wwPDB EM Validation Summary Report ⓘ

Apr 10, 2023 – 10:46 AM EDT

PDB ID	:	8CW4
EMDB ID	:	EMD-27023
Title	:	CryoEM structure of the N-pilus from Escherichia coli
Authors	:	Bui, K.H.; Black, C.S.
Deposited on	:	2022-05-18
Resolution	:	3.00 Å(reported)

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

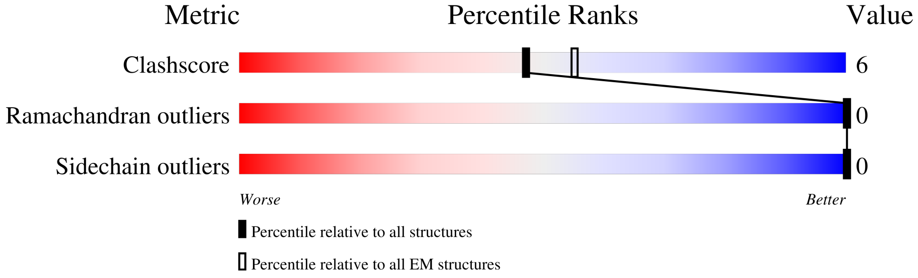
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

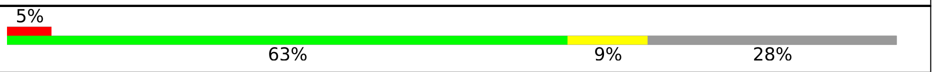
The reported resolution of this entry is 3.00 Å.

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 <=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	97	
1	1B	97	
1	1C	97	
1	1D	97	
1	1E	97	
1	1F	97	
1	1G	97	
1	1H	97	

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Mol	Chain	Length	Quality of chain
1	1I	97	• 60% 12% 28%
1	1J	97	• 60% 12% 28%
1	1K	97	• 60% 12% 28%
1	1L	97	• 61% 11% 28%
1	1M	97	• 62% 10% 28%
1	1N	97	6% 64% 8% 28%
1	2A	97	6% 62% 10% 28%
1	2B	97	• 60% 12% 28%
1	2C	97	• 60% 12% 28%
1	2D	97	• 60% 12% 28%
1	2E	97	• 60% 12% 28%
1	2F	97	• 60% 12% 28%
1	2G	97	• 60% 12% 28%
1	2H	97	• 61% 11% 28%
1	2I	97	• 60% 12% 28%
1	2J	97	• 61% 11% 28%
1	2K	97	• 61% 11% 28%
1	2L	97	• 60% 12% 28%
1	2M	97	• 62% 10% 28%
1	2N	97	6% 64% 8% 28%
1	3A	97	7% 64% 8% 28%
1	3B	97	• 59% 13% 28%
1	3C	97	• 60% 12% 28%
1	3D	97	• 60% 12% 28%
1	3E	97	• 61% 11% 28%

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Mol	Chain	Length	Quality of chain
1	3F	97	• 61% 11% 28%
1	3G	97	• 60% 12% 28%
1	3H	97	• 61% 11% 28%
1	3I	97	• 60% 12% 28%
1	3J	97	• 61% 11% 28%
1	3K	97	• 60% 12% 28%
1	3L	97	• 60% 12% 28%
1	3M	97	• 61% 11% 28%
1	3N	97	6% 63% 9% 28%
1	4A	97	6% 63% 9% 28%
1	4B	97	• 60% 12% 28%
1	4C	97	• 60% 12% 28%
1	4D	97	• 61% 11% 28%
1	4E	97	• 61% 11% 28%
1	4F	97	• 60% 12% 28%
1	4G	97	• 60% 12% 28%
1	4H	97	• 61% 11% 28%
1	4I	97	• 61% 11% 28%
1	4J	97	• 60% 12% 28%
1	4K	97	• 61% 11% 28%
1	4L	97	• 60% 12% 28%
1	4M	97	• 61% 11% 28%
1	4N	97	6% 62% 10% 28%
1	5A	97	5% 63% 9% 28%
1	5B	97	• 60% 12% 28%

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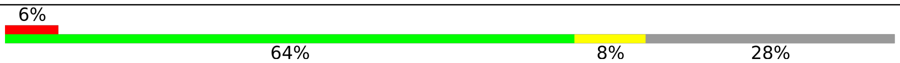
Mol	Chain	Length	Quality of chain
1	5C	97	
1	5D	97	
1	5E	97	
1	5F	97	
1	5G	97	
1	5H	97	
1	5I	97	
1	5J	97	
1	5K	97	
1	5L	97	
1	5M	97	
1	5N	97	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 44590 atoms, of which 5320 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 Conjugal transfer protein TraM.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1A	70	510	333	79	93	5	0	0
1	1B	70	510	333	79	93	5	0	0
1	1C	70	510	333	79	93	5	0	0
1	1D	70	510	333	79	93	5	0	0
1	1E	70	510	333	79	93	5	0	0
1	1F	70	510	333	79	93	5	0	0
1	1G	70	510	333	79	93	5	0	0
1	1H	70	510	333	79	93	5	0	0
1	1I	70	510	333	79	93	5	0	0
1	1J	70	510	333	79	93	5	0	0
1	1K	70	510	333	79	93	5	0	0
1	1L	70	510	333	79	93	5	0	0
1	1M	70	510	333	79	93	5	0	0
1	1N	70	510	333	79	93	5	0	0
1	2A	70	510	333	79	93	5	0	0
1	2B	70	510	333	79	93	5	0	0
1	2C	70	510	333	79	93	5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	2D	70	Total 510	C 333	N 79	O 93	S 5	0	0
1	2E	70	Total 510	C 333	N 79	O 93	S 5	0	0
1	2F	70	Total 510	C 333	N 79	O 93	S 5	0	0
1	2G	70	Total 510	C 333	N 79	O 93	S 5	0	0
1	2H	70	Total 510	C 333	N 79	O 93	S 5	0	0
1	2I	70	Total 510	C 333	N 79	O 93	S 5	0	0
1	2J	70	Total 510	C 333	N 79	O 93	S 5	0	0
1	2K	70	Total 510	C 333	N 79	O 93	S 5	0	0
1	2L	70	Total 510	C 333	N 79	O 93	S 5	0	0
1	2M	70	Total 510	C 333	N 79	O 93	S 5	0	0
1	2N	70	Total 510	C 333	N 79	O 93	S 5	0	0
1	3A	70	Total 510	C 333	N 79	O 93	S 5	0	0
1	3B	70	Total 510	C 333	N 79	O 93	S 5	0	0
1	3C	70	Total 510	C 333	N 79	O 93	S 5	0	0
1	3D	70	Total 510	C 333	N 79	O 93	S 5	0	0
1	3E	70	Total 510	C 333	N 79	O 93	S 5	0	0
1	3F	70	Total 510	C 333	N 79	O 93	S 5	0	0
1	3G	70	Total 510	C 333	N 79	O 93	S 5	0	0
1	3H	70	Total 510	C 333	N 79	O 93	S 5	0	0
1	3I	70	Total 510	C 333	N 79	O 93	S 5	0	0
1	3J	70	Total 510	C 333	N 79	O 93	S 5	0	0

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Mol	Chain	Residues	Atoms	AltConf	Trace
1	3K	70	Total C N O S 510 333 79 93 5	0	0
1	3L	70	Total C N O S 510 333 79 93 5	0	0
1	3M	70	Total C N O S 510 333 79 93 5	0	0
1	3N	70	Total C N O S 510 333 79 93 5	0	0
1	4A	70	Total C N O S 510 333 79 93 5	0	0
1	4B	70	Total C N O S 510 333 79 93 5	0	0
1	4C	70	Total C N O S 510 333 79 93 5	0	0
1	4D	70	Total C N O S 510 333 79 93 5	0	0
1	4E	70	Total C N O S 510 333 79 93 5	0	0
1	4F	70	Total C N O S 510 333 79 93 5	0	0
1	4G	70	Total C N O S 510 333 79 93 5	0	0
1	4H	70	Total C N O S 510 333 79 93 5	0	0
1	4I	70	Total C N O S 510 333 79 93 5	0	0
1	4J	70	Total C N O S 510 333 79 93 5	0	0
1	4K	70	Total C N O S 510 333 79 93 5	0	0
1	4L	70	Total C N O S 510 333 79 93 5	0	0
1	4M	70	Total C N O S 510 333 79 93 5	0	0
1	4N	70	Total C N O S 510 333 79 93 5	0	0
1	5A	70	Total C N O S 510 333 79 93 5	0	0
1	5B	70	Total C N O S 510 333 79 93 5	0	0
1	5C	70	Total C N O S 510 333 79 93 5	0	0

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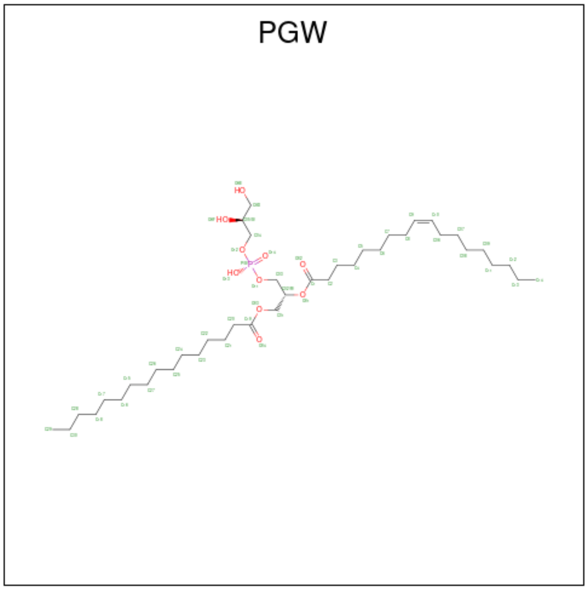
Mol	Chain	Residues	Atoms					AltConf	Trace
1	5D	70	Total 510	C 333	N 79	O 93	S 5	0	0
1	5E	70	Total 510	C 333	N 79	O 93	S 5	0	0
1	5F	70	Total 510	C 333	N 79	O 93	S 5	0	0
1	5G	70	Total 510	C 333	N 79	O 93	S 5	0	0
1	5H	70	Total 510	C 333	N 79	O 93	S 5	0	0
1	5I	70	Total 510	C 333	N 79	O 93	S 5	0	0
1	5J	70	Total 510	C 333	N 79	O 93	S 5	0	0
1	5K	70	Total 510	C 333	N 79	O 93	S 5	0	0
1	5L	70	Total 510	C 333	N 79	O 93	S 5	0	0
1	5M	70	Total 510	C 333	N 79	O 93	S 5	0	0
1	5N	70	Total 510	C 333	N 79	O 93	S 5	0	0

- Molecule 2 is (1R)-2-{[(S)-{[(2S)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-1-[(hexadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (three-letter code: PGW) (formula: $C_{40}H_{77}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
2	1B	1	Total C H O P 127 40 76 10 1	0
2	1B	1	Total C H O P 127 40 76 10 1	0
2	1C	1	Total C H O P 127 40 76 10 1	0
2	1D	1	Total C H O P 127 40 76 10 1	0
2	1E	1	Total C H O P 127 40 76 10 1	0
2	1F	1	Total C H O P 127 40 76 10 1	0
2	1G	1	Total C H O P 127 40 76 10 1	0
2	1H	1	Total C H O P 127 40 76 10 1	0
2	1I	1	Total C H O P 127 40 76 10 1	0
2	1J	1	Total C H O P 127 40 76 10 1	0
2	1K	1	Total C H O P 127 40 76 10 1	0
2	1L	1	Total C H O P 127 40 76 10 1	0
2	1M	1	Total C H O P 127 40 76 10 1	0
2	1N	1	Total C H O P 127 40 76 10 1	0
2	2B	1	Total C H O P 127 40 76 10 1	0
2	2C	1	Total C H O P 127 40 76 10 1	0
2	2D	1	Total C H O P 127 40 76 10 1	0
2	2D	1	Total C H O P 127 40 76 10 1	0
2	2E	1	Total C H O P 127 40 76 10 1	0
2	2F	1	Total C H O P 127 40 76 10 1	0
2	2G	1	Total C H O P 127 40 76 10 1	0
2	2H	1	Total C H O P 127 40 76 10 1	0

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Mol	Chain	Residues	Atoms	AltConf
2	2I	1	Total C H O P 127 40 76 10 1	0
2	2J	1	Total C H O P 127 40 76 10 1	0
2	2K	1	Total C H O P 127 40 76 10 1	0
2	2L	1	Total C H O P 127 40 76 10 1	0
2	2M	1	Total C H O P 127 40 76 10 1	0
2	2N	1	Total C H O P 127 40 76 10 1	0
2	3B	1	Total C H O P 127 40 76 10 1	0
2	3C	1	Total C H O P 127 40 76 10 1	0
2	3D	1	Total C H O P 127 40 76 10 1	0
2	3D	1	Total C H O P 127 40 76 10 1	0
2	3E	1	Total C H O P 127 40 76 10 1	0
2	3F	1	Total C H O P 127 40 76 10 1	0
2	3G	1	Total C H O P 127 40 76 10 1	0
2	3H	1	Total C H O P 127 40 76 10 1	0
2	3I	1	Total C H O P 127 40 76 10 1	0
2	3J	1	Total C H O P 127 40 76 10 1	0
2	3K	1	Total C H O P 127 40 76 10 1	0
2	3L	1	Total C H O P 127 40 76 10 1	0
2	3M	1	Total C H O P 127 40 76 10 1	0
2	3N	1	Total C H O P 127 40 76 10 1	0
2	4B	1	Total C H O P 127 40 76 10 1	0

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Mol	Chain	Residues	Atoms	AltConf
2	4C	1	Total C H O P 127 40 76 10 1	0
2	4C	1	Total C H O P 127 40 76 10 1	0
2	4D	1	Total C H O P 127 40 76 10 1	0
2	4E	1	Total C H O P 127 40 76 10 1	0
2	4F	1	Total C H O P 127 40 76 10 1	0
2	4G	1	Total C H O P 127 40 76 10 1	0
2	4H	1	Total C H O P 127 40 76 10 1	0
2	4I	1	Total C H O P 127 40 76 10 1	0
2	4J	1	Total C H O P 127 40 76 10 1	0
2	4K	1	Total C H O P 127 40 76 10 1	0
2	4L	1	Total C H O P 127 40 76 10 1	0
2	4M	1	Total C H O P 127 40 76 10 1	0
2	4N	1	Total C H O P 127 40 76 10 1	0
2	5B	1	Total C H O P 127 40 76 10 1	0
2	5C	1	Total C H O P 127 40 76 10 1	0
2	5C	1	Total C H O P 127 40 76 10 1	0
2	5D	1	Total C H O P 127 40 76 10 1	0
2	5E	1	Total C H O P 127 40 76 10 1	0
2	5F	1	Total C H O P 127 40 76 10 1	0
2	5G	1	Total C H O P 127 40 76 10 1	0
2	5H	1	Total C H O P 127 40 76 10 1	0

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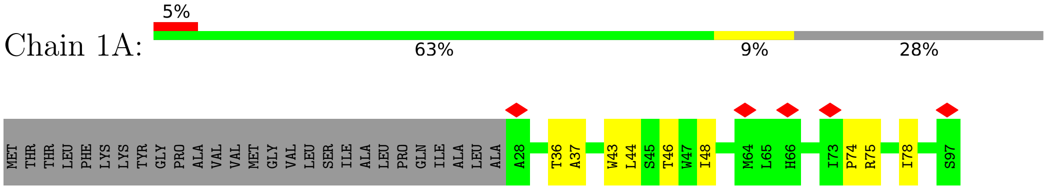
Mol	Chain	Residues	Atoms					AltConf
2	5I	1	Total 127	C 40	H 76	O 10	P 1	0
2	5J	1	Total 127	C 40	H 76	O 10	P 1	0
2	5K	1	Total 127	C 40	H 76	O 10	P 1	0
2	5L	1	Total 127	C 40	H 76	O 10	P 1	0
2	5M	1	Total 127	C 40	H 76	O 10	P 1	0
2	5N	1	Total 127	C 40	H 76	O 10	P 1	0

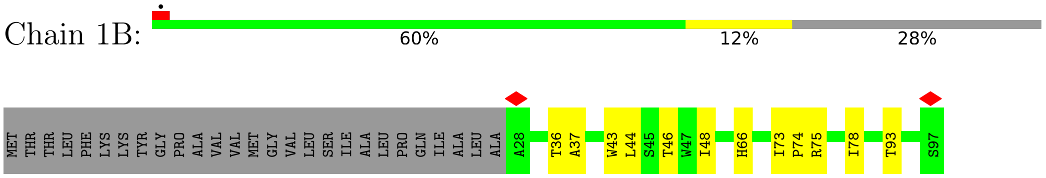
3 Residue-property plots ⓘ

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

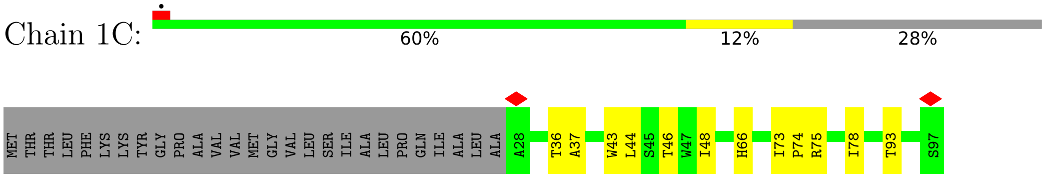
- Molecule 1: Conjugal transfer protein TraM



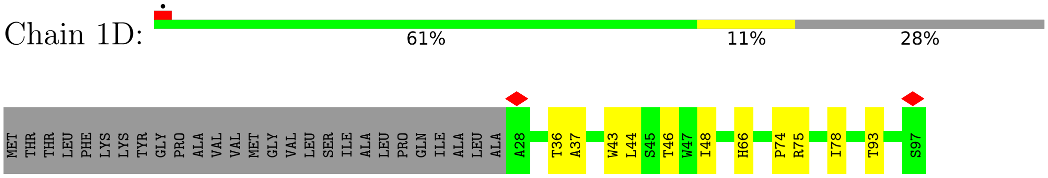
- Molecule 1: Conjugal transfer protein TraM



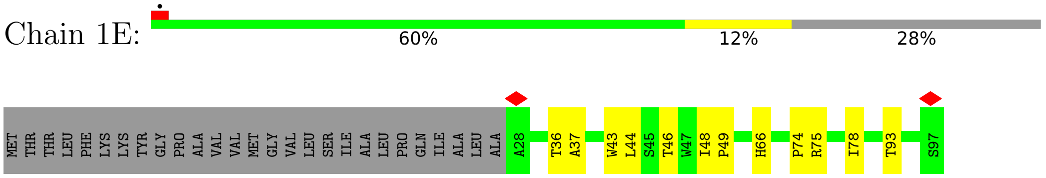
- Molecule 1: Conjugal transfer protein TraM



- Molecule 1: Conjugal transfer protein TraM

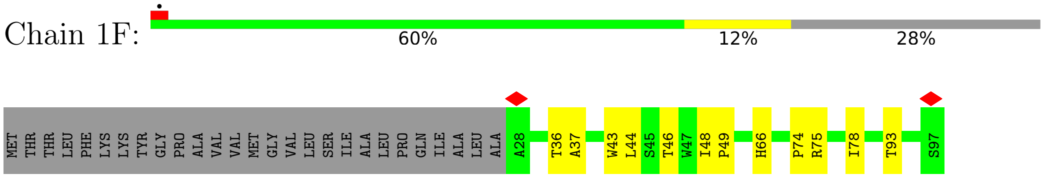


- Molecule 1: Conjugal transfer protein TraM



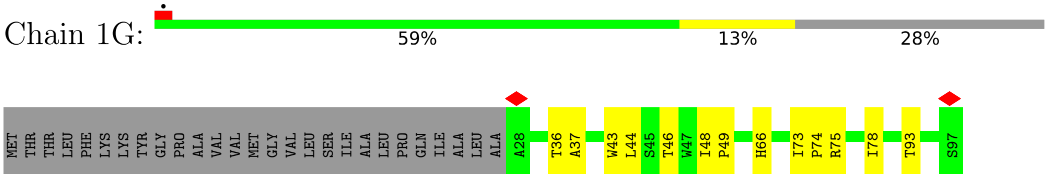
- Molecule 1: Conjugal transfer protein TraM

Chain 1F:



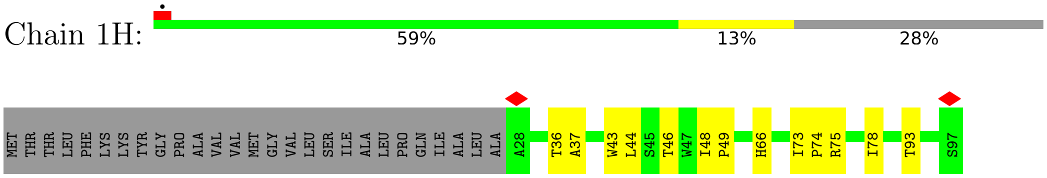
- Molecule 1: Conjugal transfer protein TraM

Chain 1G:



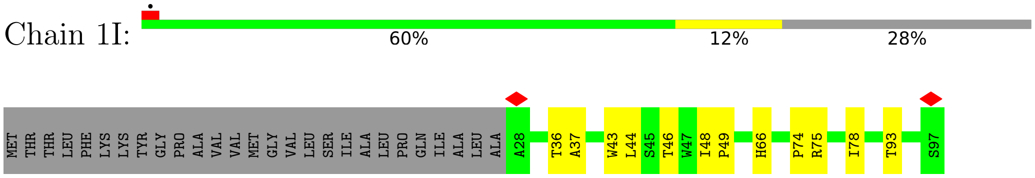
- Molecule 1: Conjugal transfer protein TraM

Chain 1H:



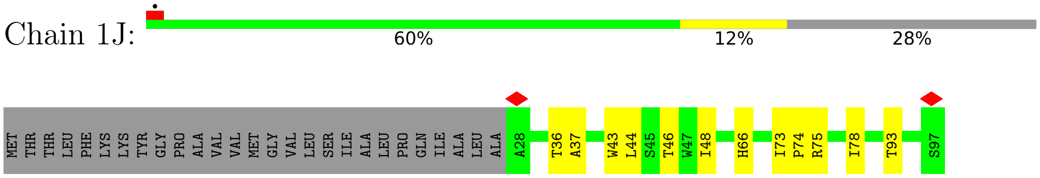
- Molecule 1: Conjugal transfer protein TraM

Chain 1I:



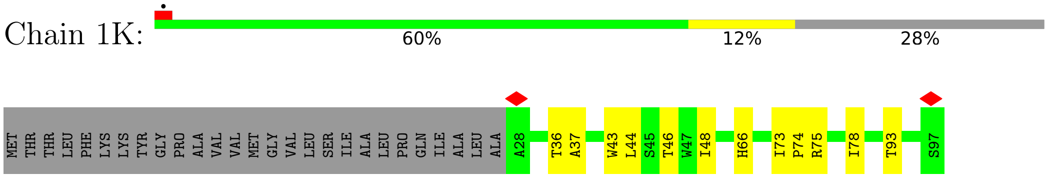
- Molecule 1: Conjugal transfer protein TraM

Chain 1J:



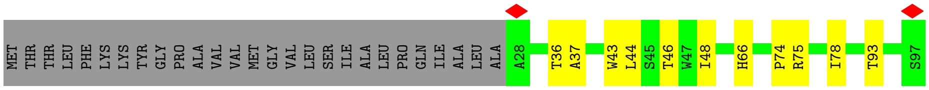
- Molecule 1: Conjugal transfer protein TraM

Chain 1K:



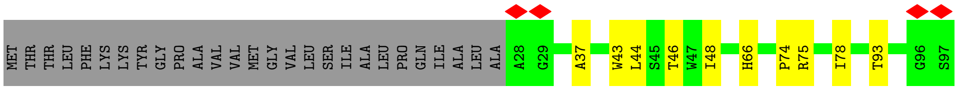
- Molecule 1: Conjugal transfer protein TraM

Chain 1L:



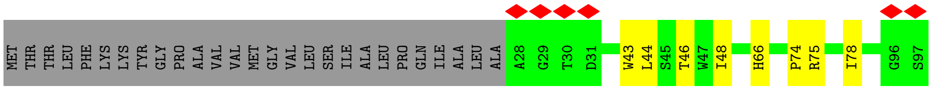
• Molecule 1: Conjugal transfer protein TraM

Chain 1M:

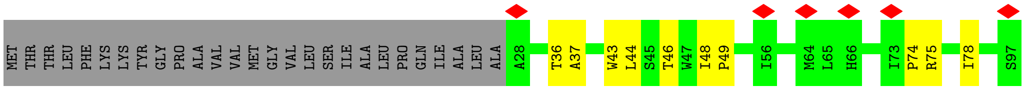
• Molecule 1: Conjugal transfer protein TraM

Chain 1N:

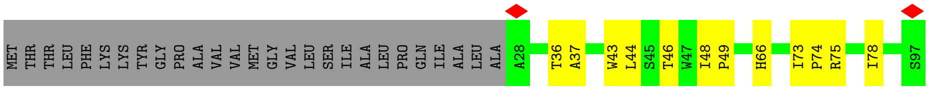
• Molecule 1: Conjugal transfer protein TraM

Chain 2A:

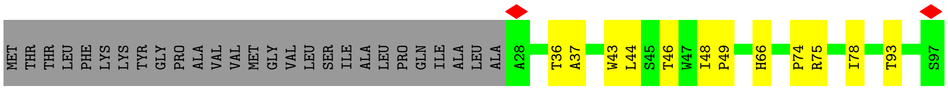
• Molecule 1: Conjugal transfer protein TraM

Chain 2B:

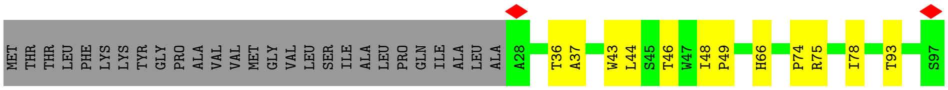
• Molecule 1: Conjugal transfer protein TraM

Chain 2C:

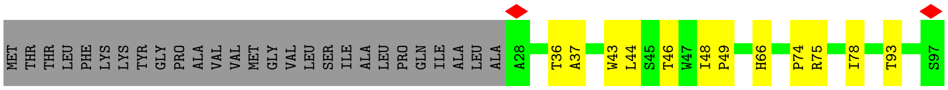
• Molecule 1: Conjugal transfer protein TraM

Chain 2D:

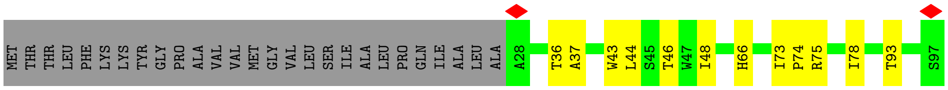
• Molecule 1: Conjugal transfer protein TraM

Chain 2E:



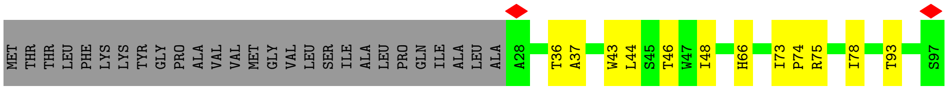
- Molecule 1: Conjugal transfer protein TraM

Chain 2F:



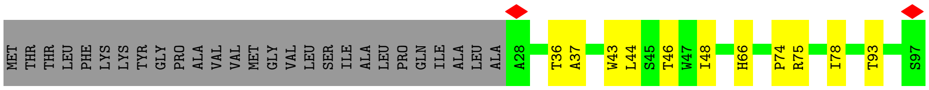
- Molecule 1: Conjugal transfer protein TraM

Chain 2G:



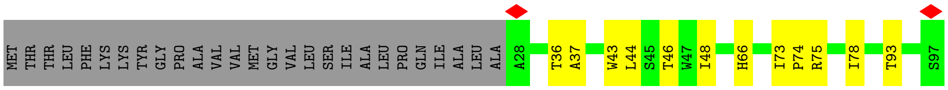
- Molecule 1: Conjugal transfer protein TraM

Chain 2H:



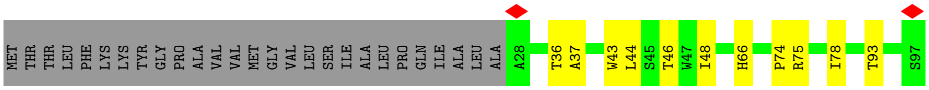
- Molecule 1: Conjugal transfer protein TraM

Chain 2I:



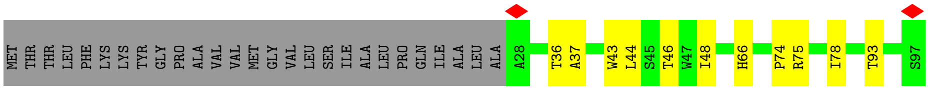
- Molecule 1: Conjugal transfer protein TraM

Chain 2J:



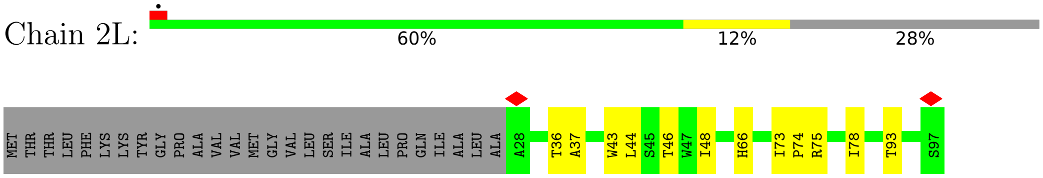
- Molecule 1: Conjugal transfer protein TraM

Chain 2K:



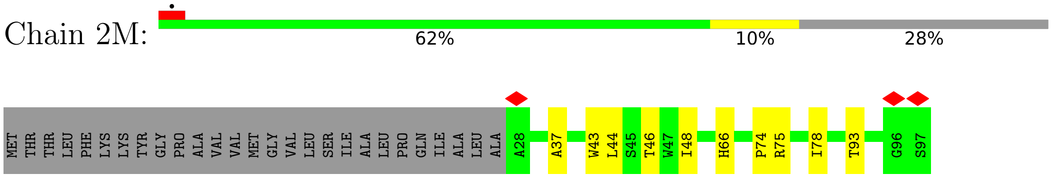
- Molecule 1: Conjugal transfer protein TraM

Chain 2L:



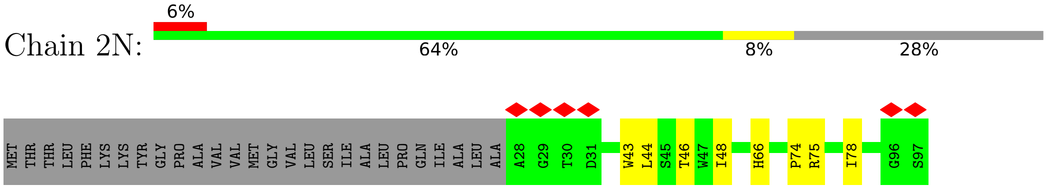
- Molecule 1: Conjugal transfer protein TraM

Chain 2M:



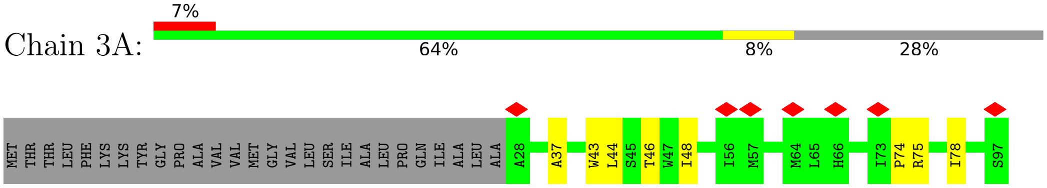
- Molecule 1: Conjugal transfer protein TraM

Chain 2N:



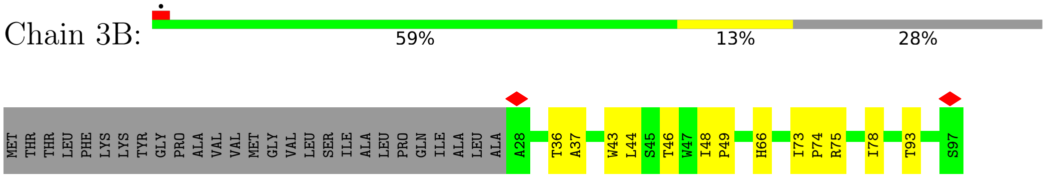
- Molecule 1: Conjugal transfer protein TraM

Chain 3A:



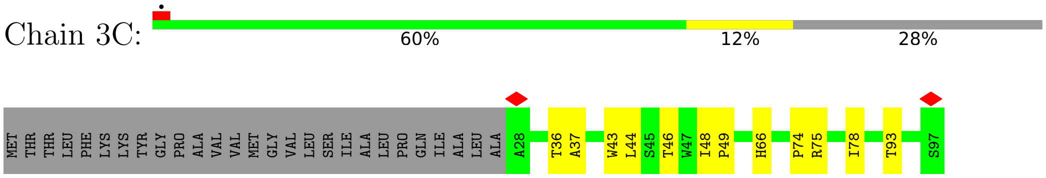
- Molecule 1: Conjugal transfer protein TraM

Chain 3B:



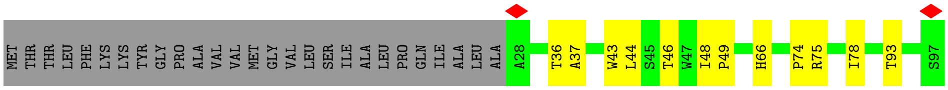
- Molecule 1: Conjugal transfer protein TraM

Chain 3C:



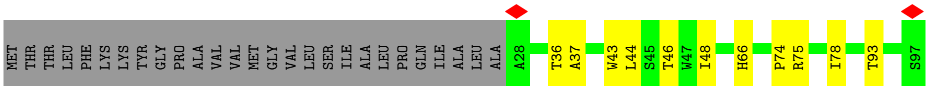
- Molecule 1: Conjugal transfer protein TraM

Chain 3D:



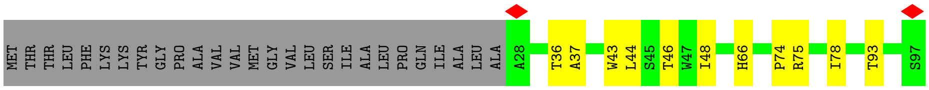
- Molecule 1: Conjugal transfer protein TraM

Chain 3E:



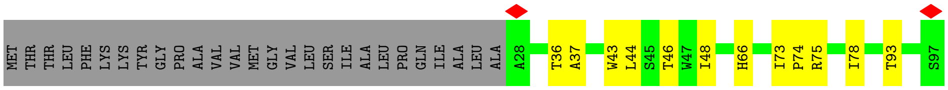
- Molecule 1: Conjugal transfer protein TraM

Chain 3F:



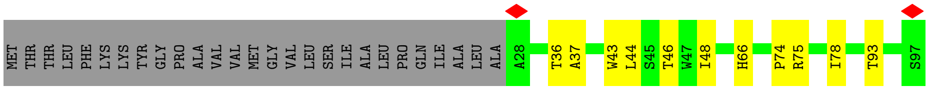
- Molecule 1: Conjugal transfer protein TraM

Chain 3G:



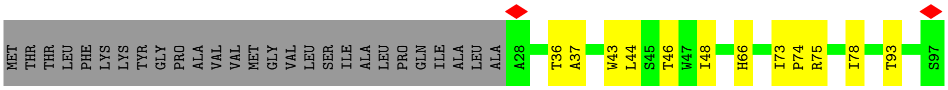
- Molecule 1: Conjugal transfer protein TraM

Chain 3H:



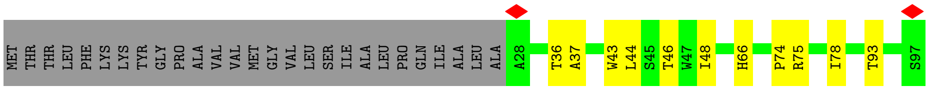
- Molecule 1: Conjugal transfer protein TraM

Chain 3I:



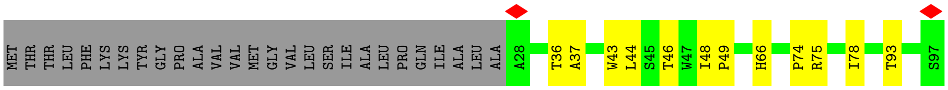
- Molecule 1: Conjugal transfer protein TraM

Chain 3J:



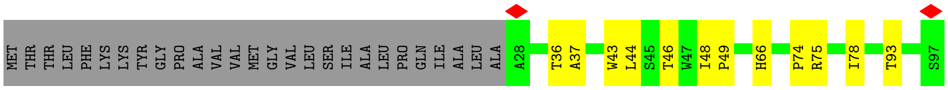
- Molecule 1: Conjugal transfer protein TraM

Chain 3K:



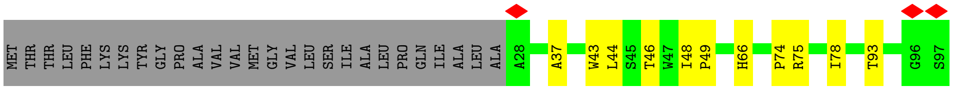
• Molecule 1: Conjugal transfer protein TraM

Chain 3L:



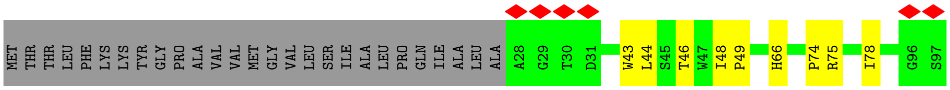
• Molecule 1: Conjugal transfer protein TraM

Chain 3M:



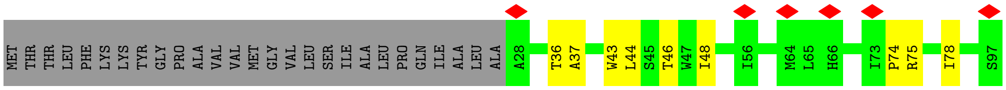
• Molecule 1: Conjugal transfer protein TraM

Chain 3N:



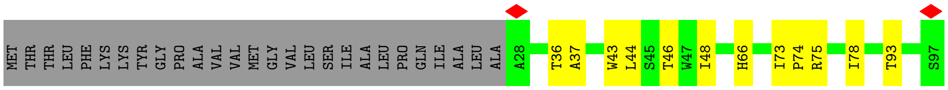
• Molecule 1: Conjugal transfer protein TraM

Chain 4A:



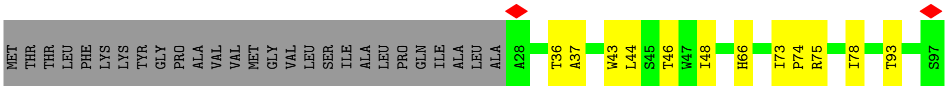
• Molecule 1: Conjugal transfer protein TraM

Chain 4B:



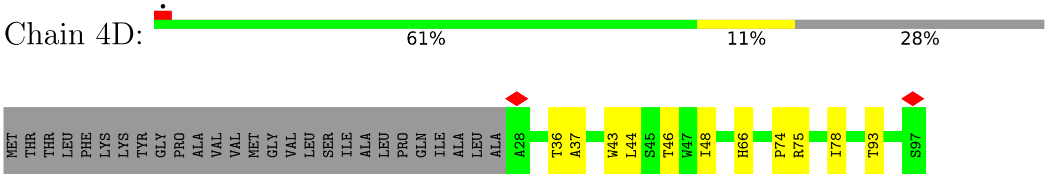
• Molecule 1: Conjugal transfer protein TraM

Chain 4C:



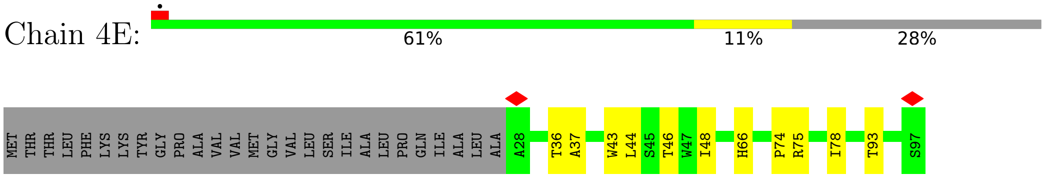
- Molecule 1: Conjugal transfer protein TraM

Chain 4D:



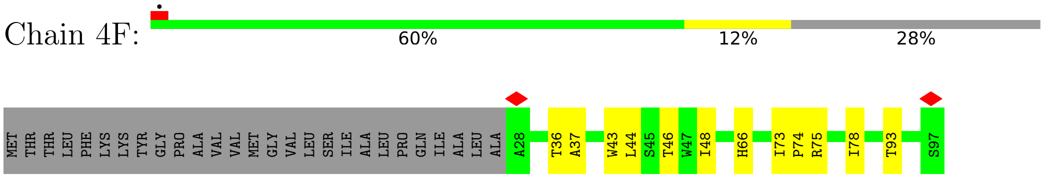
- Molecule 1: Conjugal transfer protein TraM

Chain 4E:



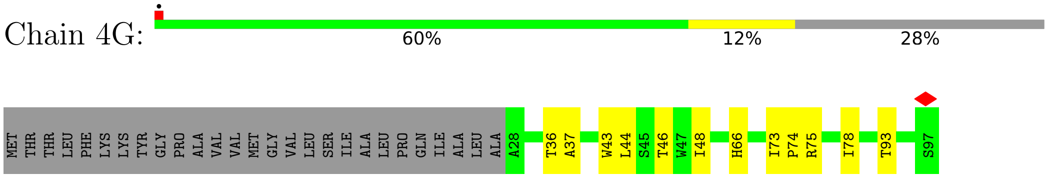
- Molecule 1: Conjugal transfer protein TraM

Chain 4F:



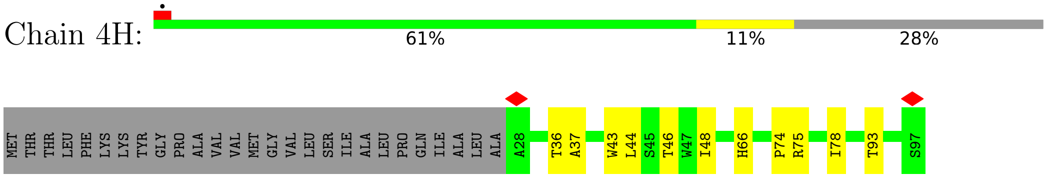
- Molecule 1: Conjugal transfer protein TraM

