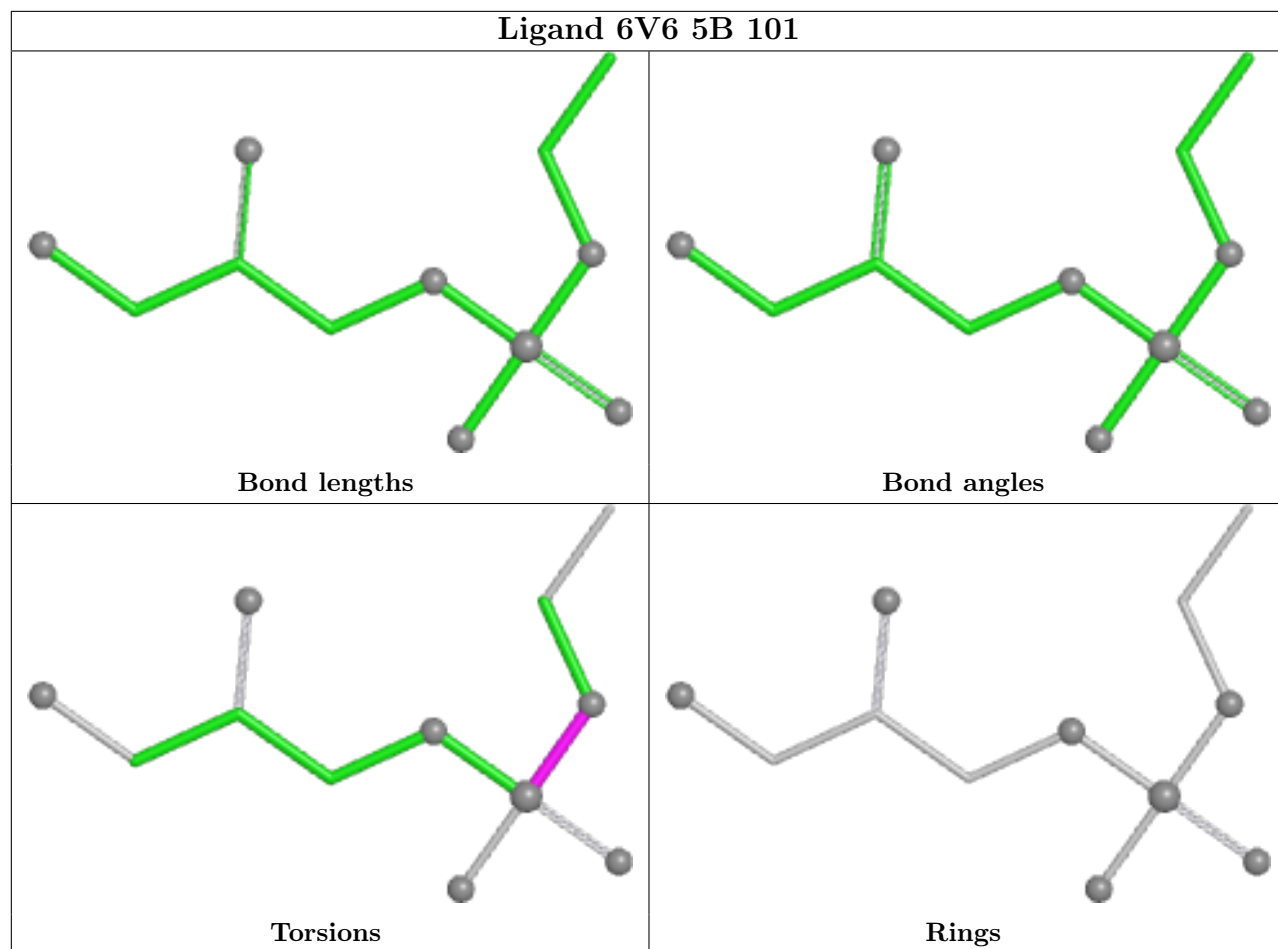


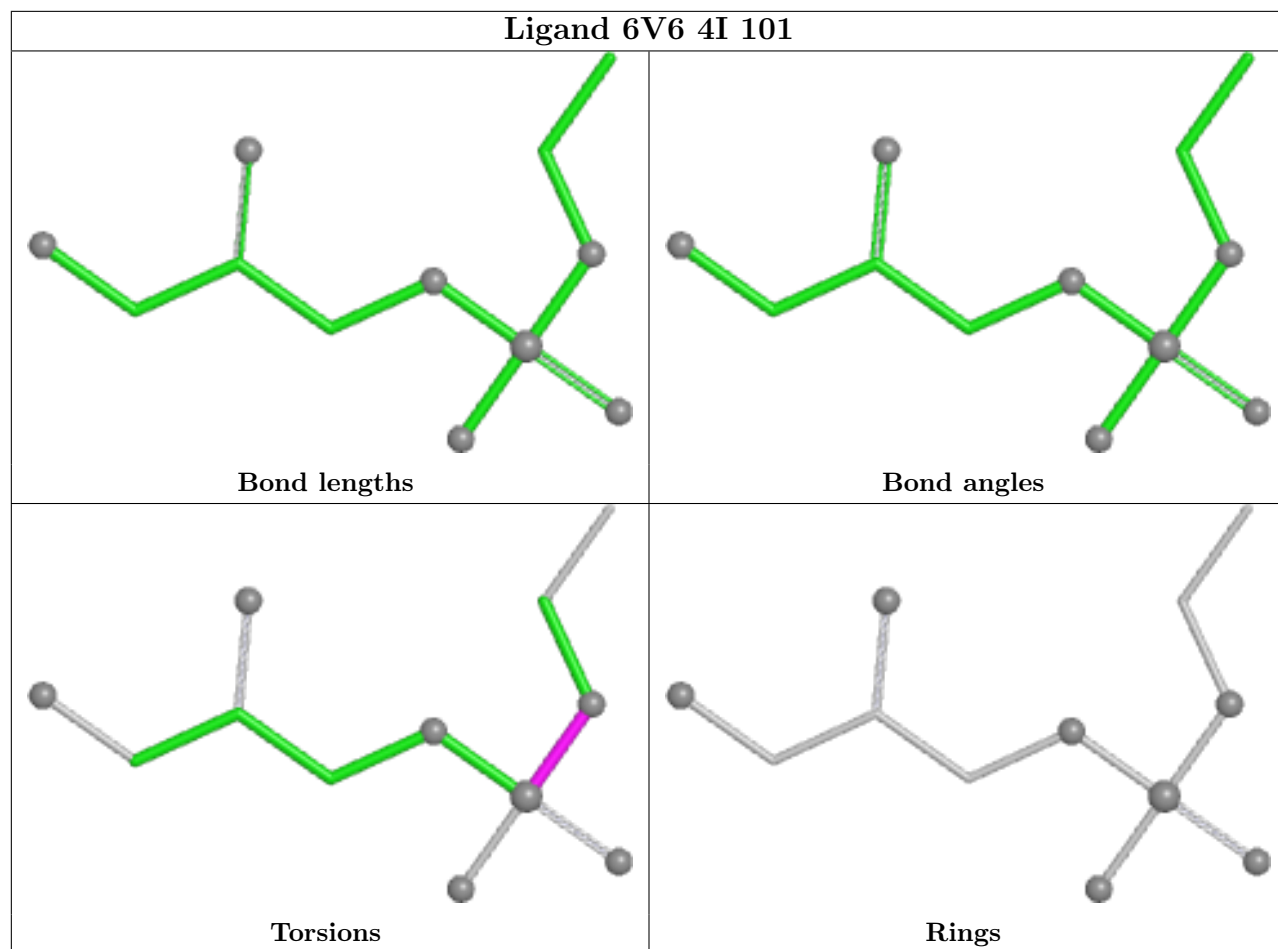


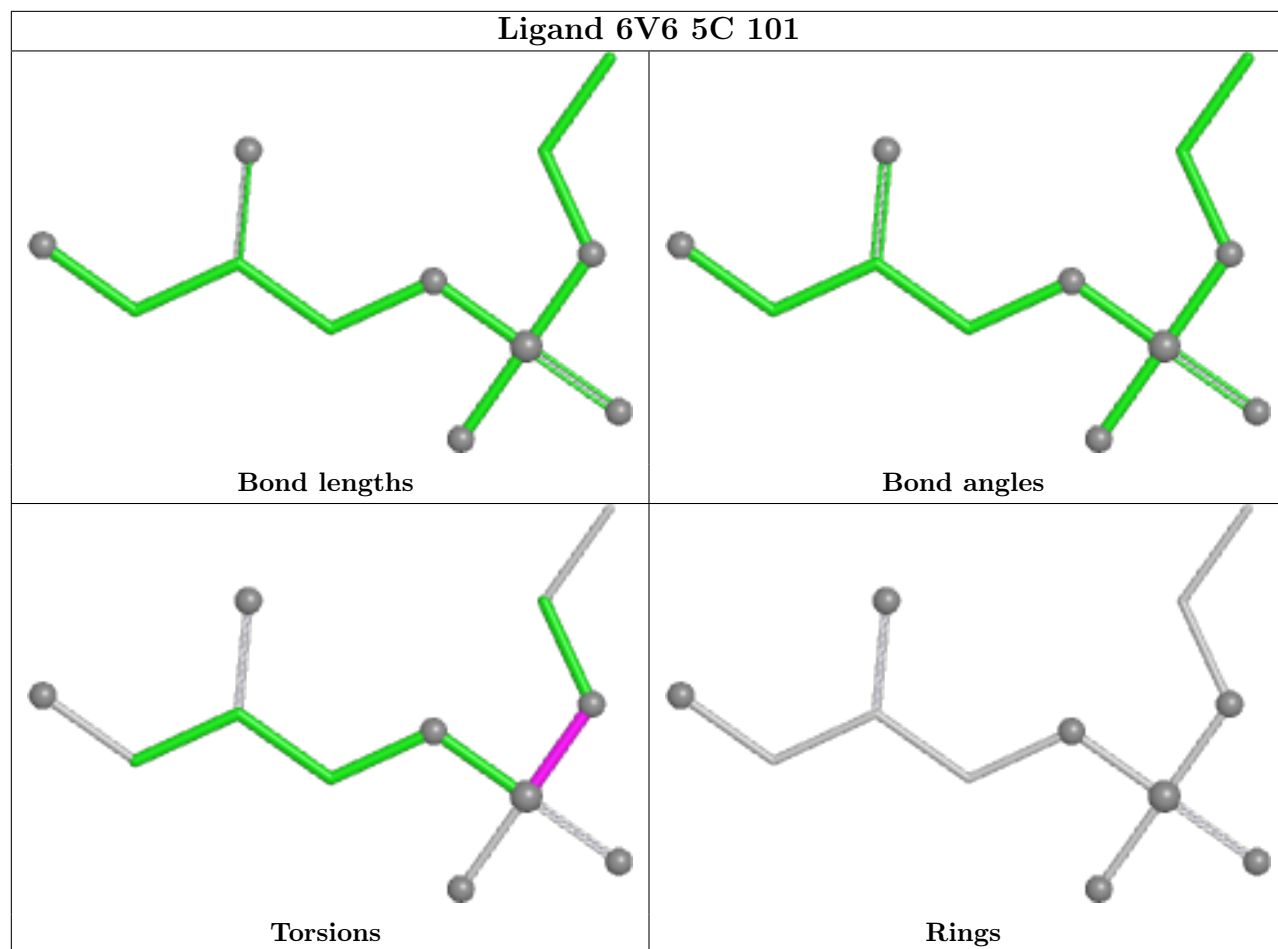