Chain 4G:



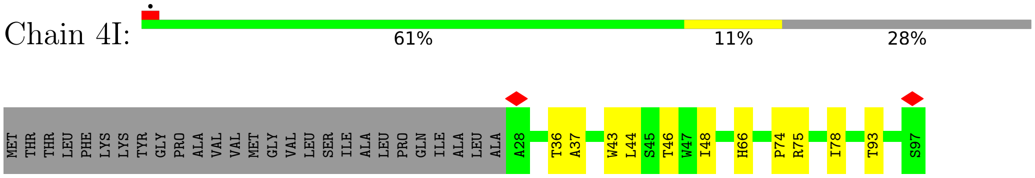
- Molecule 1: Conjugal transfer protein TraM

Chain 4H:



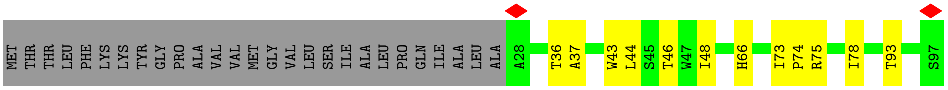
- Molecule 1: Conjugal transfer protein TraM

Chain 4I:



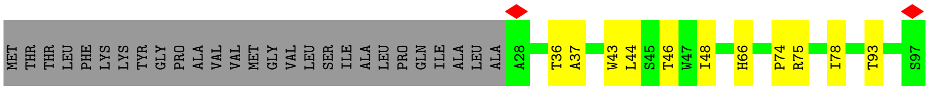
- Molecule 1: Conjugal transfer protein TraM

Chain 4J:



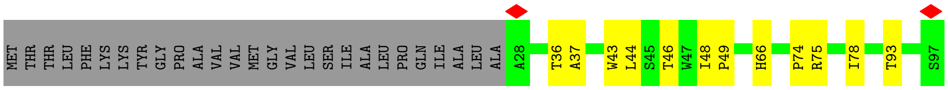
- Molecule 1: Conjugal transfer protein TraM

Chain 4K:



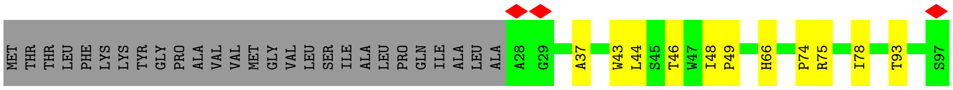
- Molecule 1: Conjugal transfer protein TraM

Chain 4L:



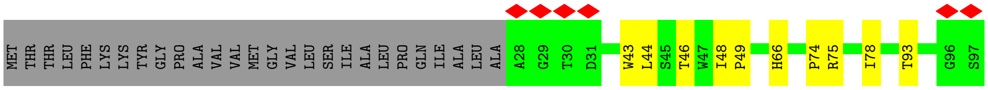
- Molecule 1: Conjugal transfer protein TraM

Chain 4M:



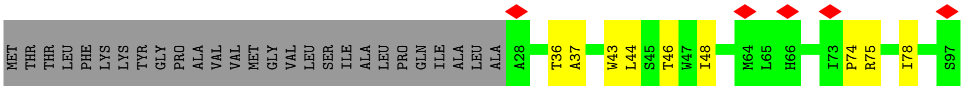
- Molecule 1: Conjugal transfer protein TraM

Chain 4N:



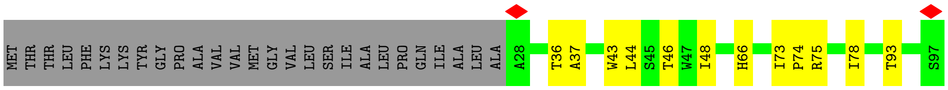
- Molecule 1: Conjugal transfer protein TraM

Chain 5A:



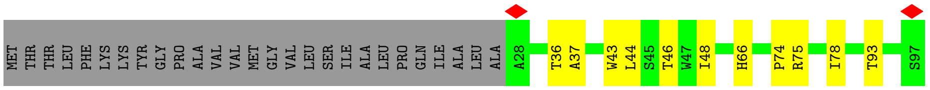
- Molecule 1: Conjugal transfer protein TraM

Chain 5B:



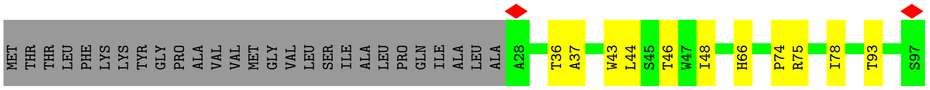
- Molecule 1: Conjugal transfer protein TraM

Chain 5C:



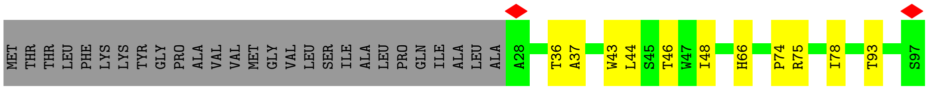
- Molecule 1: Conjugal transfer protein TraM

Chain 5D:



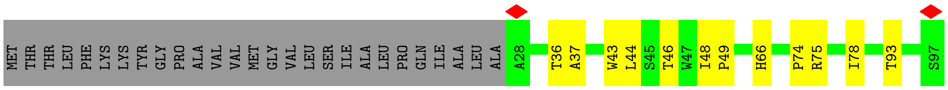
- Molecule 1: Conjugal transfer protein TraM

Chain 5E:



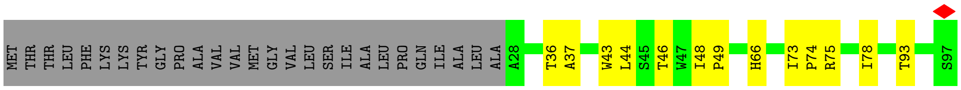
- Molecule 1: Conjugal transfer protein TraM

Chain 5F:



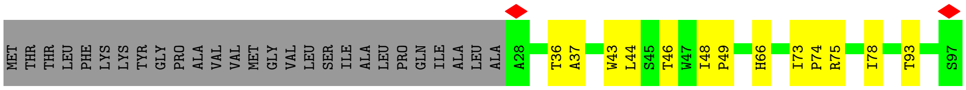
- Molecule 1: Conjugal transfer protein TraM

Chain 5G:



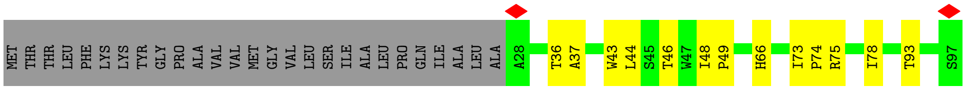
- Molecule 1: Conjugal transfer protein TraM

Chain 5H:

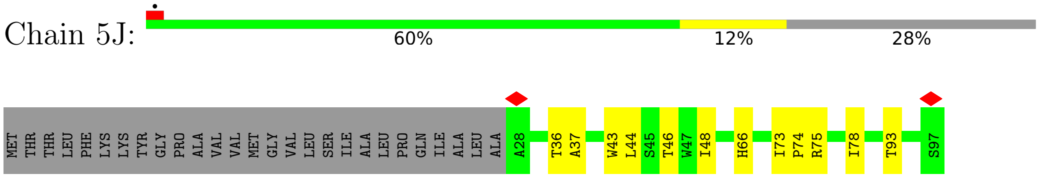


- Molecule 1: Conjugal transfer protein TraM

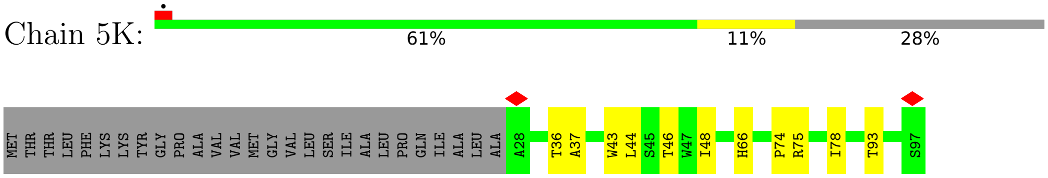
Chain 5I:



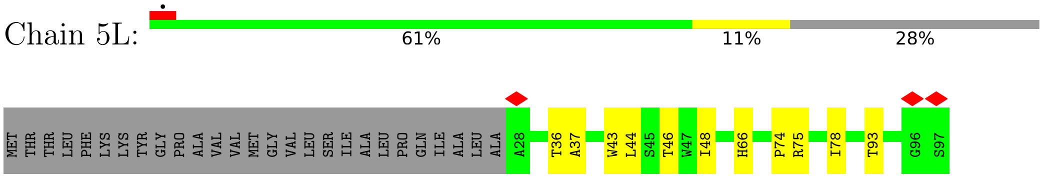
- Molecule 1: Conjugal transfer protein TraM



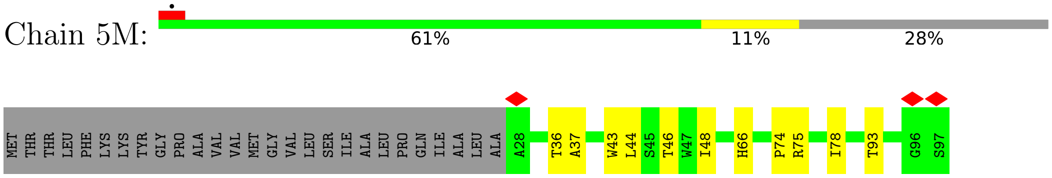
- Molecule 1: Conjugal transfer protein TraM



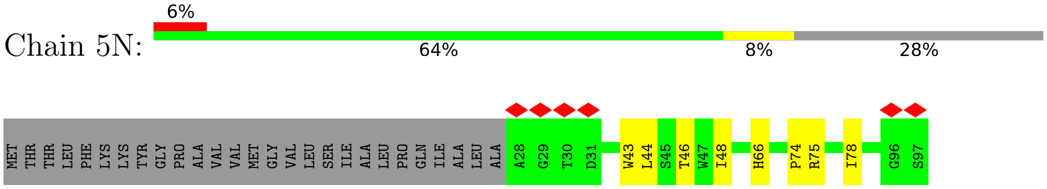
- Molecule 1: Conjugal transfer protein TraM



- Molecule 1: Conjugal transfer protein TraM



- Molecule 1: Conjugal transfer protein TraM



4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	134660	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 ($e^-/\text{Å}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.009	Depositor
Minimum map value	-0.964	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.094	Depositor
Recommended contour level	0.364	Depositor
Map size (Å)	279.04, 279.04, 279.04	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.25	0/522	0.41	0/715
1	1B	0.26	0/522	0.41	0/715
1	1C	0.25	0/522	0.41	0/715
1	1D	0.25	0/522	0.41	0/715
1	1E	0.25	0/522	0.41	0/715
1	1F	0.26	0/522	0.41	0/715
1	1G	0.25	0/522	0.41	0/715
1	1H	0.25	0/522	0.41	0/715
1	1I	0.26	0/522	0.41	0/715
1	1J	0.25	0/522	0.41	0/715
1	1K	0.25	0/522	0.41	0/715
1	1L	0.25	0/522	0.41	0/715
1	1M	0.25	0/522	0.41	0/715
1	1N	0.26	0/522	0.41	0/715
1	2A	0.25	0/522	0.41	0/715
1	2B	0.25	0/522	0.41	0/715
1	2C	0.25	0/522	0.41	0/715
1	2D	0.26	0/522	0.41	0/715
1	2E	0.25	0/522	0.41	0/715
1	2F	0.26	0/522	0.41	0/715
1	2G	0.25	0/522	0.41	0/715
1	2H	0.25	0/522	0.41	0/715
1	2I	0.26	0/522	0.41	0/715
1	2J	0.25	0/522	0.41	0/715
1	2K	0.25	0/522	0.41	0/715
1	2L	0.25	0/522	0.41	0/715
1	2M	0.25	0/522	0.41	0/715
1	2N	0.25	0/522	0.41	0/715
1	3A	0.25	0/522	0.41	0/715
1	3B	0.25	0/522	0.41	0/715
1	3C	0.25	0/522	0.41	0/715
1	3D	0.25	0/522	0.41	0/715

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	3E	0.25	0/522	0.41	0/715
1	3F	0.26	0/522	0.41	0/715
1	3G	0.25	0/522	0.41	0/715
1	3H	0.25	0/522	0.41	0/715
1	3I	0.26	0/522	0.41	0/715
1	3J	0.25	0/522	0.41	0/715
1	3K	0.25	0/522	0.41	0/715
1	3L	0.26	0/522	0.41	0/715
1	3M	0.25	0/522	0.41	0/715
1	3N	0.25	0/522	0.41	0/715
1	4A	0.26	0/522	0.41	0/715
1	4B	0.26	0/522	0.41	0/715
1	4C	0.26	0/522	0.41	0/715
1	4D	0.25	0/522	0.41	0/715
1	4E	0.26	0/522	0.41	0/715
1	4F	0.25	0/522	0.41	0/715
1	4G	0.25	0/522	0.41	0/715
1	4H	0.26	0/522	0.41	0/715
1	4I	0.25	0/522	0.41	0/715
1	4J	0.26	0/522	0.41	0/715
1	4K	0.25	0/522	0.41	0/715
1	4L	0.25	0/522	0.41	0/715
1	4M	0.26	0/522	0.41	0/715
1	4N	0.25	0/522	0.41	0/715
1	5A	0.25	0/522	0.41	0/715
1	5B	0.25	0/522	0.41	0/715
1	5C	0.25	0/522	0.41	0/715
1	5D	0.25	0/522	0.41	0/715
1	5E	0.26	0/522	0.41	0/715
1	5F	0.25	0/522	0.41	0/715
1	5G	0.26	0/522	0.41	0/715
1	5H	0.26	0/522	0.41	0/715
1	5I	0.25	0/522	0.41	0/715
1	5J	0.26	0/522	0.41	0/715
1	5K	0.25	0/522	0.41	0/715
1	5L	0.25	0/522	0.41	0/715
1	5M	0.25	0/522	0.41	0/715
1	5N	0.26	0/522	0.41	0/715
All	All	0.25	0/36540	0.41	0/50050

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	510	0	523	7	0
1	1B	510	0	523	10	0
1	1C	510	0	523	10	0
1	1D	510	0	523	9	0
1	1E	510	0	523	10	0
1	1F	510	0	523	10	0
1	1G	510	0	523	11	0
1	1H	510	0	523	11	0
1	1I	510	0	523	10	0
1	1J	510	0	523	10	0
1	1K	510	0	523	10	0
1	1L	510	0	523	9	0
1	1M	510	0	523	8	0
1	1N	510	0	523	5	0
1	2A	510	0	523	8	0
1	2B	510	0	523	10	0
1	2C	510	0	523	10	0
1	2D	510	0	523	10	0
1	2E	510	0	523	10	0
1	2F	510	0	523	10	0
1	2G	510	0	523	10	0
1	2H	510	0	523	9	0
1	2I	510	0	523	10	0
1	2J	510	0	523	9	0
1	2K	510	0	523	9	0
1	2L	510	0	523	10	0
1	2M	510	0	523	8	0
1	2N	510	0	523	5	0
1	3A	510	0	523	6	0
1	3B	510	0	523	11	0
1	3C	510	0	523	10	0
1	3D	510	0	523	10	0
1	3E	510	0	523	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	3F	510	0	523	9	0
1	3G	510	0	523	10	0
1	3H	510	0	523	9	0
1	3I	510	0	523	10	0
1	3J	510	0	523	9	0
1	3K	510	0	523	10	0
1	3L	510	0	523	10	0
1	3M	510	0	523	9	0
1	3N	510	0	523	6	0
1	4A	510	0	523	7	0
1	4B	510	0	523	10	0
1	4C	510	0	523	10	0
1	4D	510	0	523	9	0
1	4E	510	0	523	9	0
1	4F	510	0	523	10	0
1	4G	510	0	523	10	0
1	4H	510	0	523	9	0
1	4I	510	0	523	9	0
1	4J	510	0	523	10	0
1	4K	510	0	523	9	0
1	4L	510	0	523	10	0
1	4M	510	0	523	9	0
1	4N	510	0	523	7	0
1	5A	510	0	523	7	0
1	5B	510	0	523	10	0
1	5C	510	0	523	9	0
1	5D	510	0	523	9	0
1	5E	510	0	523	9	0
1	5F	510	0	523	10	0
1	5G	510	0	523	11	0
1	5H	510	0	523	11	0
1	5I	510	0	523	11	0
1	5J	510	0	523	10	0
1	5K	510	0	523	9	0
1	5L	510	0	523	9	0
1	5M	510	0	523	9	0
1	5N	510	0	523	5	0
2	1B	102	152	152	5	0
2	1C	51	76	76	2	0
2	1D	51	76	76	2	0
2	1E	51	76	76	2	0
2	1F	51	76	76	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	1G	51	76	76	3	0
2	1H	51	76	76	2	0
2	1I	51	76	76	3	0
2	1J	51	76	76	3	0
2	1K	51	76	76	2	0
2	1L	51	76	76	2	0
2	1M	51	76	76	2	0
2	1N	51	76	76	2	0
2	2B	51	76	76	2	0
2	2C	51	76	76	2	0
2	2D	102	152	152	4	0
2	2E	51	76	76	3	0
2	2F	51	76	76	3	0
2	2G	51	76	76	2	0
2	2H	51	76	76	3	0
2	2I	51	76	76	2	0
2	2J	51	76	76	2	0
2	2K	51	76	76	3	0
2	2L	51	76	76	2	0
2	2M	51	76	76	2	0
2	2N	51	76	76	2	0
2	3B	51	76	76	2	0
2	3C	51	76	76	2	0
2	3D	102	152	152	4	0
2	3E	51	76	76	2	0
2	3F	51	76	76	3	0
2	3G	51	76	76	2	0
2	3H	51	76	76	3	0
2	3I	51	76	76	2	0
2	3J	51	76	76	2	0
2	3K	51	76	76	2	0
2	3L	51	76	76	2	0
2	3M	51	76	76	2	0
2	3N	51	76	76	2	0
2	4B	51	76	76	2	0
2	4C	102	152	152	5	0
2	4D	51	76	76	2	0
2	4E	51	76	76	3	0
2	4F	51	76	76	3	0
2	4G	51	76	76	2	0
2	4H	51	76	76	2	0
2	4I	51	76	76	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	4J	51	76	76	2	0
2	4K	51	76	76	2	0
2	4L	51	76	76	2	0
2	4M	51	76	76	2	0
2	4N	51	76	76	2	0
2	5B	51	76	76	2	0
2	5C	102	152	152	4	0
2	5D	51	76	76	2	0
2	5E	51	76	76	2	0
2	5F	51	76	76	3	0
2	5G	51	76	76	3	0
2	5H	51	76	76	3	0
2	5I	51	76	76	3	0
2	5J	51	76	76	2	0
2	5K	51	76	76	2	0
2	5L	51	76	76	2	0
2	5M	51	76	76	2	0
2	5N	51	76	76	2	0
All	All	39270	5320	41930	518	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 6.

The worst 5 of 518 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)
1:4L:43:TRP:O	1:4L:46:THR:OG1	2.11	0.69
1:3A:43:TRP:O	1:3A:46:THR:OG1	2.11	0.69
1:4N:43:TRP:O	1:4N:46:THR:OG1	2.11	0.69
1:5L:43:TRP:O	1:5L:46:THR:OG1	2.11	0.69
1:4A:43:TRP:O	1:4A:46:THR:OG1	2.11	0.69

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	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	1B	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	1C	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	1D	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	1E	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	1F	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	1G	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	1H	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	1I	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	1J	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	1K	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	1L	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	1M	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	1N	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	2A	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	2B	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	2C	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	2D	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	2E	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	2F	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	2G	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	2H	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	2I	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	2J	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	2K	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	2L	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	2M	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	2N	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	3A	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	3B	68/97 (70%)	66 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	3C	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	3D	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	3E	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	3F	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	3G	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	3H	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	3I	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	3J	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	3K	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	3L	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	3M	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	3N	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	4A	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	4B	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	4C	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	4D	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	4E	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	4F	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	4G	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	4H	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	4I	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	4J	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	4K	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	4L	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	4M	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	4N	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	5A	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	5B	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	5C	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	5D	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	5E	68/97 (70%)	66 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	5F	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	5G	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	5H	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	5I	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	5J	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	5K	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	5L	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	5M	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
1	5N	68/97 (70%)	66 (97%)	2 (3%)	0	100	100
All	All	4760/6790 (70%)	4620 (97%)	140 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1A	57/78 (73%)	57 (100%)	0	100	100
1	1B	57/78 (73%)	57 (100%)	0	100	100
1	1C	57/78 (73%)	57 (100%)	0	100	100
1	1D	57/78 (73%)	57 (100%)	0	100	100
1	1E	57/78 (73%)	57 (100%)	0	100	100
1	1F	57/78 (73%)	57 (100%)	0	100	100
1	1G	57/78 (73%)	57 (100%)	0	100	100
1	1H	57/78 (73%)	57 (100%)	0	100	100
1	1I	57/78 (73%)	57 (100%)	0	100	100
1	1J	57/78 (73%)	57 (100%)	0	100	100
1	1K	57/78 (73%)	57 (100%)	0	100	100
1	1L	57/78 (73%)	57 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1M	57/78 (73%)	57 (100%)	0	100	100
1	1N	57/78 (73%)	57 (100%)	0	100	100
1	2A	57/78 (73%)	57 (100%)	0	100	100
1	2B	57/78 (73%)	57 (100%)	0	100	100
1	2C	57/78 (73%)	57 (100%)	0	100	100
1	2D	57/78 (73%)	57 (100%)	0	100	100
1	2E	57/78 (73%)	57 (100%)	0	100	100
1	2F	57/78 (73%)	57 (100%)	0	100	100
1	2G	57/78 (73%)	57 (100%)	0	100	100
1	2H	57/78 (73%)	57 (100%)	0	100	100
1	2I	57/78 (73%)	57 (100%)	0	100	100
1	2J	57/78 (73%)	57 (100%)	0	100	100
1	2K	57/78 (73%)	57 (100%)	0	100	100
1	2L	57/78 (73%)	57 (100%)	0	100	100
1	2M	57/78 (73%)	57 (100%)	0	100	100
1	2N	57/78 (73%)	57 (100%)	0	100	100
1	3A	57/78 (73%)	57 (100%)	0	100	100
1	3B	57/78 (73%)	57 (100%)	0	100	100
1	3C	57/78 (73%)	57 (100%)	0	100	100
1	3D	57/78 (73%)	57 (100%)	0	100	100
1	3E	57/78 (73%)	57 (100%)	0	100	100
1	3F	57/78 (73%)	57 (100%)	0	100	100
1	3G	57/78 (73%)	57 (100%)	0	100	100
1	3H	57/78 (73%)	57 (100%)	0	100	100
1	3I	57/78 (73%)	57 (100%)	0	100	100
1	3J	57/78 (73%)	57 (100%)	0	100	100
1	3K	57/78 (73%)	57 (100%)	0	100	100
1	3L	57/78 (73%)	57 (100%)	0	100	100
1	3M	57/78 (73%)	57 (100%)	0	100	100
1	3N	57/78 (73%)	57 (100%)	0	100	100
1	4A	57/78 (73%)	57 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	4B	57/78 (73%)	57 (100%)	0	100	100
1	4C	57/78 (73%)	57 (100%)	0	100	100
1	4D	57/78 (73%)	57 (100%)	0	100	100
1	4E	57/78 (73%)	57 (100%)	0	100	100
1	4F	57/78 (73%)	57 (100%)	0	100	100
1	4G	57/78 (73%)	57 (100%)	0	100	100
1	4H	57/78 (73%)	57 (100%)	0	100	100
1	4I	57/78 (73%)	57 (100%)	0	100	100
1	4J	57/78 (73%)	57 (100%)	0	100	100
1	4K	57/78 (73%)	57 (100%)	0	100	100
1	4L	57/78 (73%)	57 (100%)	0	100	100
1	4M	57/78 (73%)	57 (100%)	0	100	100
1	4N	57/78 (73%)	57 (100%)	0	100	100
1	5A	57/78 (73%)	57 (100%)	0	100	100
1	5B	57/78 (73%)	57 (100%)	0	100	100
1	5C	57/78 (73%)	57 (100%)	0	100	100
1	5D	57/78 (73%)	57 (100%)	0	100	100
1	5E	57/78 (73%)	57 (100%)	0	100	100
1	5F	57/78 (73%)	57 (100%)	0	100	100
1	5G	57/78 (73%)	57 (100%)	0	100	100
1	5H	57/78 (73%)	57 (100%)	0	100	100
1	5I	57/78 (73%)	57 (100%)	0	100	100
1	5J	57/78 (73%)	57 (100%)	0	100	100
1	5K	57/78 (73%)	57 (100%)	0	100	100
1	5L	57/78 (73%)	57 (100%)	0	100	100
1	5M	57/78 (73%)	57 (100%)	0	100	100
1	5N	57/78 (73%)	57 (100%)	0	100	100
All	All	3990/5460 (73%)	3990 (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. There are no such sidechains identified.

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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

70 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	PGW	3B	101	-	50,50,50	0.47	0	53,56,56	0.42	0
2	PGW	2D	101	-	50,50,50	0.47	0	53,56,56	0.43	0
2	PGW	1I	101	-	50,50,50	0.47	0	53,56,56	0.42	0
2	PGW	1C	101	-	50,50,50	0.47	0	53,56,56	0.43	0
2	PGW	2C	101	-	50,50,50	0.47	0	53,56,56	0.43	0
2	PGW	4D	101	-	50,50,50	0.47	0	53,56,56	0.43	0
2	PGW	3N	101	-	50,50,50	0.48	0	53,56,56	0.43	0
2	PGW	4C	101	-	50,50,50	0.47	0	53,56,56	0.42	0
2	PGW	4I	101	-	50,50,50	0.47	0	53,56,56	0.43	0
2	PGW	4G	101	-	50,50,50	0.48	0	53,56,56	0.42	0
2	PGW	5C	102	-	50,50,50	0.47	0	53,56,56	0.43	0
2	PGW	2E	101	-	50,50,50	0.48	0	53,56,56	0.43	0
2	PGW	2F	101	-	50,50,50	0.47	0	53,56,56	0.43	0
2	PGW	4F	101	-	50,50,50	0.47	0	53,56,56	0.43	0
2	PGW	1N	101	-	50,50,50	0.47	0	53,56,56	0.43	0
2	PGW	3D	101	-	50,50,50	0.47	0	53,56,56	0.43	0
2	PGW	1B	101	-	50,50,50	0.47	0	53,56,56	0.43	0
2	PGW	4N	101	-	50,50,50	0.48	0	53,56,56	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	PGW	5F	101	-	50,50,50	0.47	0	53,56,56	0.43	0
2	PGW	5I	101	-	50,50,50	0.47	0	53,56,56	0.43	0
2	PGW	2B	101	-	50,50,50	0.47	0	53,56,56	0.43	0
2	PGW	2G	101	-	50,50,50	0.47	0	53,56,56	0.43	0
2	PGW	3C	101	-	50,50,50	0.47	0	53,56,56	0.43	0
2	PGW	4J	101	-	50,50,50	0.47	0	53,56,56	0.43	0
2	PGW	4C	102	-	50,50,50	0.47	0	53,56,56	0.43	0
2	PGW	5C	101	-	50,50,50	0.47	0	53,56,56	0.43	0
2	PGW	4L	101	-	50,50,50	0.47	0	53,56,56	0.43	0
2	PGW	5K	101	-	50,50,50	0.47	0	53,56,56	0.42	0
2	PGW	5N	101	-	50,50,50	0.48	0	53,56,56	0.43	0
2	PGW	5G	101	-	50,50,50	0.48	0	53,56,56	0.42	0
2	PGW	1E	101	-	50,50,50	0.48	0	53,56,56	0.43	0
2	PGW	1B	102	-	50,50,50	0.47	0	53,56,56	0.43	0
2	PGW	1H	101	-	50,50,50	0.47	0	53,56,56	0.42	0
2	PGW	3D	102	-	50,50,50	0.47	0	53,56,56	0.43	0
2	PGW	3G	101	-	50,50,50	0.47	0	53,56,56	0.42	0
2	PGW	4B	101	-	50,50,50	0.47	0	53,56,56	0.42	0
2	PGW	5M	101	-	50,50,50	0.47	0	53,56,56	0.42	0
2	PGW	4M	101	-	50,50,50	0.48	0	53,56,56	0.43	0
2	PGW	5L	101	-	50,50,50	0.48	0	53,56,56	0.42	0
2	PGW	3E	101	-	50,50,50	0.47	0	53,56,56	0.42	0
2	PGW	1J	101	-	50,50,50	0.47	0	53,56,56	0.43	0
2	PGW	3H	101	-	50,50,50	0.47	0	53,56,56	0.42	0
2	PGW	2H	101	-	50,50,50	0.47	0	53,56,56	0.43	0
2	PGW	3M	101	-	50,50,50	0.47	0	53,56,56	0.43	0
2	PGW	2K	101	-	50,50,50	0.47	0	53,56,56	0.42	0
2	PGW	2M	101	-	50,50,50	0.47	0	53,56,56	0.42	0
2	PGW	2I	101	-	50,50,50	0.48	0	53,56,56	0.42	0
2	PGW	3I	101	-	50,50,50	0.47	0	53,56,56	0.43	0
2	PGW	3K	101	-	50,50,50	0.47	0	53,56,56	0.43	0
2	PGW	2D	102	-	50,50,50	0.47	0	53,56,56	0.43	0
2	PGW	1K	101	-	50,50,50	0.47	0	53,56,56	0.43	0
2	PGW	4E	101	-	50,50,50	0.47	0	53,56,56	0.43	0
2	PGW	5H	101	-	50,50,50	0.47	0	53,56,56	0.43	0
2	PGW	2L	101	-	50,50,50	0.47	0	53,56,56	0.42	0
2	PGW	5B	101	-	50,50,50	0.47	0	53,56,56	0.43	0
2	PGW	3J	101	-	50,50,50	0.47	0	53,56,56	0.42	0
2	PGW	1F	101	-	50,50,50	0.48	0	53,56,56	0.42	0
2	PGW	1D	101	-	50,50,50	0.47	0	53,56,56	0.43	0
2	PGW	2J	101	-	50,50,50	0.47	0	53,56,56	0.42	0
2	PGW	5E	101	-	50,50,50	0.48	0	53,56,56	0.42	0
2	PGW	1M	101	-	50,50,50	0.48	0	53,56,56	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	PGW	5D	101	-	50,50,50	0.47	0	53,56,56	0.43	0
2	PGW	3L	101	-	50,50,50	0.47	0	53,56,56	0.43	0
2	PGW	1L	101	-	50,50,50	0.47	0	53,56,56	0.42	0
2	PGW	3F	101	-	50,50,50	0.47	0	53,56,56	0.43	0
2	PGW	1G	101	-	50,50,50	0.47	0	53,56,56	0.43	0
2	PGW	4H	101	-	50,50,50	0.47	0	53,56,56	0.42	0
2	PGW	2N	101	-	50,50,50	0.47	0	53,56,56	0.42	0
2	PGW	4K	101	-	50,50,50	0.47	0	53,56,56	0.43	0
2	PGW	5J	101	-	50,50,50	0.47	0	53,56,56	0.43	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	PGW	3B	101	-	-	17/55/55/55	-
2	PGW	2D	101	-	-	17/55/55/55	-
2	PGW	1I	101	-	-	17/55/55/55	-
2	PGW	1C	101	-	-	17/55/55/55	-
2	PGW	2C	101	-	-	17/55/55/55	-
2	PGW	4D	101	-	-	17/55/55/55	-
2	PGW	3N	101	-	-	17/55/55/55	-
2	PGW	4C	101	-	-	17/55/55/55	-
2	PGW	4I	101	-	-	17/55/55/55	-
2	PGW	4G	101	-	-	17/55/55/55	-
2	PGW	5C	102	-	-	17/55/55/55	-
2	PGW	2E	101	-	-	17/55/55/55	-
2	PGW	2F	101	-	-	17/55/55/55	-
2	PGW	4F	101	-	-	17/55/55/55	-
2	PGW	1N	101	-	-	17/55/55/55	-
2	PGW	3D	101	-	-	17/55/55/55	-
2	PGW	1B	101	-	-	17/55/55/55	-
2	PGW	4N	101	-	-	17/55/55/55	-
2	PGW	5F	101	-	-	17/55/55/55	-
2	PGW	5I	101	-	-	17/55/55/55	-
2	PGW	2B	101	-	-	17/55/55/55	-
2	PGW	2G	101	-	-	17/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PGW	3C	101	-	-	17/55/55/55	-
2	PGW	4J	101	-	-	17/55/55/55	-
2	PGW	4C	102	-	-	17/55/55/55	-
2	PGW	5C	101	-	-	17/55/55/55	-
2	PGW	4L	101	-	-	17/55/55/55	-
2	PGW	5K	101	-	-	17/55/55/55	-
2	PGW	5N	101	-	-	17/55/55/55	-
2	PGW	5G	101	-	-	17/55/55/55	-
2	PGW	1E	101	-	-	17/55/55/55	-
2	PGW	1B	102	-	-	17/55/55/55	-
2	PGW	1H	101	-	-	17/55/55/55	-
2	PGW	3D	102	-	-	17/55/55/55	-
2	PGW	3G	101	-	-	17/55/55/55	-
2	PGW	4B	101	-	-	17/55/55/55	-
2	PGW	5M	101	-	-	17/55/55/55	-
2	PGW	4M	101	-	-	17/55/55/55	-
2	PGW	5L	101	-	-	17/55/55/55	-
2	PGW	3E	101	-	-	17/55/55/55	-
2	PGW	1J	101	-	-	17/55/55/55	-
2	PGW	3H	101	-	-	17/55/55/55	-
2	PGW	2H	101	-	-	17/55/55/55	-
2	PGW	3M	101	-	-	17/55/55/55	-
2	PGW	2K	101	-	-	17/55/55/55	-
2	PGW	2M	101	-	-	17/55/55/55	-
2	PGW	2I	101	-	-	17/55/55/55	-
2	PGW	3I	101	-	-	17/55/55/55	-
2	PGW	3K	101	-	-	17/55/55/55	-
2	PGW	2D	102	-	-	17/55/55/55	-
2	PGW	1K	101	-	-	17/55/55/55	-
2	PGW	4E	101	-	-	17/55/55/55	-
2	PGW	5H	101	-	-	17/55/55/55	-
2	PGW	2L	101	-	-	17/55/55/55	-
2	PGW	5B	101	-	-	17/55/55/55	-
2	PGW	3J	101	-	-	17/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PGW	1F	101	-	-	17/55/55/55	-
2	PGW	1D	101	-	-	17/55/55/55	-
2	PGW	2J	101	-	-	17/55/55/55	-
2	PGW	5E	101	-	-	17/55/55/55	-
2	PGW	1M	101	-	-	17/55/55/55	-
2	PGW	5D	101	-	-	17/55/55/55	-
2	PGW	3L	101	-	-	17/55/55/55	-
2	PGW	1L	101	-	-	17/55/55/55	-
2	PGW	3F	101	-	-	17/55/55/55	-
2	PGW	1G	101	-	-	17/55/55/55	-
2	PGW	4H	101	-	-	17/55/55/55	-
2	PGW	2N	101	-	-	17/55/55/55	-
2	PGW	4K	101	-	-	17/55/55/55	-
2	PGW	5J	101	-	-	17/55/55/55	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 1190 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	1B	101	PGW	O04-C19-O03-C01
2	1B	102	PGW	O04-C19-O03-C01
2	1C	101	PGW	O04-C19-O03-C01
2	1D	101	PGW	O04-C19-O03-C01
2	1E	101	PGW	O04-C19-O03-C01

There are no ring outliers.

70 monomers are involved in 159 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	3B	101	PGW	2	0
2	2D	101	PGW	2	0
2	1I	101	PGW	3	0
2	1C	101	PGW	2	0
2	2C	101	PGW	2	0
2	4D	101	PGW	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	3N	101	PGW	2	0
2	4C	101	PGW	3	0
2	4I	101	PGW	3	0
2	4G	101	PGW	2	0
2	5C	102	PGW	2	0
2	2E	101	PGW	3	0
2	2F	101	PGW	3	0
2	4F	101	PGW	3	0
2	1N	101	PGW	2	0
2	3D	101	PGW	2	0
2	1B	101	PGW	2	0
2	4N	101	PGW	2	0
2	5F	101	PGW	3	0
2	5I	101	PGW	3	0
2	2B	101	PGW	2	0
2	2G	101	PGW	2	0
2	3C	101	PGW	2	0
2	4J	101	PGW	2	0
2	4C	102	PGW	2	0
2	5C	101	PGW	2	0
2	4L	101	PGW	2	0
2	5K	101	PGW	2	0
2	5N	101	PGW	2	0
2	5G	101	PGW	3	0
2	1E	101	PGW	2	0
2	1B	102	PGW	3	0
2	1H	101	PGW	2	0
2	3D	102	PGW	2	0
2	3G	101	PGW	2	0
2	4B	101	PGW	2	0
2	5M	101	PGW	2	0
2	4M	101	PGW	2	0
2	5L	101	PGW	2	0
2	3E	101	PGW	2	0
2	1J	101	PGW	3	0
2	3H	101	PGW	3	0
2	2H	101	PGW	3	0
2	3M	101	PGW	2	0
2	2K	101	PGW	3	0
2	2M	101	PGW	2	0
2	2I	101	PGW	2	0
2	3I	101	PGW	2	0

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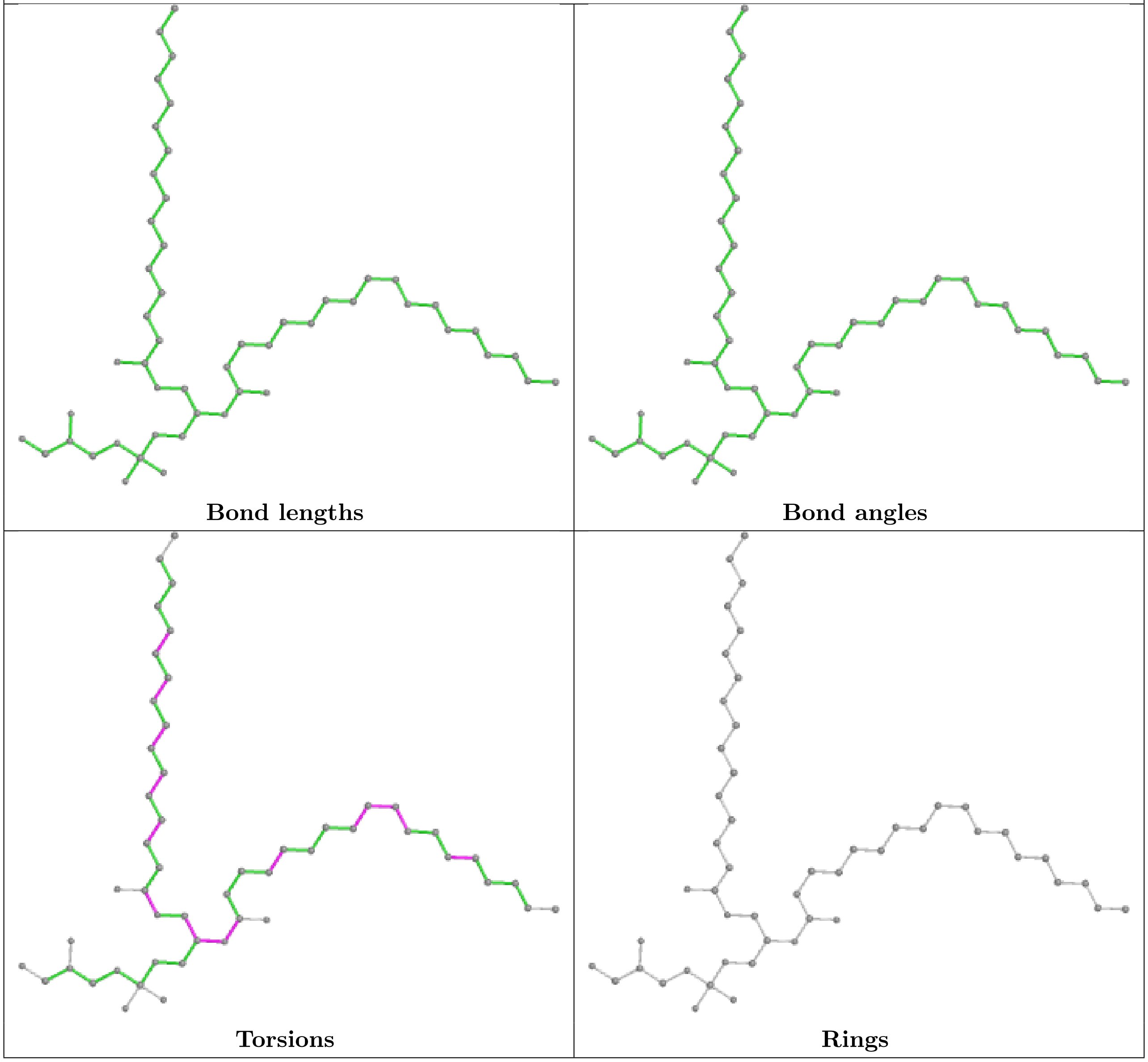
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	3K	101	PGW	2	0
2	2D	102	PGW	2	0
2	1K	101	PGW	2	0
2	4E	101	PGW	3	0
2	5H	101	PGW	3	0
2	2L	101	PGW	2	0
2	5B	101	PGW	2	0
2	3J	101	PGW	2	0
2	1F	101	PGW	3	0
2	1D	101	PGW	2	0
2	2J	101	PGW	2	0
2	5E	101	PGW	2	0
2	1M	101	PGW	2	0
2	5D	101	PGW	2	0
2	3L	101	PGW	2	0
2	1L	101	PGW	2	0
2	3F	101	PGW	3	0
2	1G	101	PGW	3	0
2	4H	101	PGW	2	0
2	2N	101	PGW	2	0
2	4K	101	PGW	2	0
2	5J	101	PGW	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 then 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 PGW 3B 101



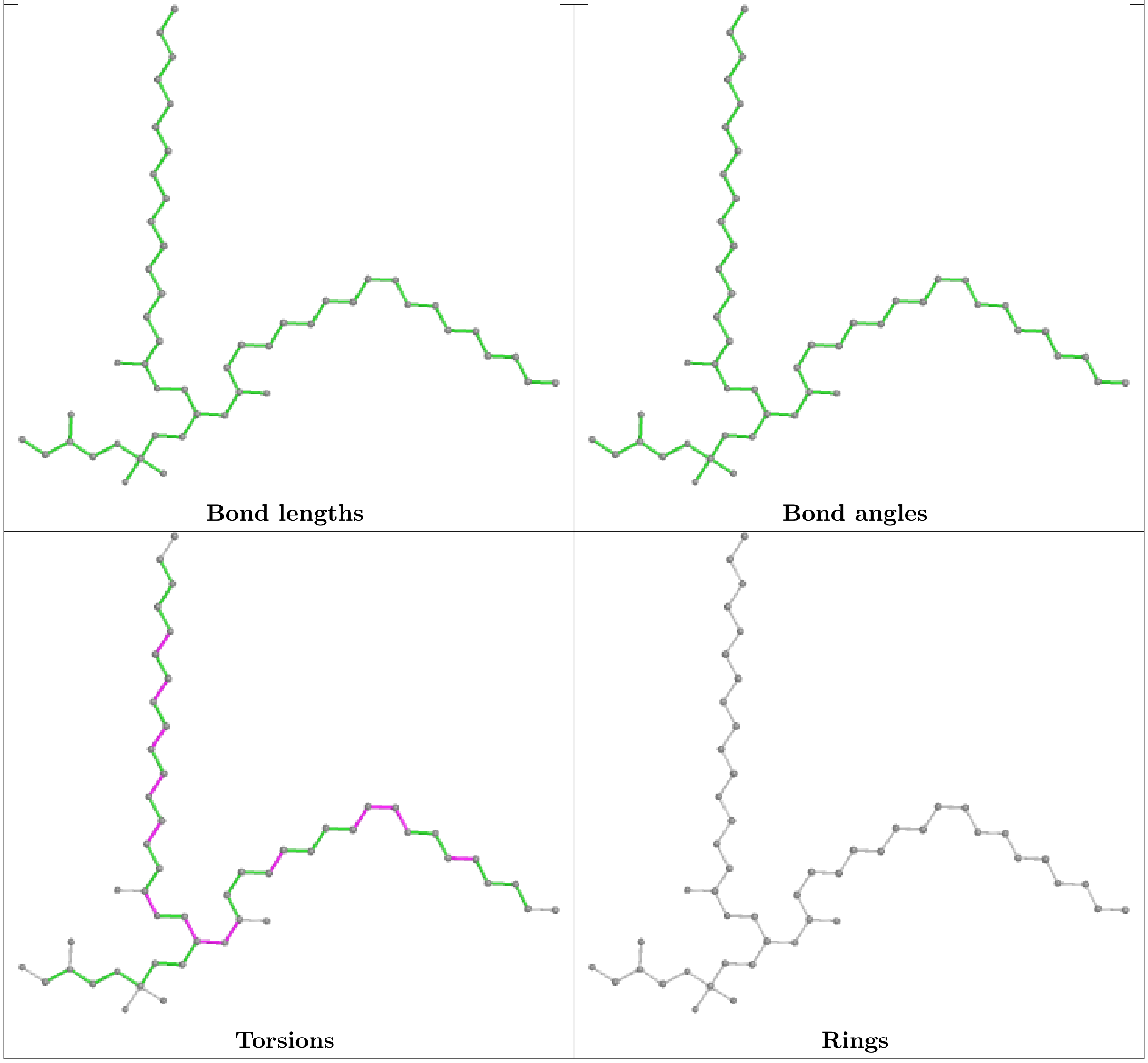
Bond lengths

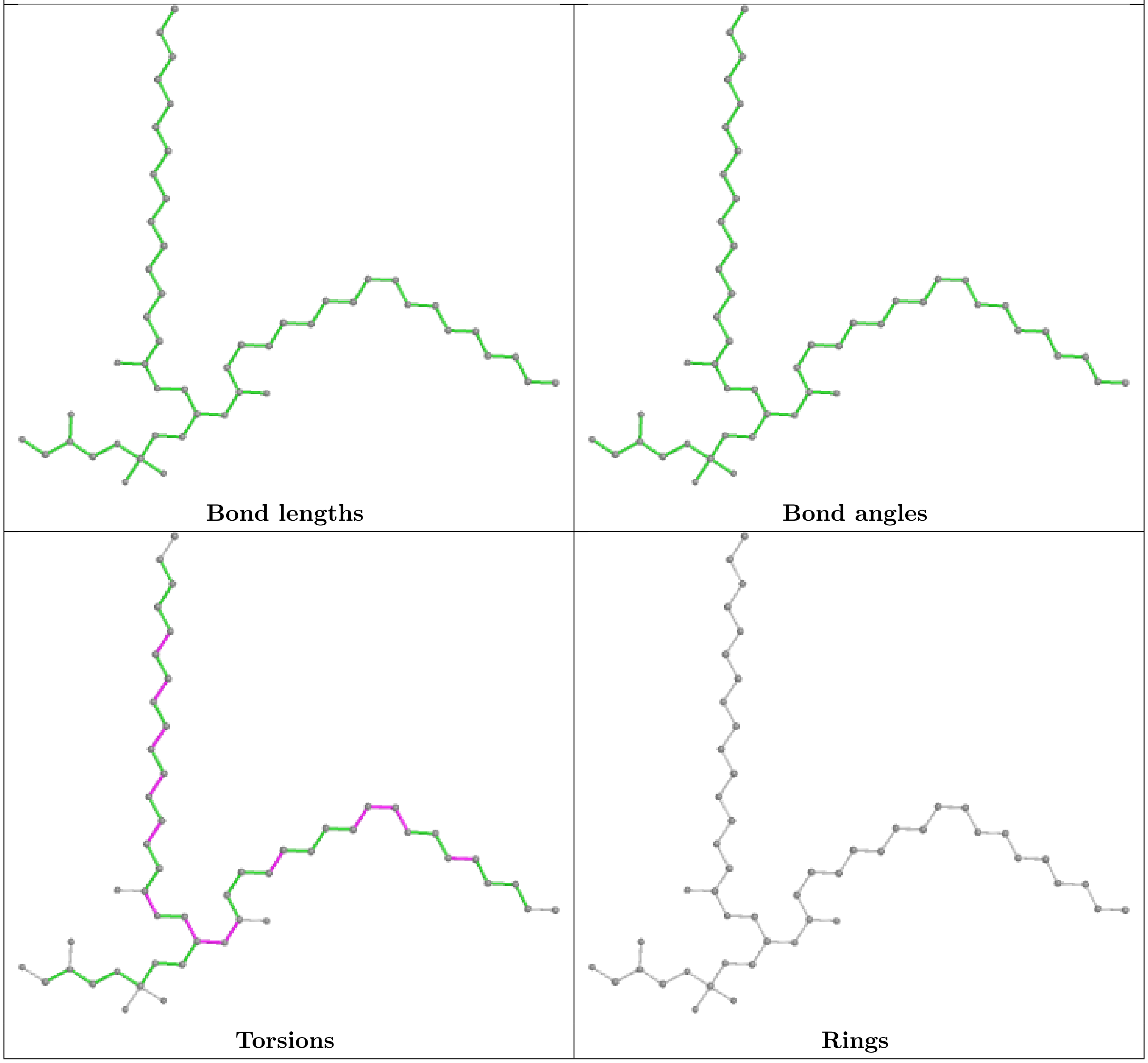
Bond angles

Torsions

Rings

Ligand PGW 2D 101





Ligand PGW 1I 101

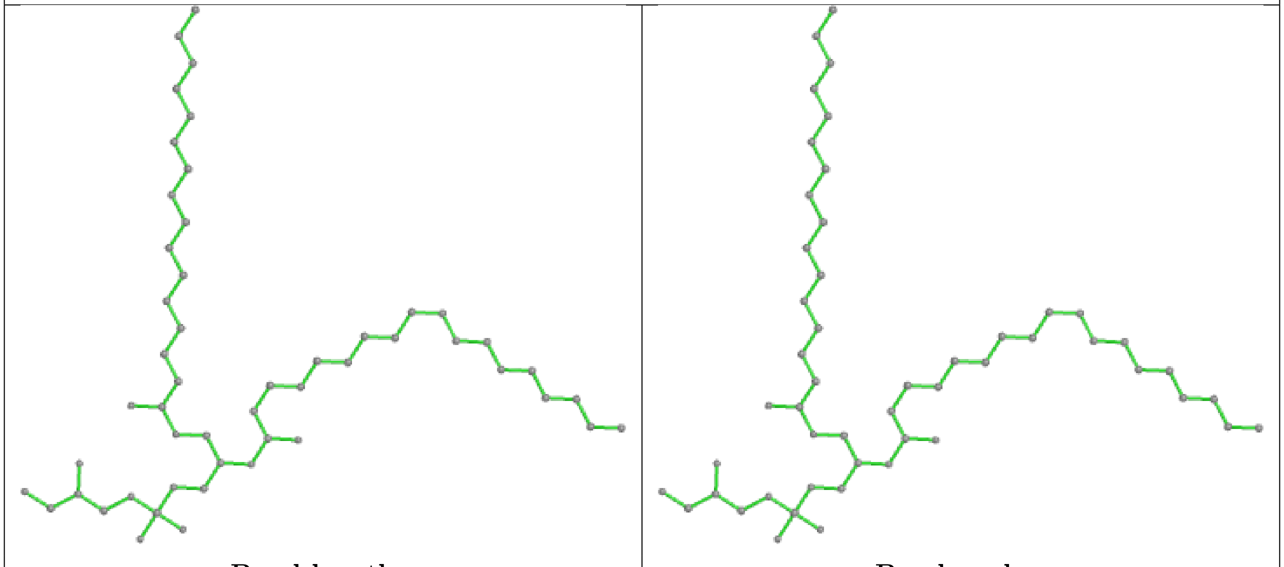
Bond lengths

Bond angles

Torsions

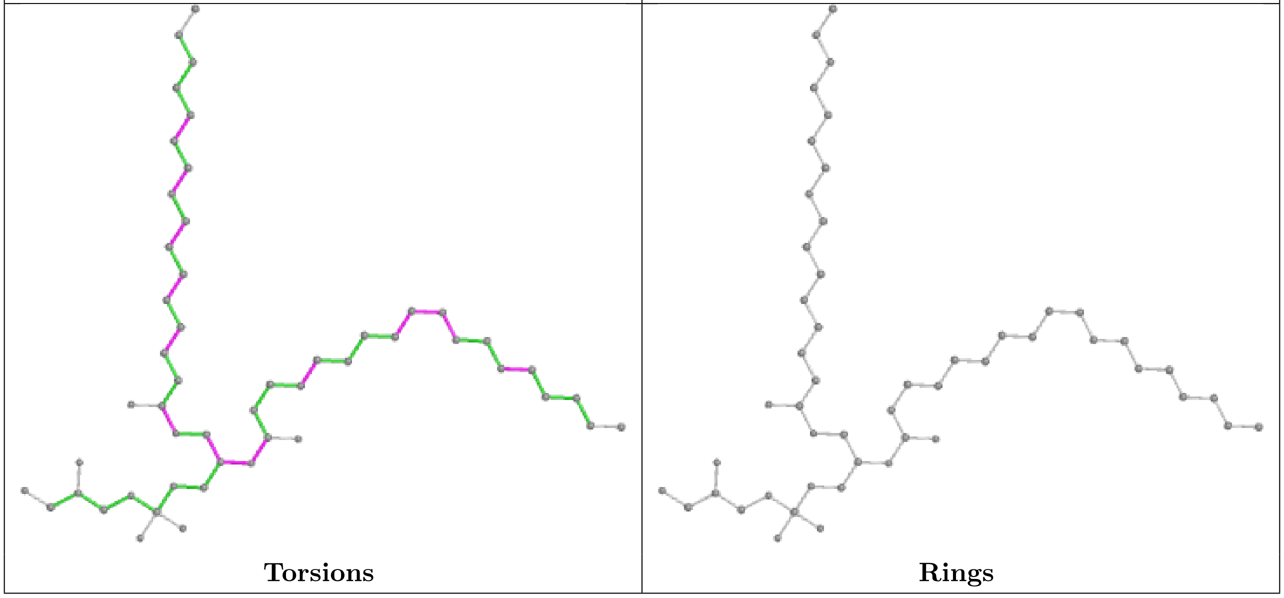
Rings

Ligand PGW 1C 101



Bond lengths

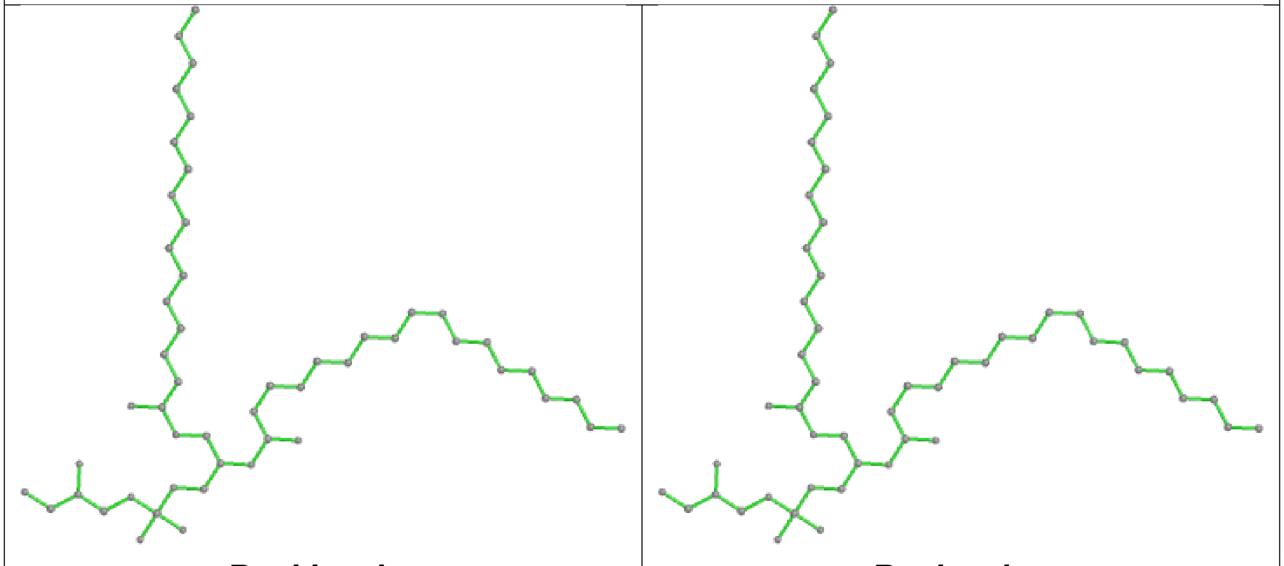
Bond angles



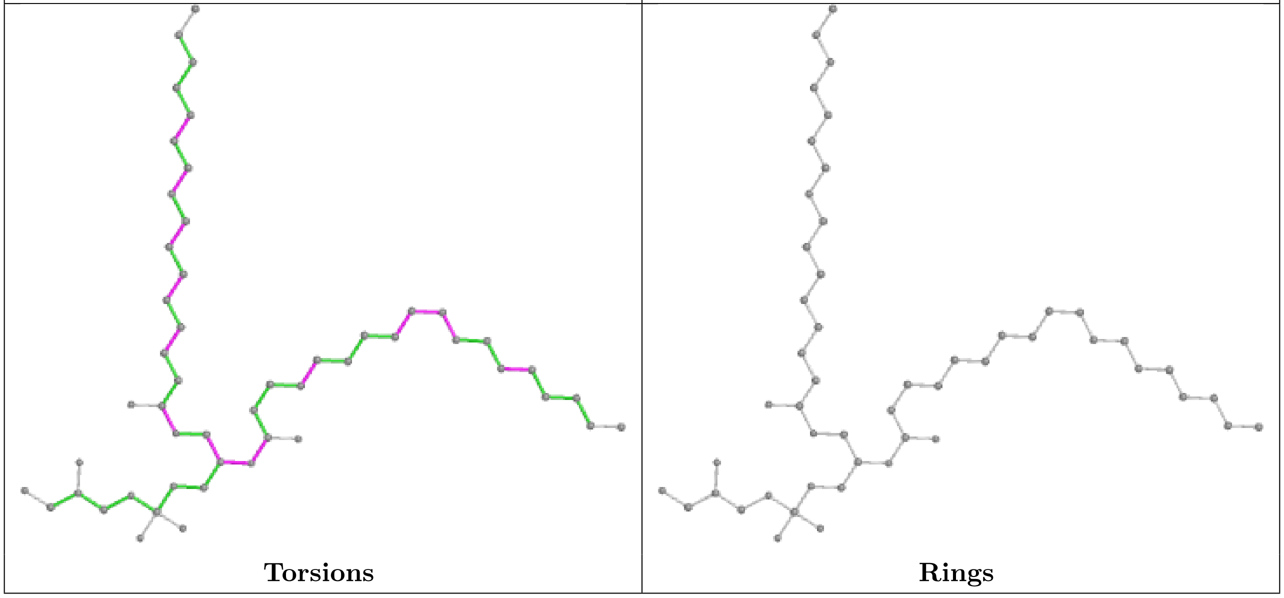
Torsions

Rings

Ligand PGW 2C 101

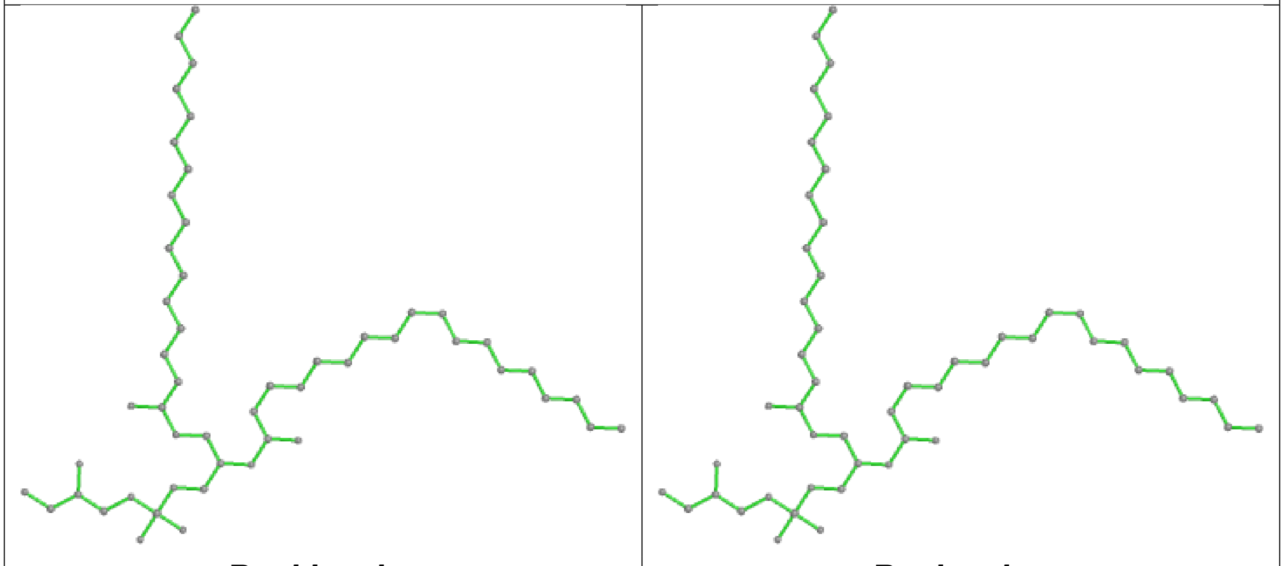


Bond lengths **Bond angles**



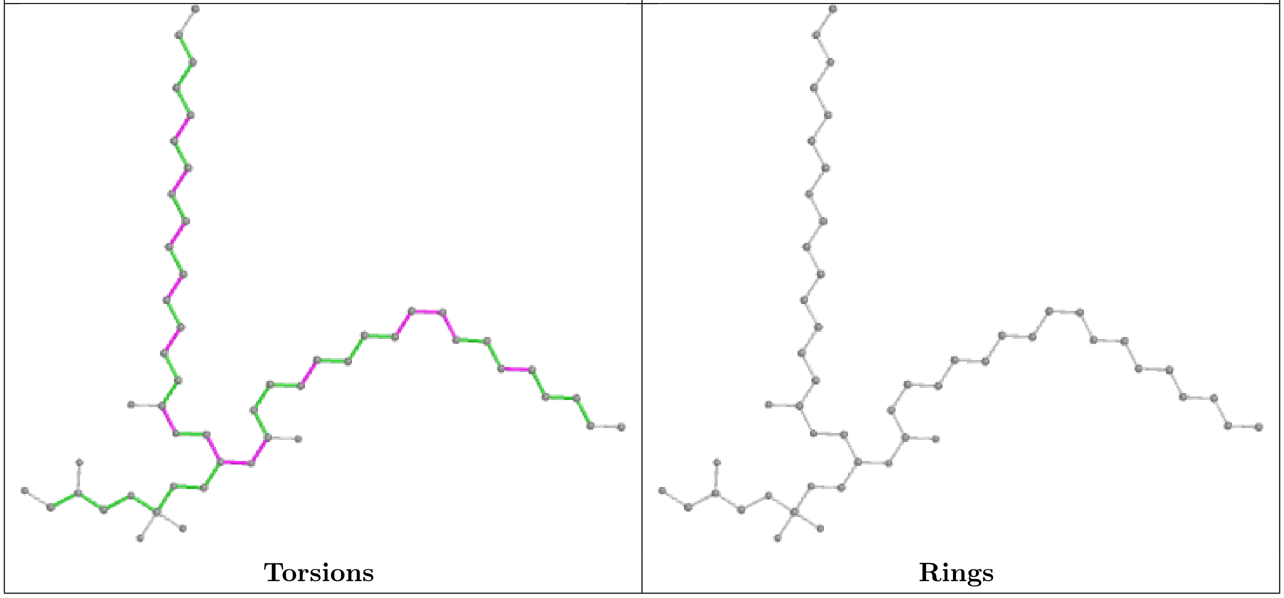
Torsions **Rings**

Ligand PGW 4D 101



Bond lengths

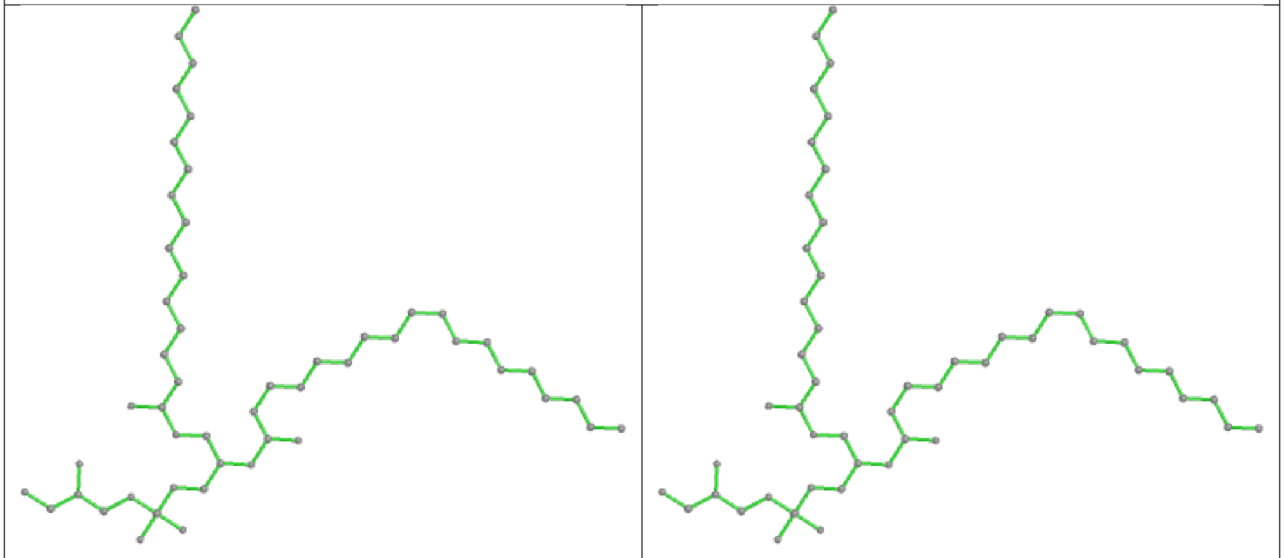
Bond angles



Torsions

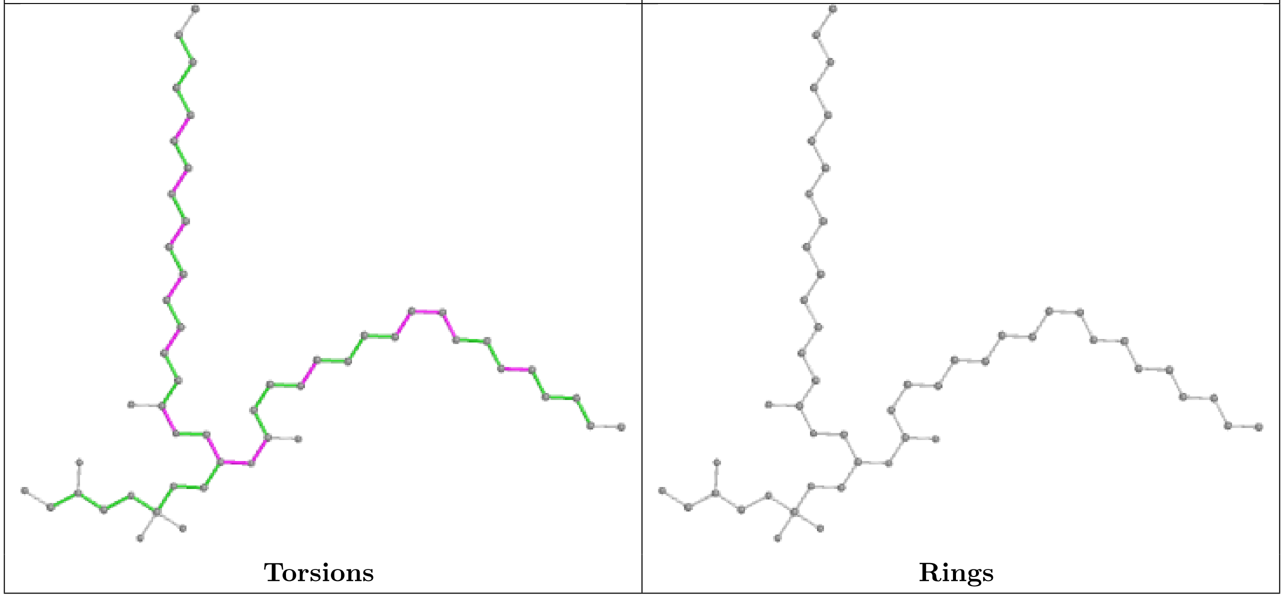
Rings

Ligand PGW 3N 101



Bond lengths

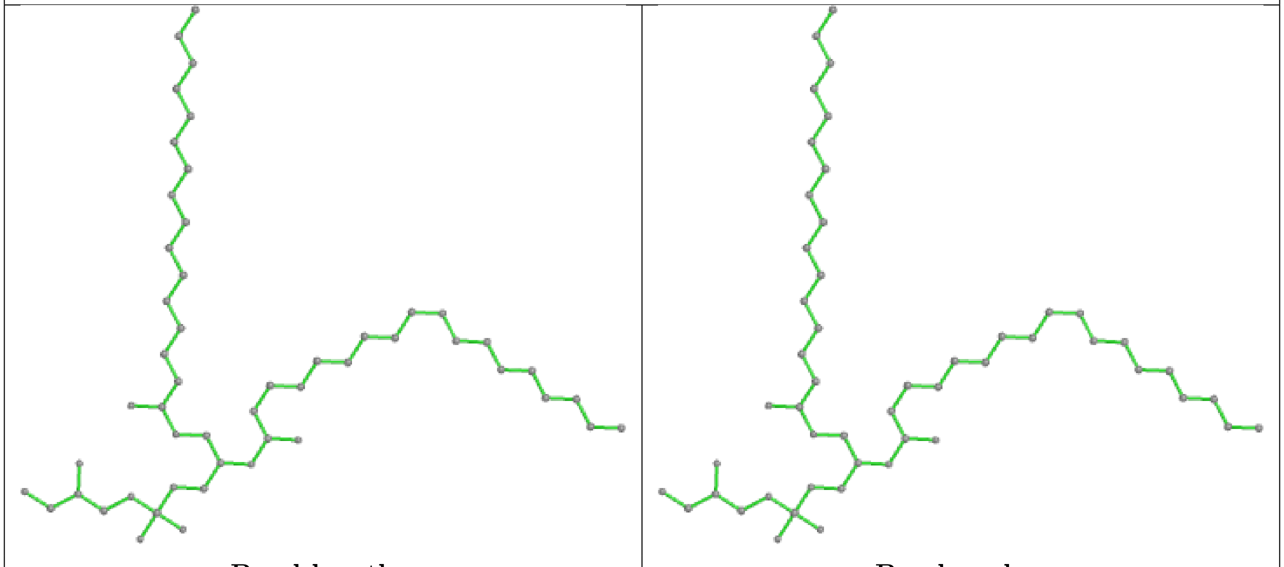
Bond angles



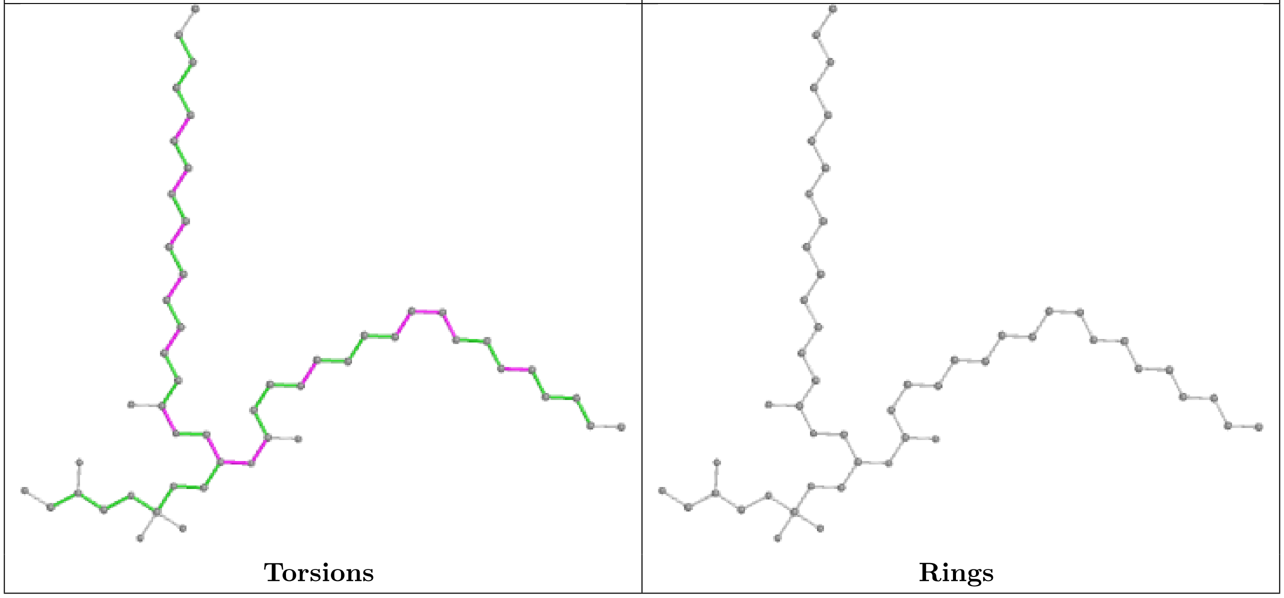
Torsions

Rings

Ligand PGW 4C 101

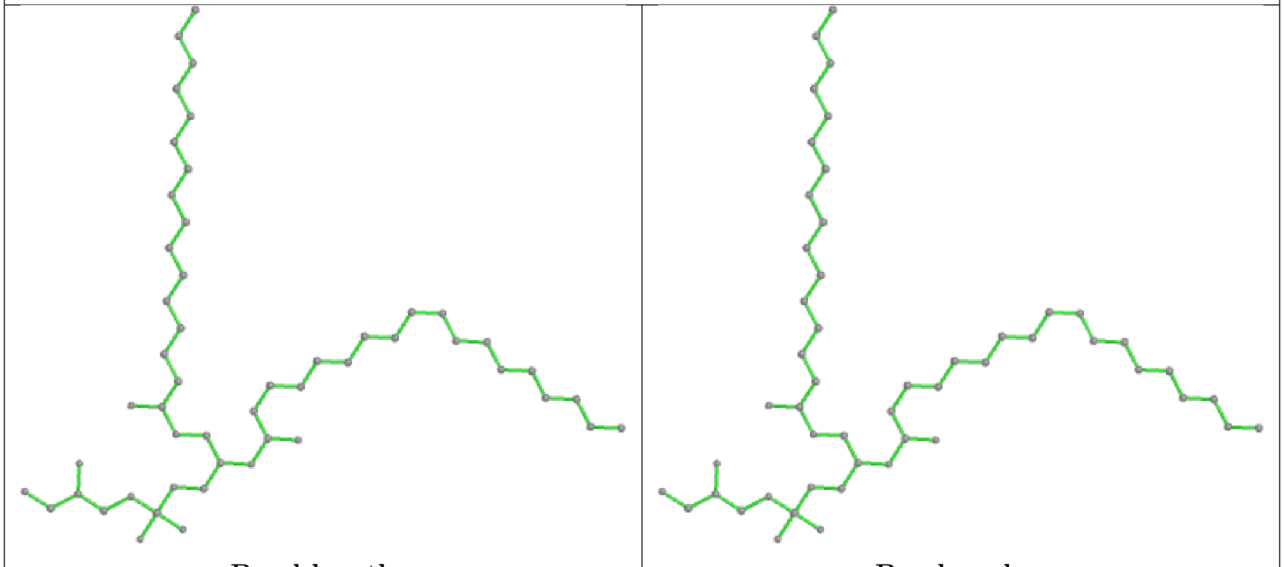


Bond lengths **Bond angles**

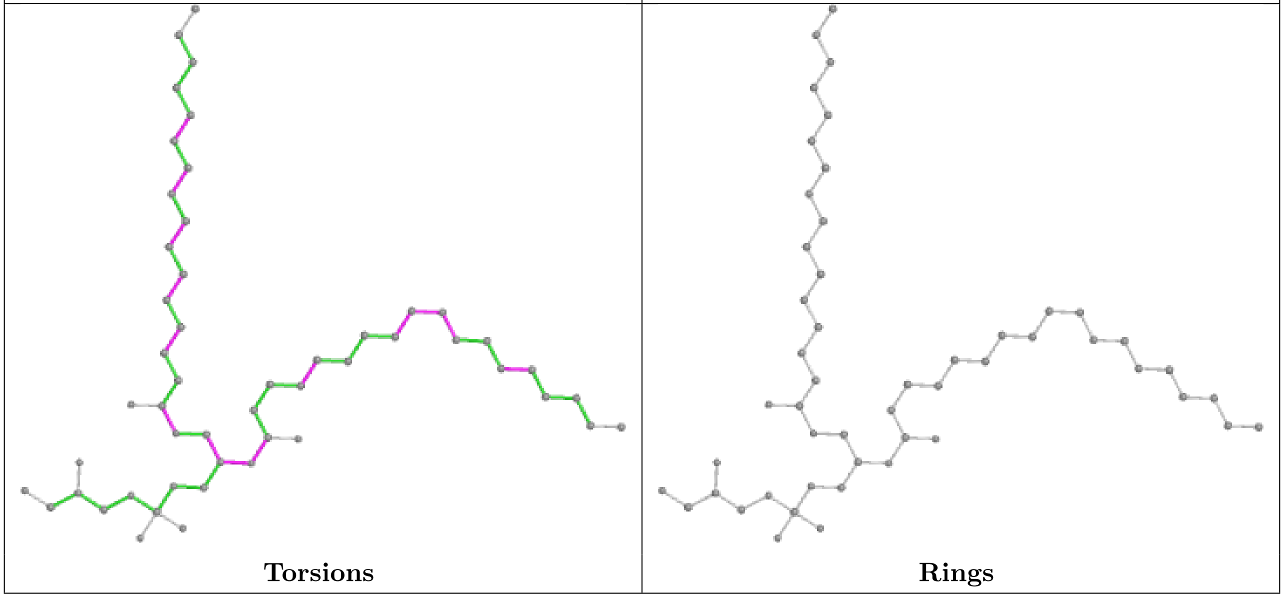


Torsions **Rings**

Ligand PGW 4I 101

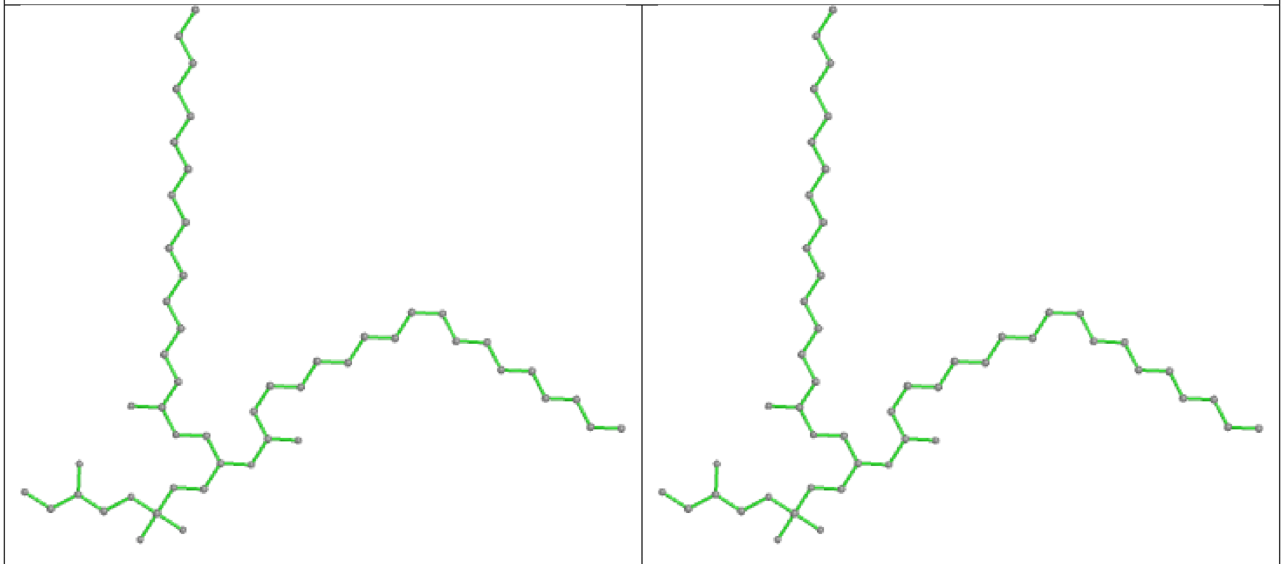


Bond lengths **Bond angles**

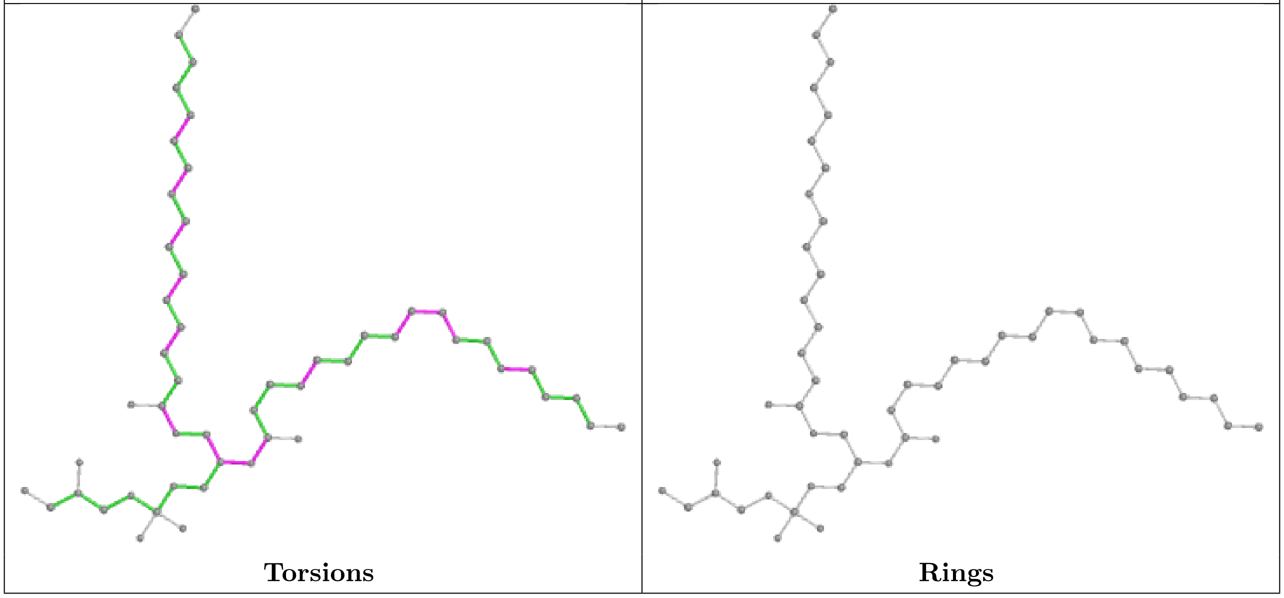


Torsions **Rings**

Ligand PGW 4G 101

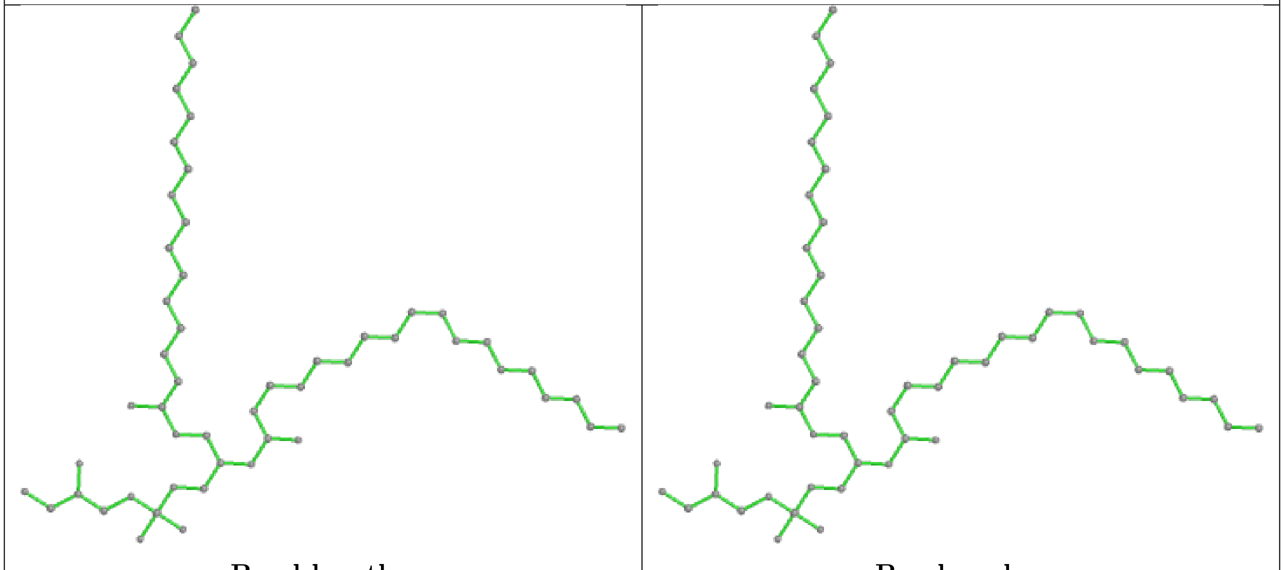