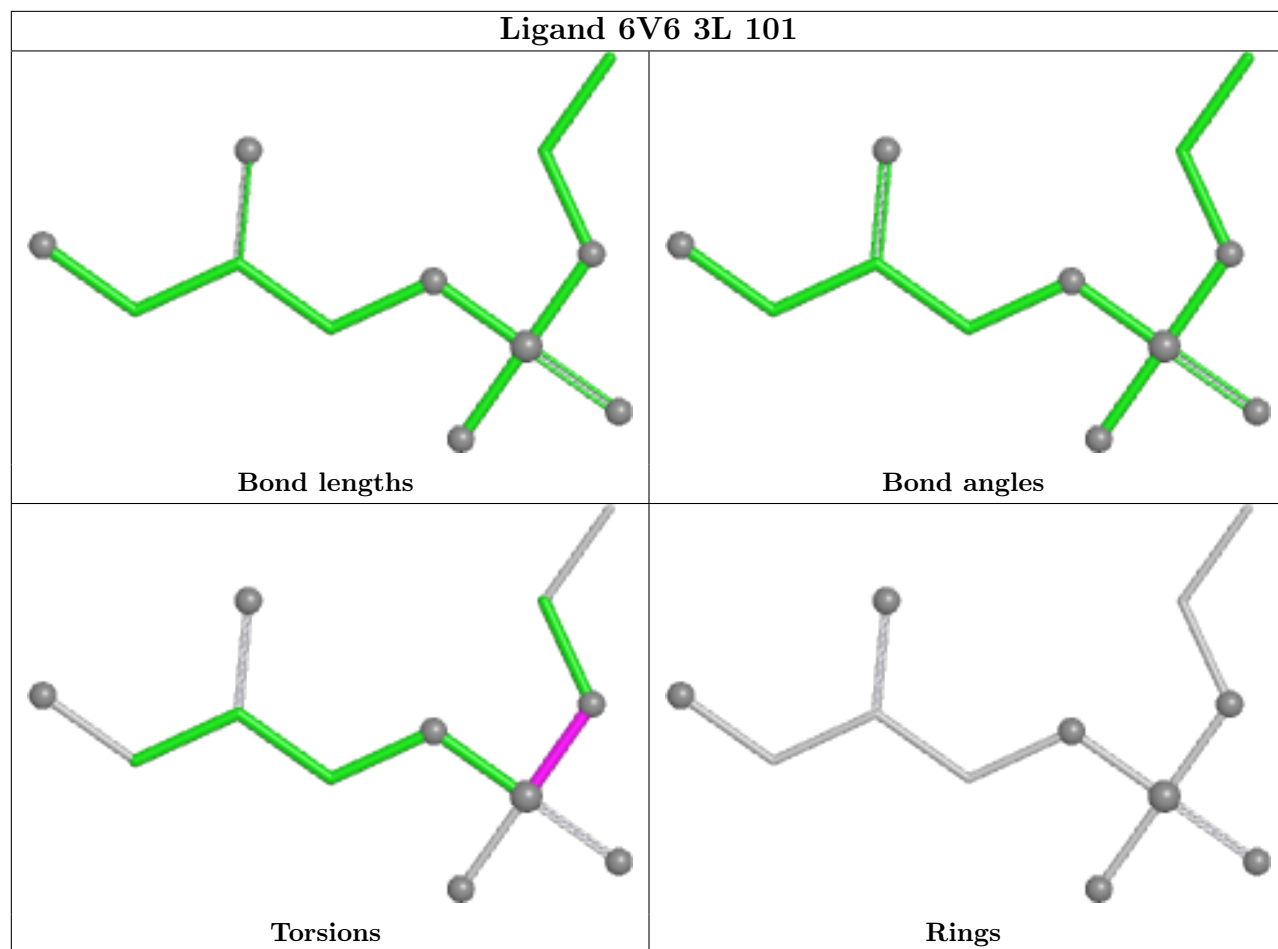


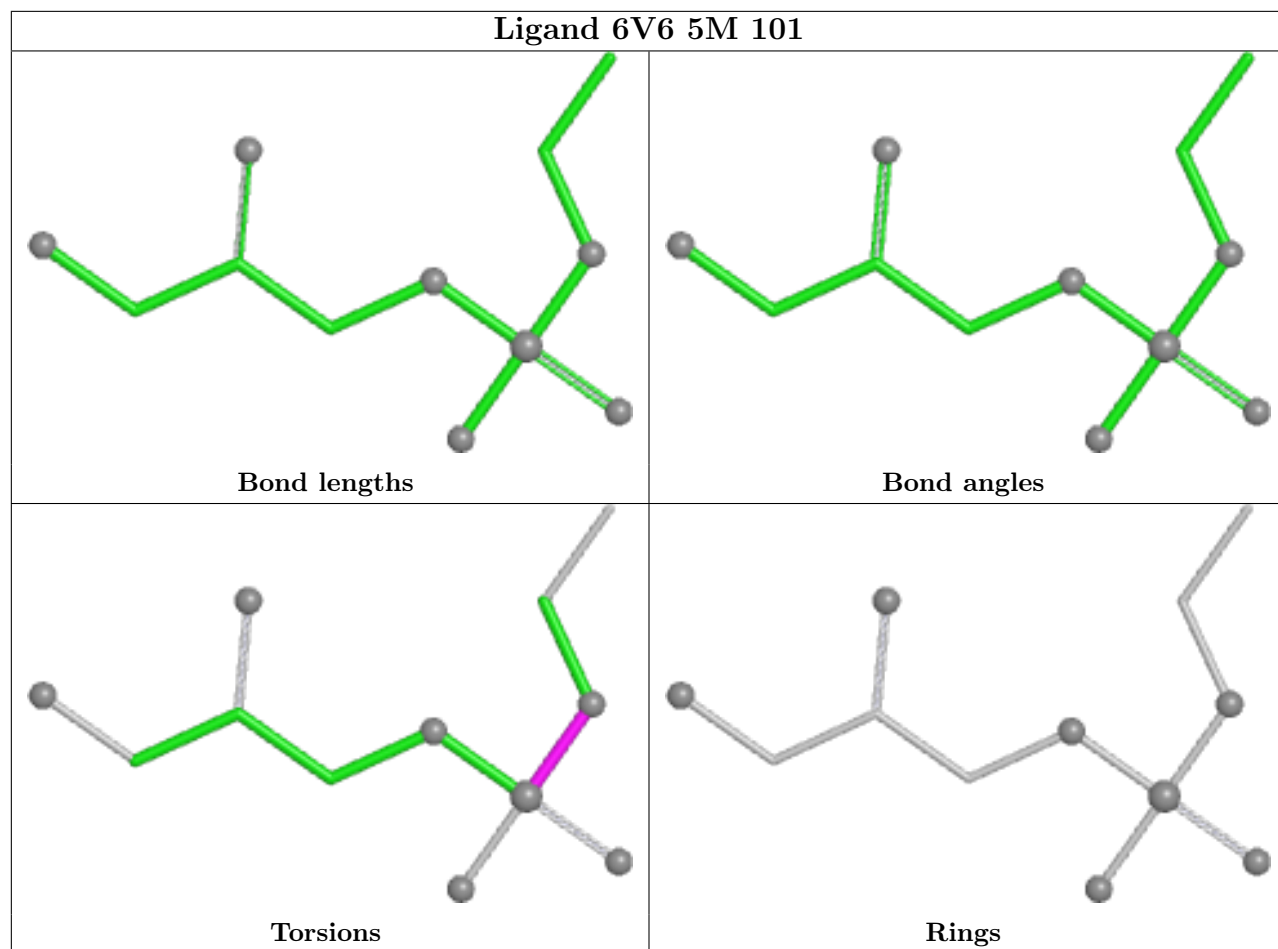


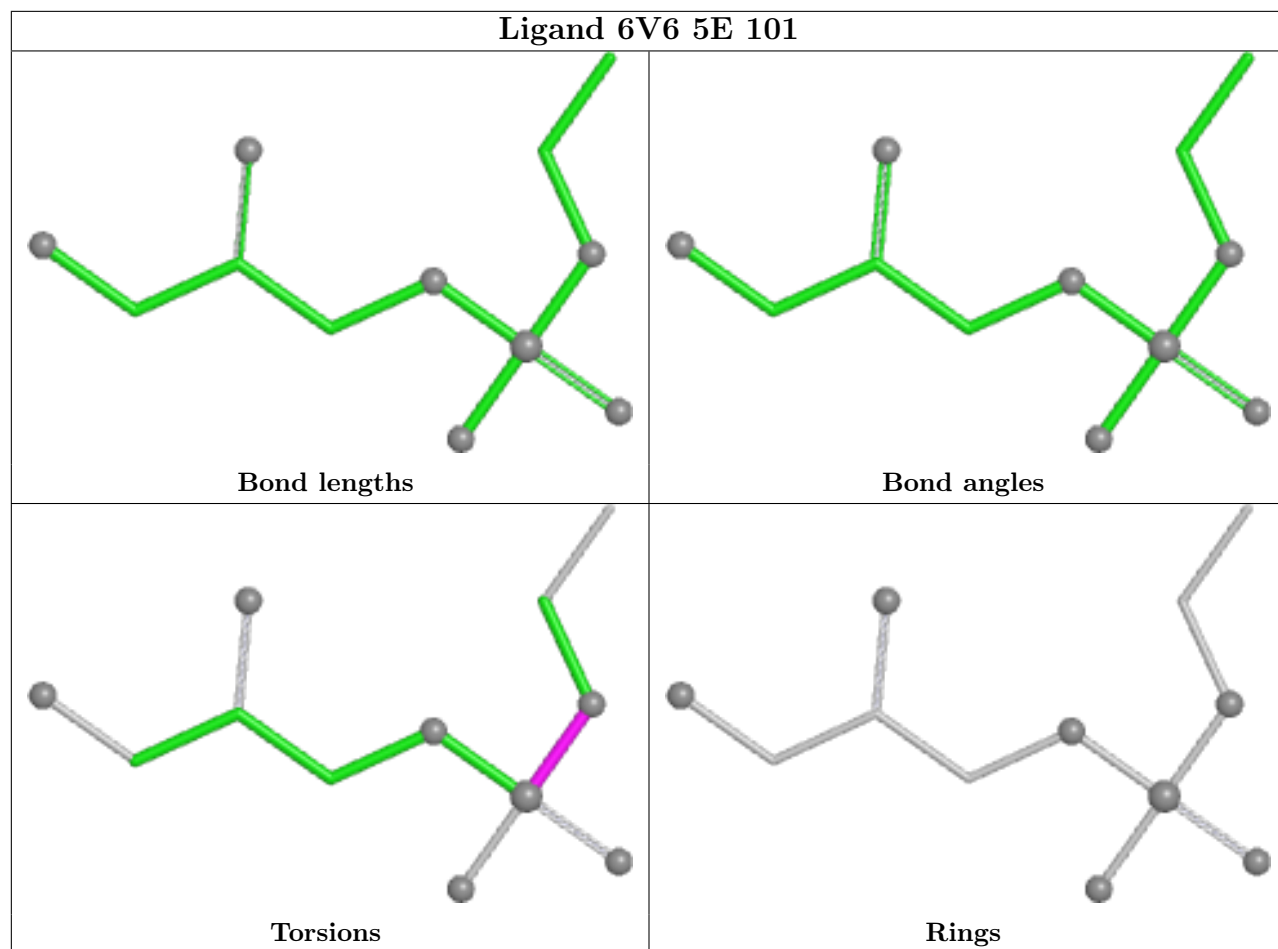


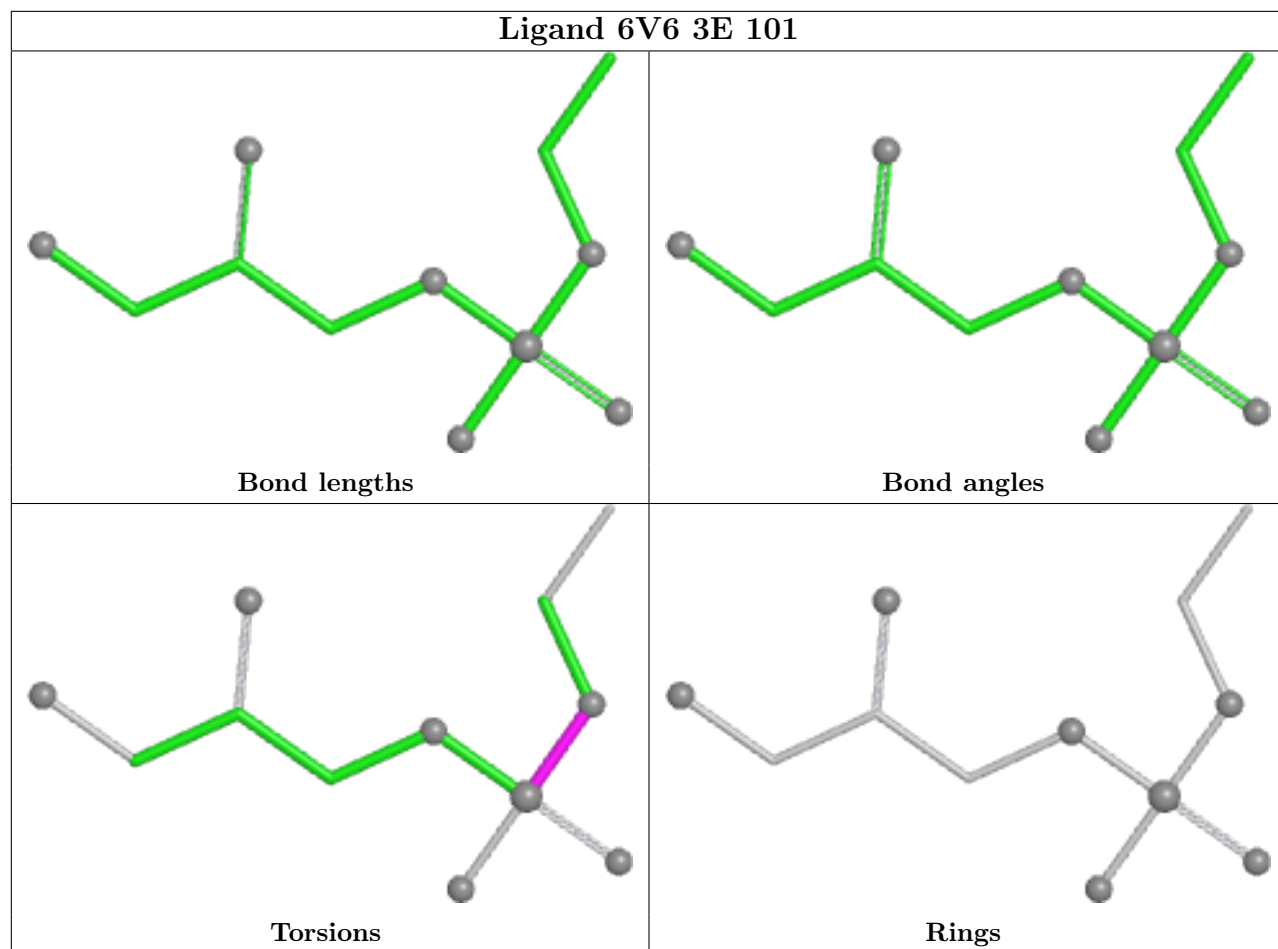












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

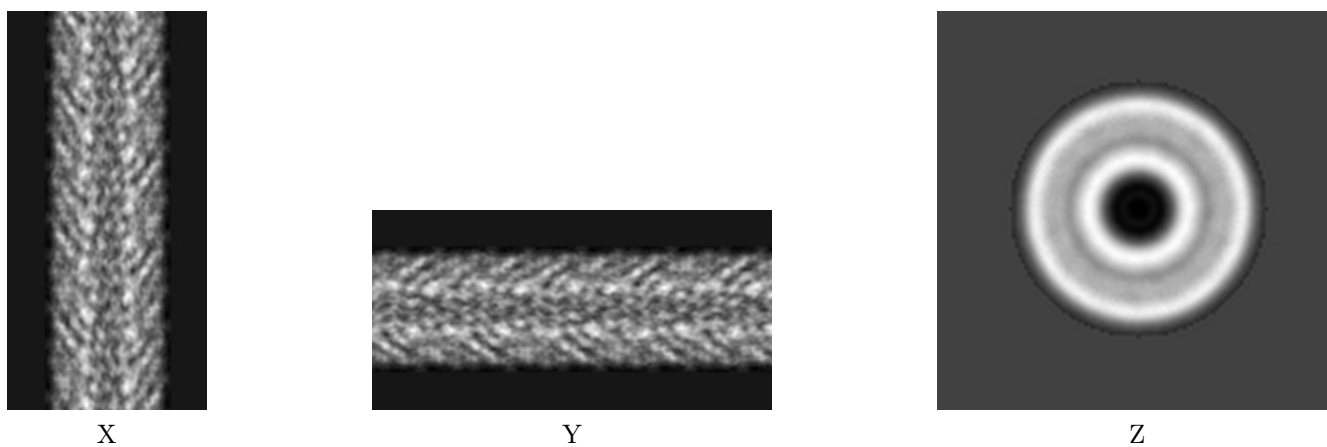
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4046. 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](#)