Bond lengths **Bond angles**



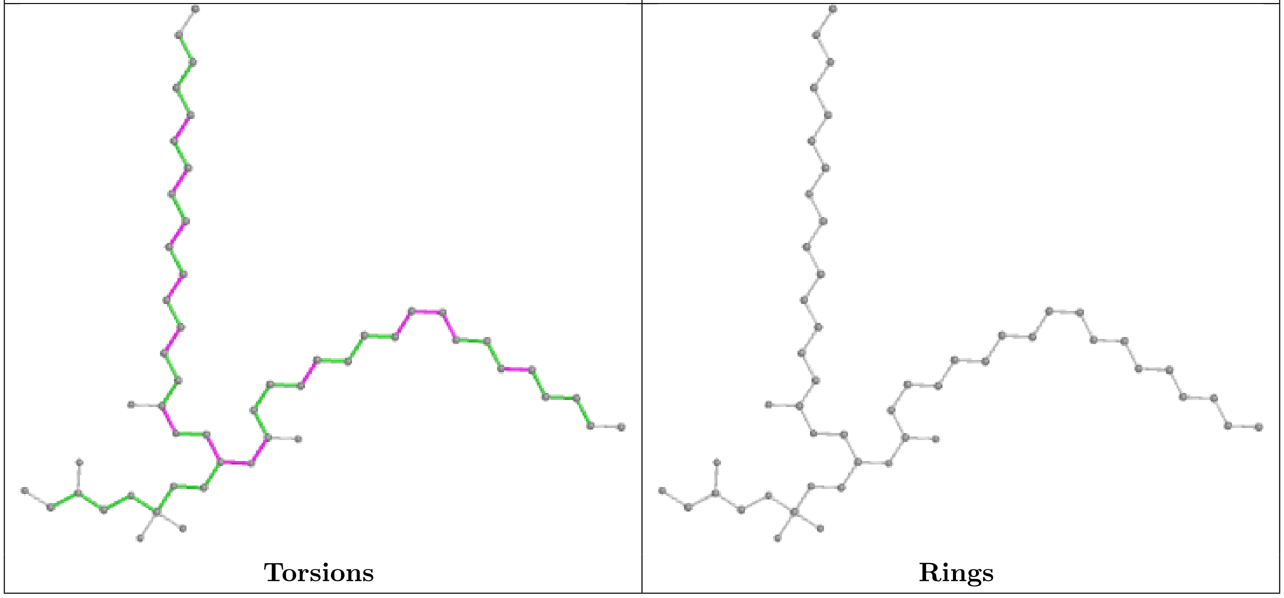
Torsions **Rings**

Ligand PGW 5C 102



Bond lengths

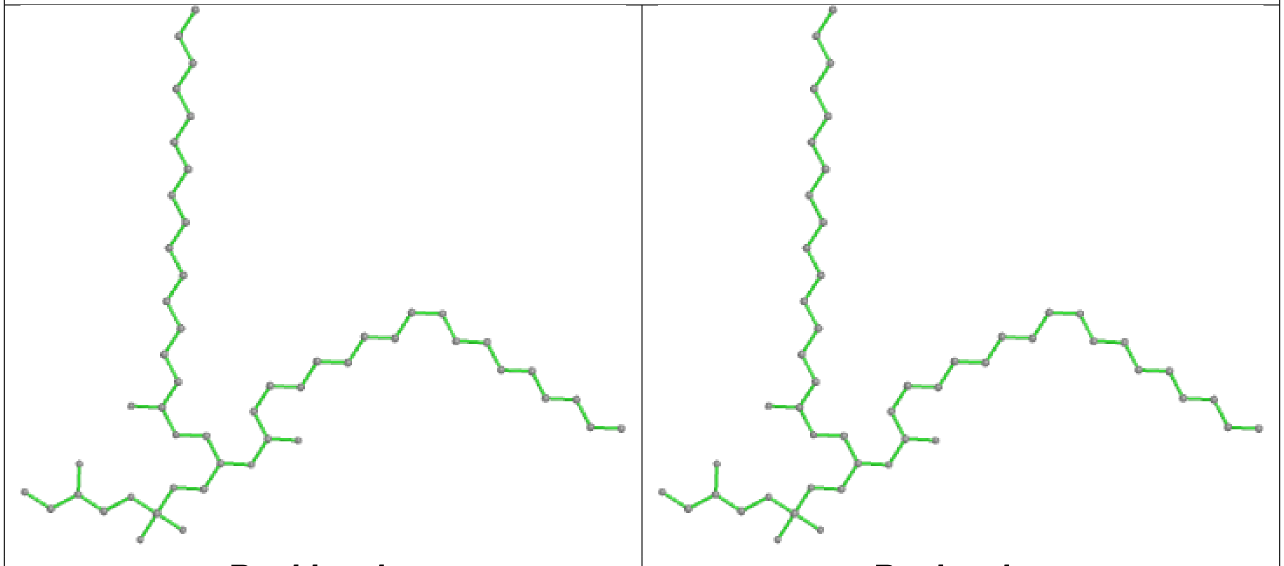
Bond angles



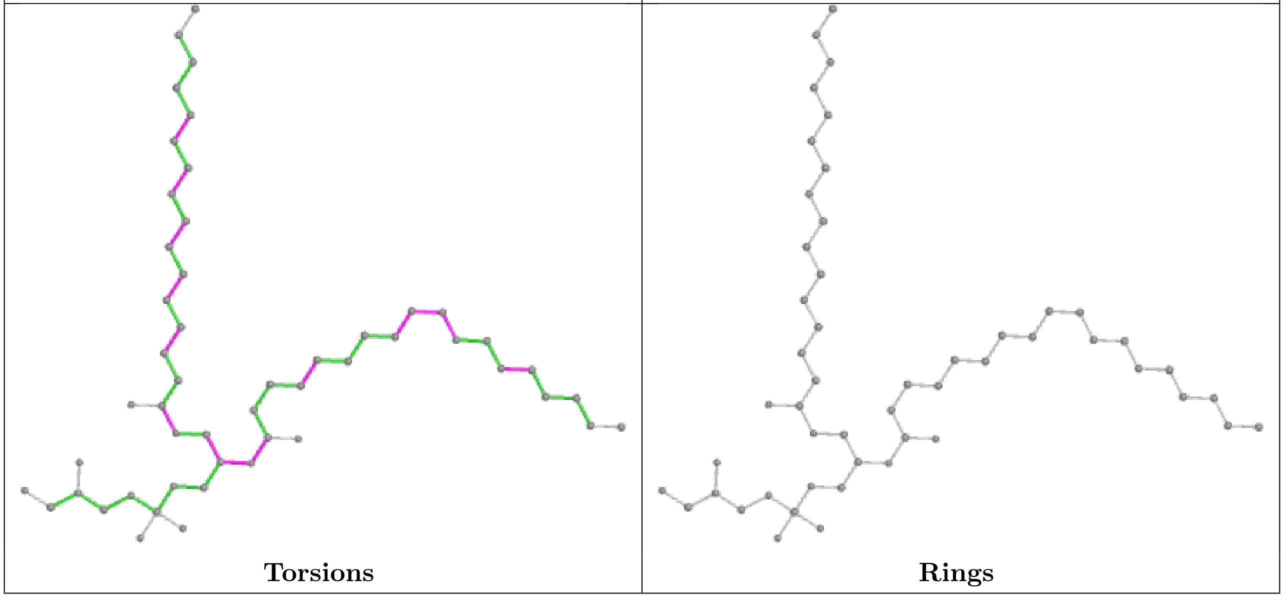
Torsions

Rings

Ligand PGW 2E 101

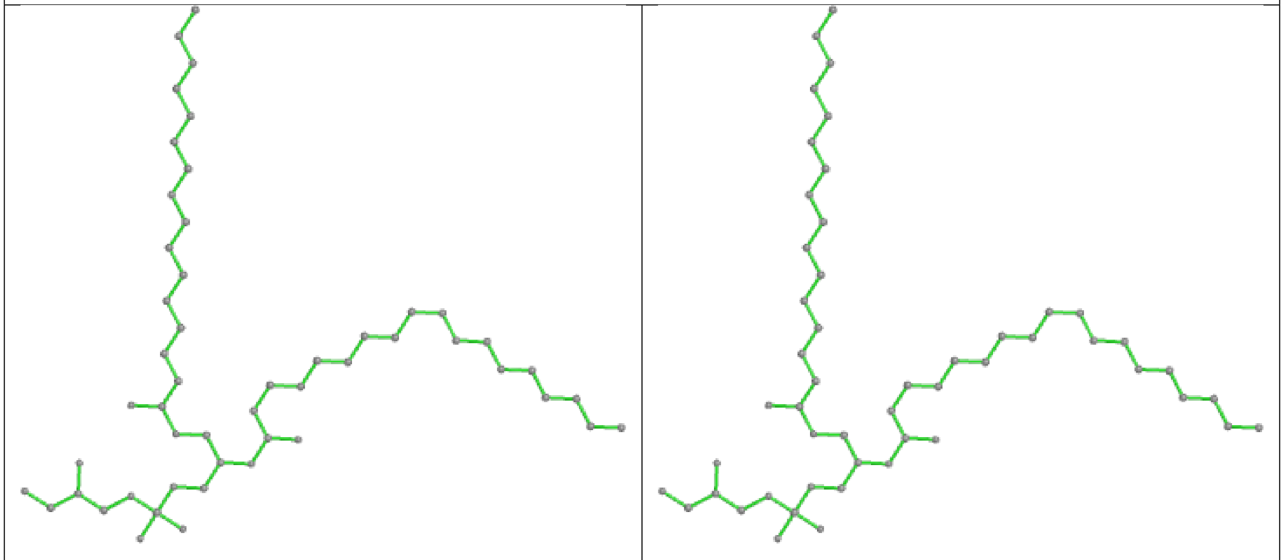


Bond lengths **Bond angles**

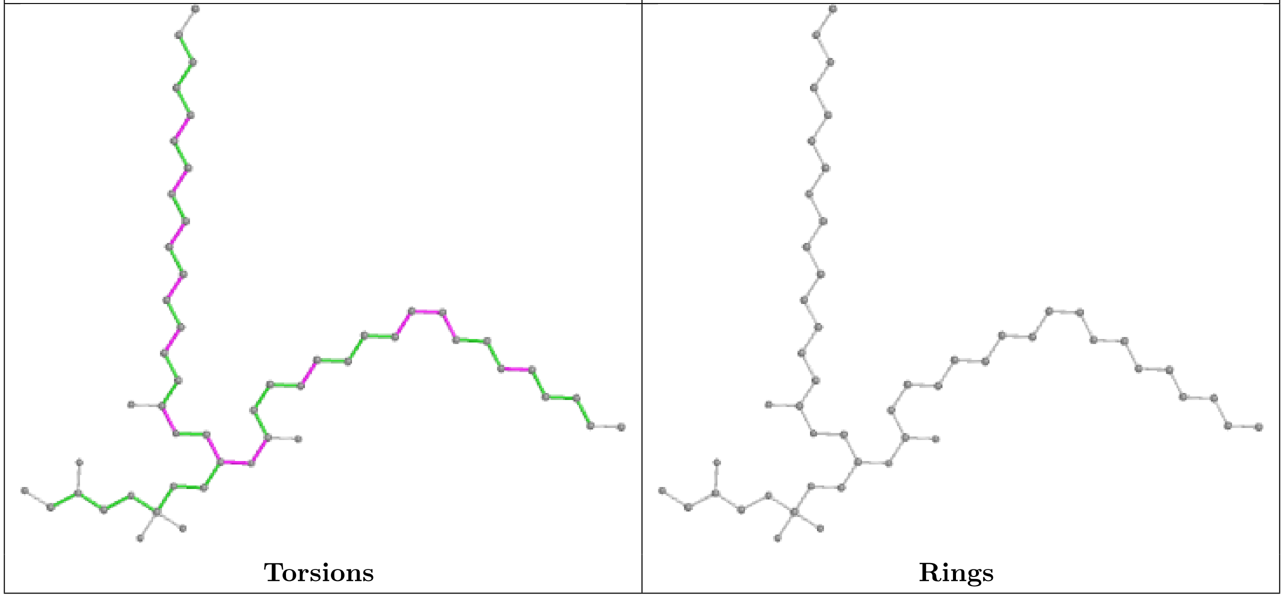


Torsions **Rings**

Ligand PGW 2F 101

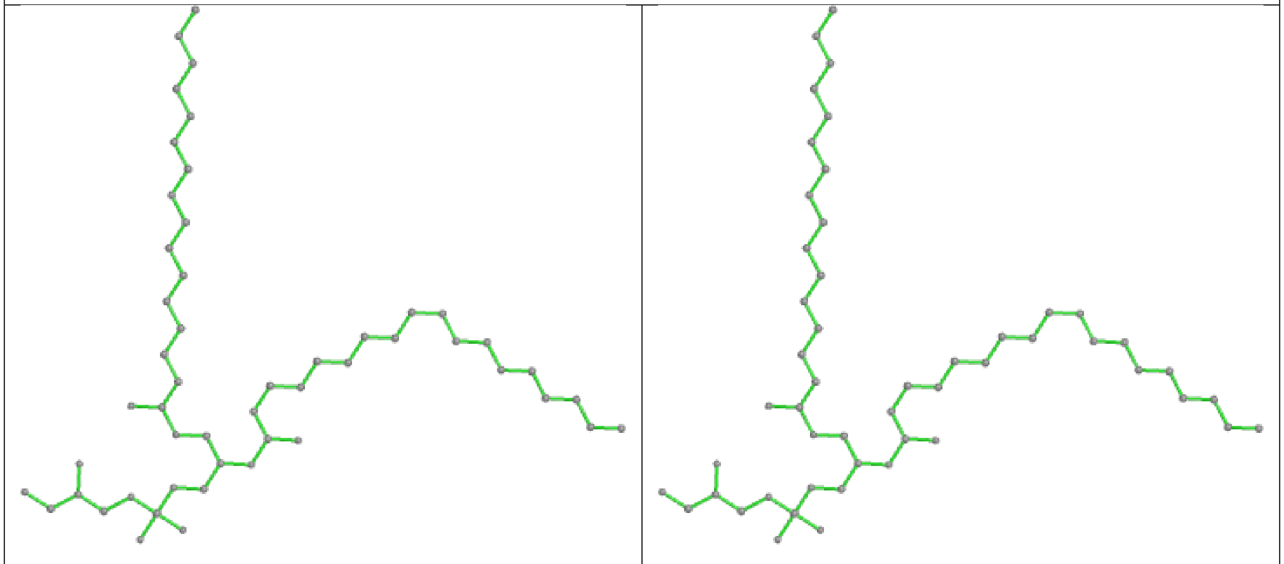


Bond lengths **Bond angles**

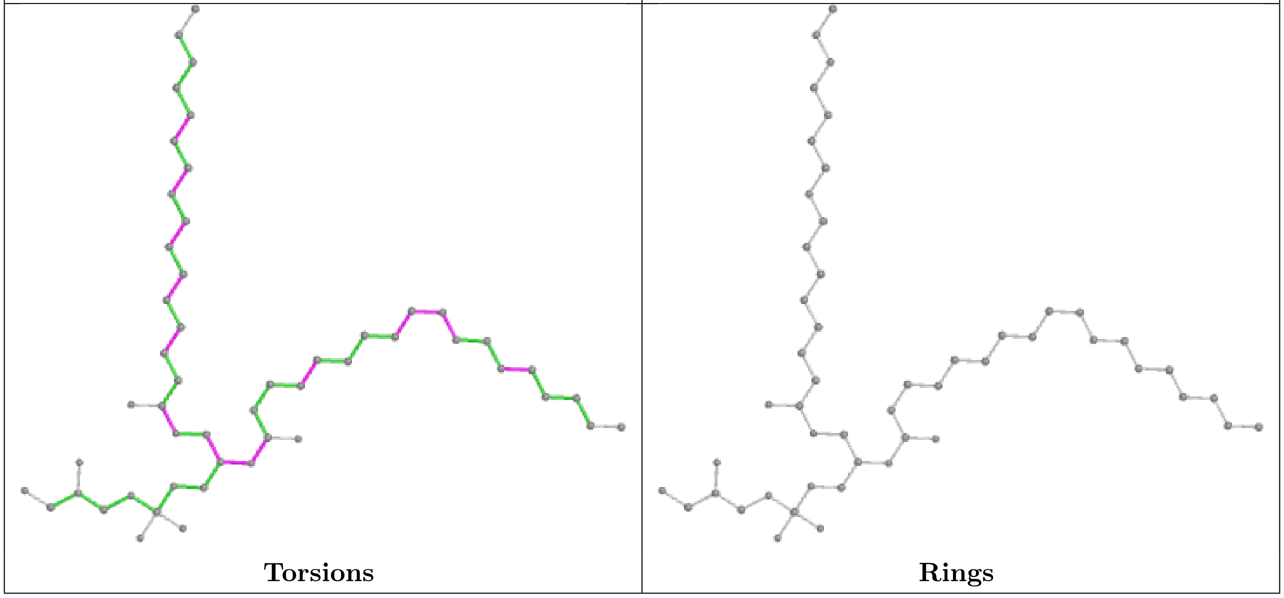


Torsions **Rings**

Ligand PGW 4F 101

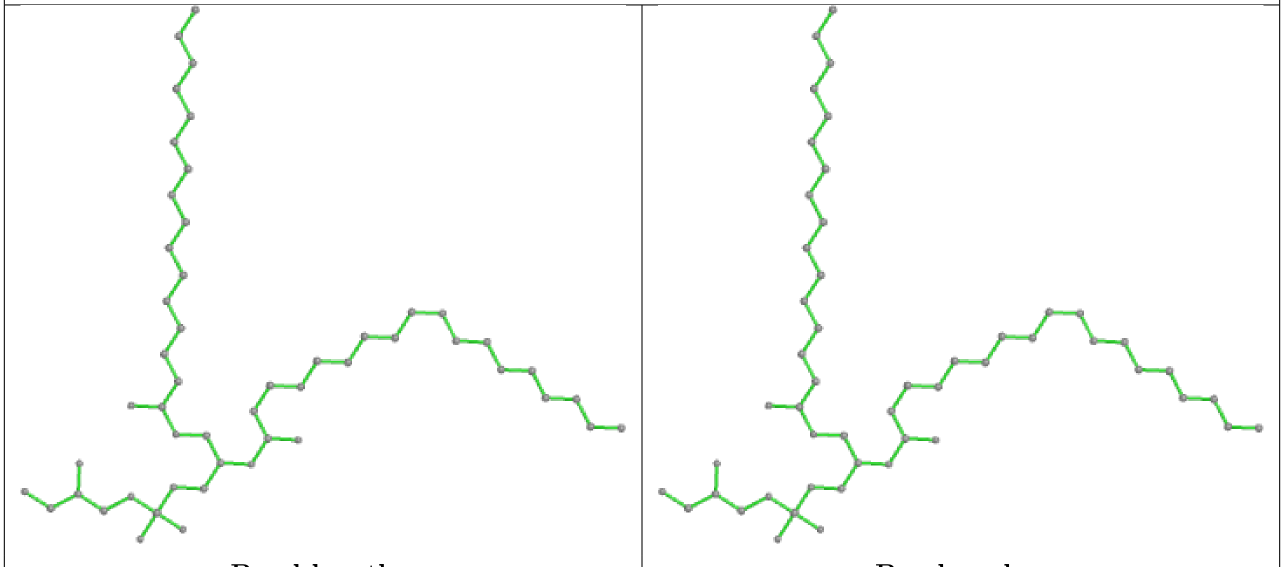


Bond lengths **Bond angles**

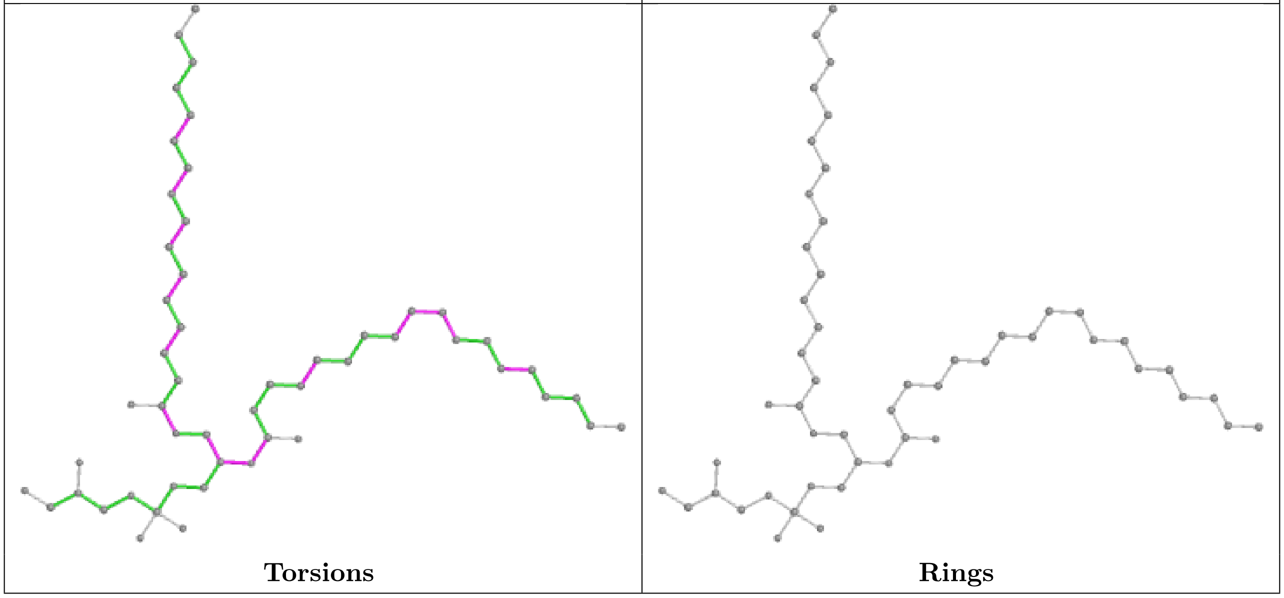


Torsions **Rings**

Ligand PGW 1N 101

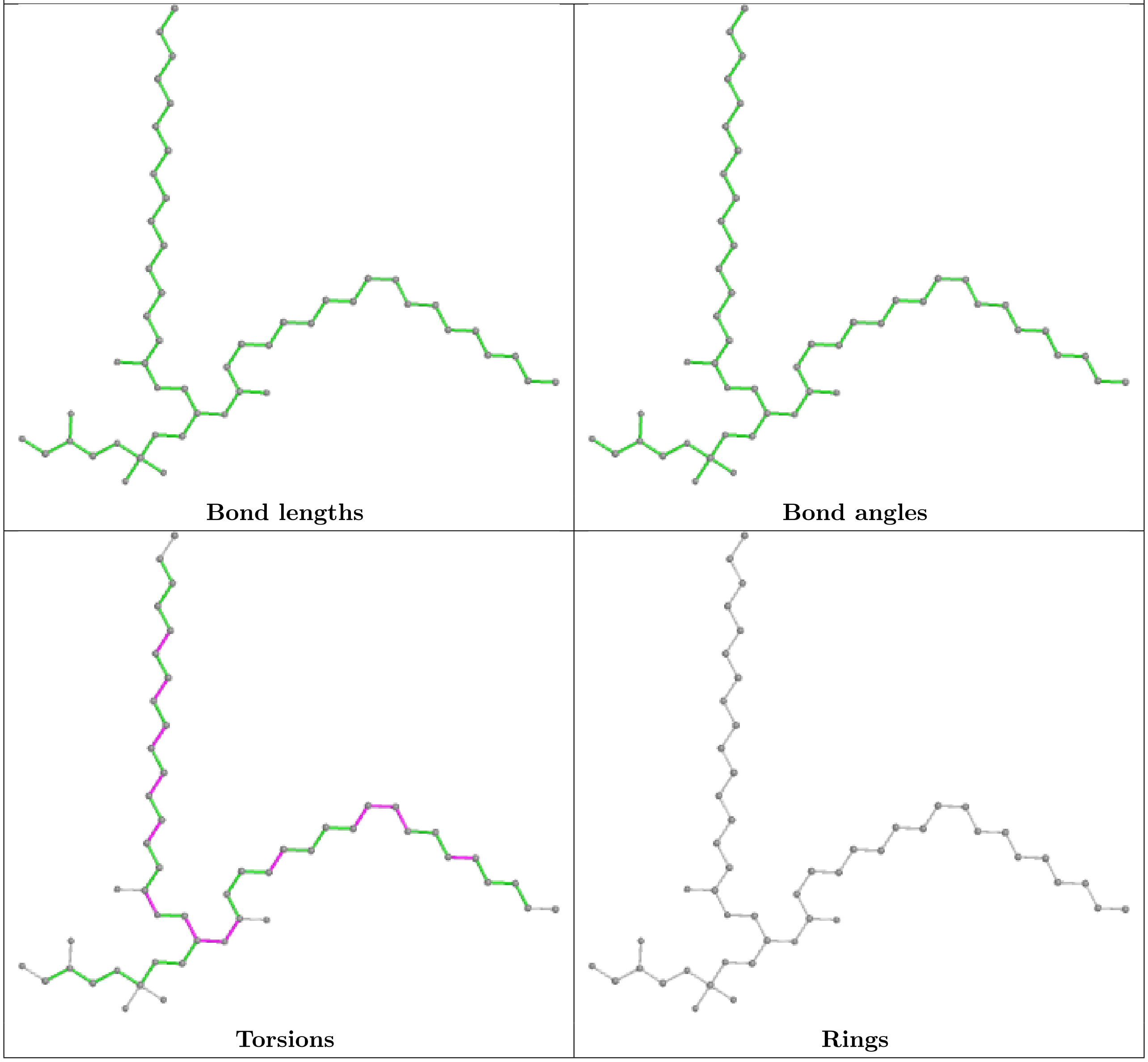


Bond lengths Bond angles



Torsions Rings

Ligand PGW 3D 101



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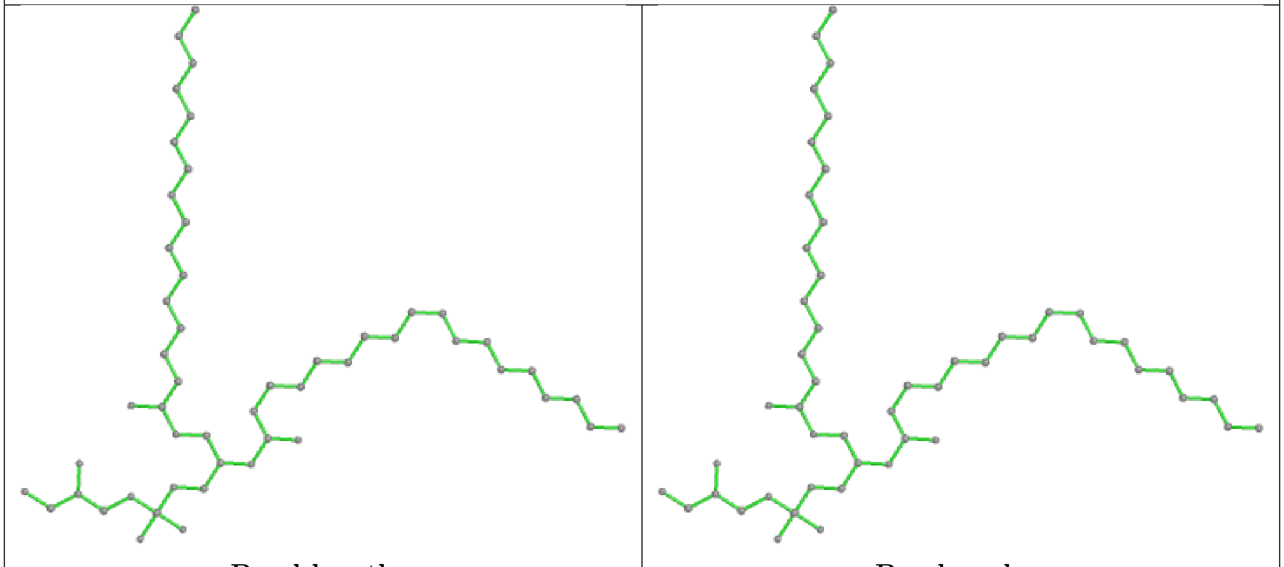
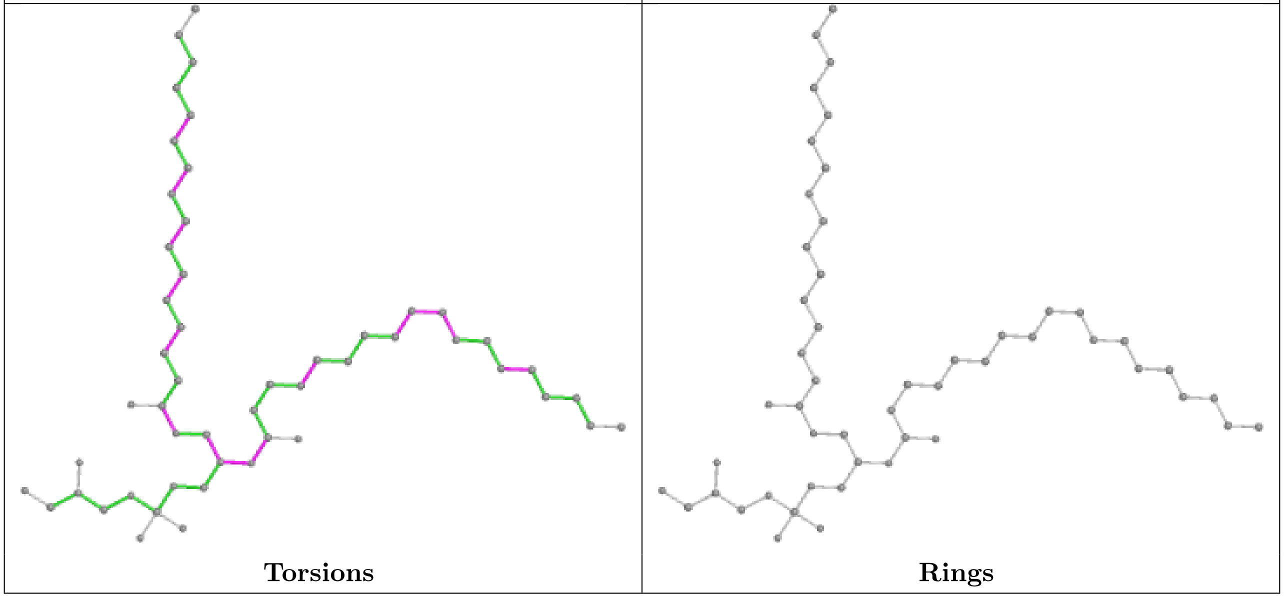


Bond lengths

Bond angles



Torsions

Rings

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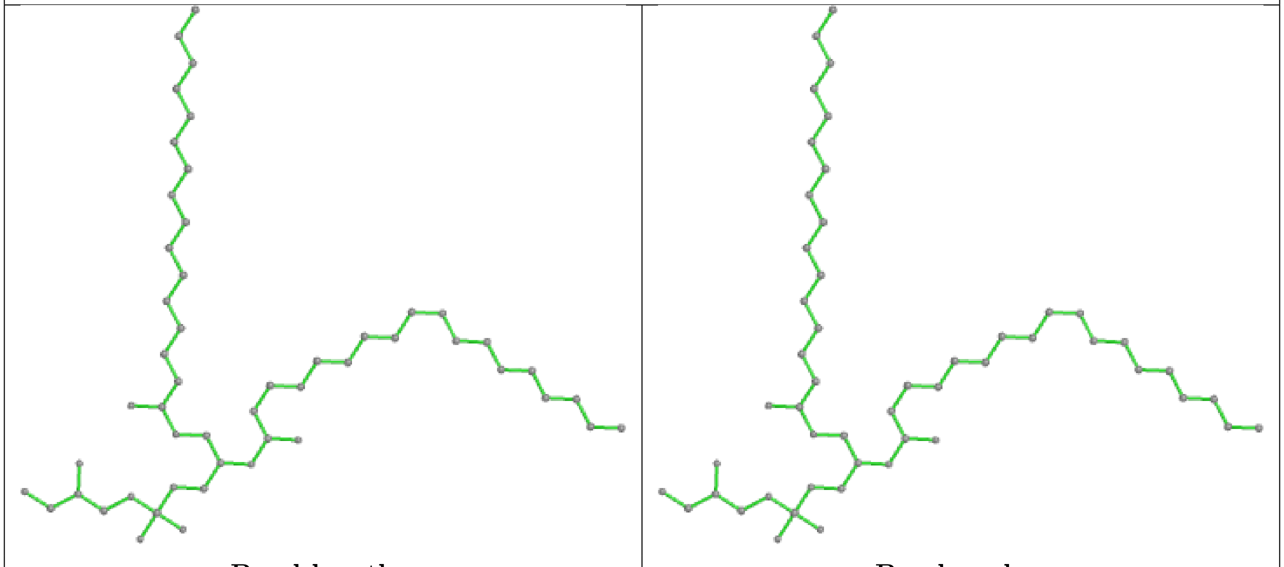
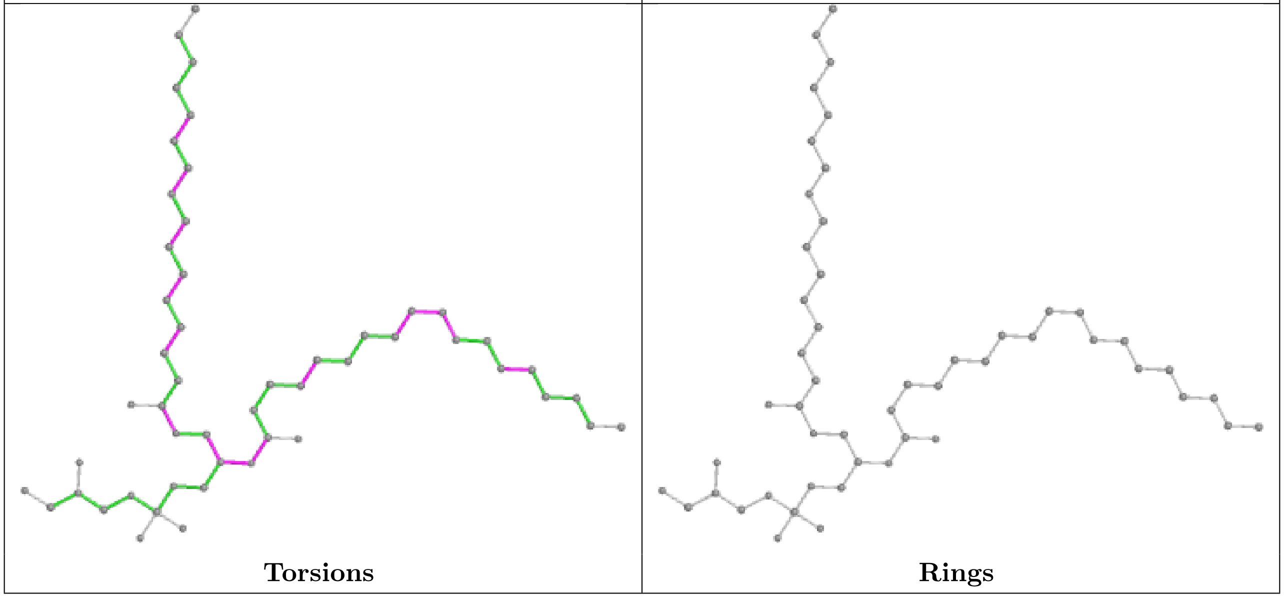


Bond lengths

Bond angles



Torsions

Rings

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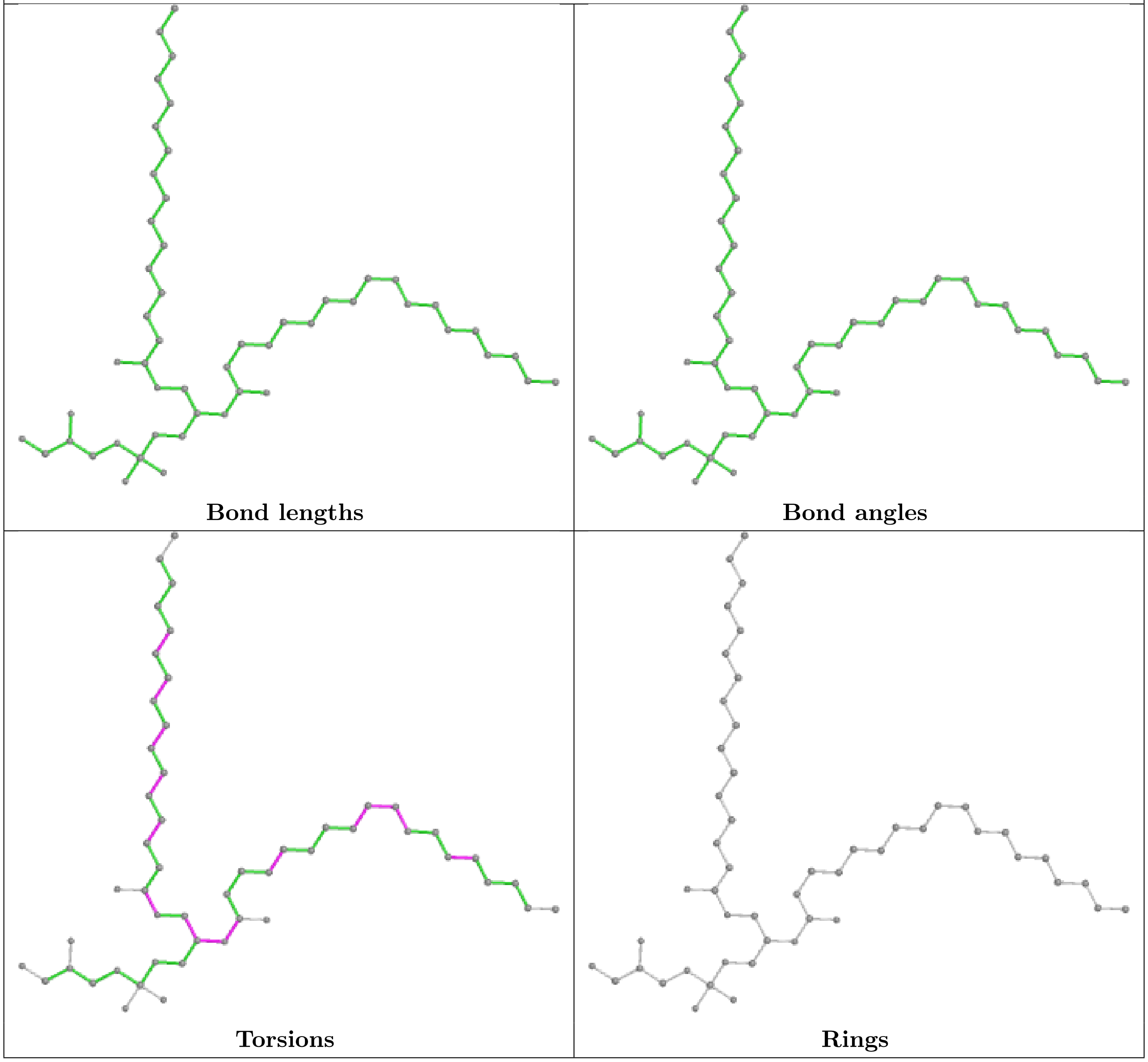