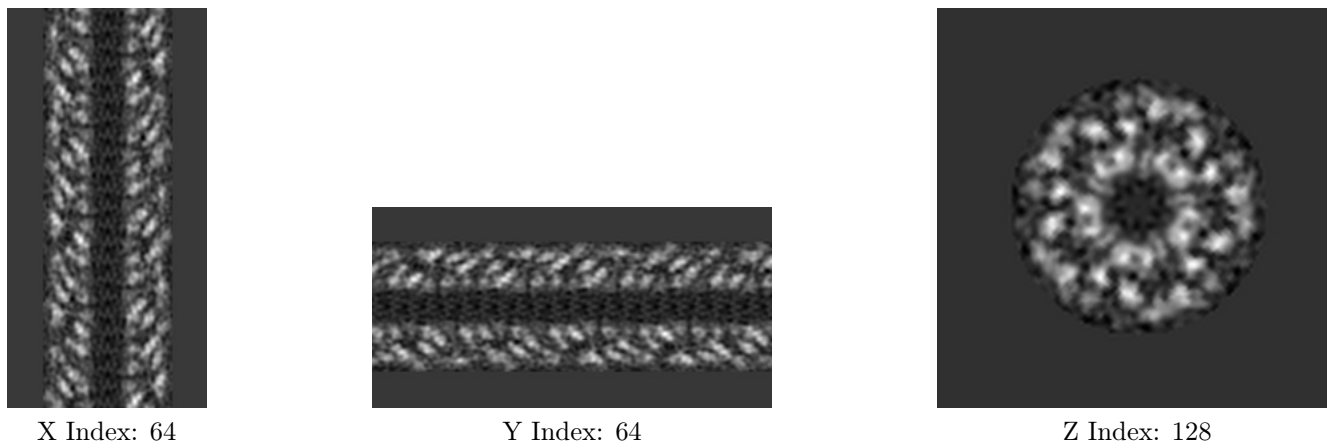
6.1.1 Primary map



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

6.2 Central slices [i](#)

6.2.1 Primary map



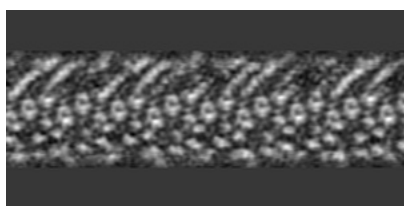
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

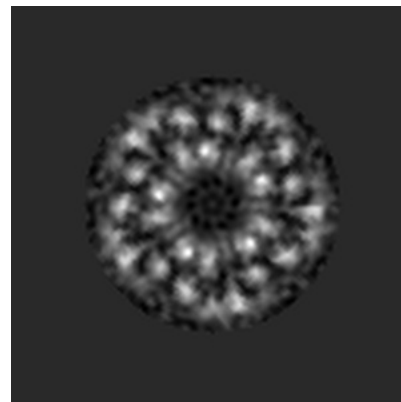
6.3.1 Primary map



X Index: 80



Y Index: 48



Z Index: 95

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 44.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