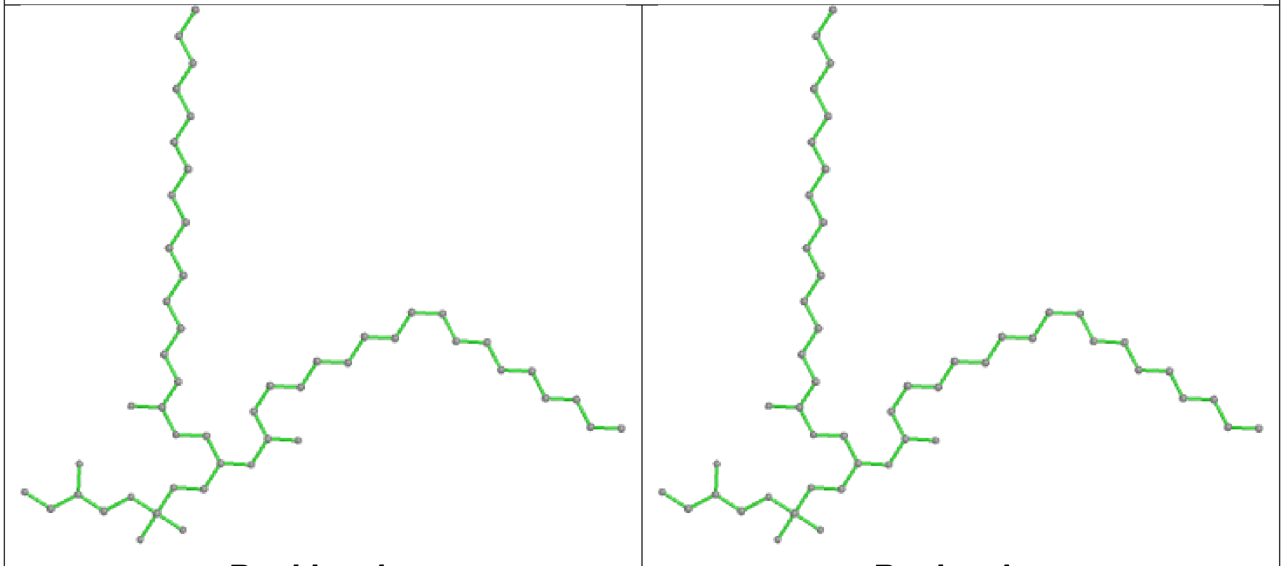
Bond lengths

Bond angles

Torsions

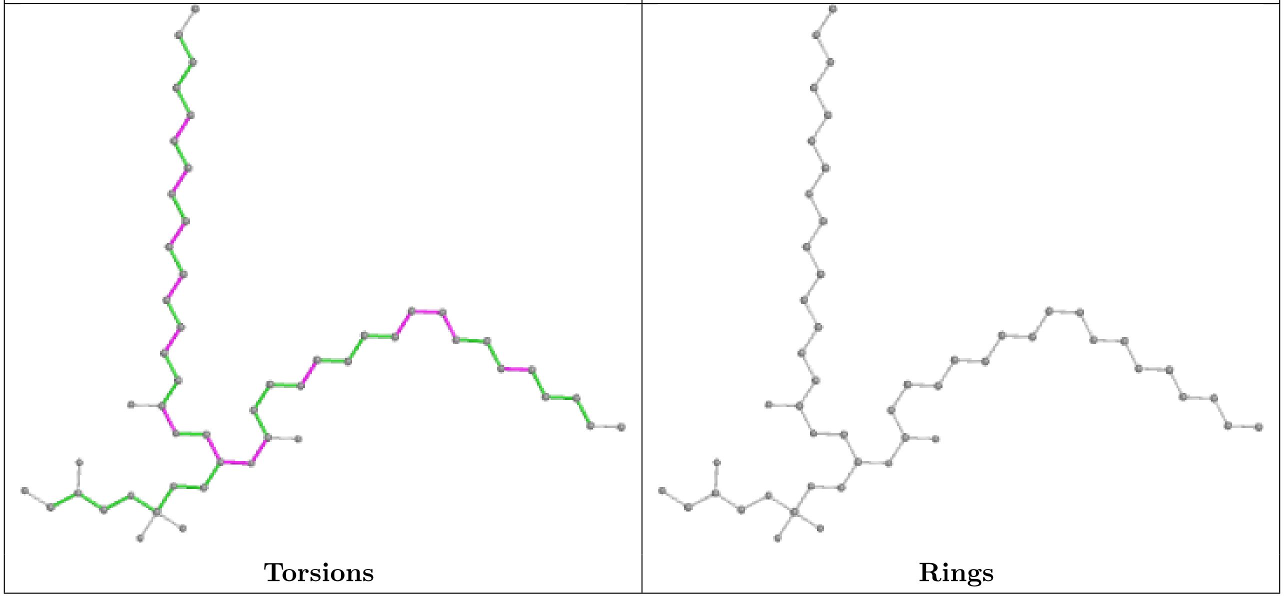
Rings

Ligand PGW 5I 101



Bond lengths

Bond angles



Torsions

Rings

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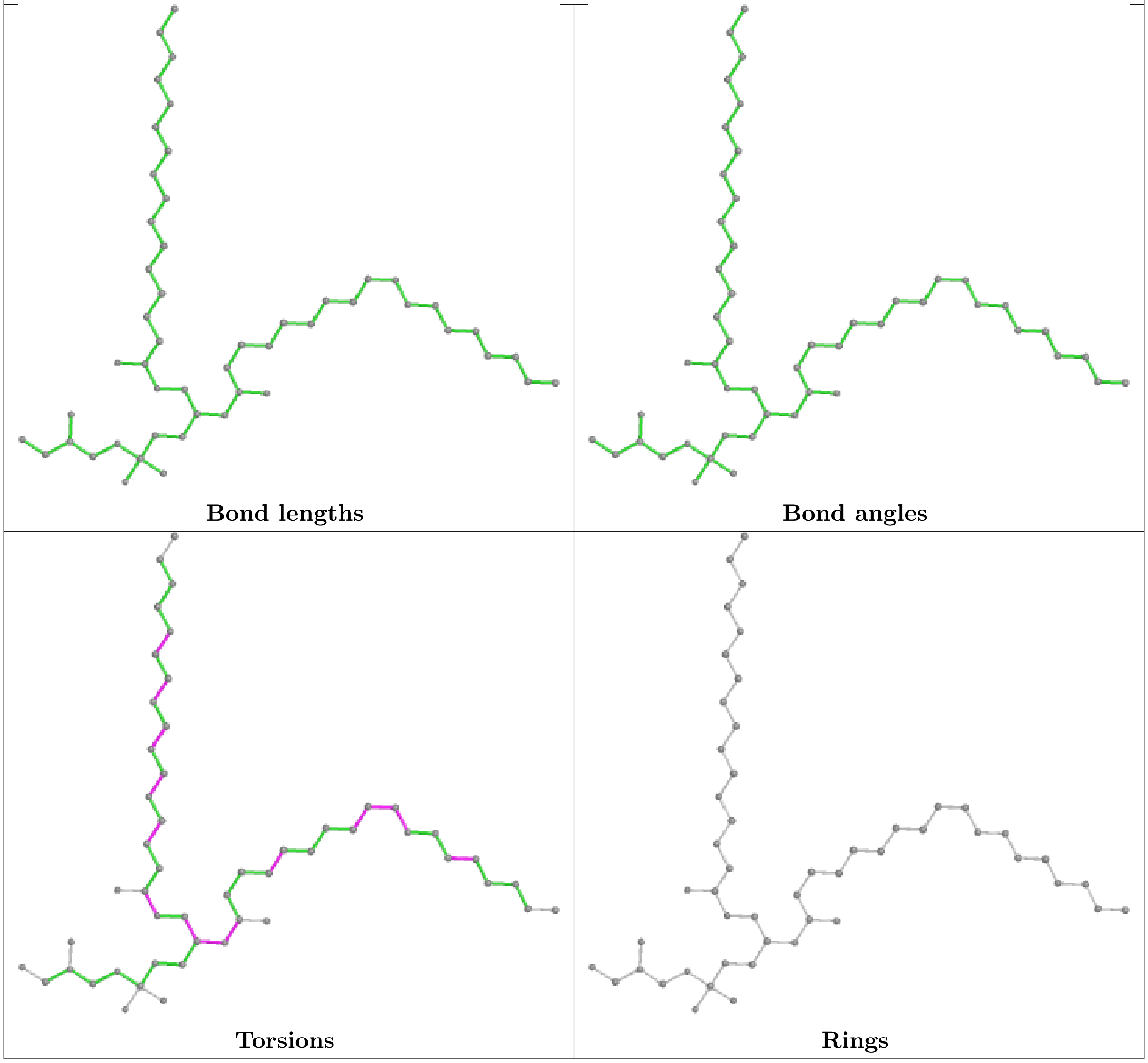

Bond lengths

Bond angles

Torsions

Rings

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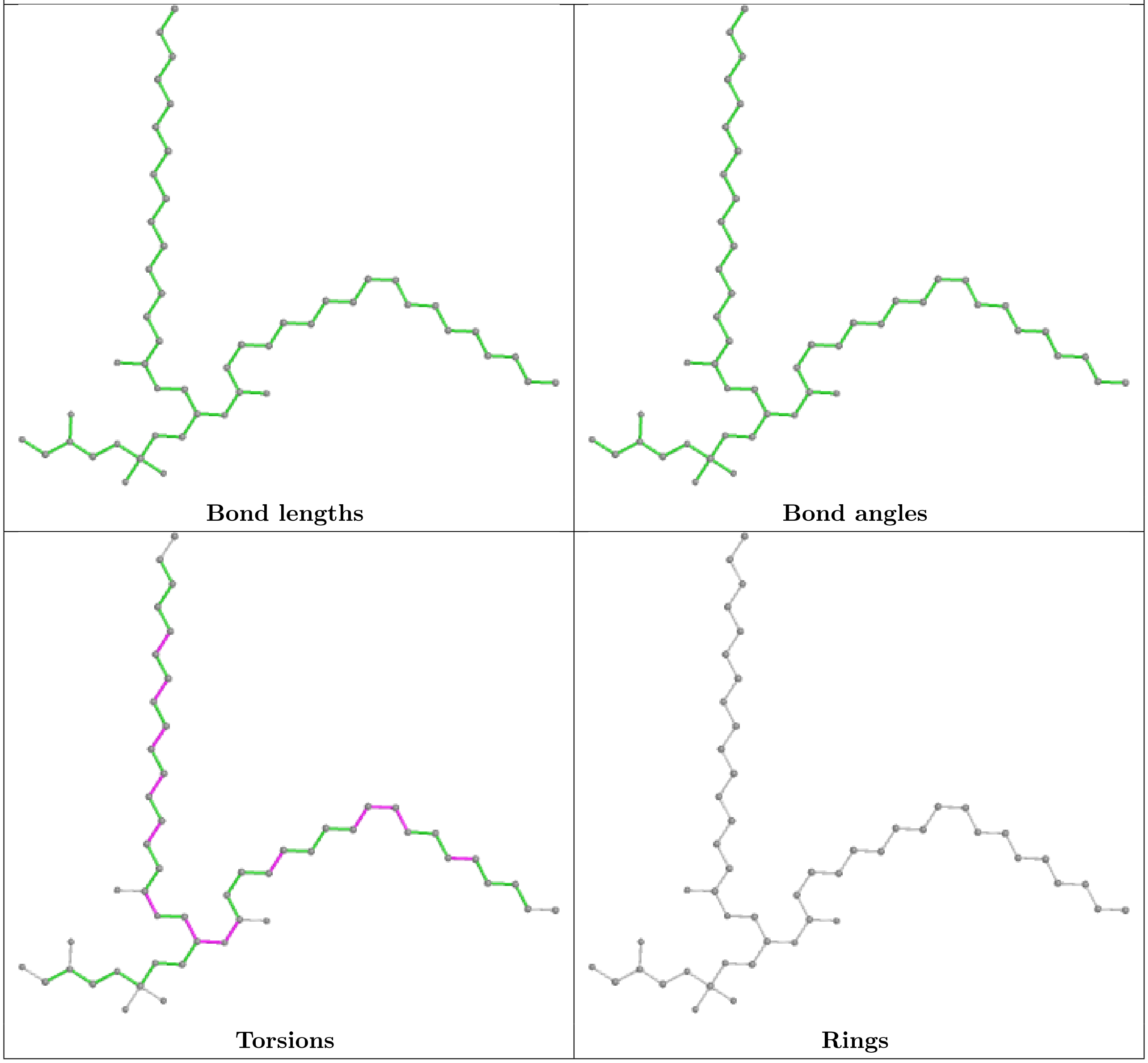


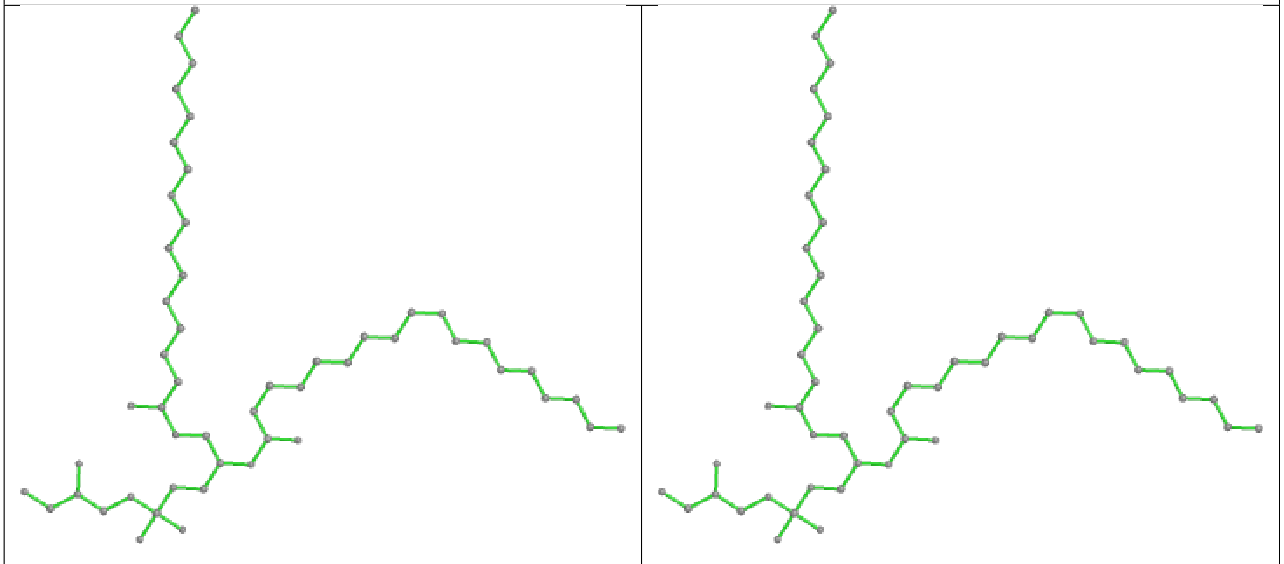
Bond lengths

Bond angles

Torsions

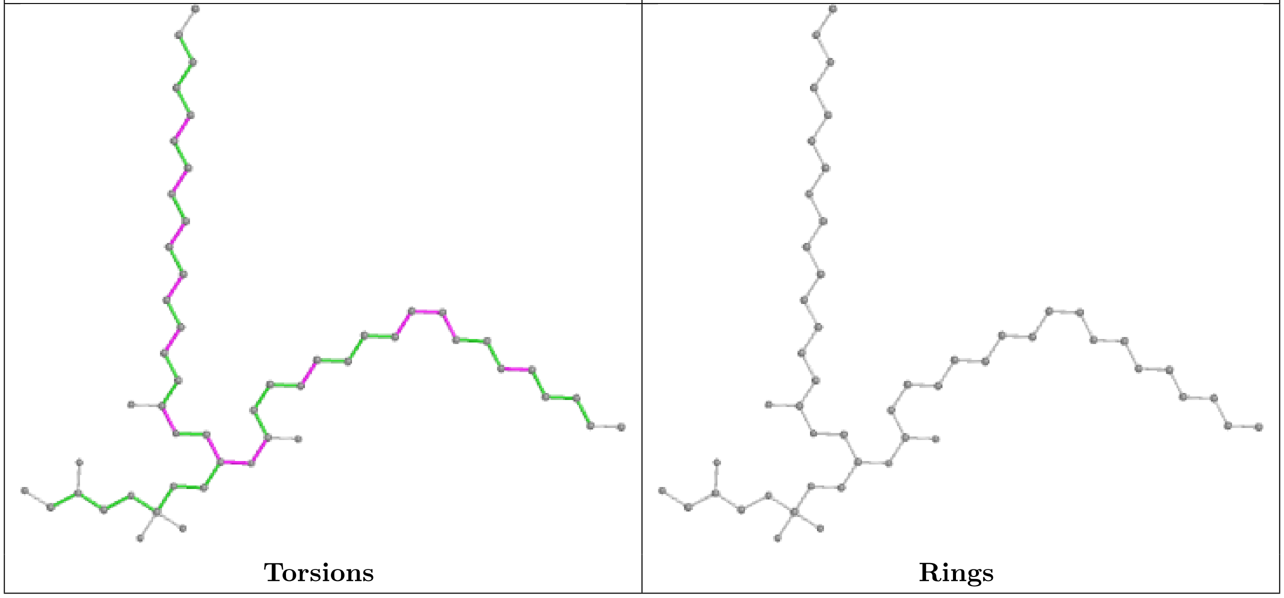
Rings

Ligand PGW 3C 101



Bond lengths

Bond angles



Torsions

Rings

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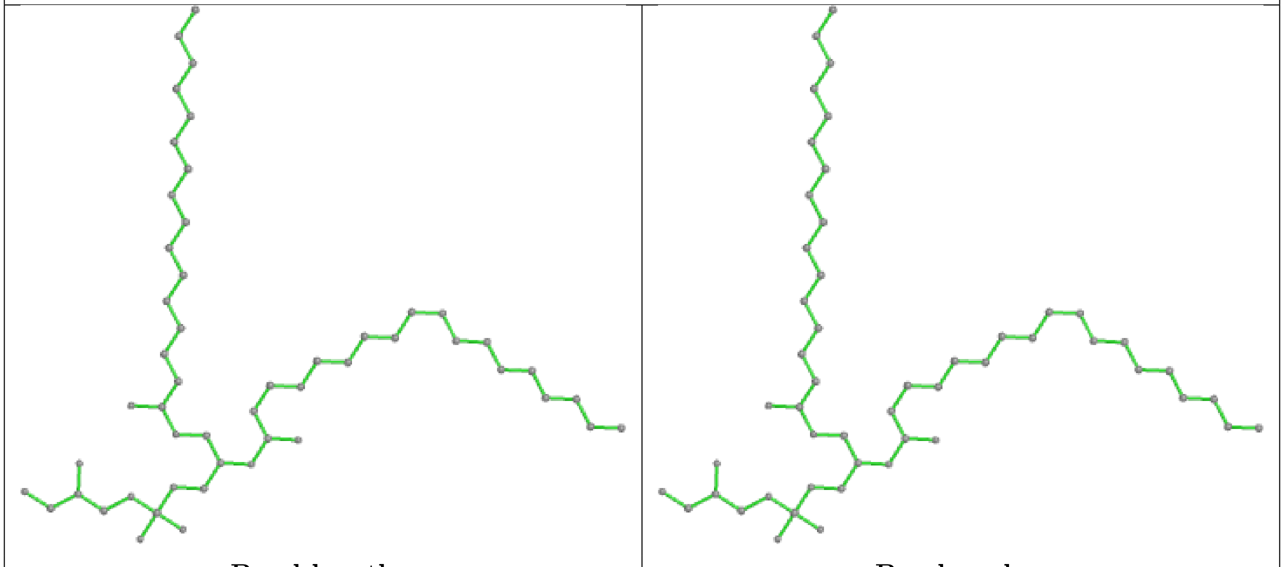
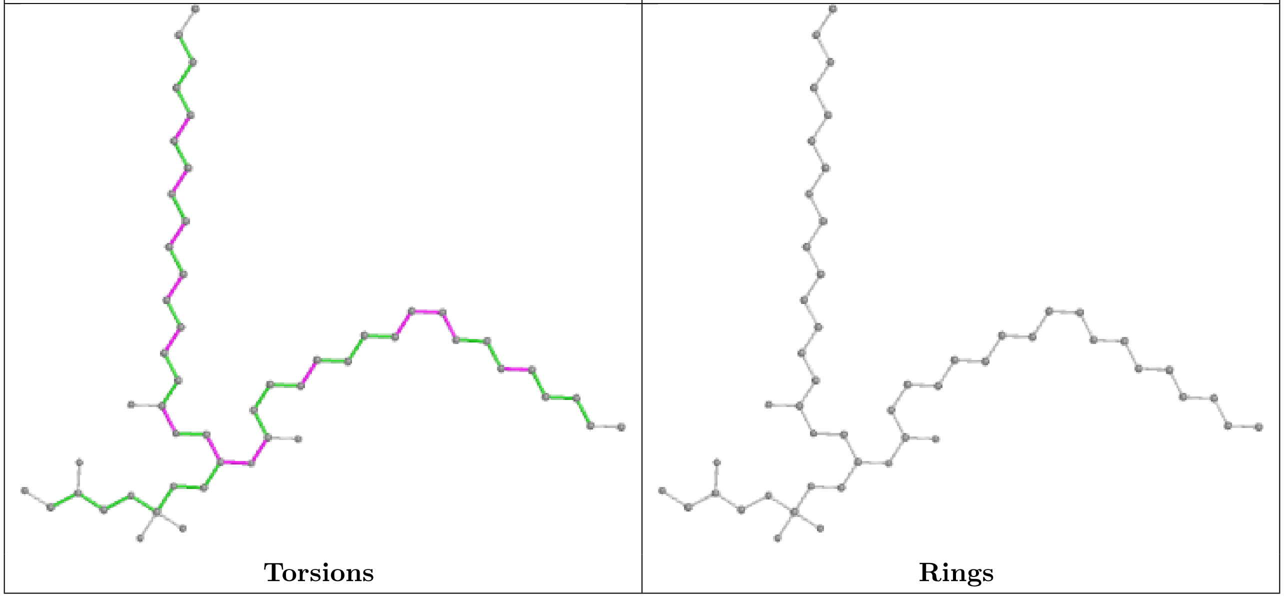


Bond lengths **Bond angles**



Torsions **Rings**

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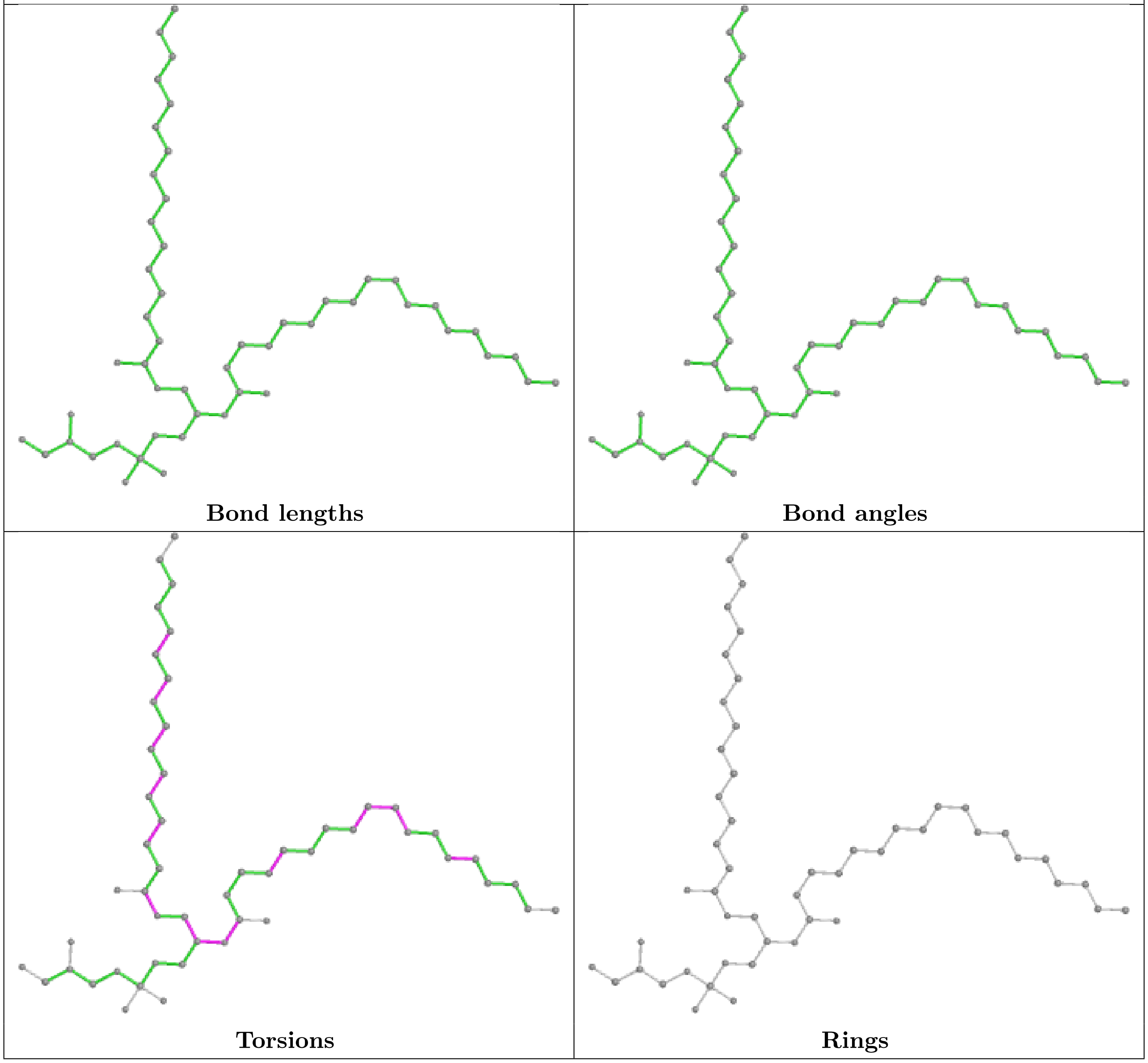

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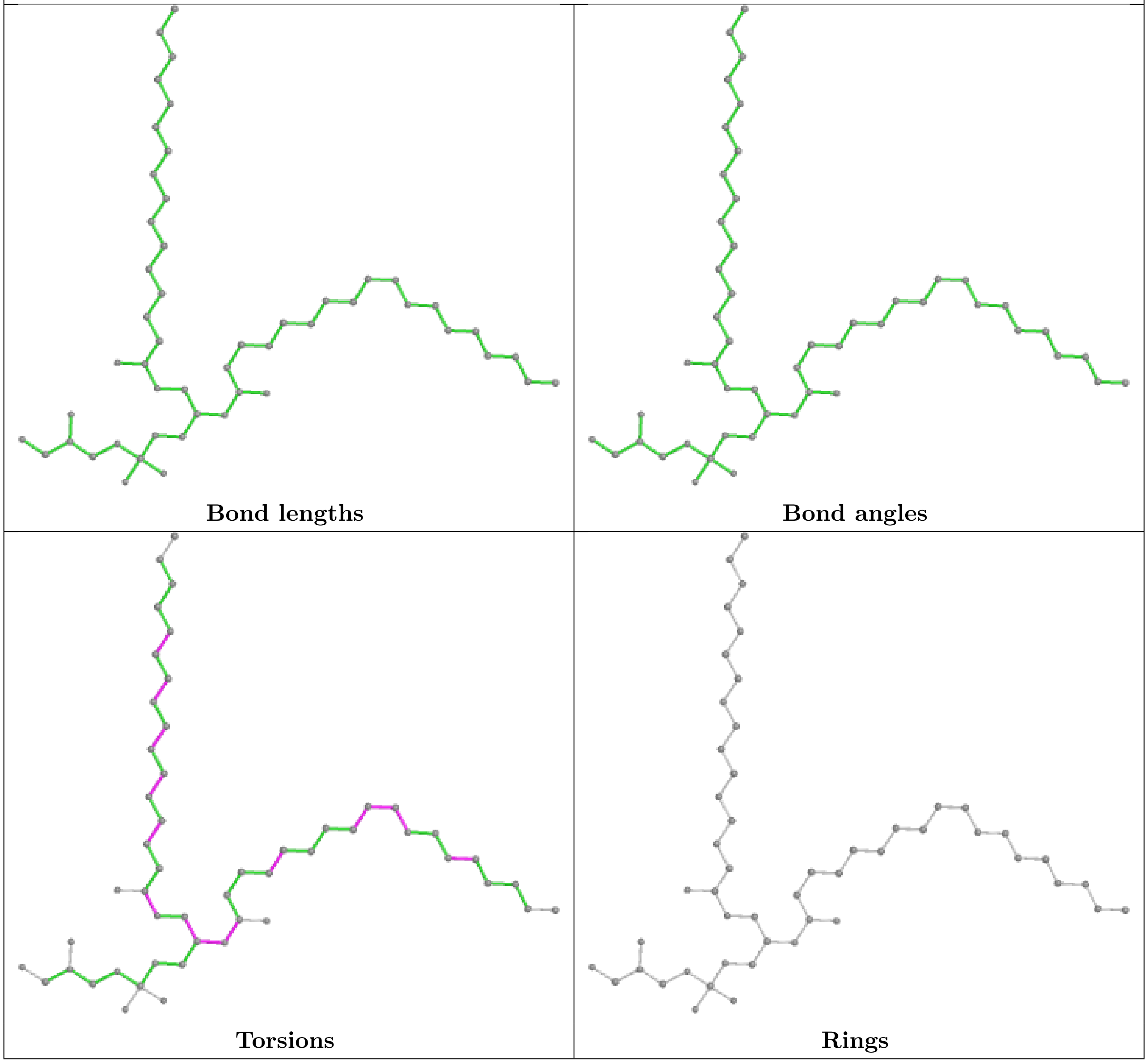


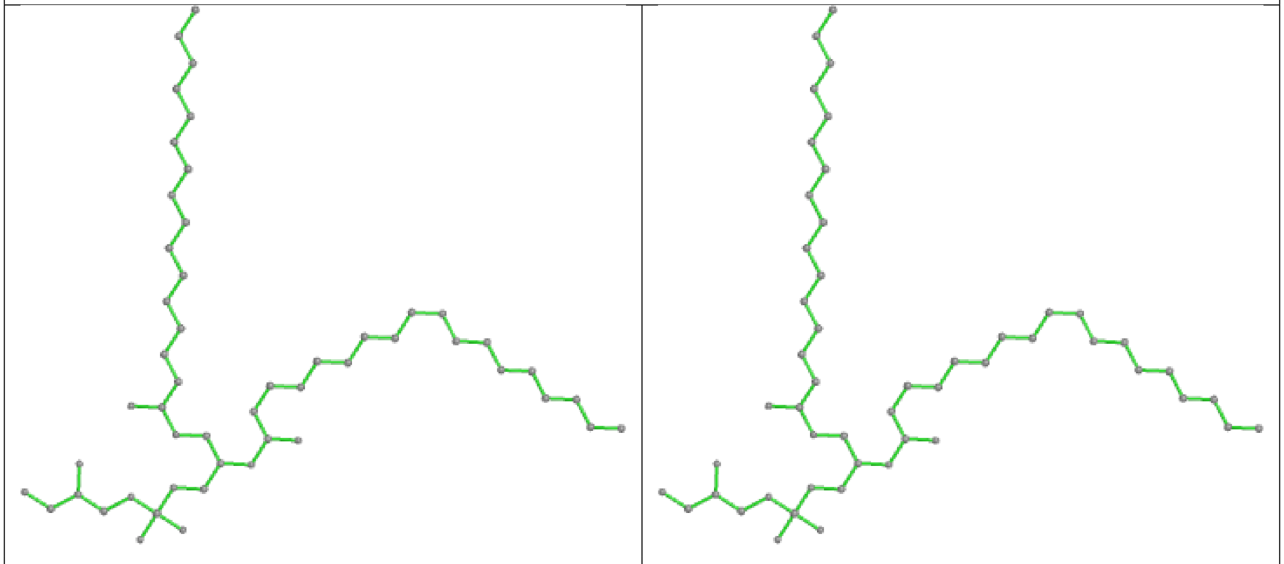
Bond lengths

Bond angles

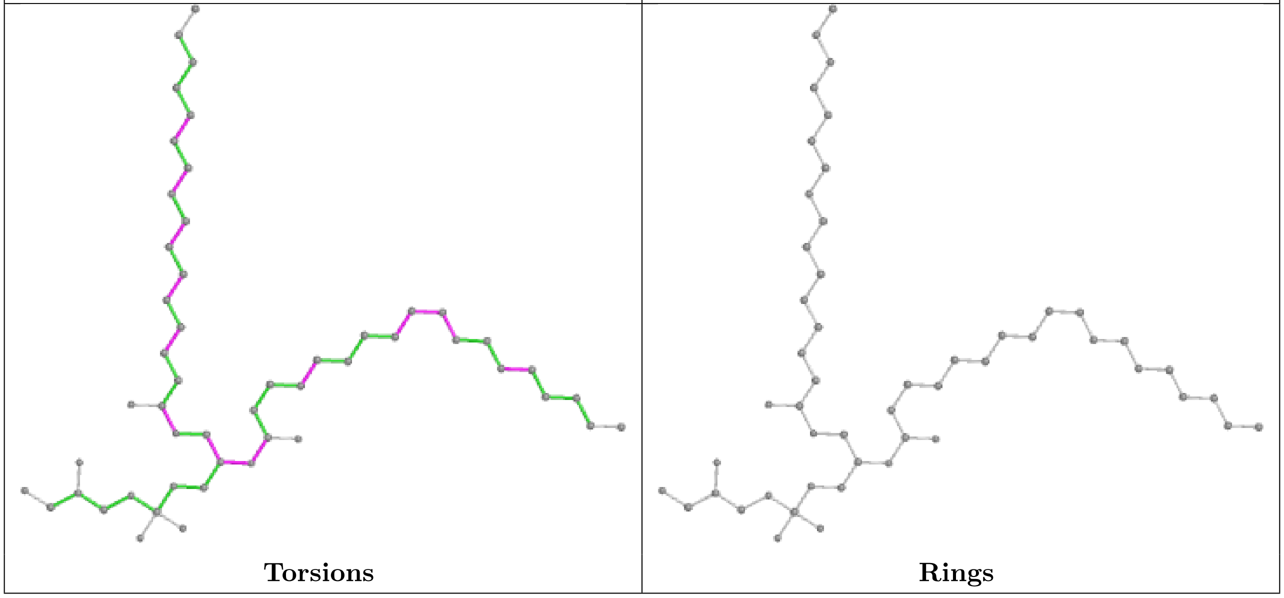
Torsions

Rings

Ligand PGW 4L 101



Bond lengths Bond angles



Torsions Rings

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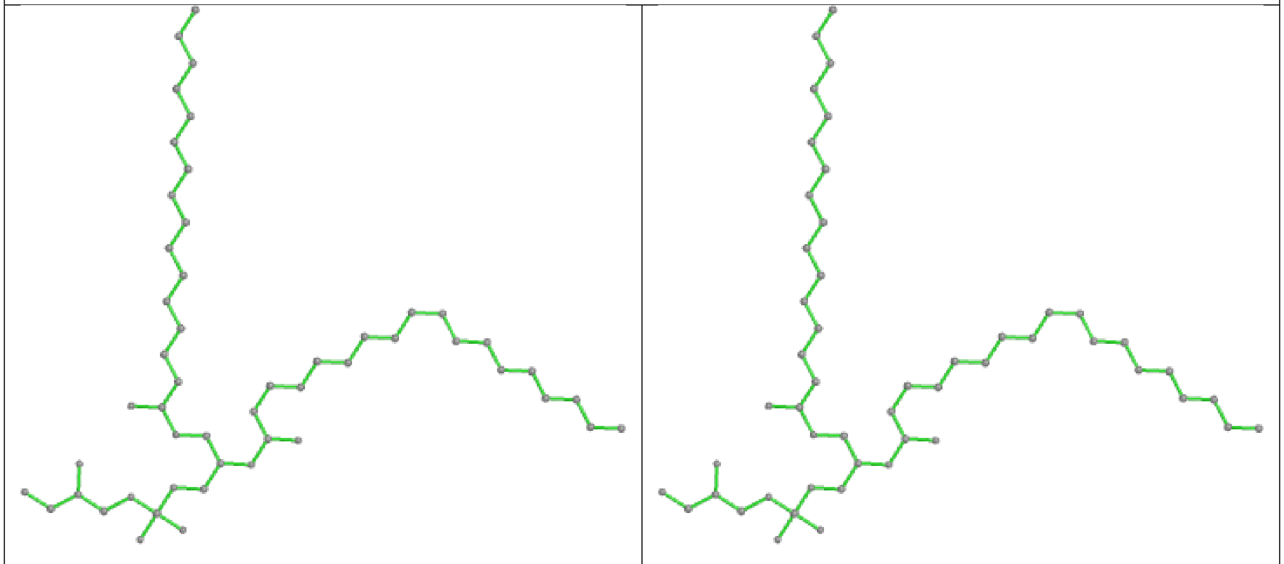
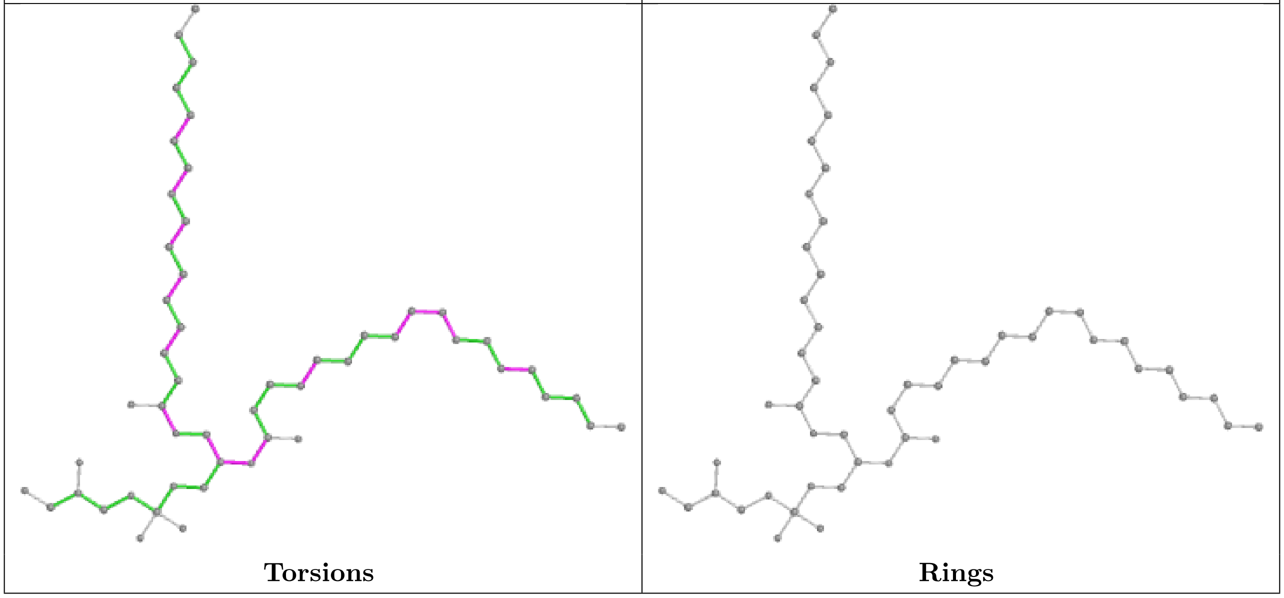
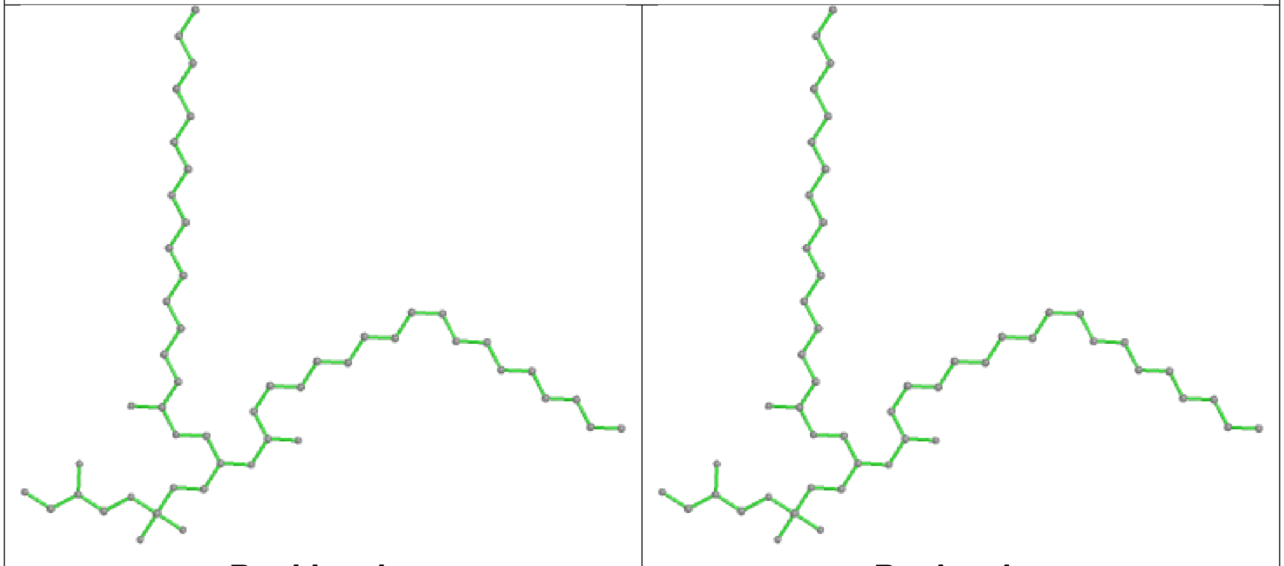