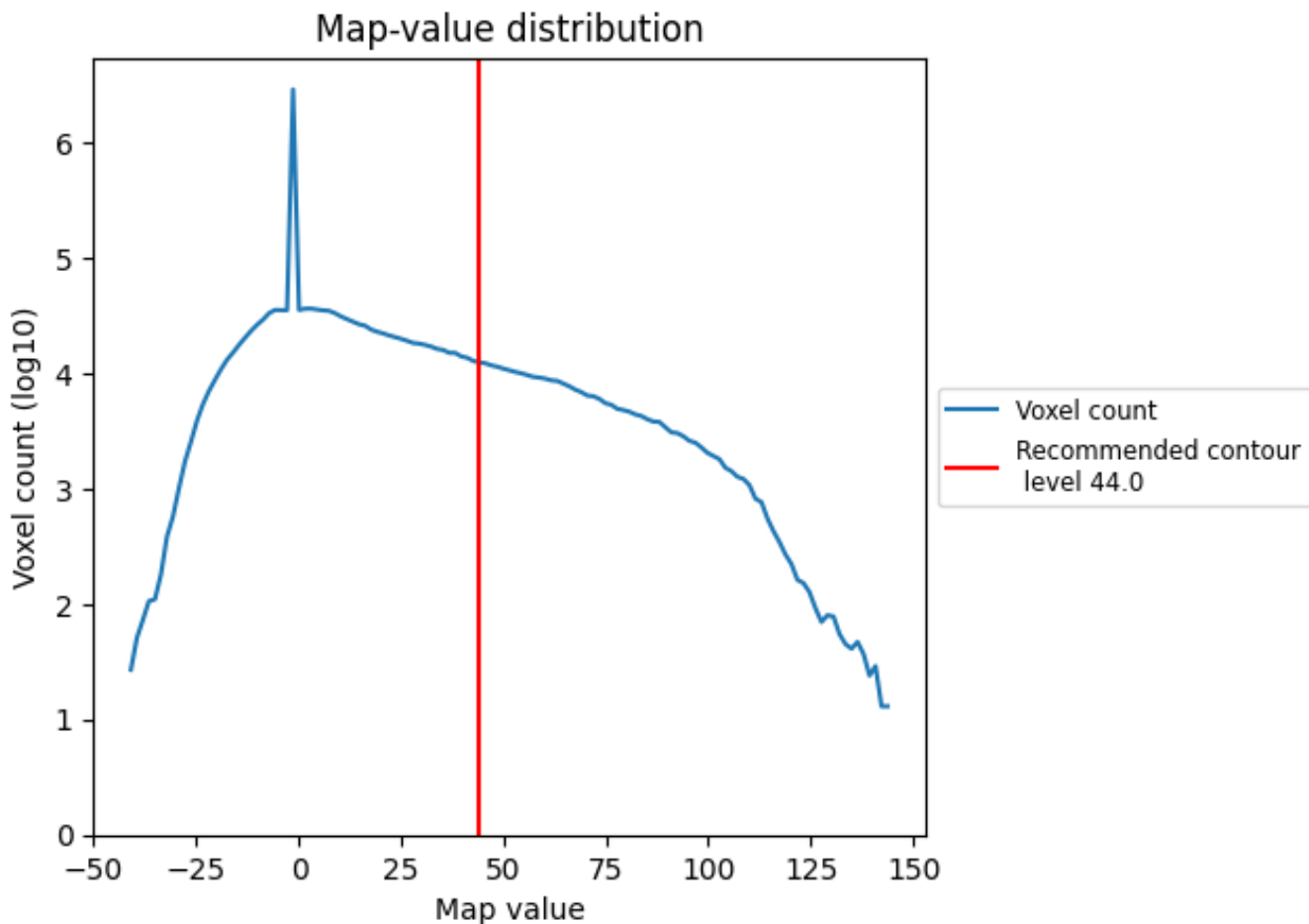
6.5 Mask visualisation

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

7 Map analysis [i](#)

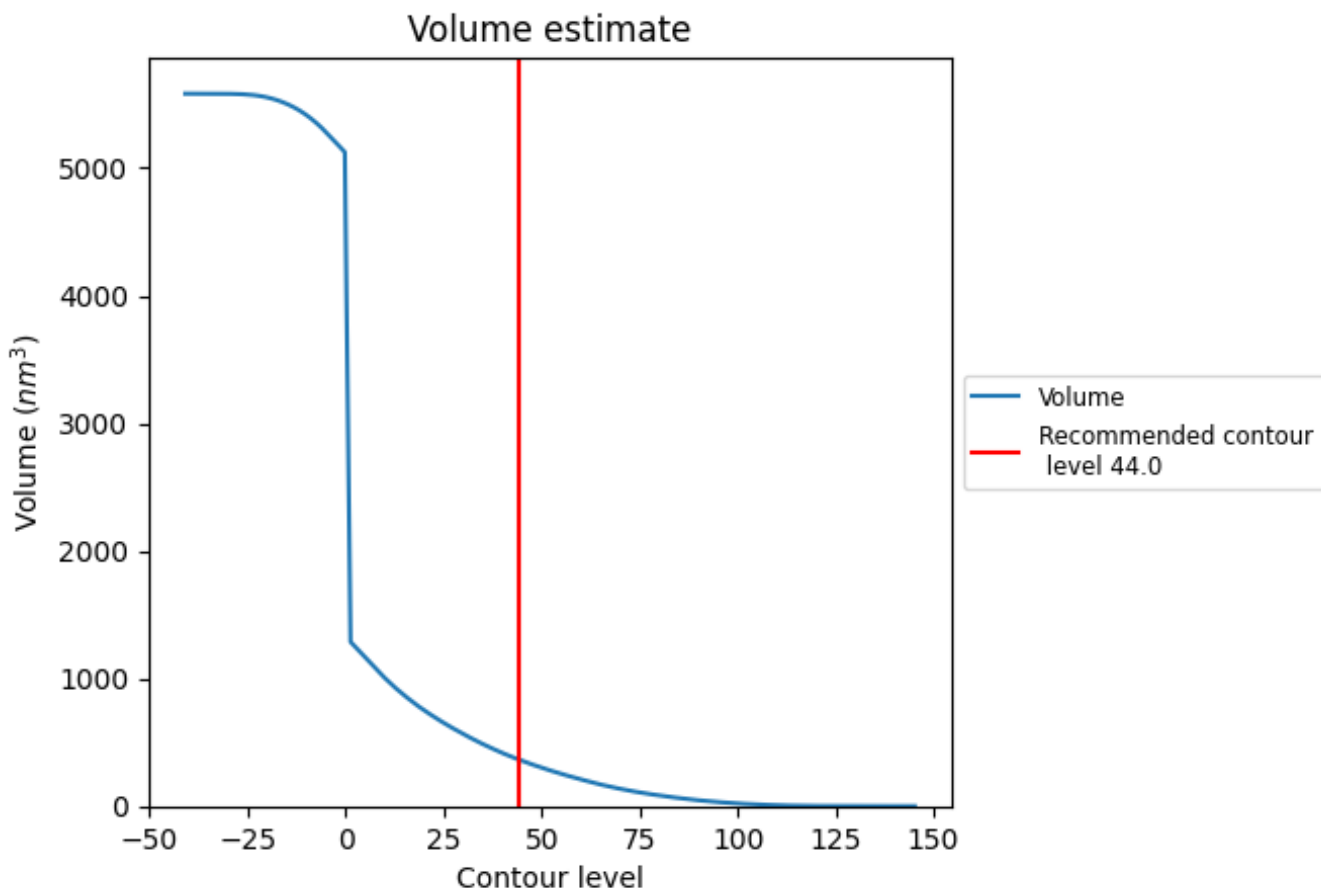
This section contains the results of statistical analysis of the map.

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 368 nm^3 ; this corresponds to an approximate mass of 332 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.

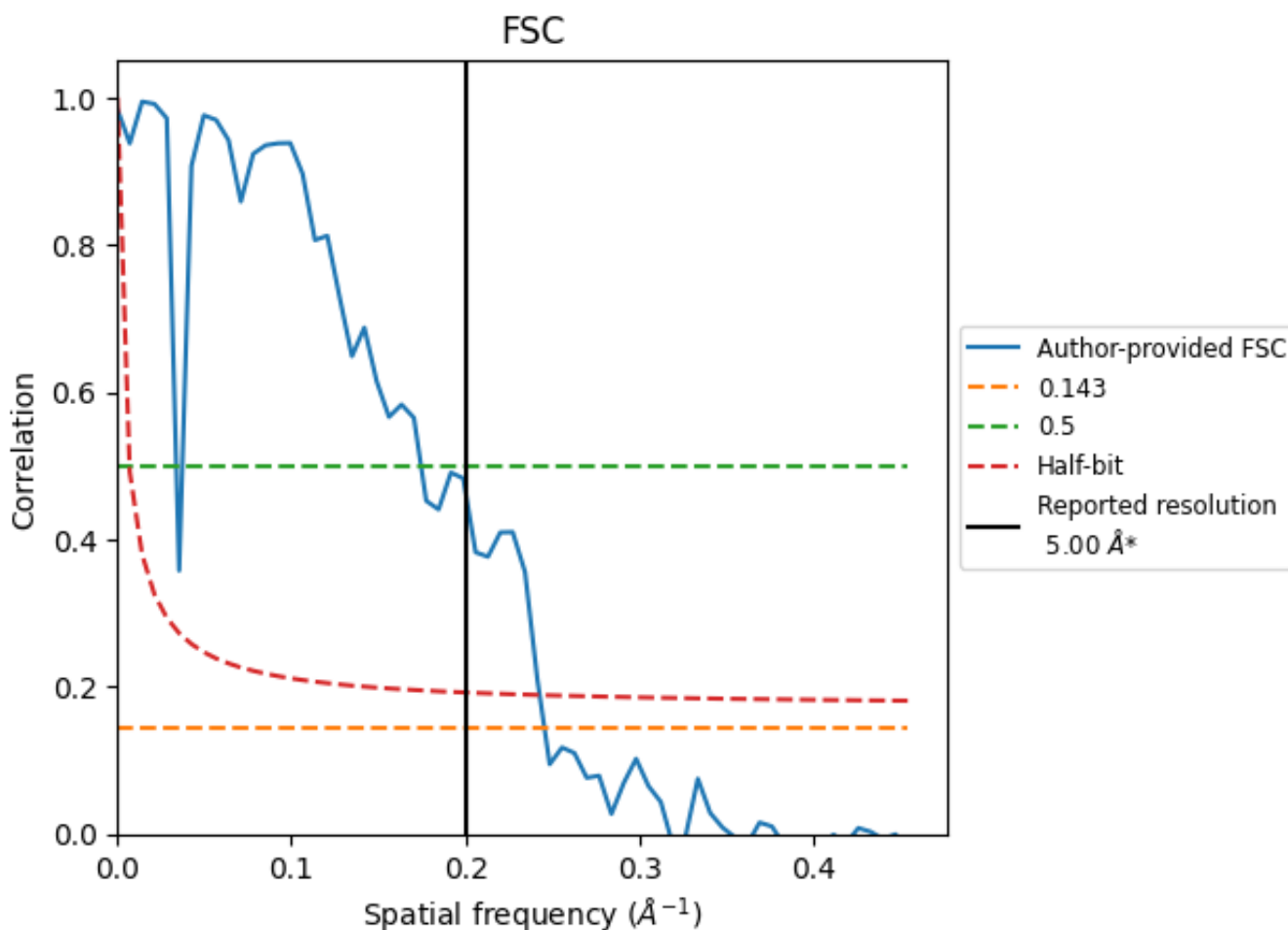
7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

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 0.200 Å⁻¹

8.2 Resolution estimates [i](#)

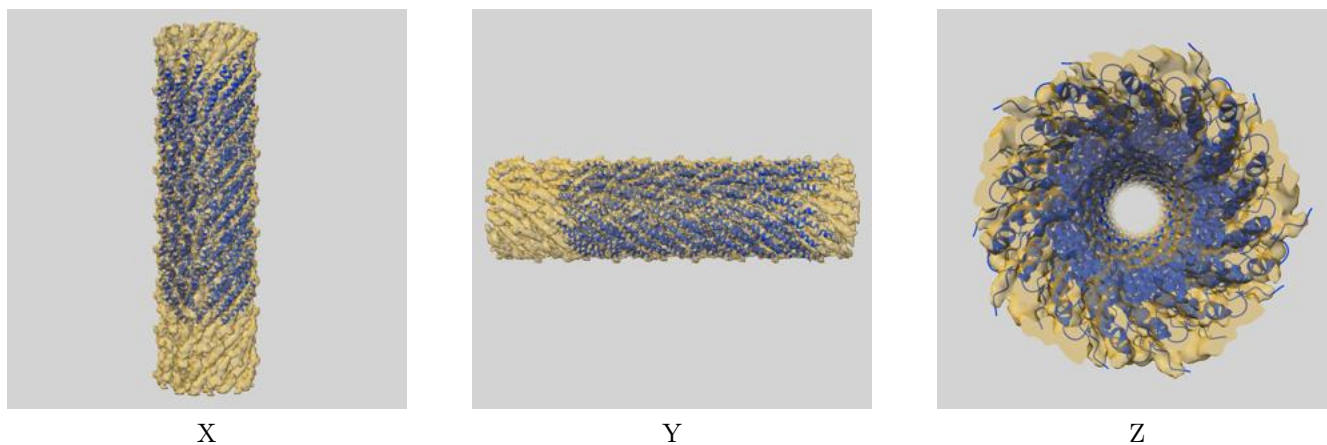
Resolution estimate (Å)	Estimation criterion (FSC cut-off)			
	0.143	0.5	Half-bit	Other
Reported by author	-	-	-	5.00
Author-provided FSC curve	4.07	29.50	4.12	-
Unmasked-calculated*	-	-	-	-

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

9 Map-model fit [i](#)

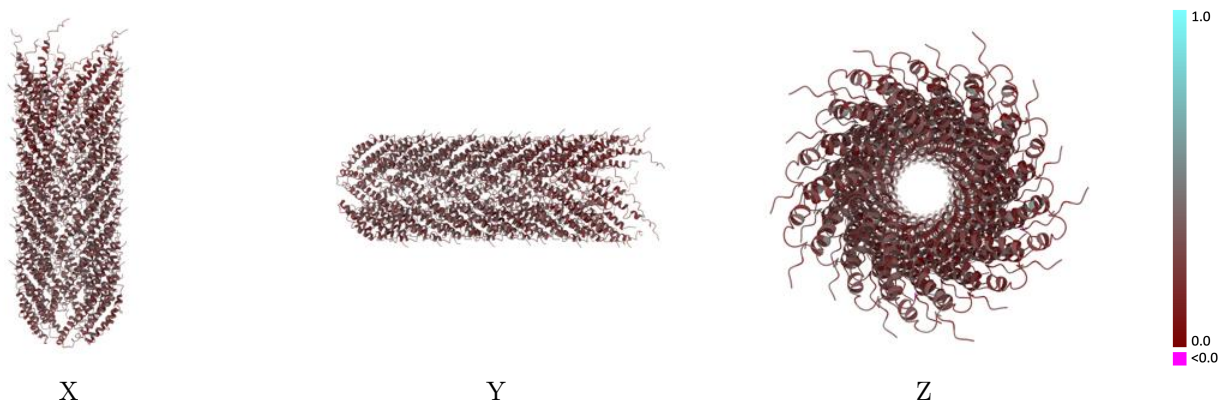
This section contains information regarding the fit between EMDB map EMD-4046 and PDB model 5LFB. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



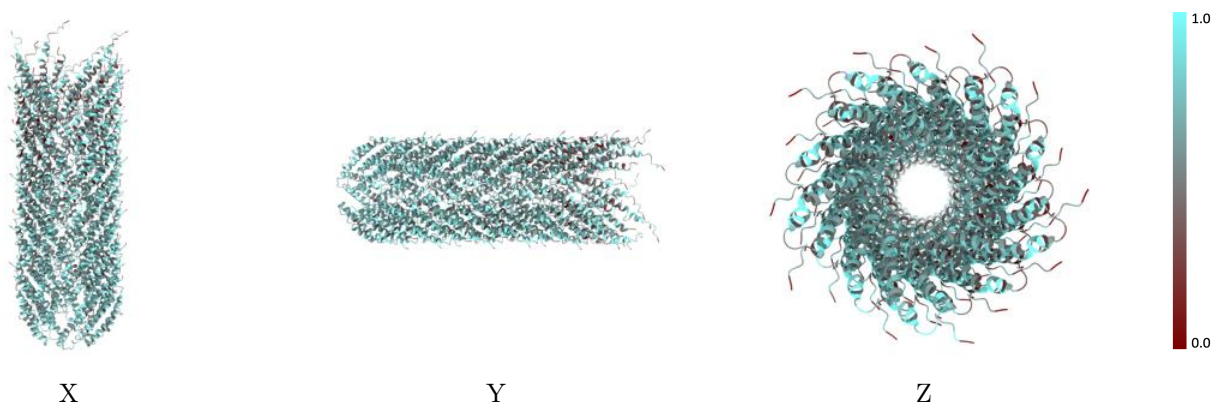
The images above show the 3D surface view of the map at the recommended contour level 44.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