Bond lengths **Bond angles**



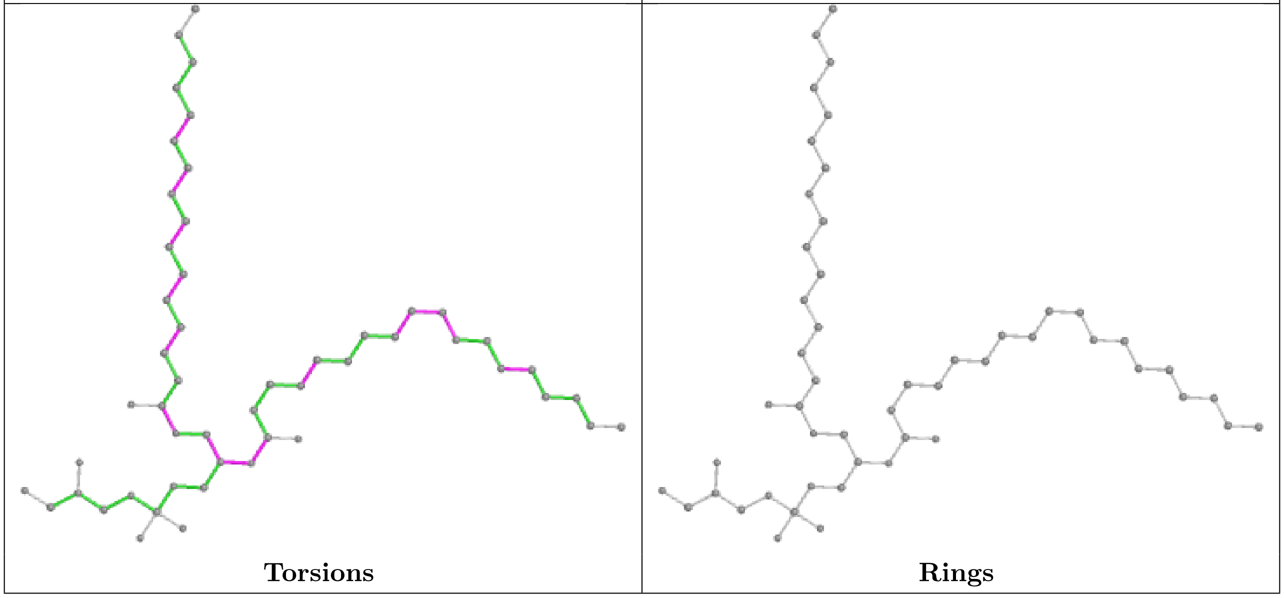
Torsions **Rings**

Ligand PGW 5N 101



Bond lengths

Bond angles



Torsions

Rings

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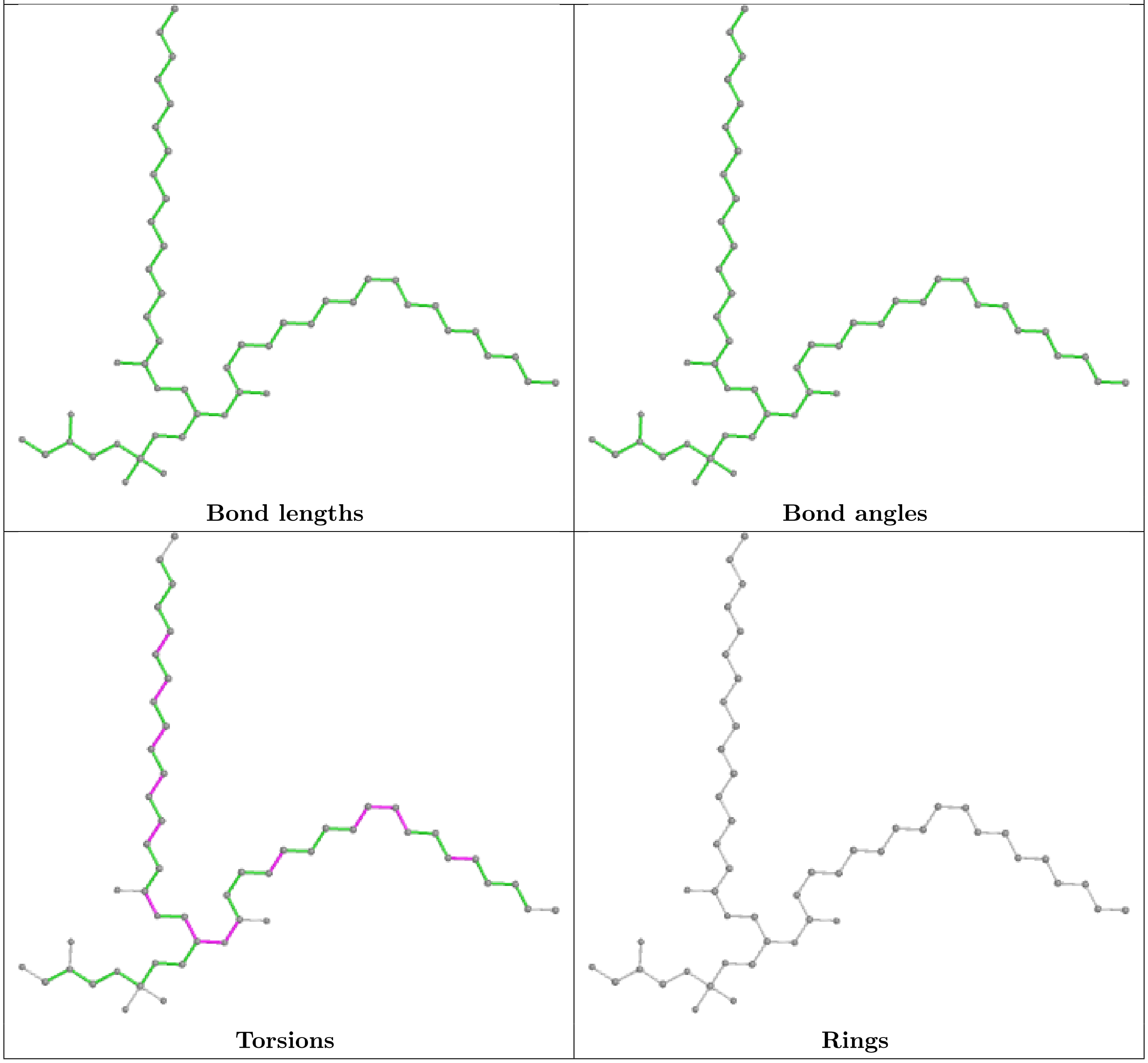


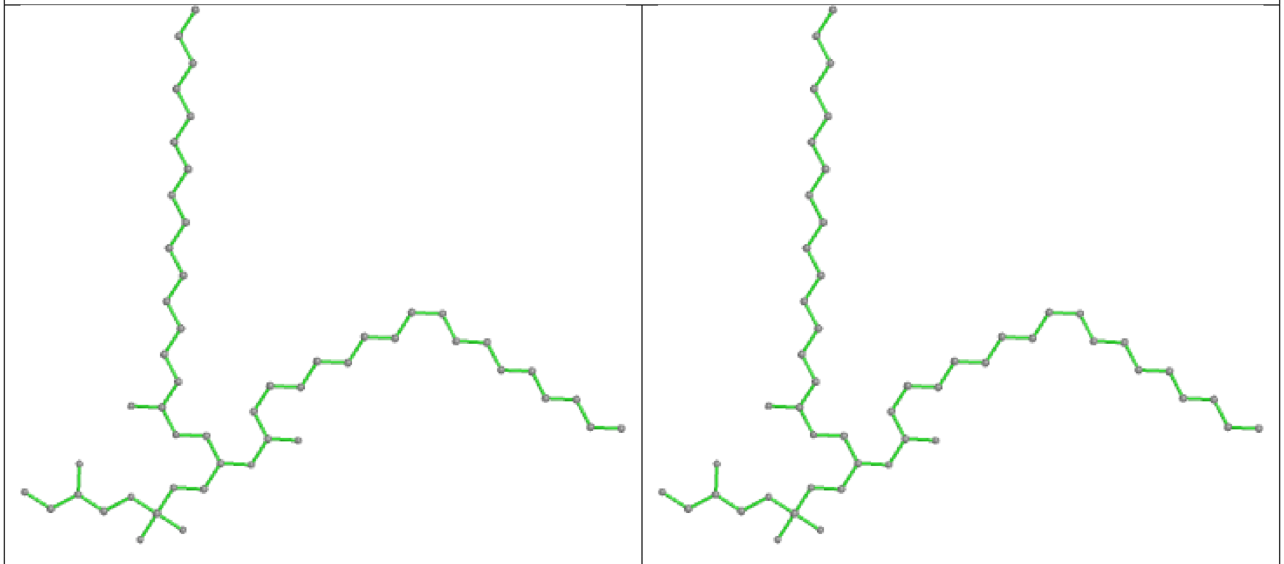
Bond lengths

Bond angles

Torsions

Rings

Ligand PGW 1E 101



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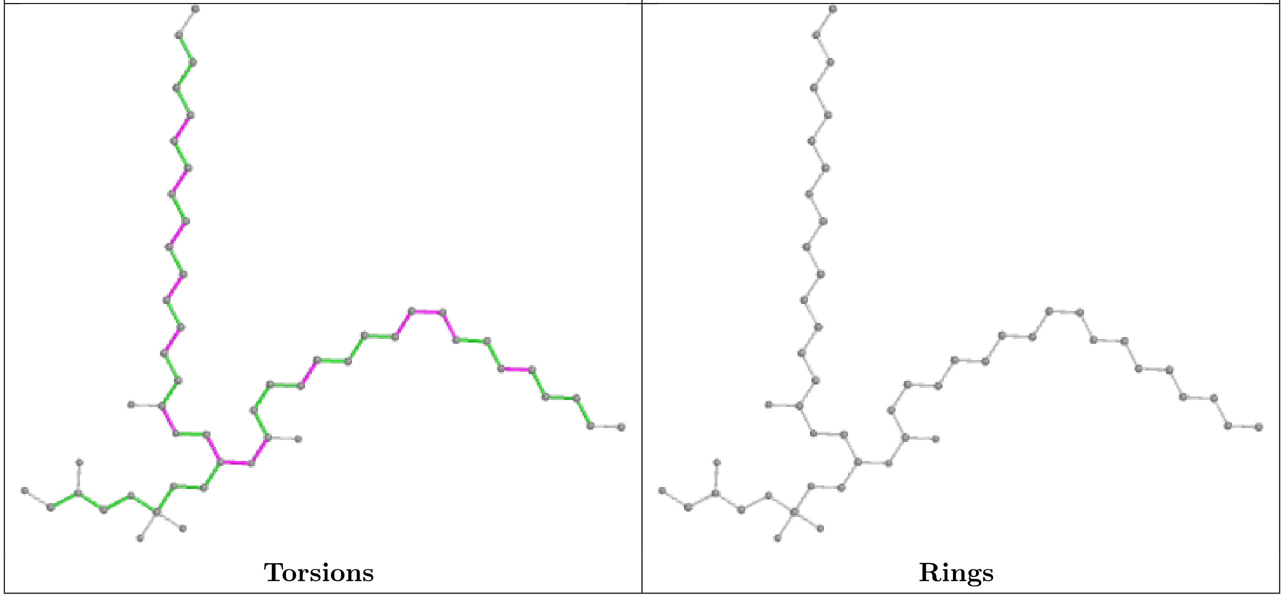
Bond angles



Torsions

Rings

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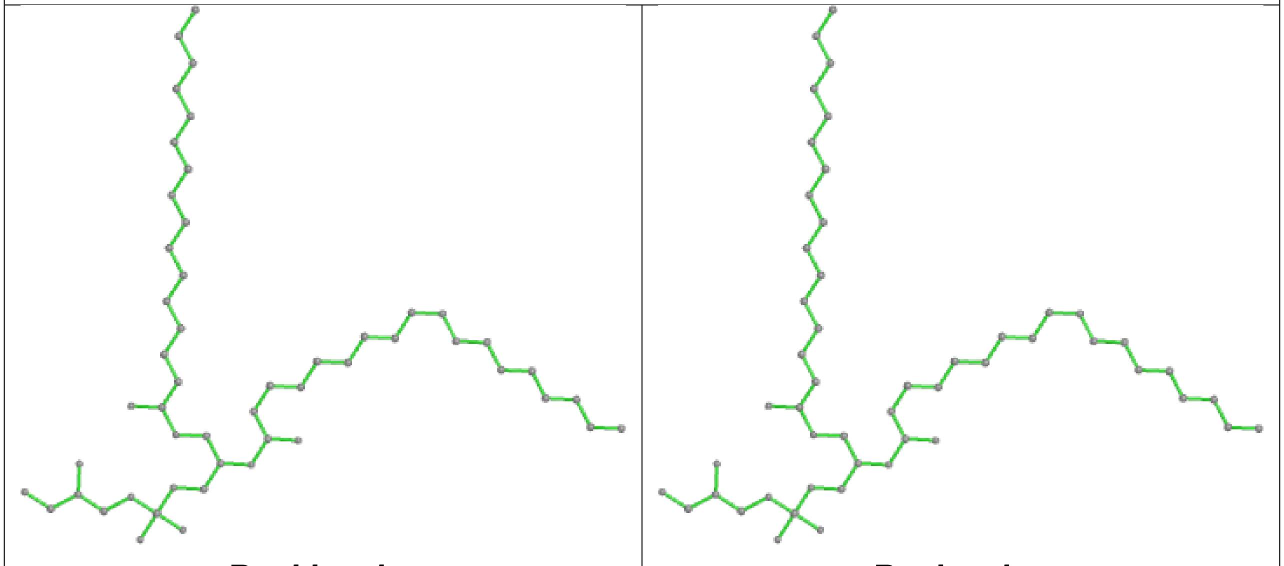
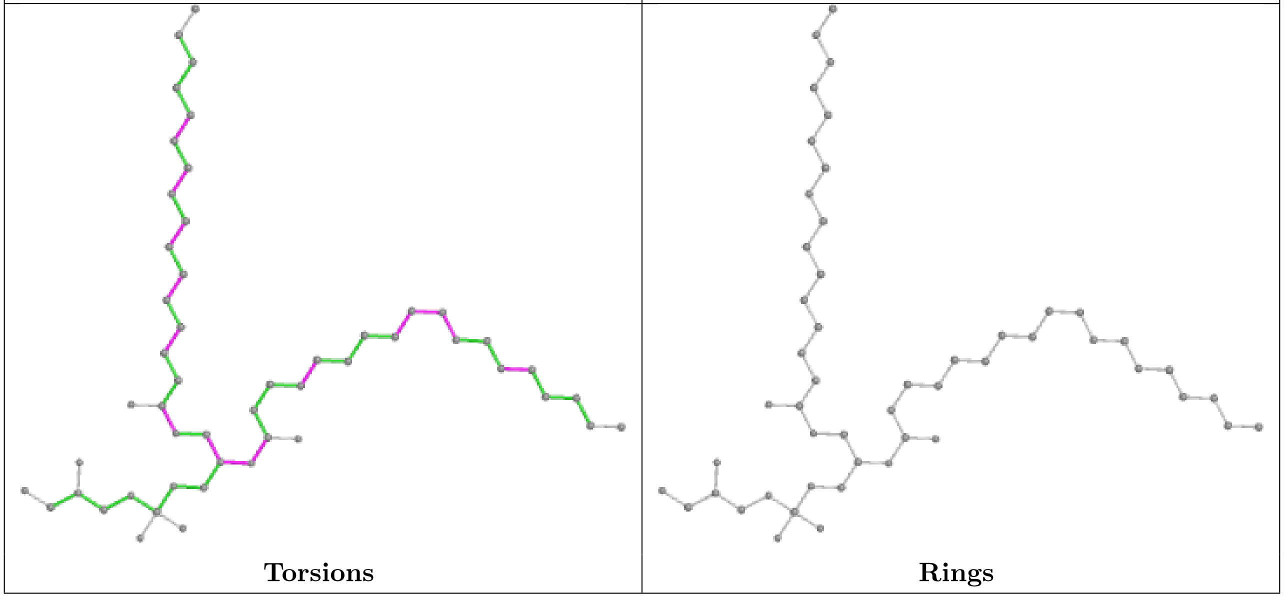


Bond lengths **Bond angles**



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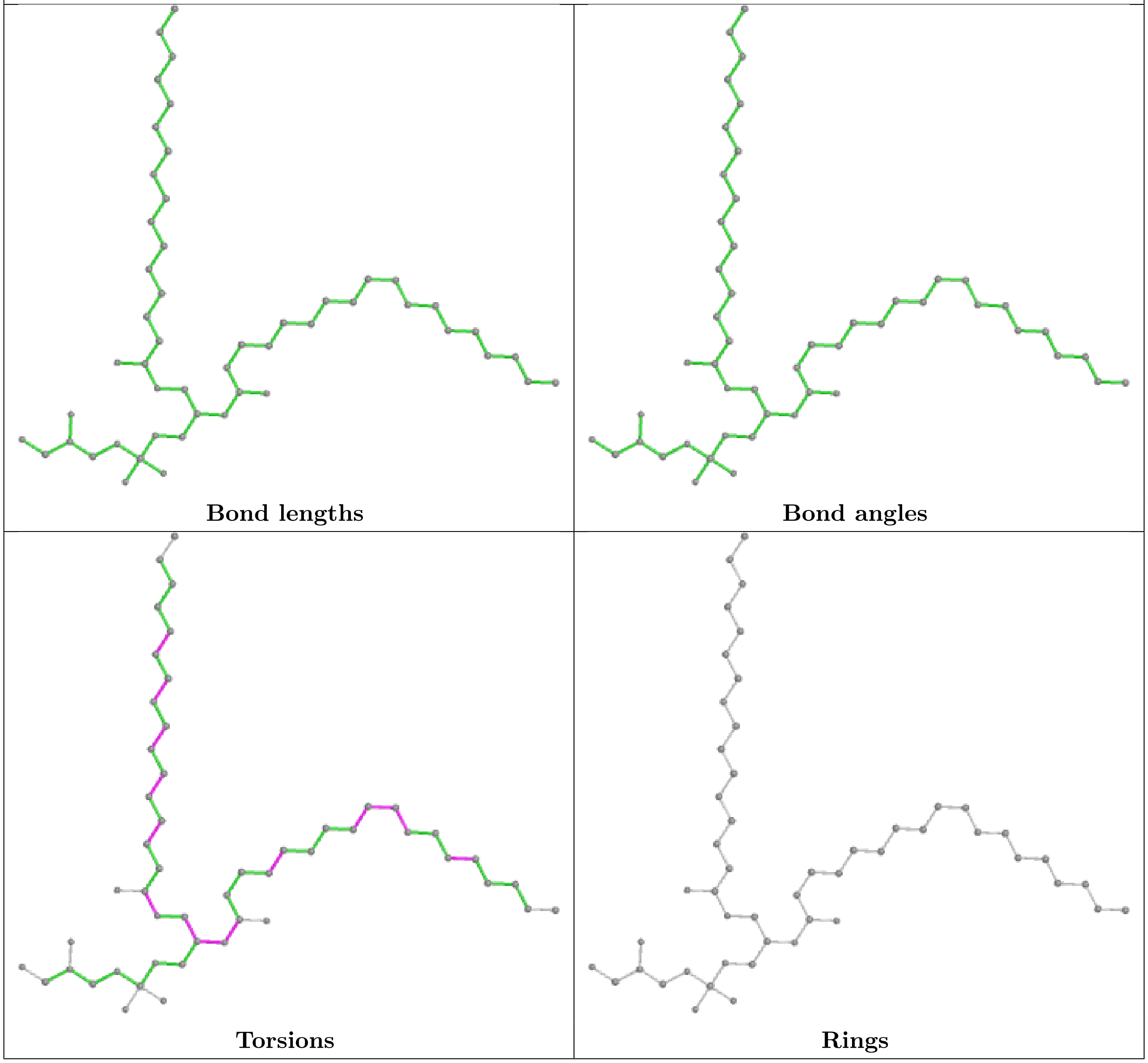

Bond lengths

Bond angles

Torsions

Rings

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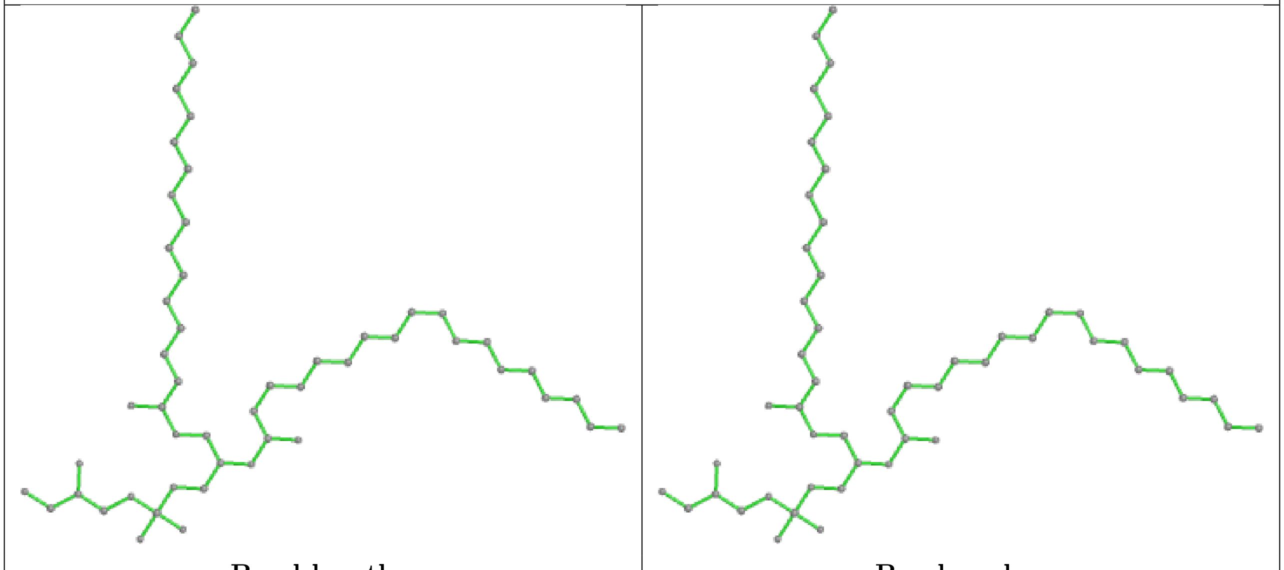
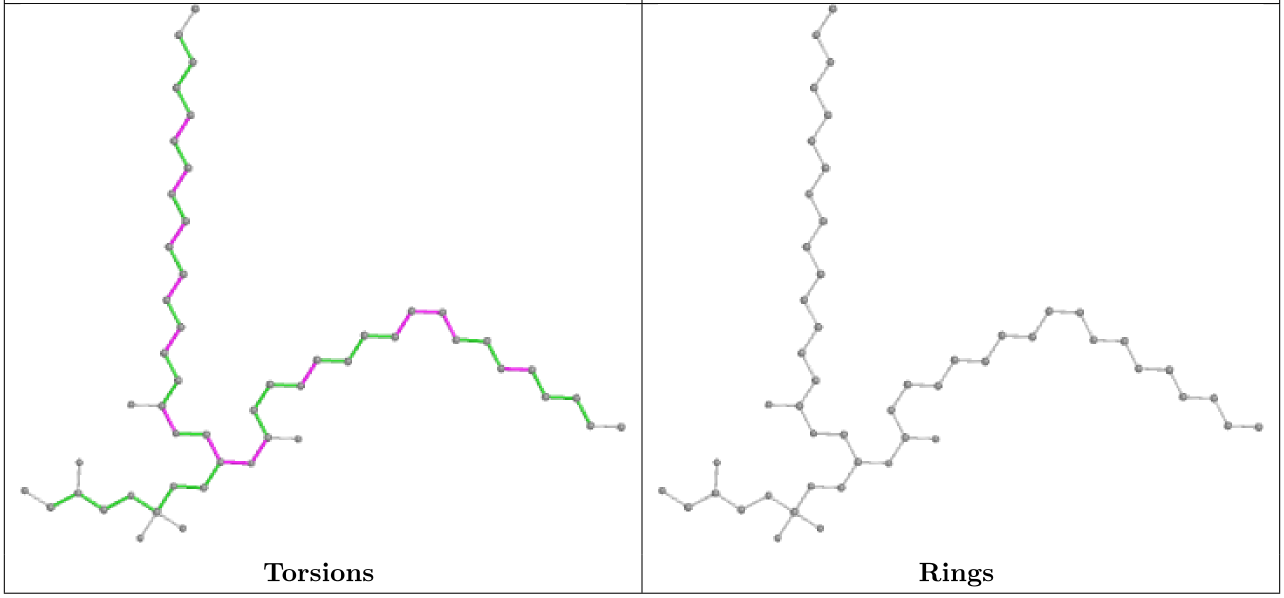
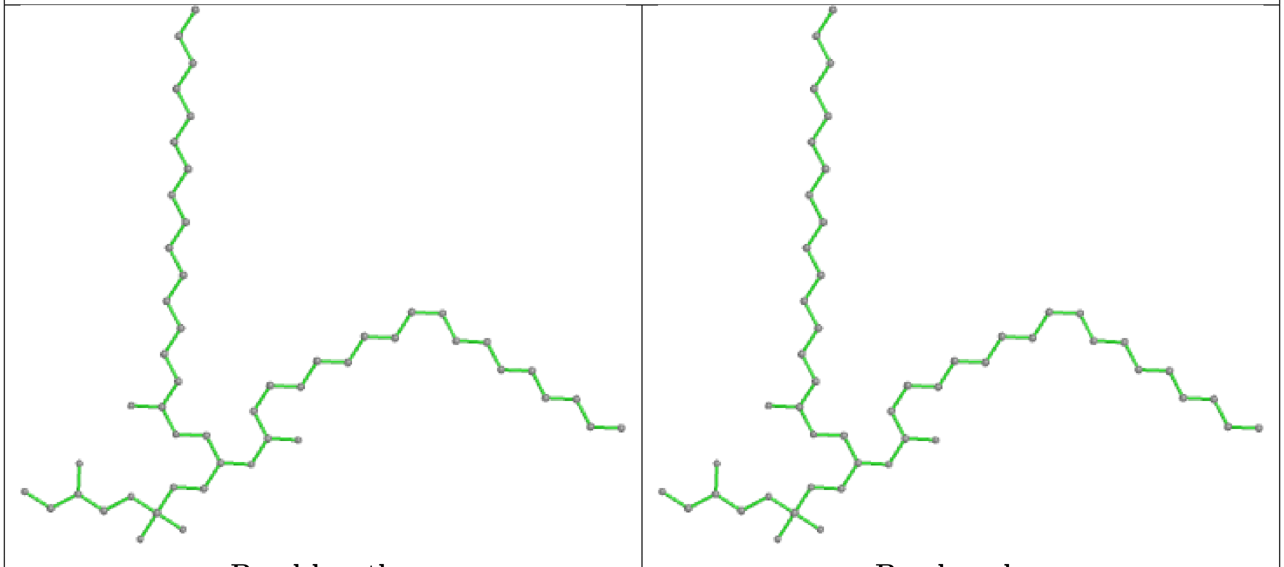


Bond lengths **Bond angles**



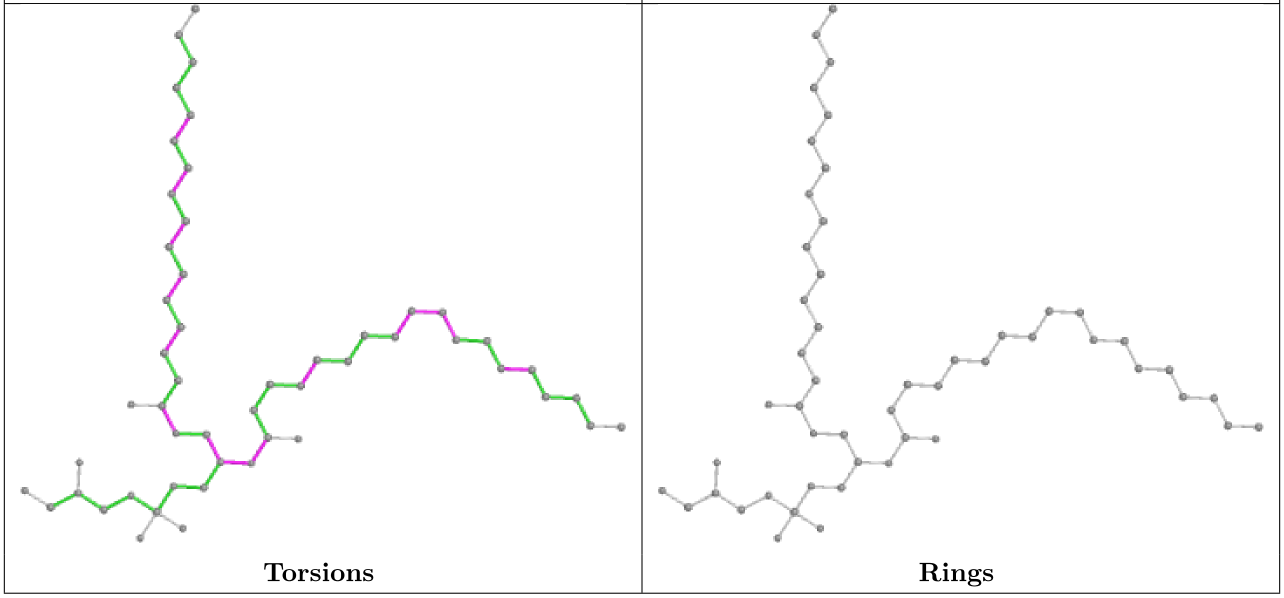
Torsions **Rings**

Ligand PGW 3G 101



Bond lengths

Bond angles



Torsions

Rings

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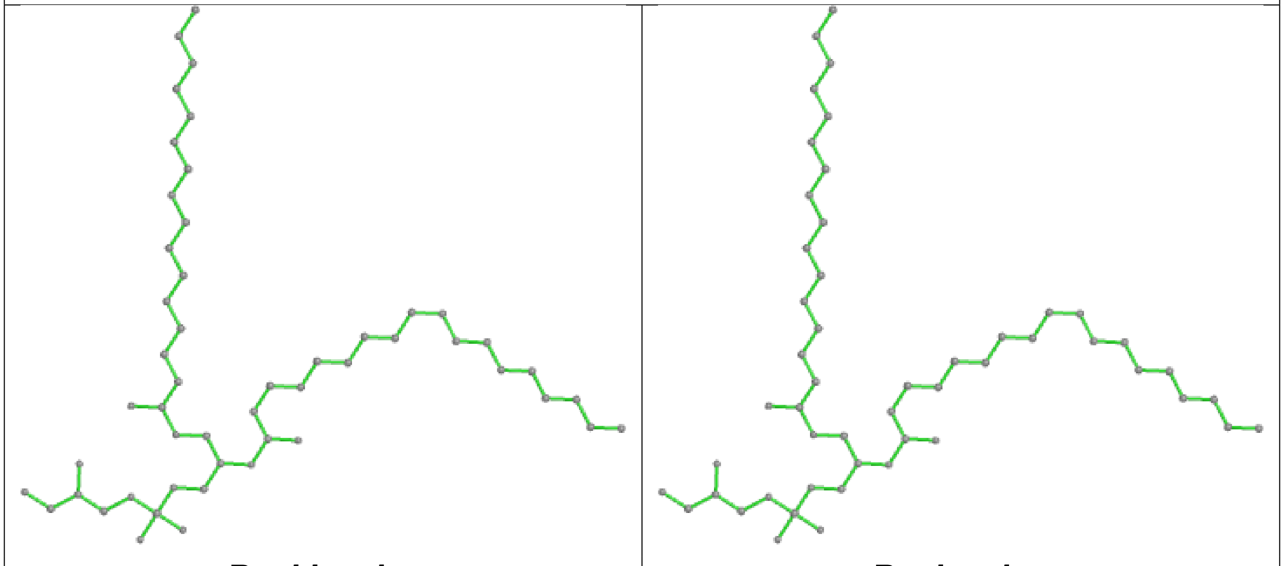
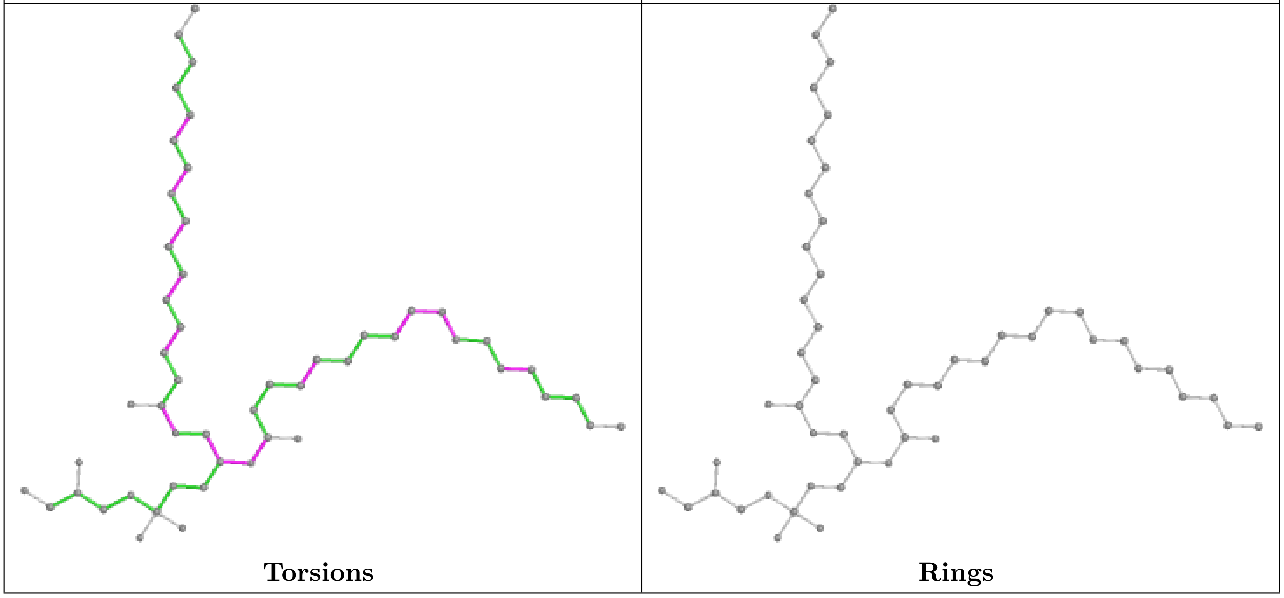


Bond lengths

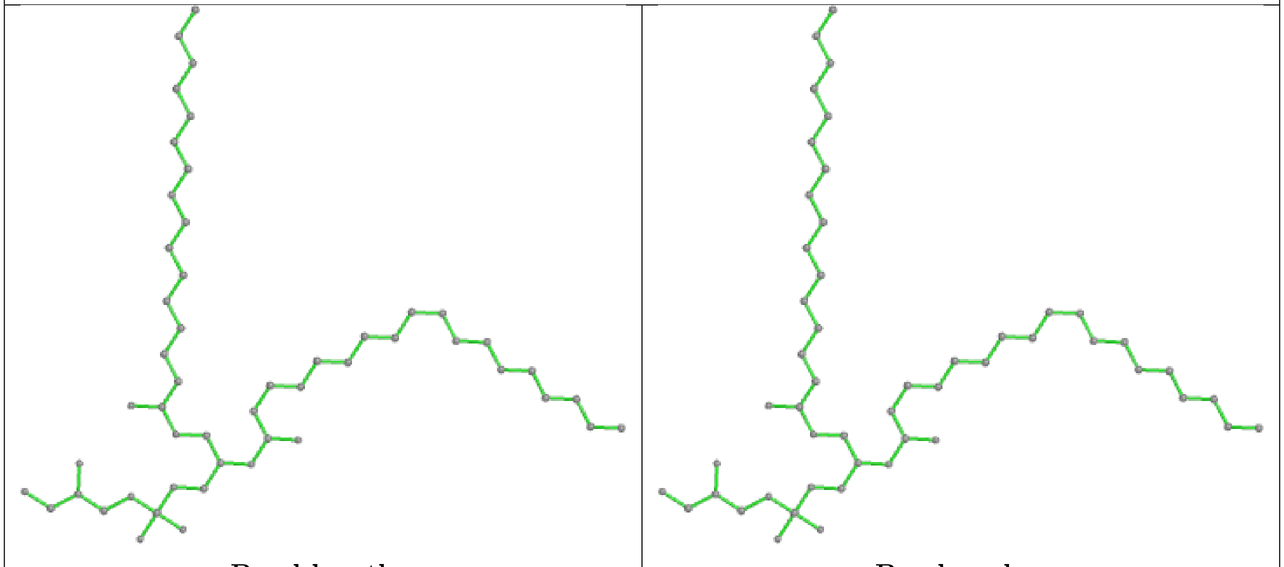
Bond angles



Torsions

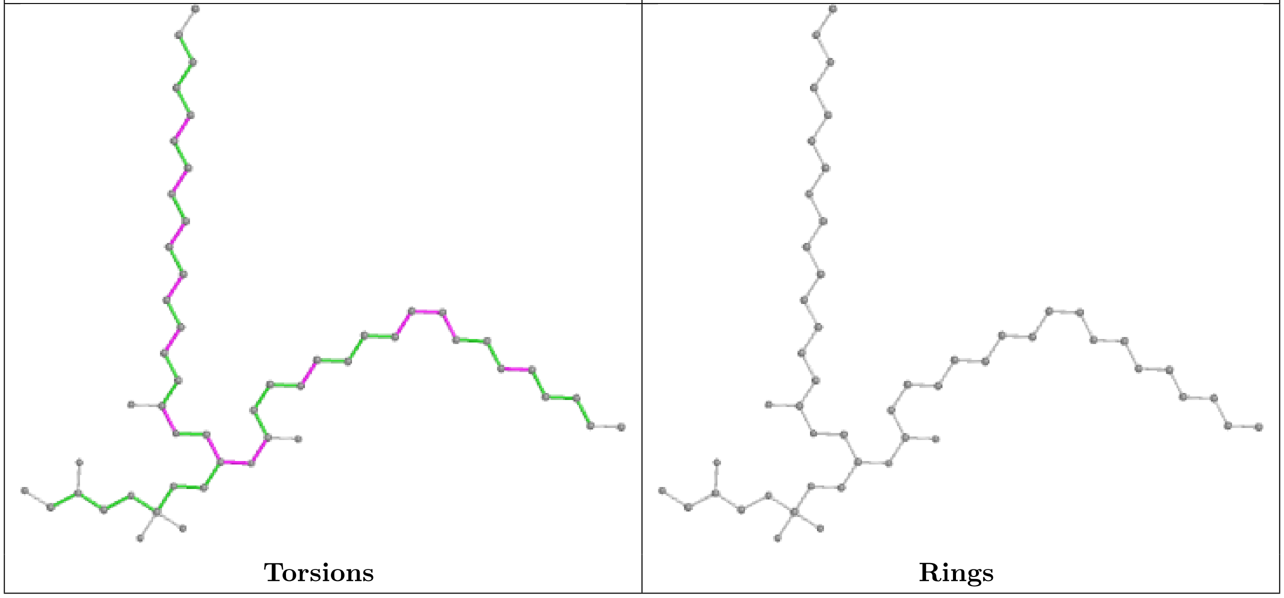
Rings

Ligand PGW 5M 101



Bond lengths

Bond angles



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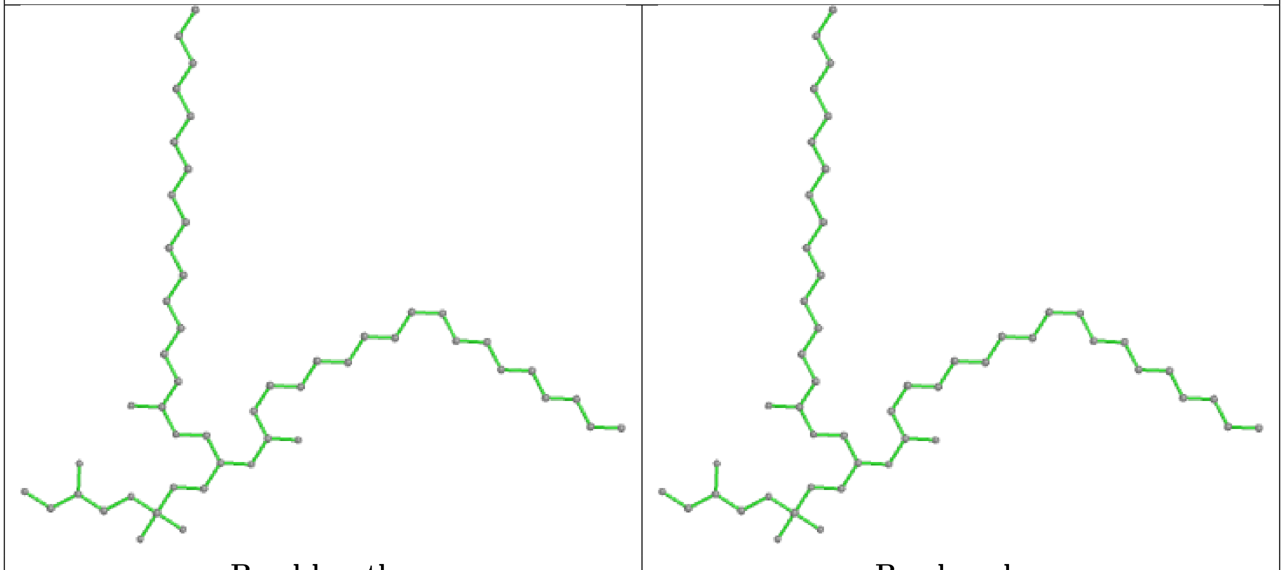
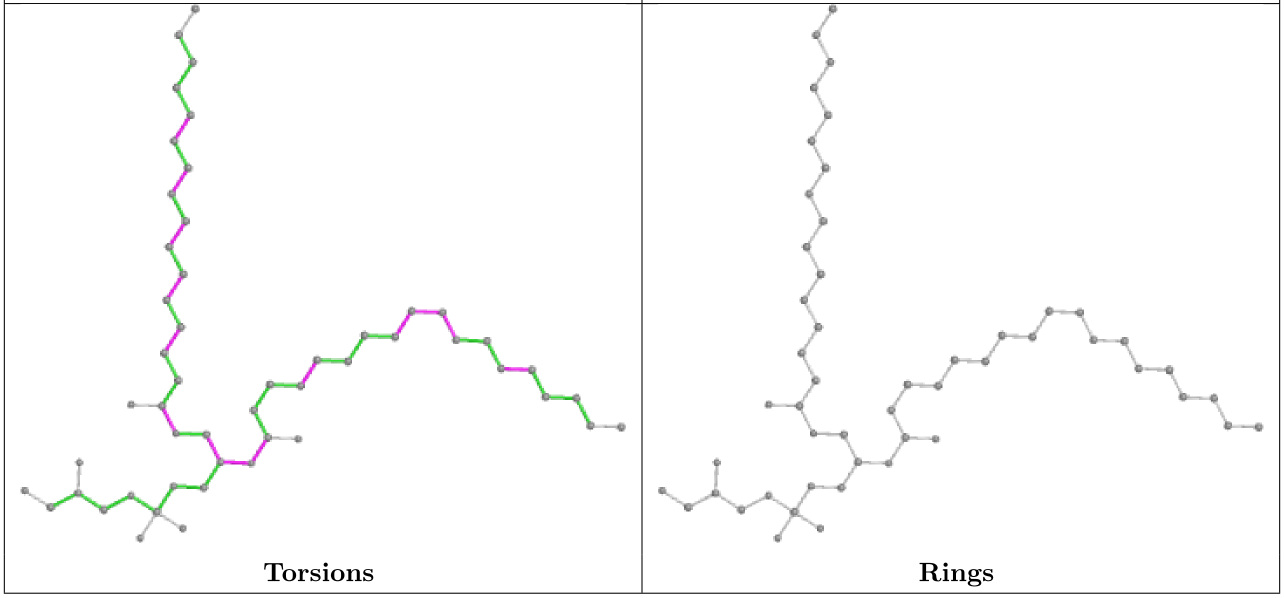


Bond lengths **Bond angles**



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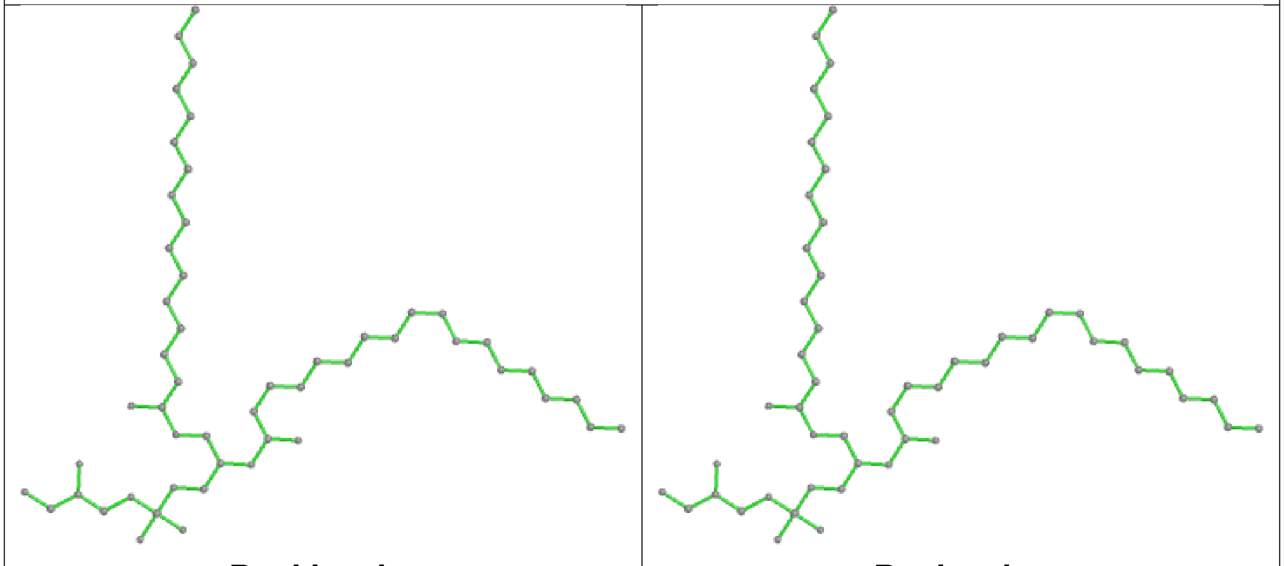
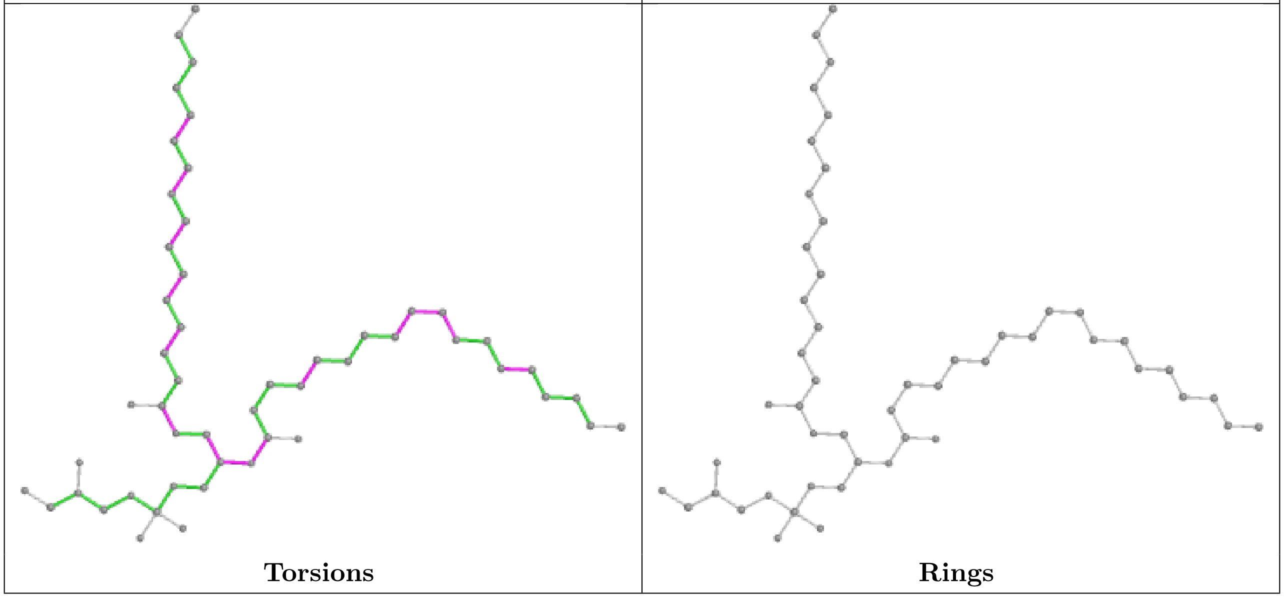


Bond lengths

Bond angles



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Rings

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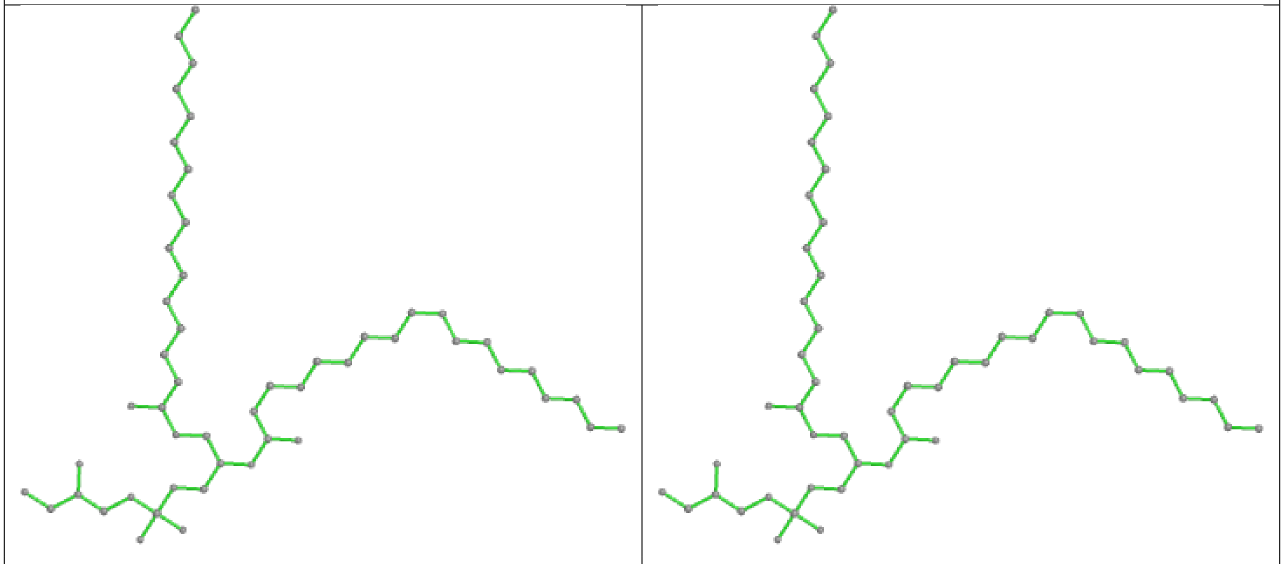
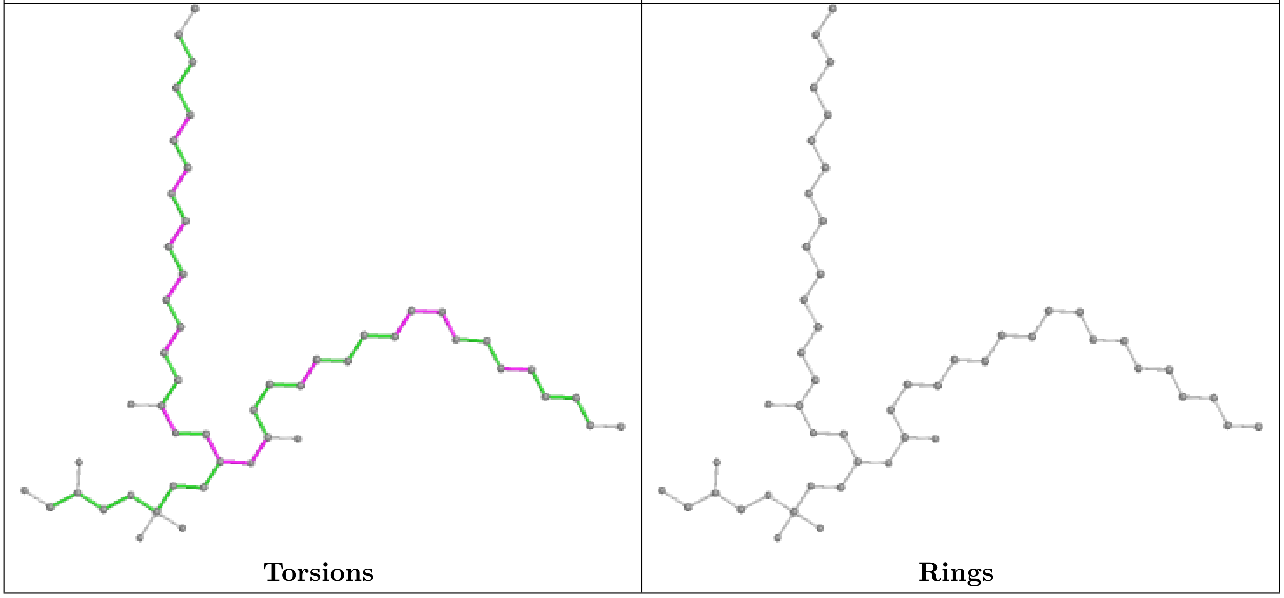


Bond lengths **Bond angles**



Torsions **Rings**

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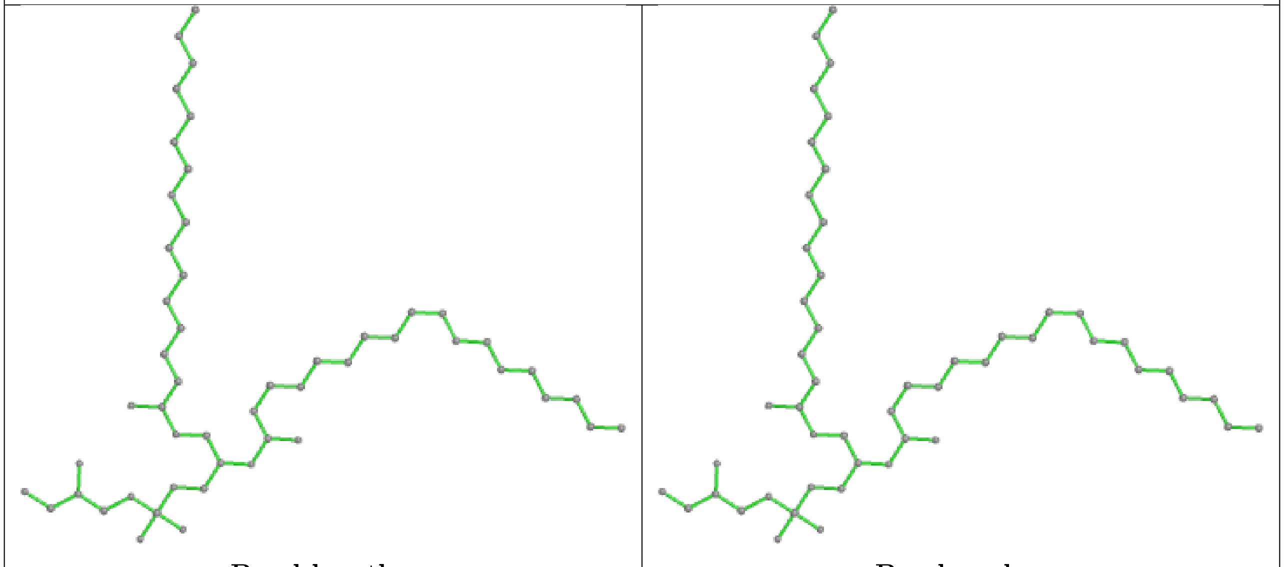
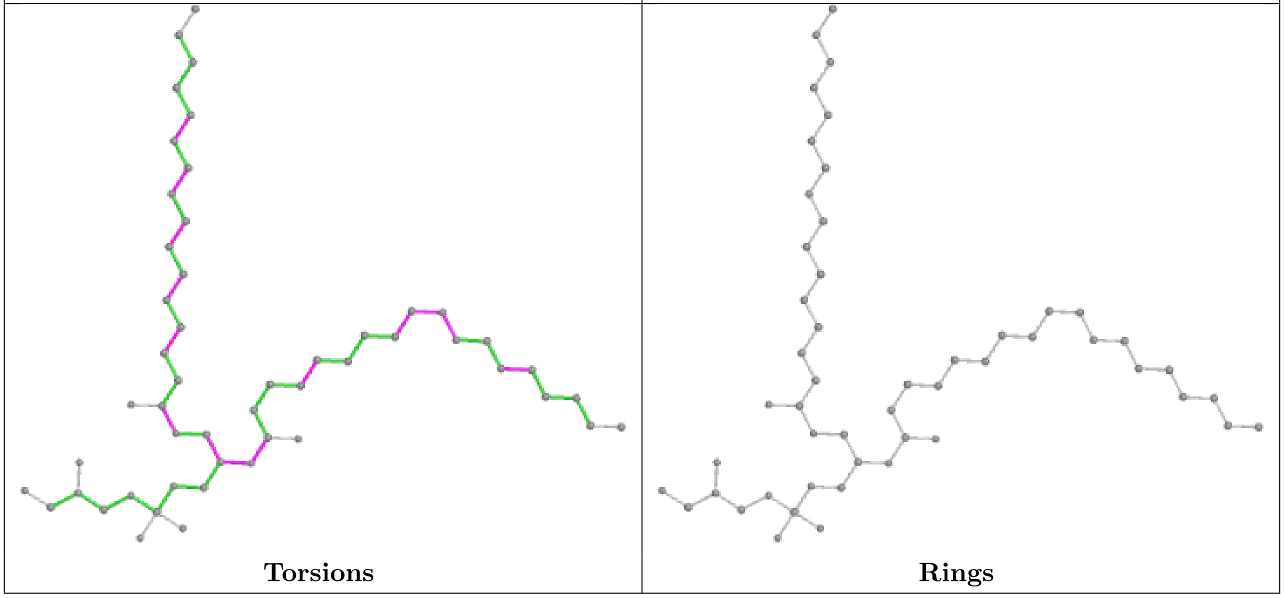
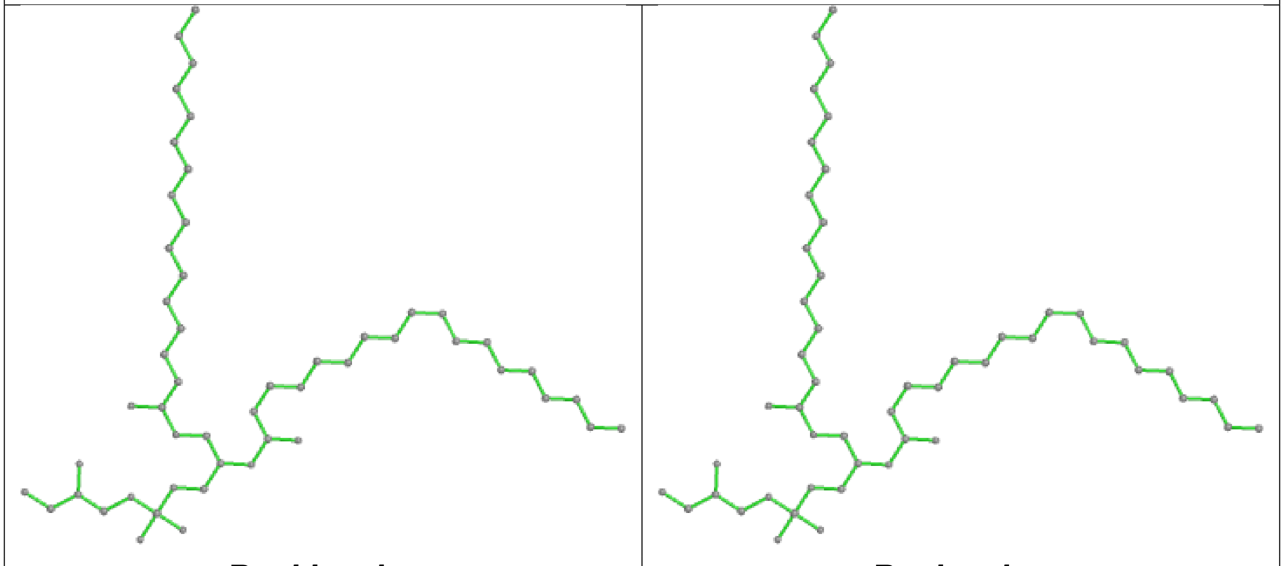


Bond lengths **Bond angles**



Torsions **Rings**

Ligand PGW 3H 101



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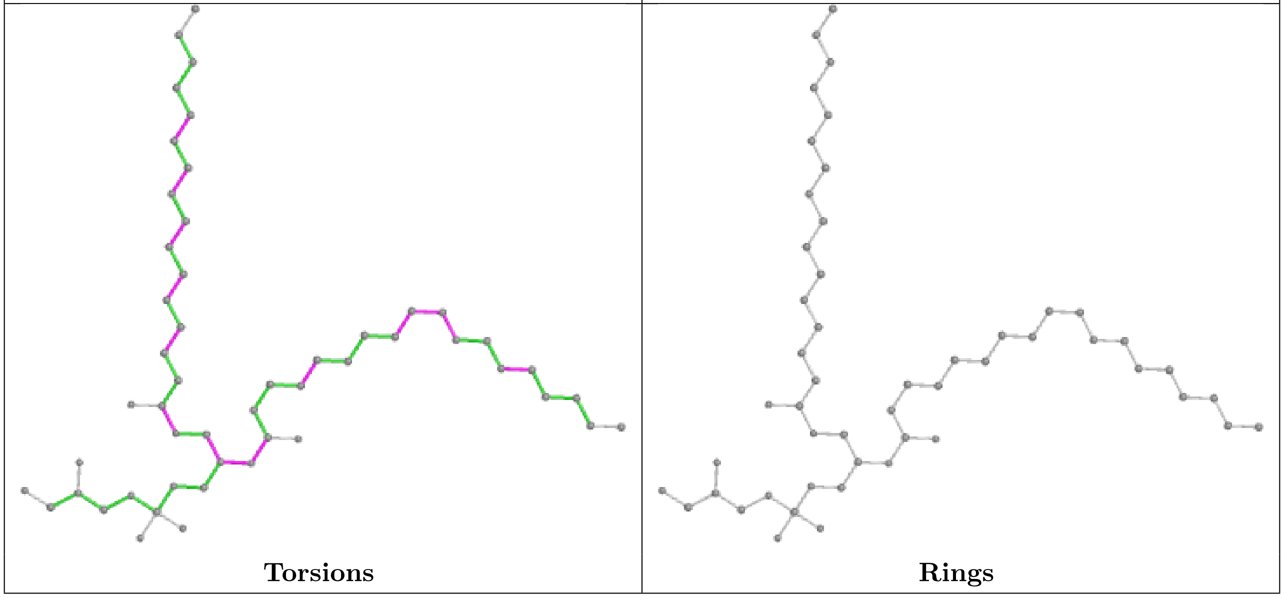
Bond angles



Torsions

Rings

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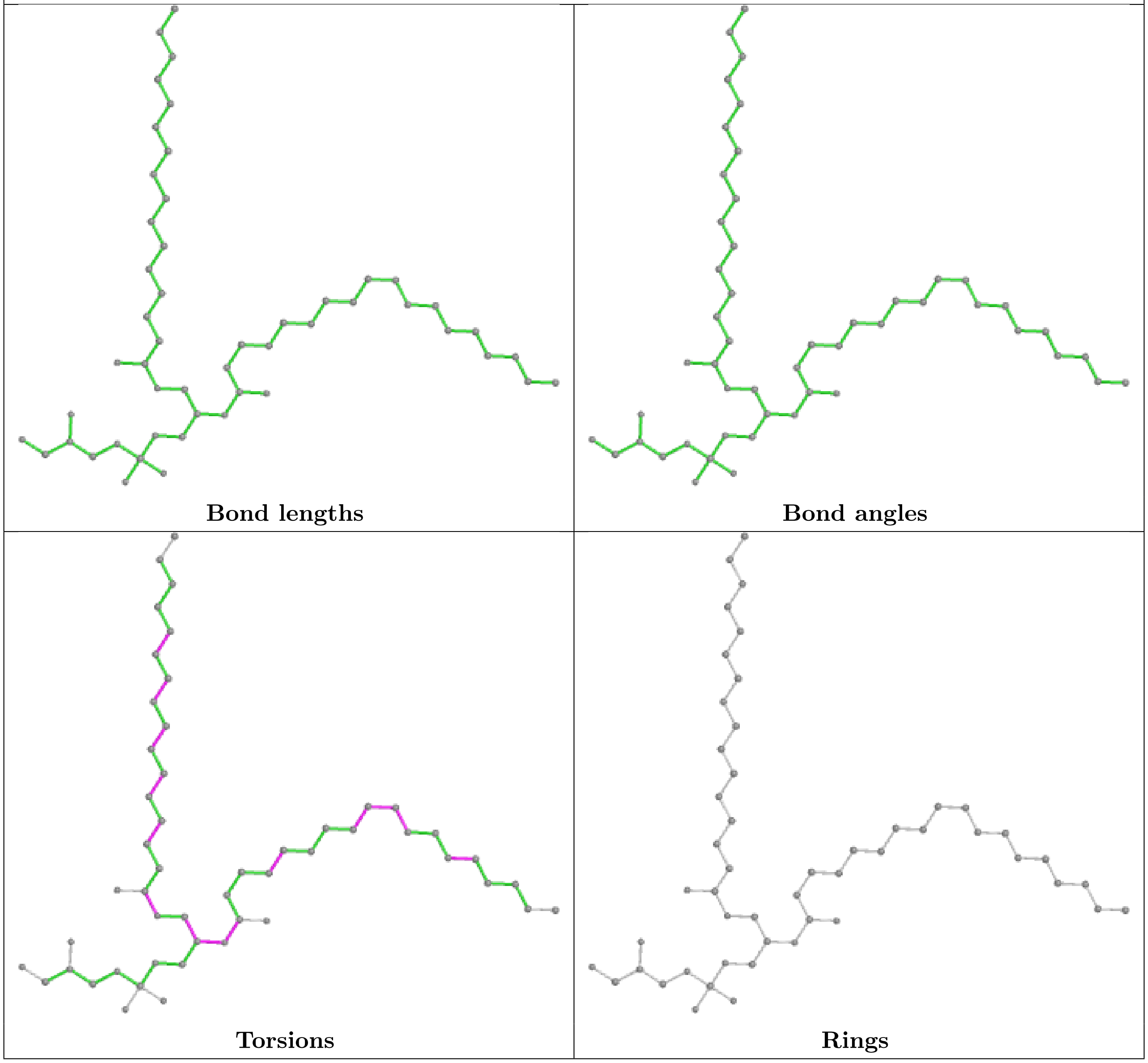

Bond lengths

Bond angles

Torsions

Rings

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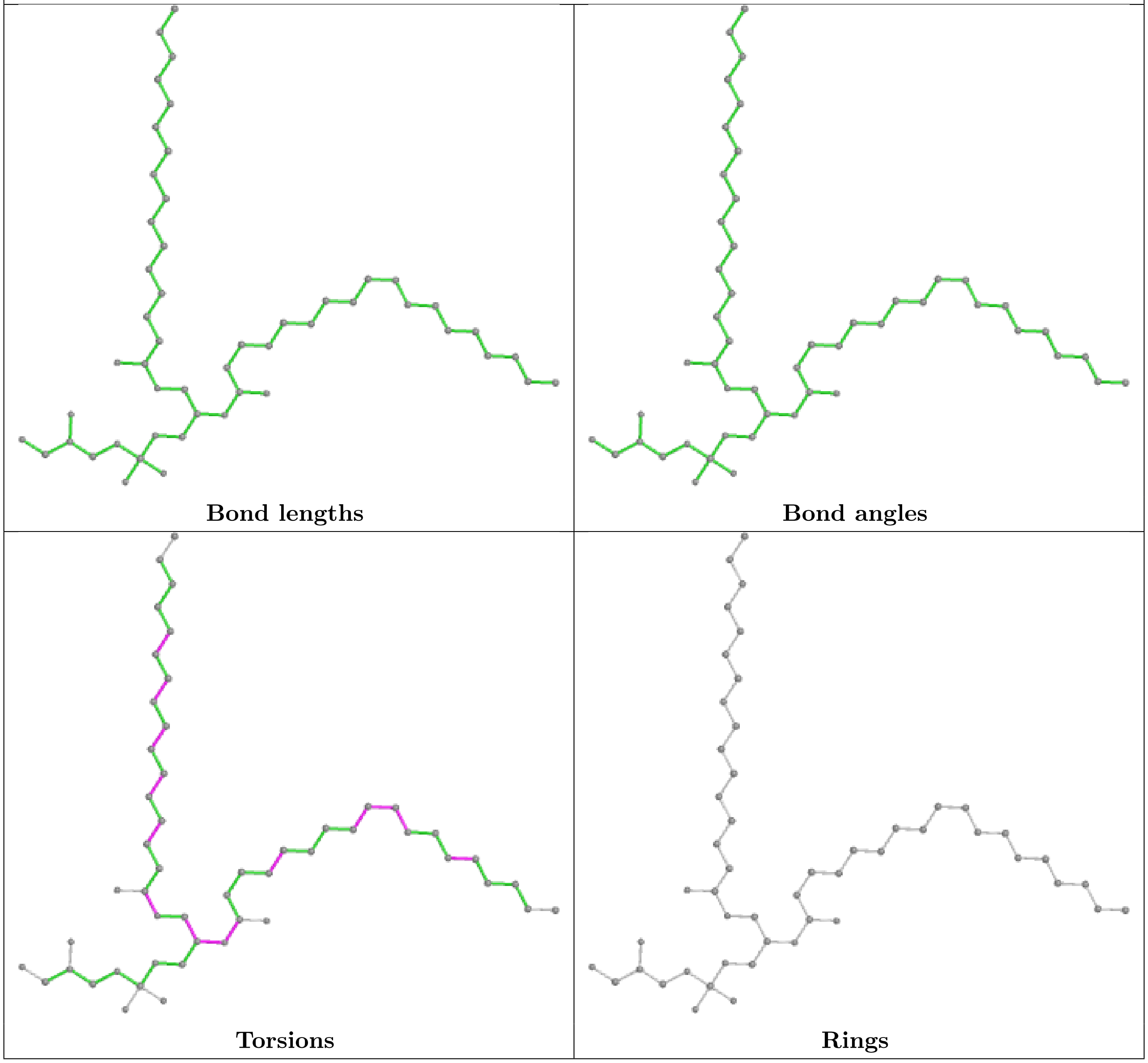

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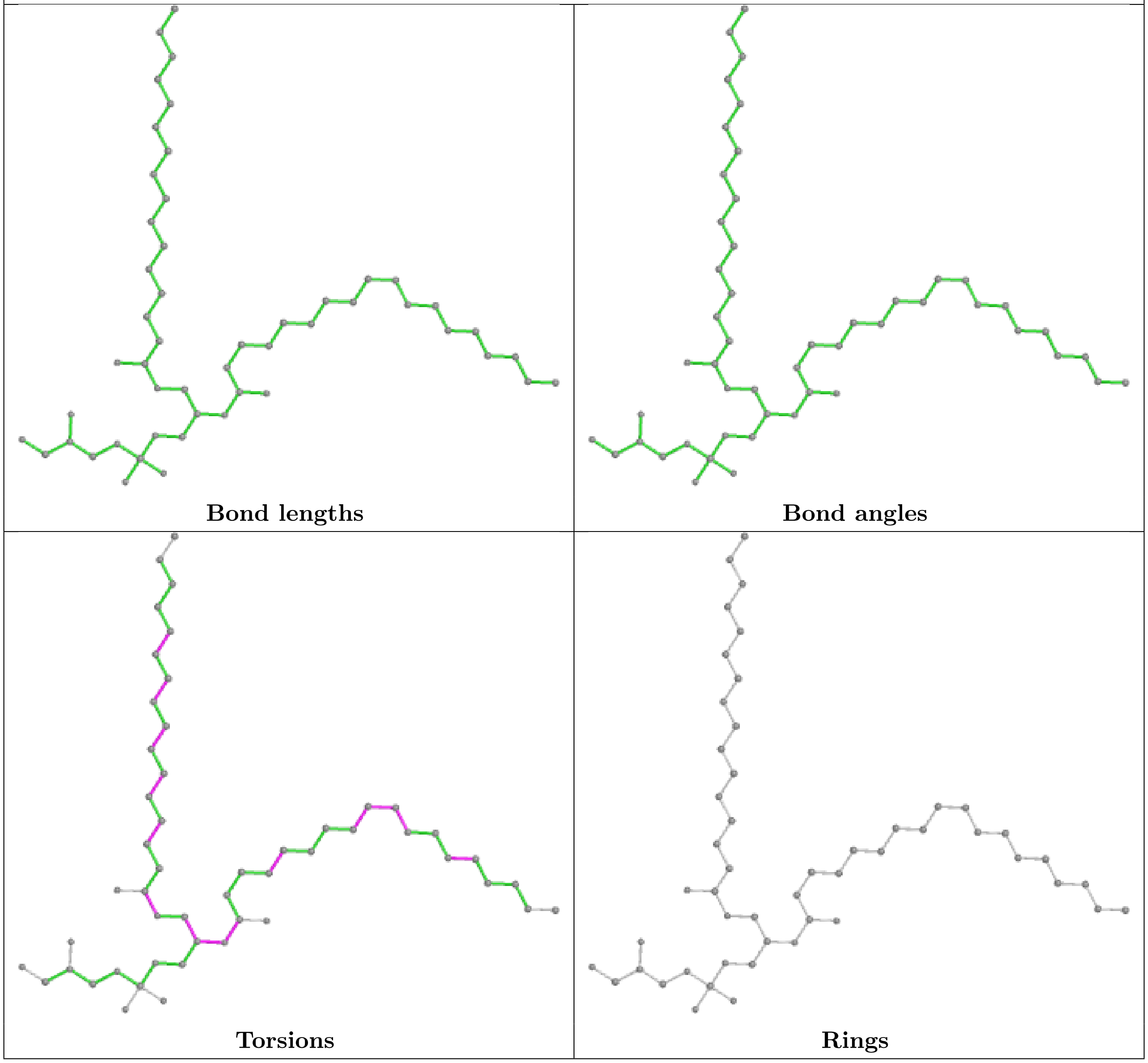

Bond lengths

Bond angles

Torsions

Rings

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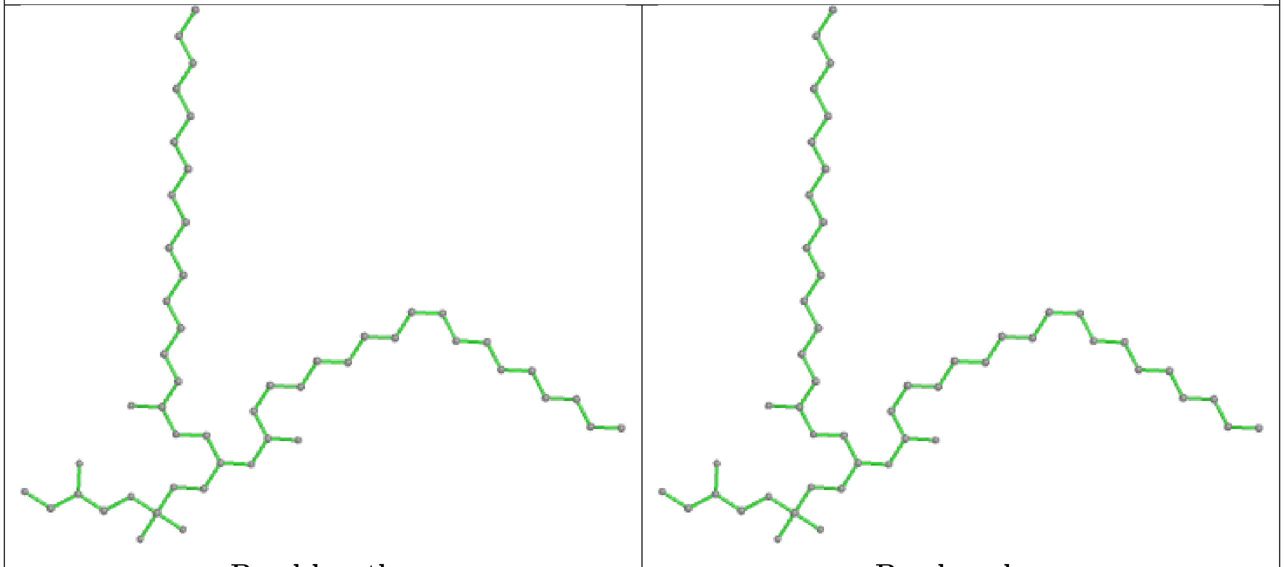
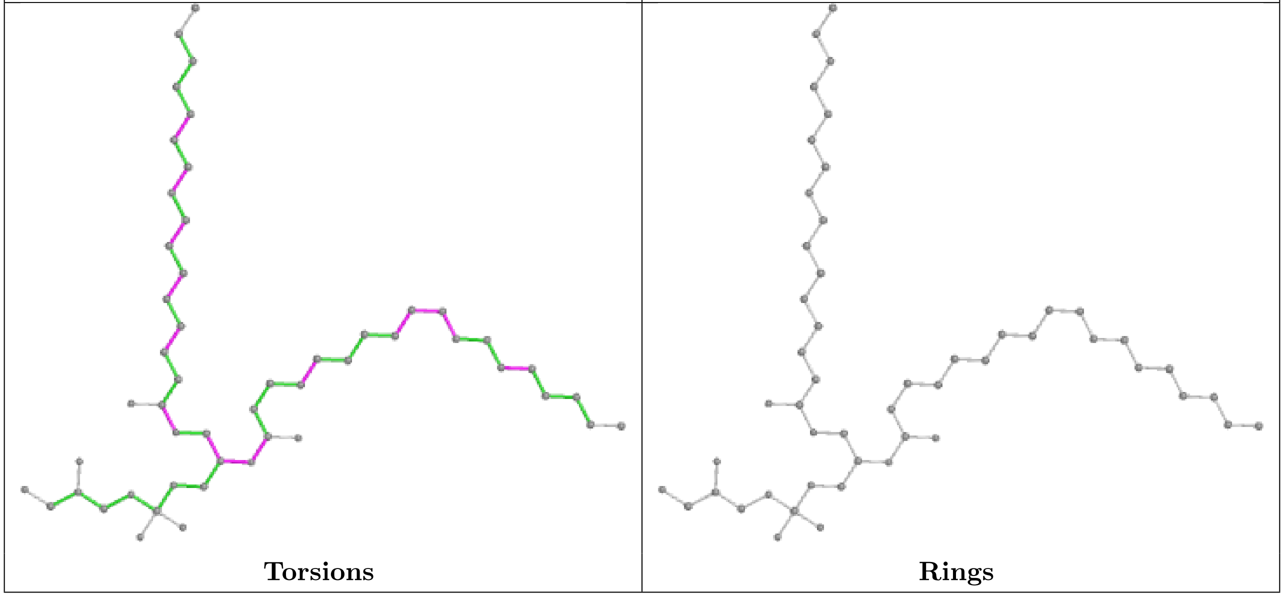


Bond lengths

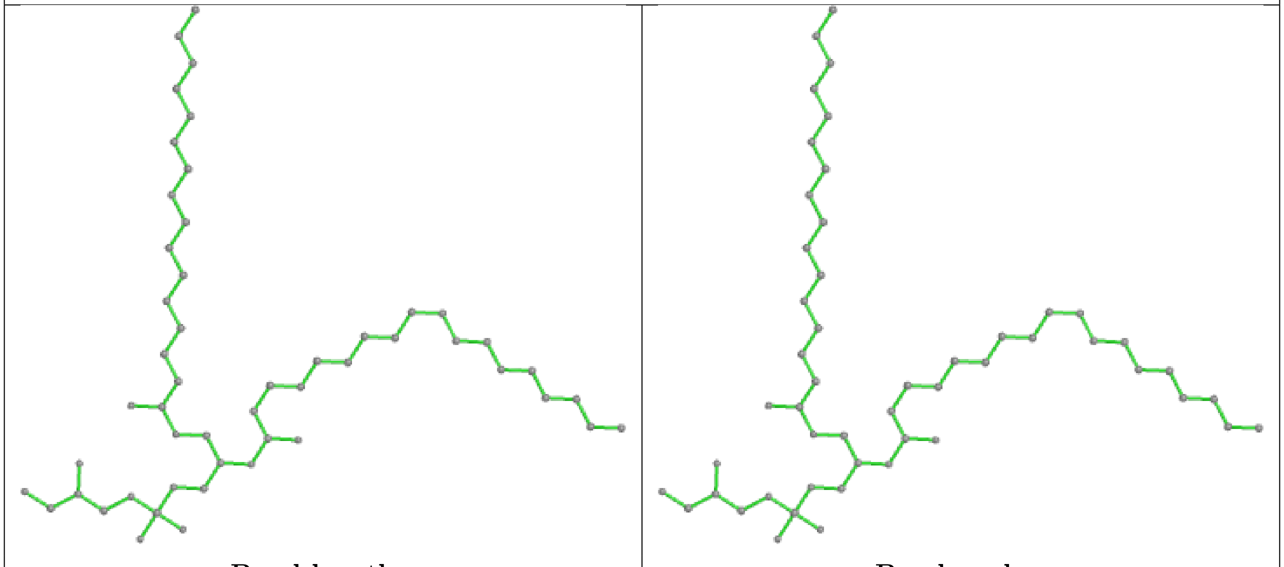
Bond angles



Torsions

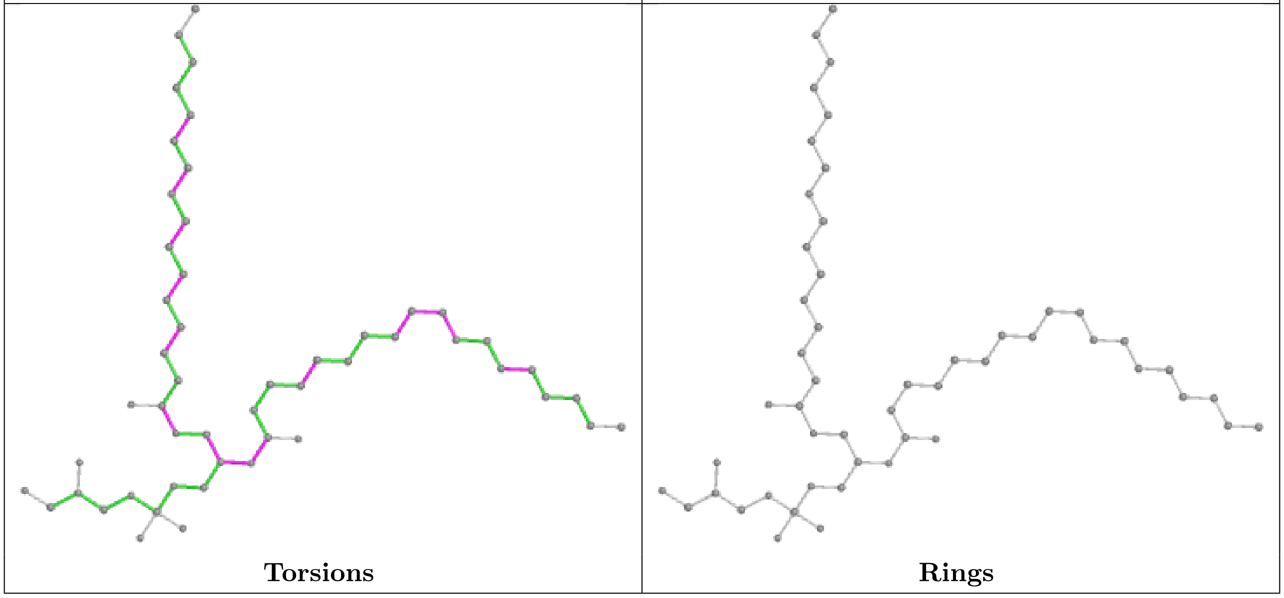
Rings

Ligand PGW 2I 101



Bond lengths

Bond angles



Torsions

Rings

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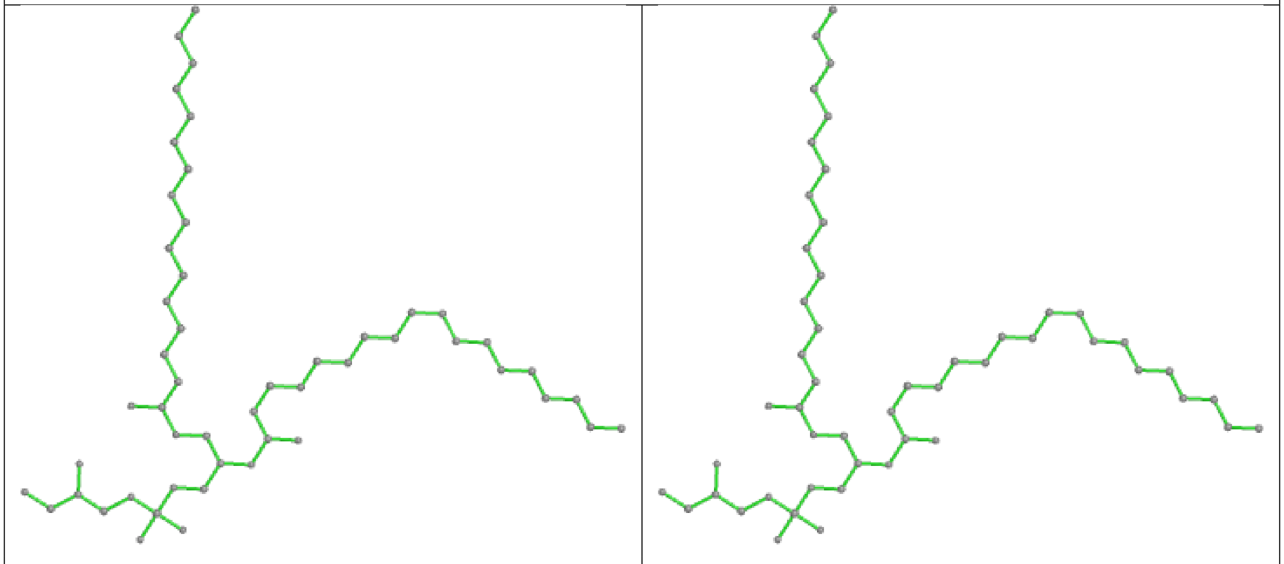
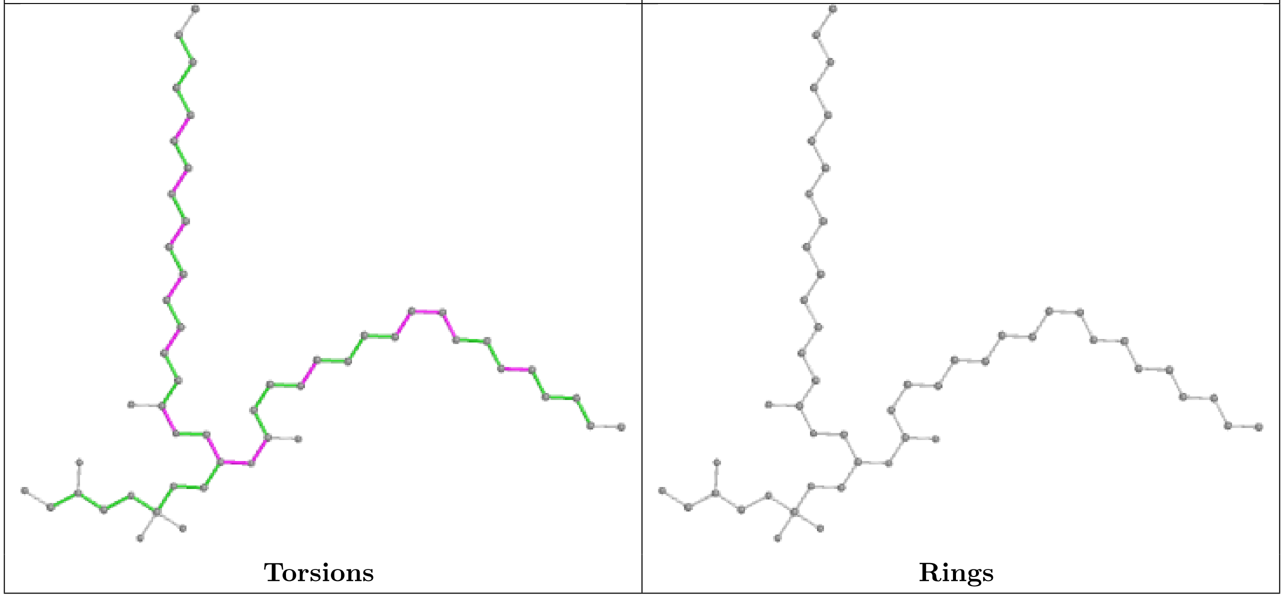
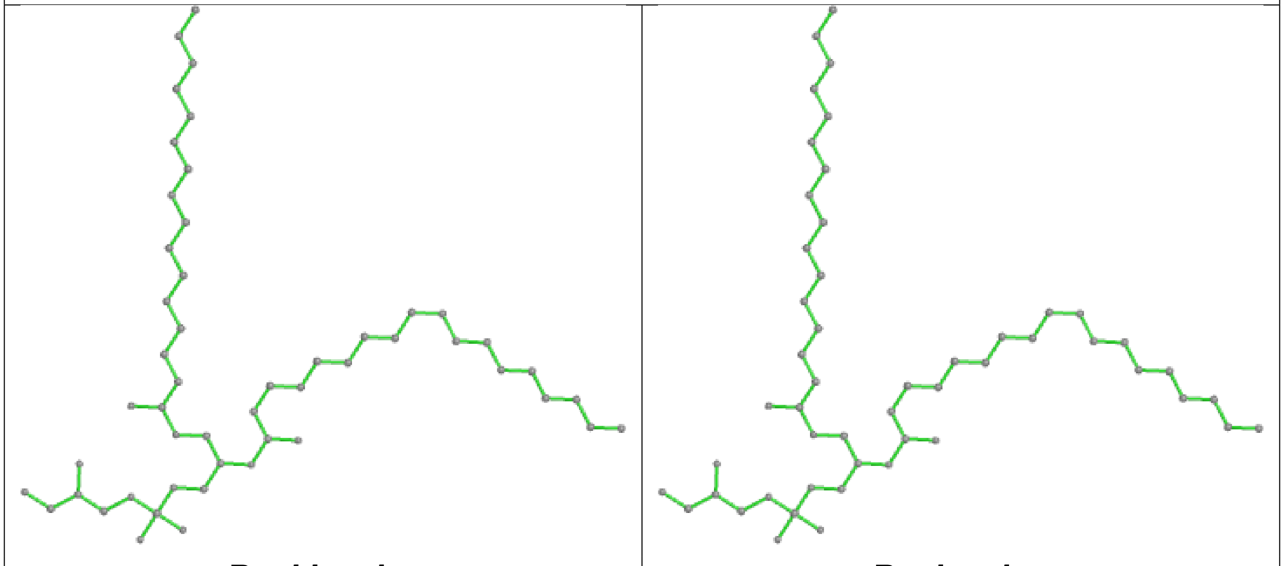