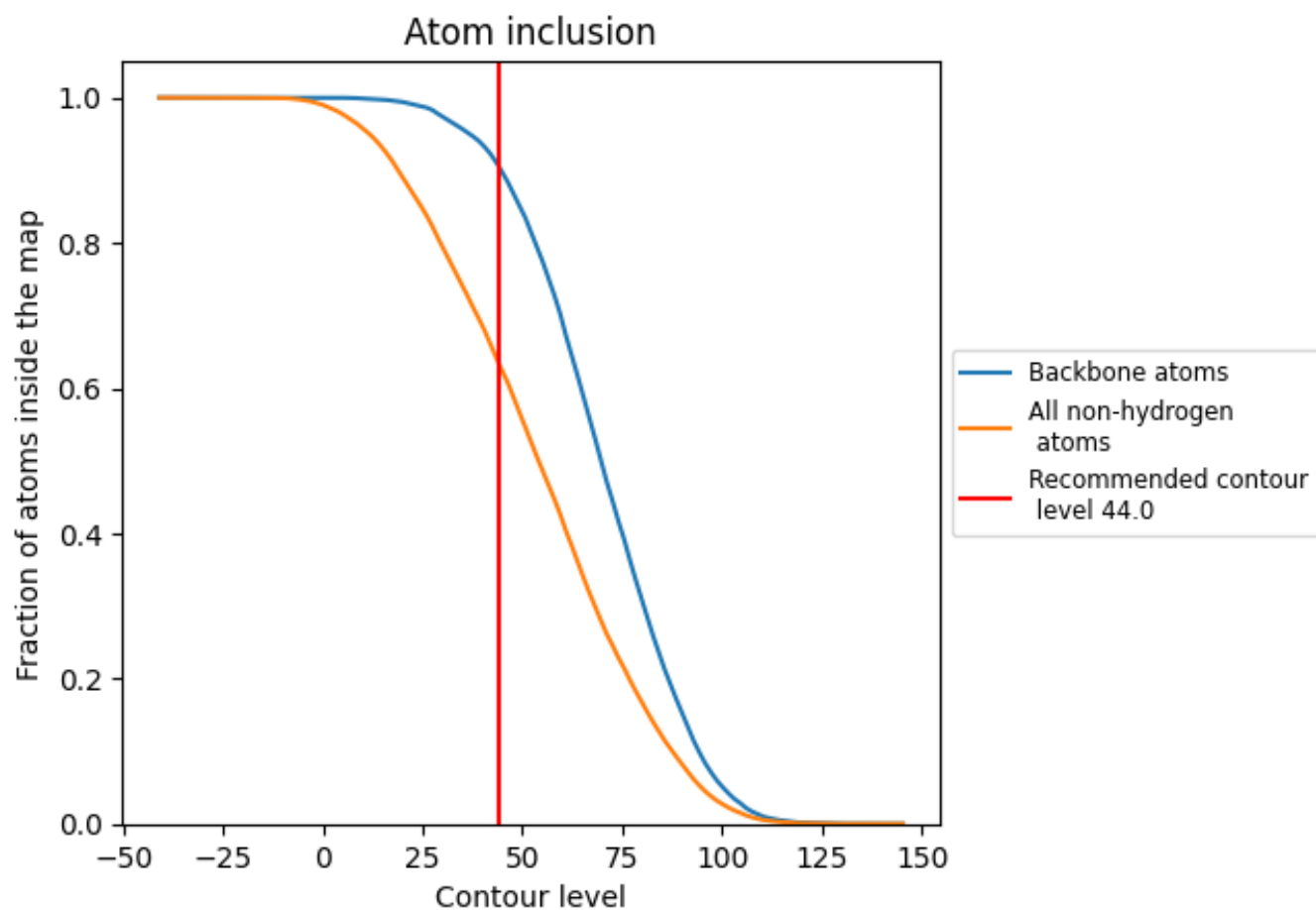
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (44.0).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 63% 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 (44.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6347	 0.2850
1A	 0.6543	 0.3090
1B	 0.6564	 0.3140
1C	 0.6708	 0.3200
1D	 0.6626	 0.3210
1E	 0.6728	 0.3170
1F	 0.6667	 0.3210
1G	 0.6523	 0.3190
1H	 0.6667	 0.3200
1I	 0.6708	 0.3210
1J	 0.6584	 0.3170
1K	 0.6564	 0.3210
1L	 0.6687	 0.3170
1M	 0.6770	 0.3190
1N	 0.6646	 0.3170
1O	 0.6626	 0.3130
2A	 0.6481	 0.2960
2B	 0.6626	 0.3140
2C	 0.6749	 0.3130
2D	 0.6502	 0.3110
2E	 0.6543	 0.3120
2F	 0.6440	 0.3080
2G	 0.6502	 0.3060
2H	 0.6337	 0.2890
2I	 0.6235	 0.2760
2J	 0.6132	 0.2630
2K	 0.6193	 0.2510
2L	 0.6070	 0.2500
2M	 0.5905	 0.2460
2N	 0.5967	 0.2560
2O	 0.6235	 0.2730
3A	 0.6481	 0.2980
3B	 0.6687	 0.3150
3C	 0.6708	 0.3100
3D	 0.6605	 0.3130



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Chain	Atom inclusion	Q-score
3E	 0.6502	 0.3140
3F	 0.6502	 0.2990
3G	 0.6481	 0.2940
3H	 0.6399	 0.2840
3I	 0.6132	 0.2640
3J	 0.6091	 0.2480
3K	 0.6193	 0.2430
3L	 0.5926	 0.2450
3M	 0.5782	 0.2410
3N	 0.5988	 0.2430
3O	 0.6152	 0.2730
4A	 0.6420	 0.3000
4B	 0.6646	 0.3130
4C	 0.6626	 0.3130
4D	 0.6646	 0.3130
4E	 0.6605	 0.3130
4F	 0.6461	 0.3040
4G	 0.6461	 0.2920
4H	 0.6337	 0.2720
4I	 0.6132	 0.2540
4J	 0.5947	 0.2350
4K	 0.5988	 0.2280
4L	 0.5617	 0.2220
4M	 0.5638	 0.2230
4N	 0.5679	 0.2250
4O	 0.5967	 0.2530
5A	 0.6461	 0.2960
5B	 0.6605	 0.3120
5C	 0.6687	 0.3120
5D	 0.6687	 0.3200
5E	 0.6543	 0.3160
5F	 0.6502	 0.3080
5G	 0.6440	 0.2990
5H	 0.6337	 0.2850
5I	 0.6152	 0.2600
5J	 0.5988	 0.2500
5K	 0.6049	 0.2400
5L	 0.5864	 0.2260
5M	 0.5720	 0.2230
5N	 0.5720	 0.2260
5O	 0.5926	 0.2460