Bond lengths **Bond angles**



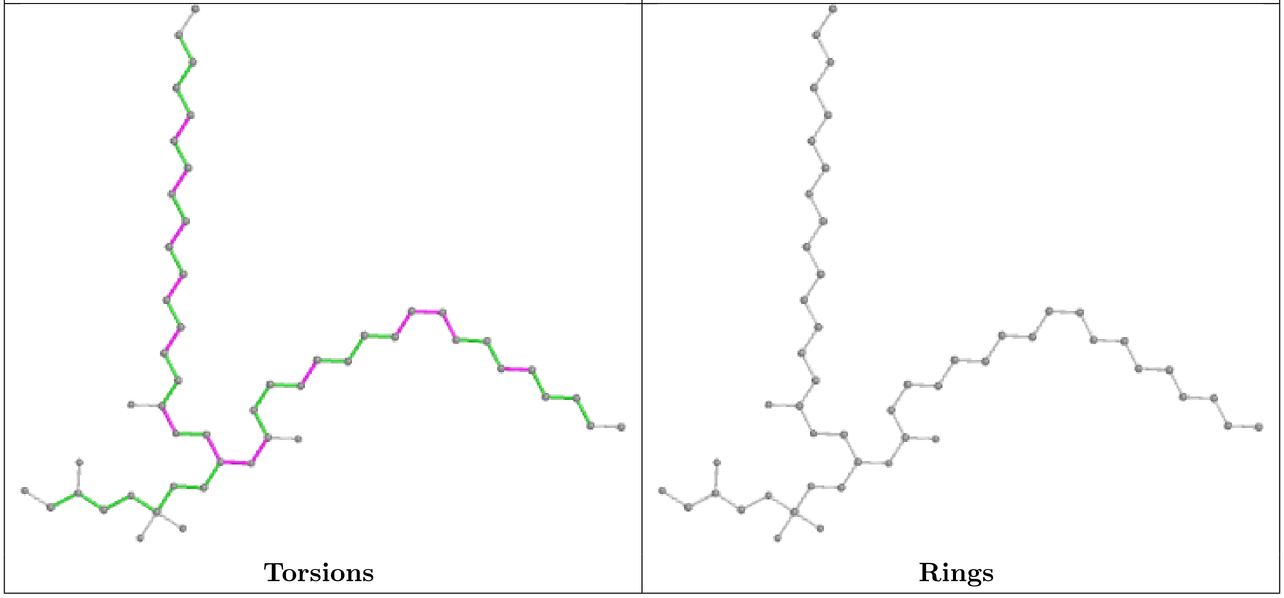
Torsions **Rings**

Ligand PGW 3K 101



Bond lengths

Bond angles



Torsions

Rings

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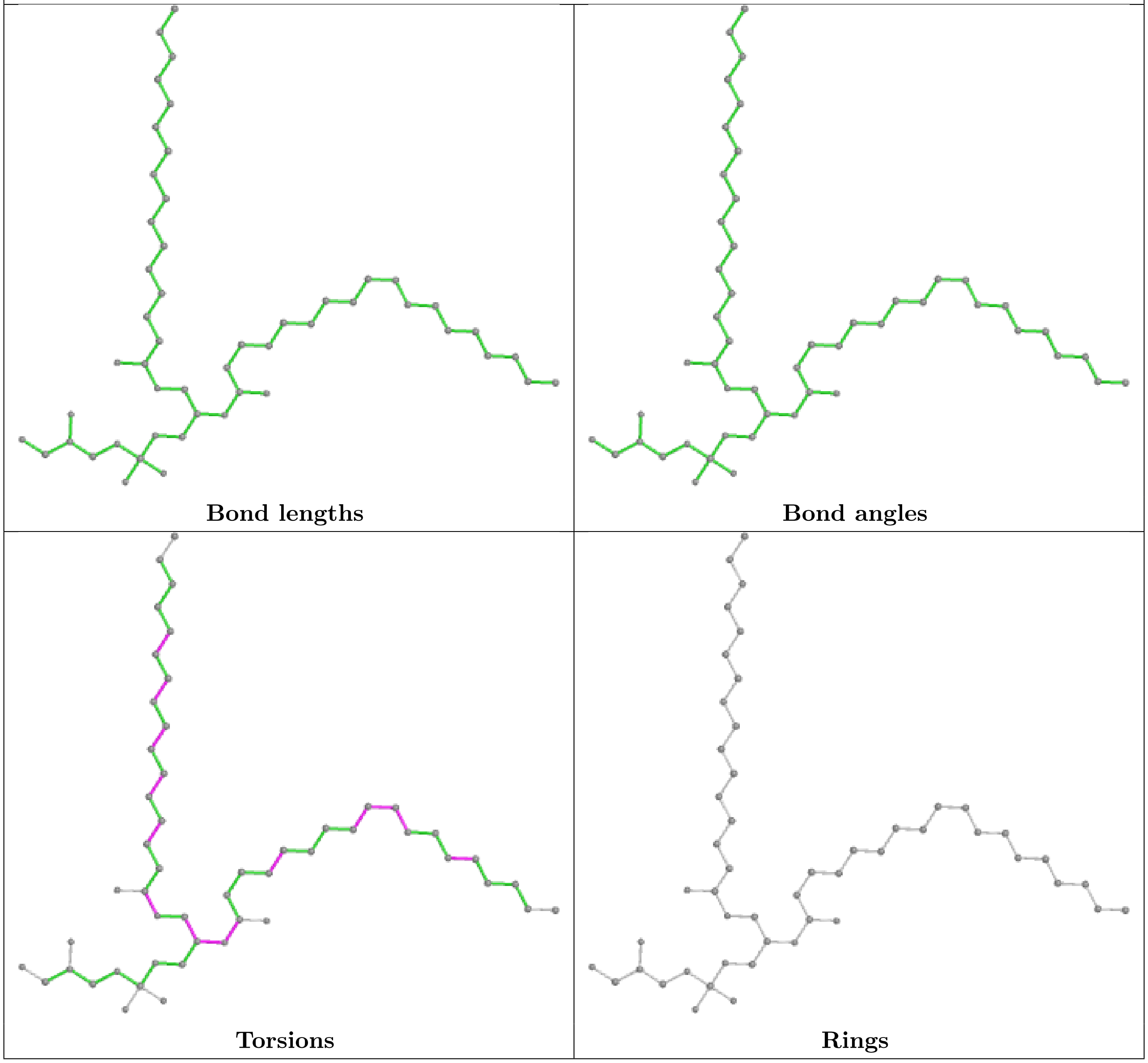


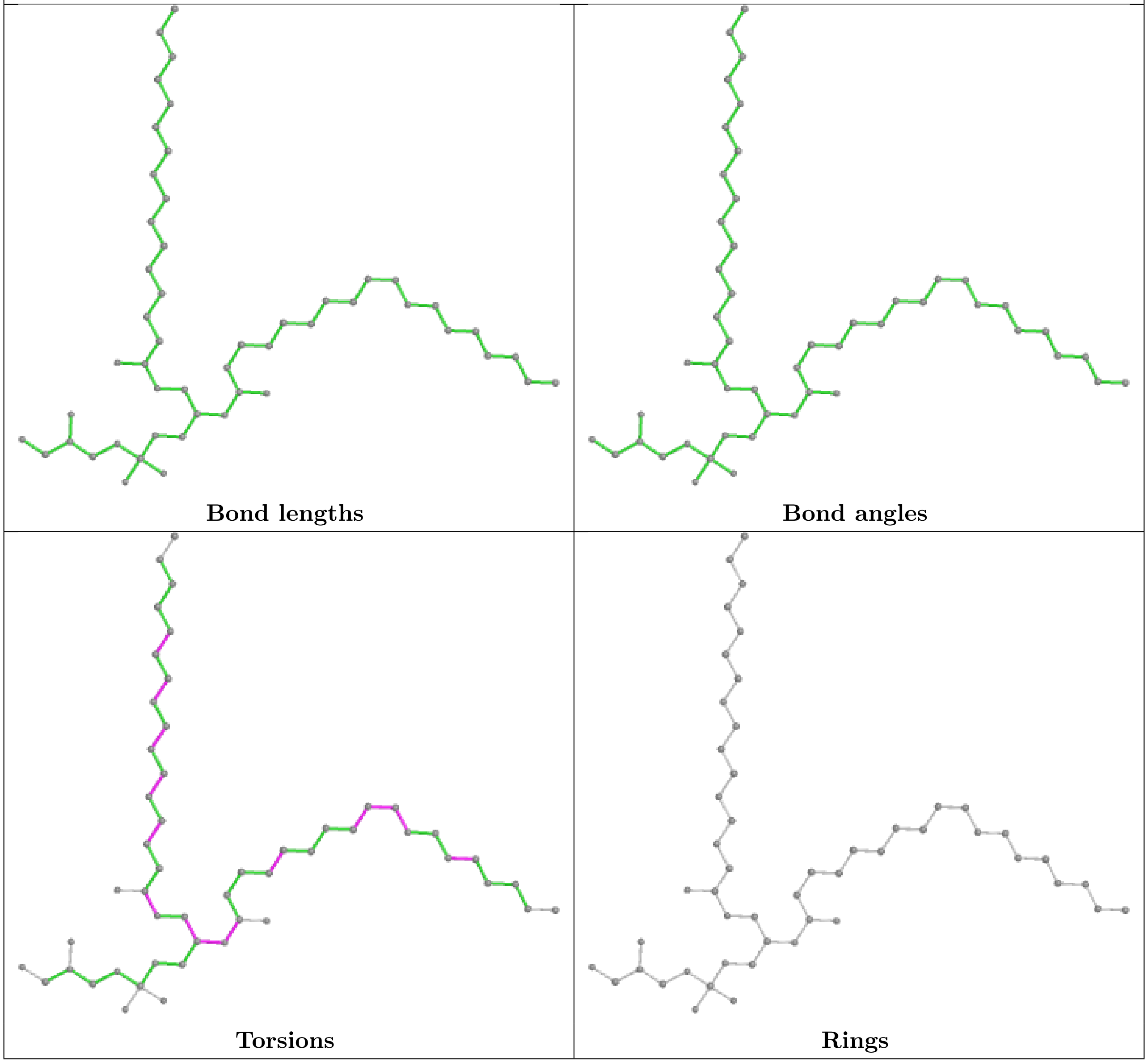
Bond lengths

Bond angles

Torsions

Rings

Ligand PGW 1K 101



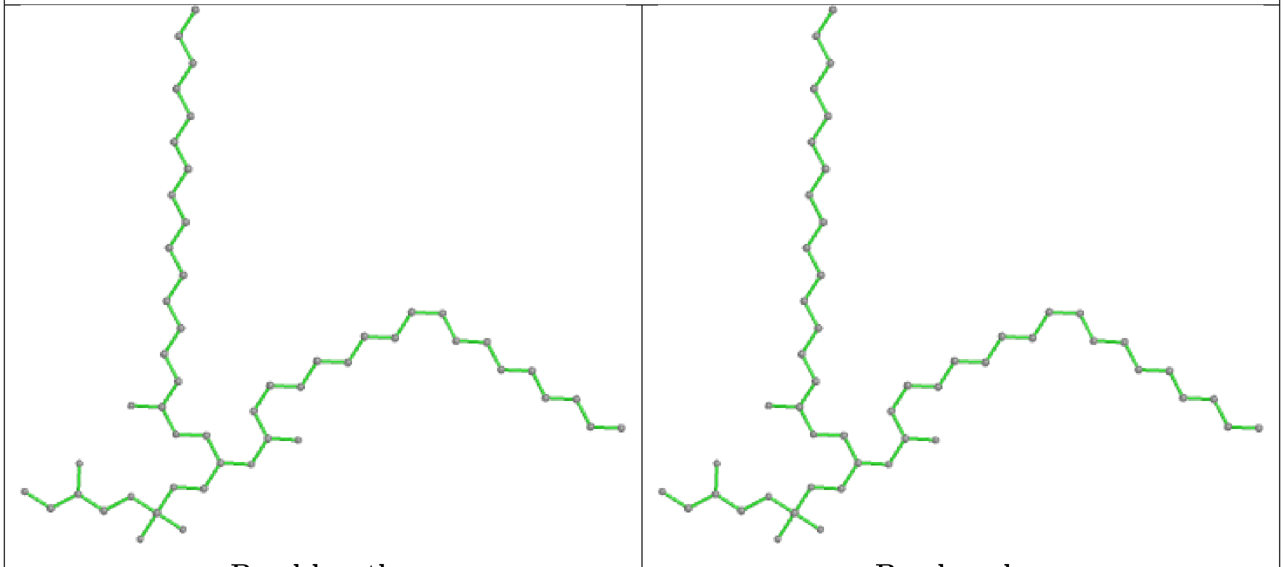
Bond lengths

Bond angles

Torsions

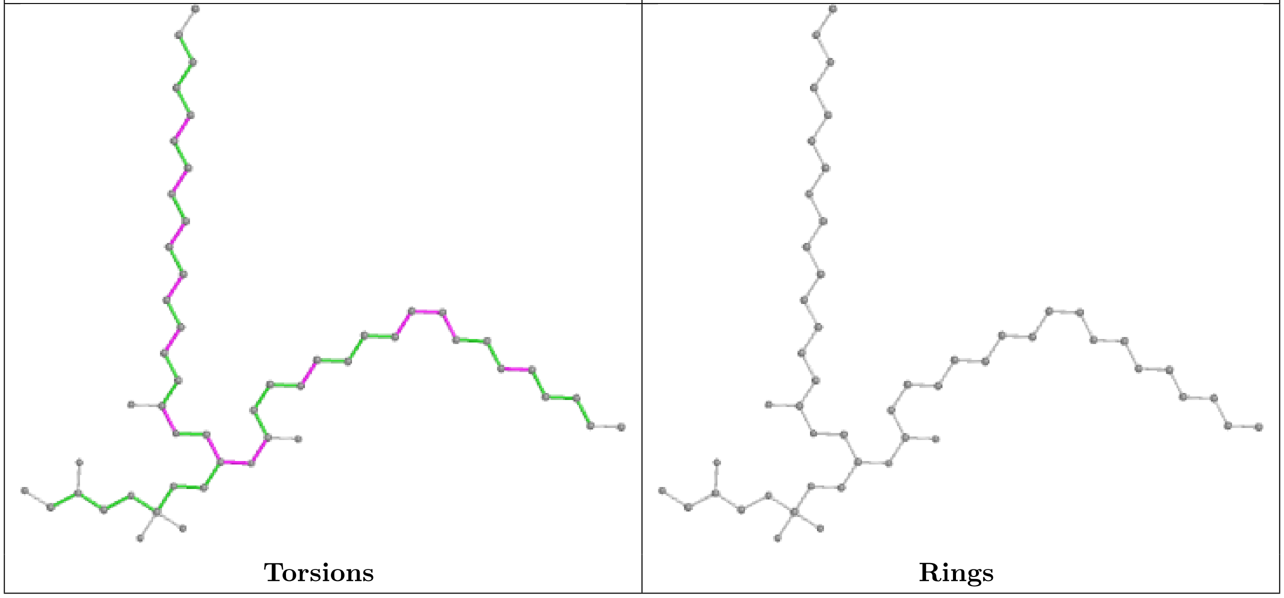
Rings

Ligand PGW 4E 101



Bond lengths

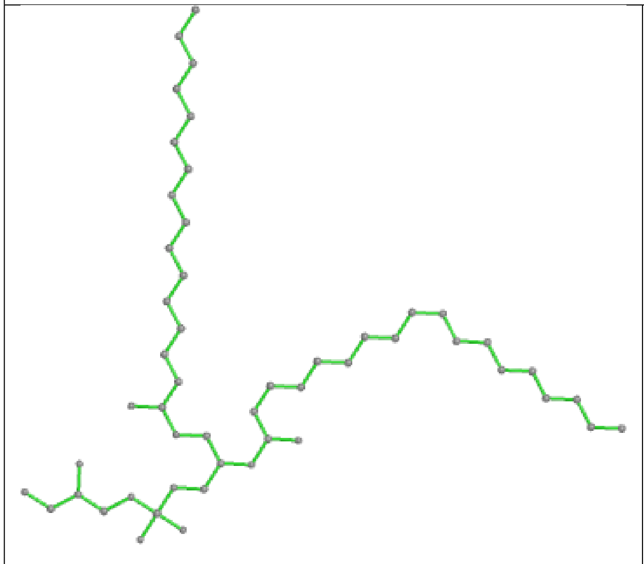
Bond angles



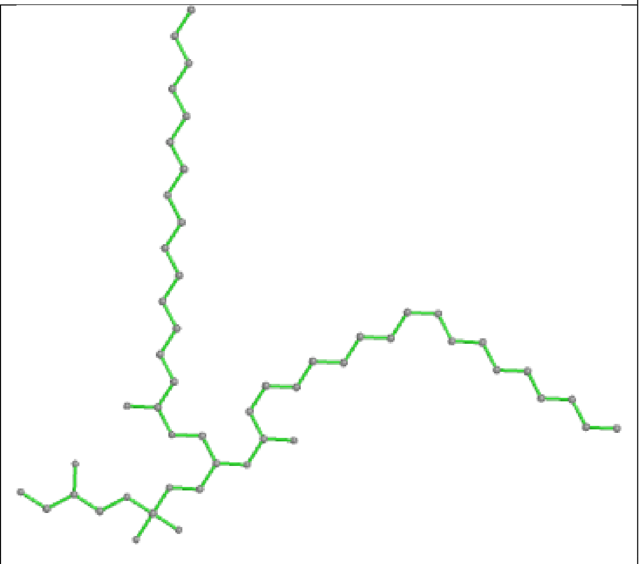
Torsions

Rings

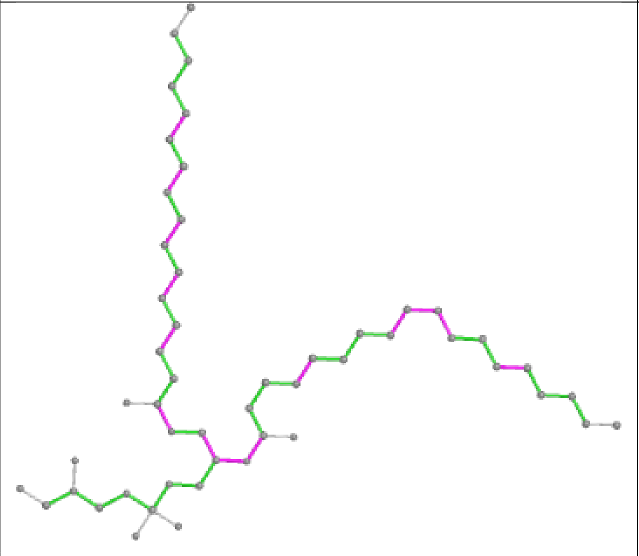
Ligand PGW 5H 101



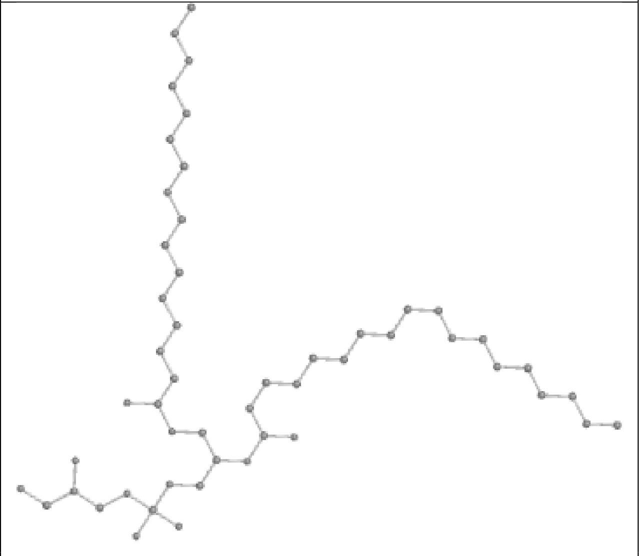
Bond lengths



Bond angles

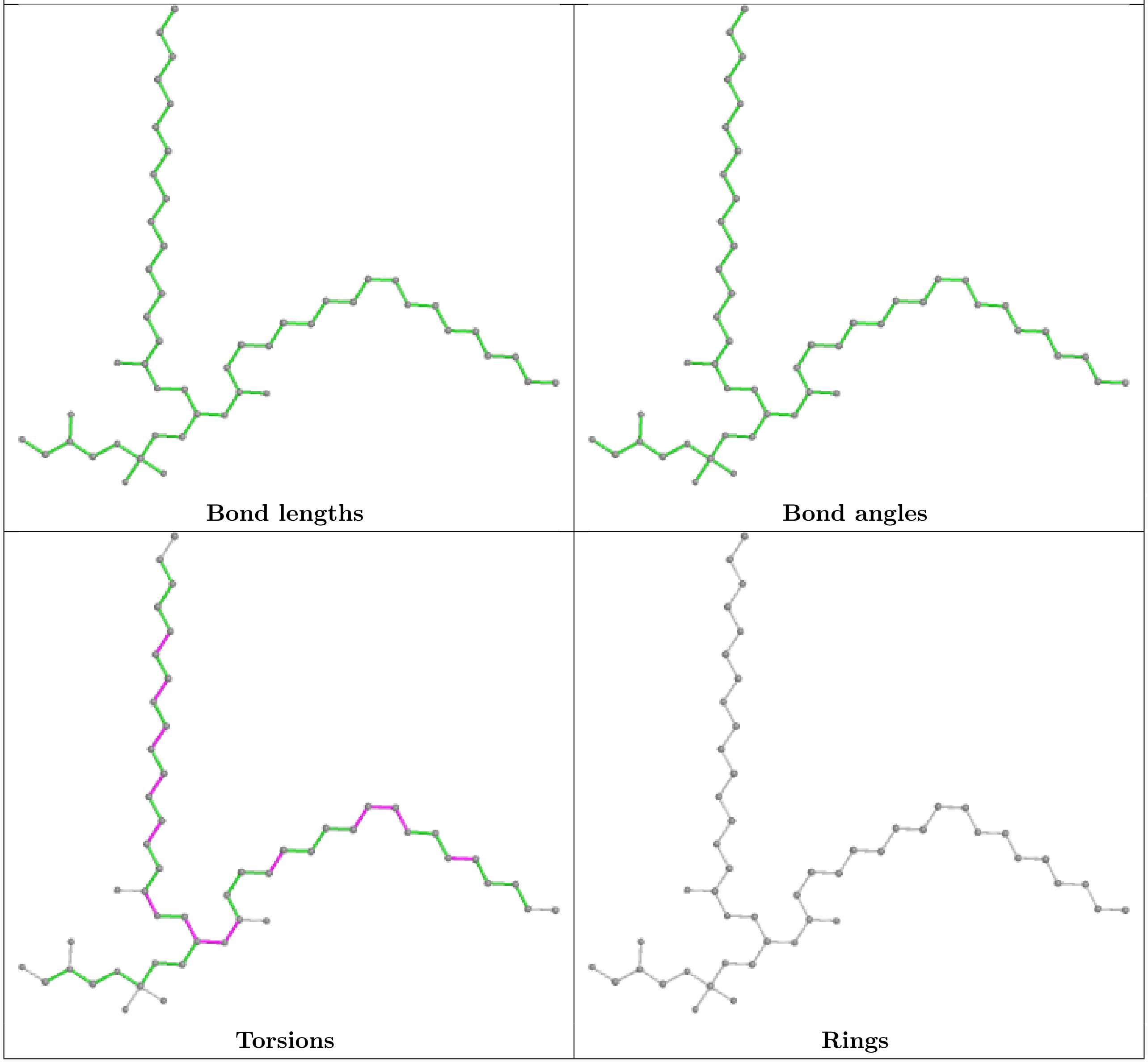


Torsions



Rings

Ligand PGW 2L 101



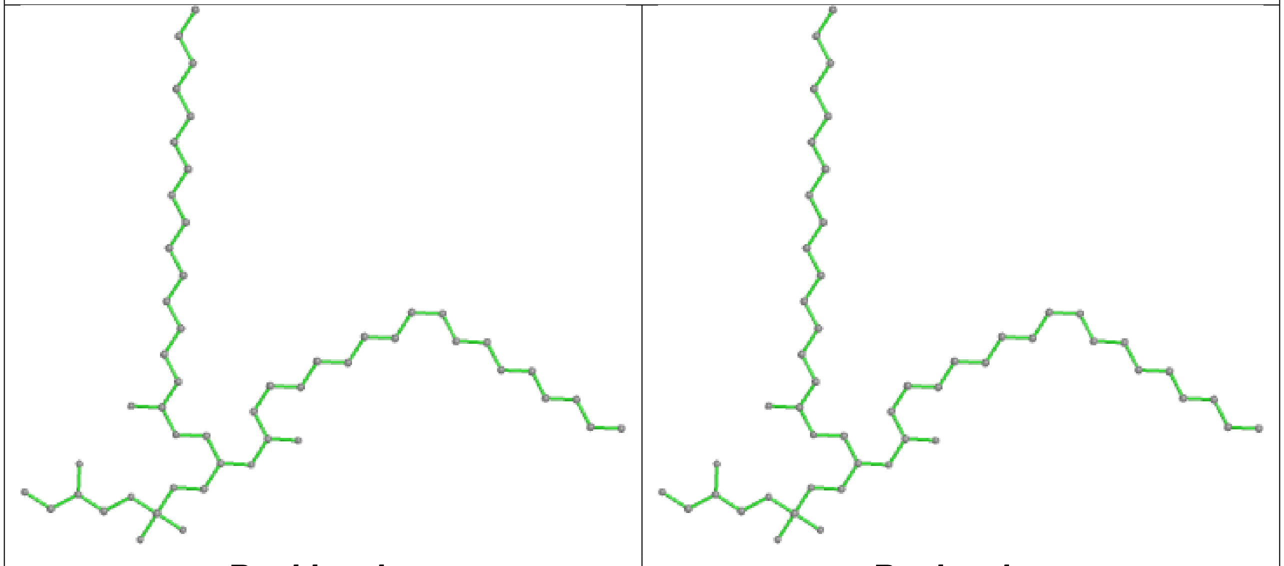
Bond lengths

Bond angles

Torsions

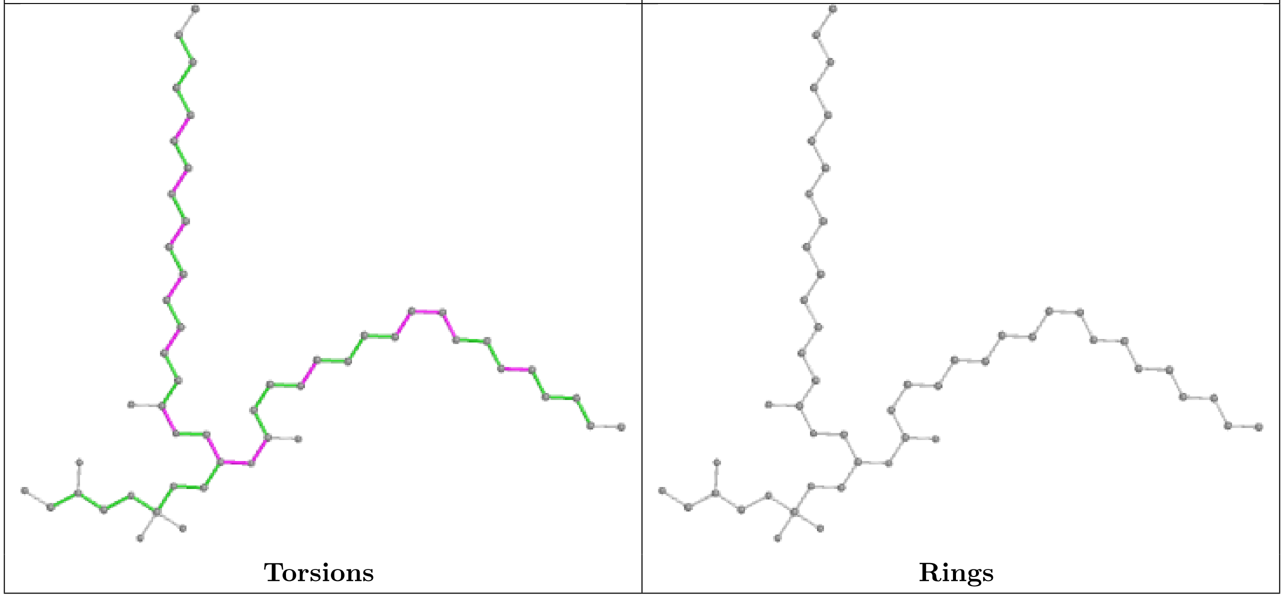
Rings

Ligand PGW 5B 101



Bond lengths

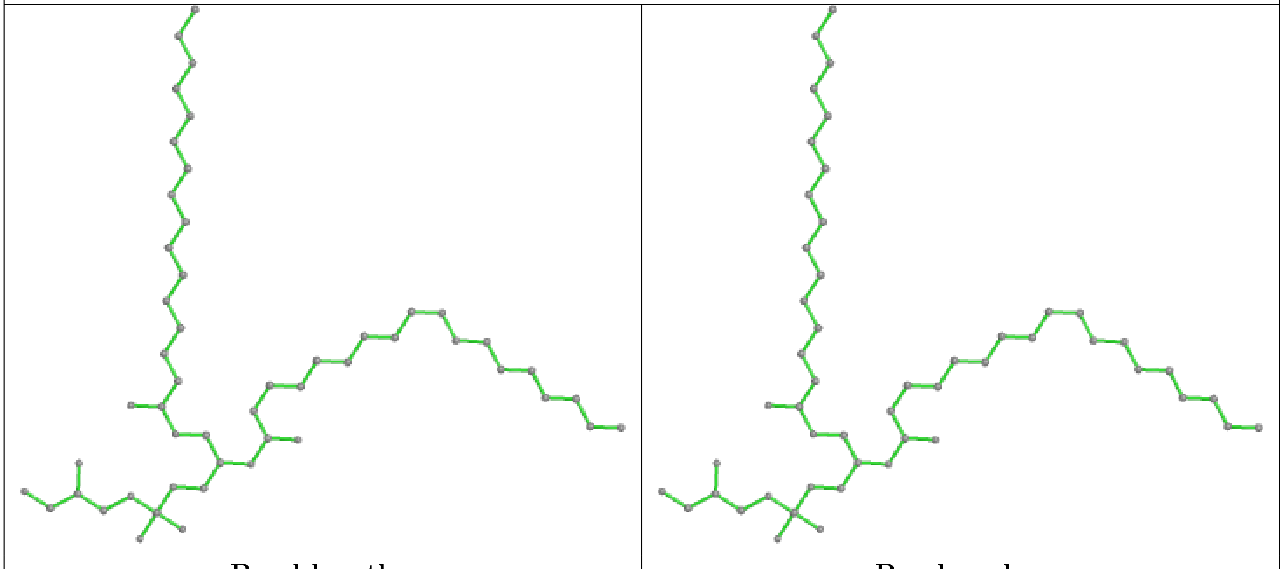
Bond angles



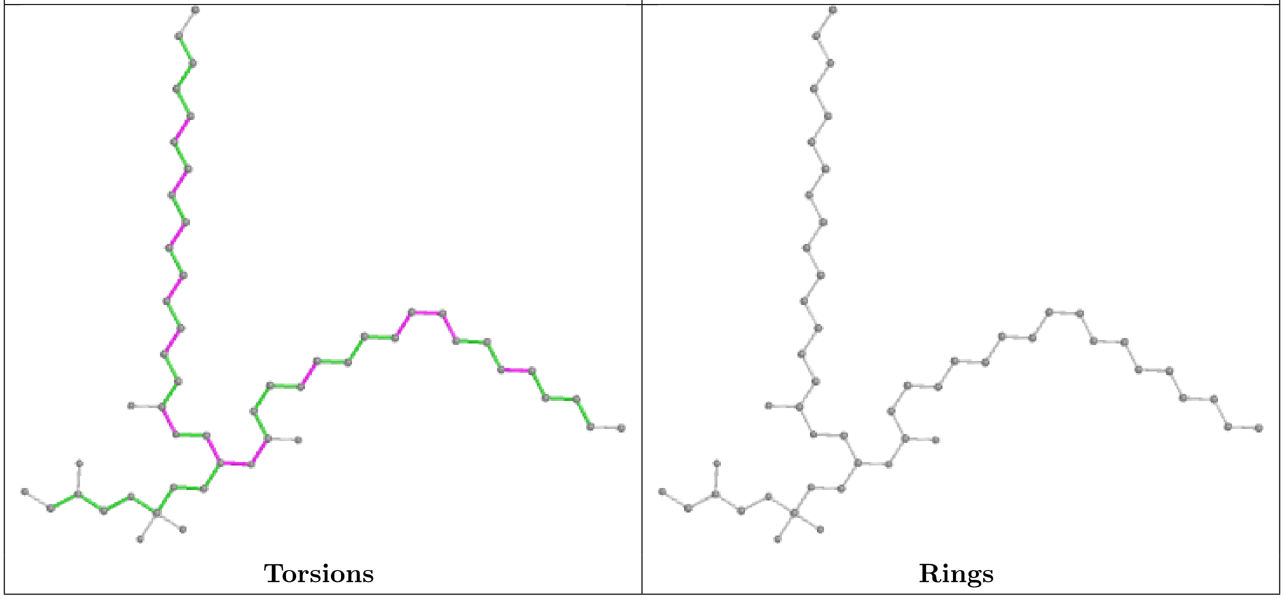
Torsions

Rings

Ligand PGW 3J 101

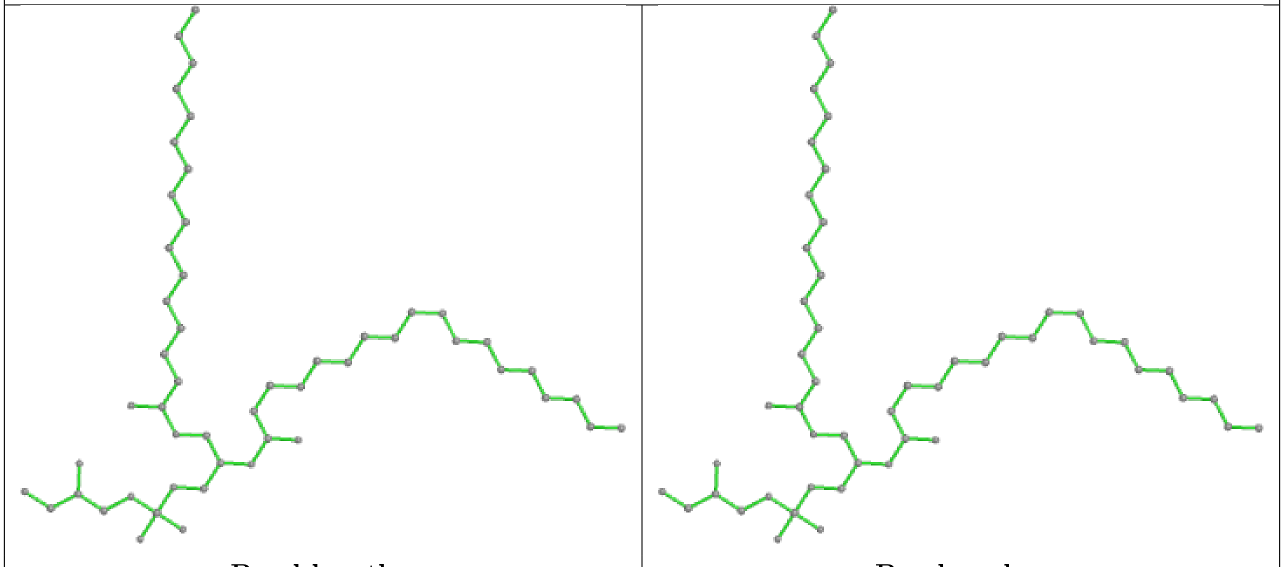


Bond lengths **Bond angles**

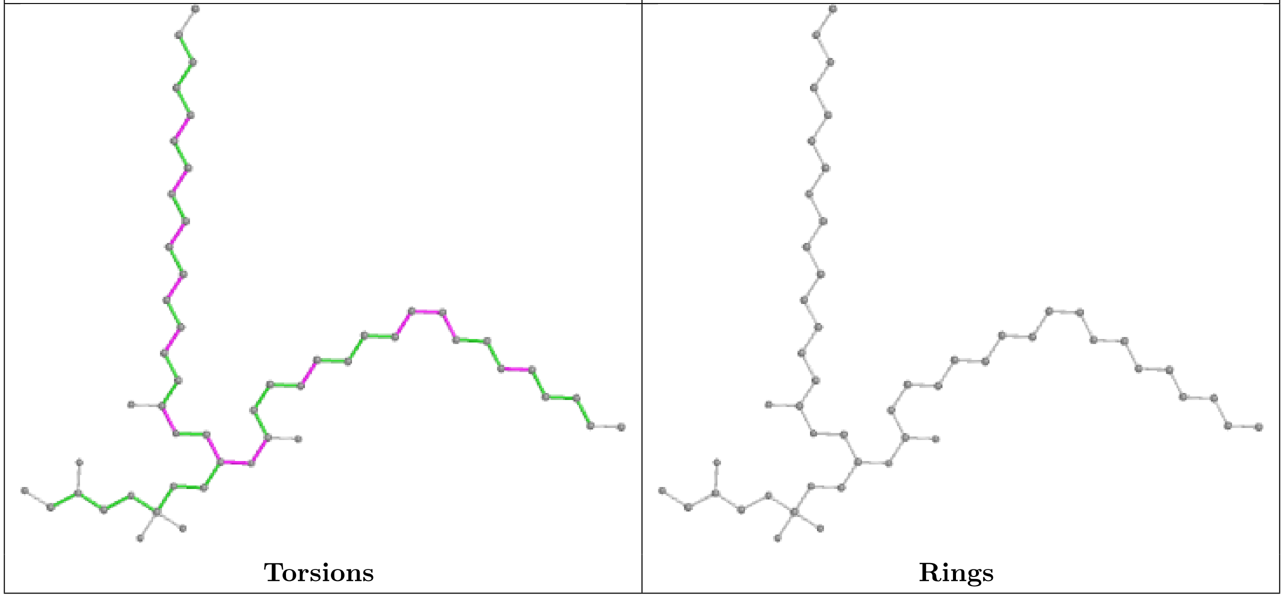


Torsions **Rings**

Ligand PGW 1F 101

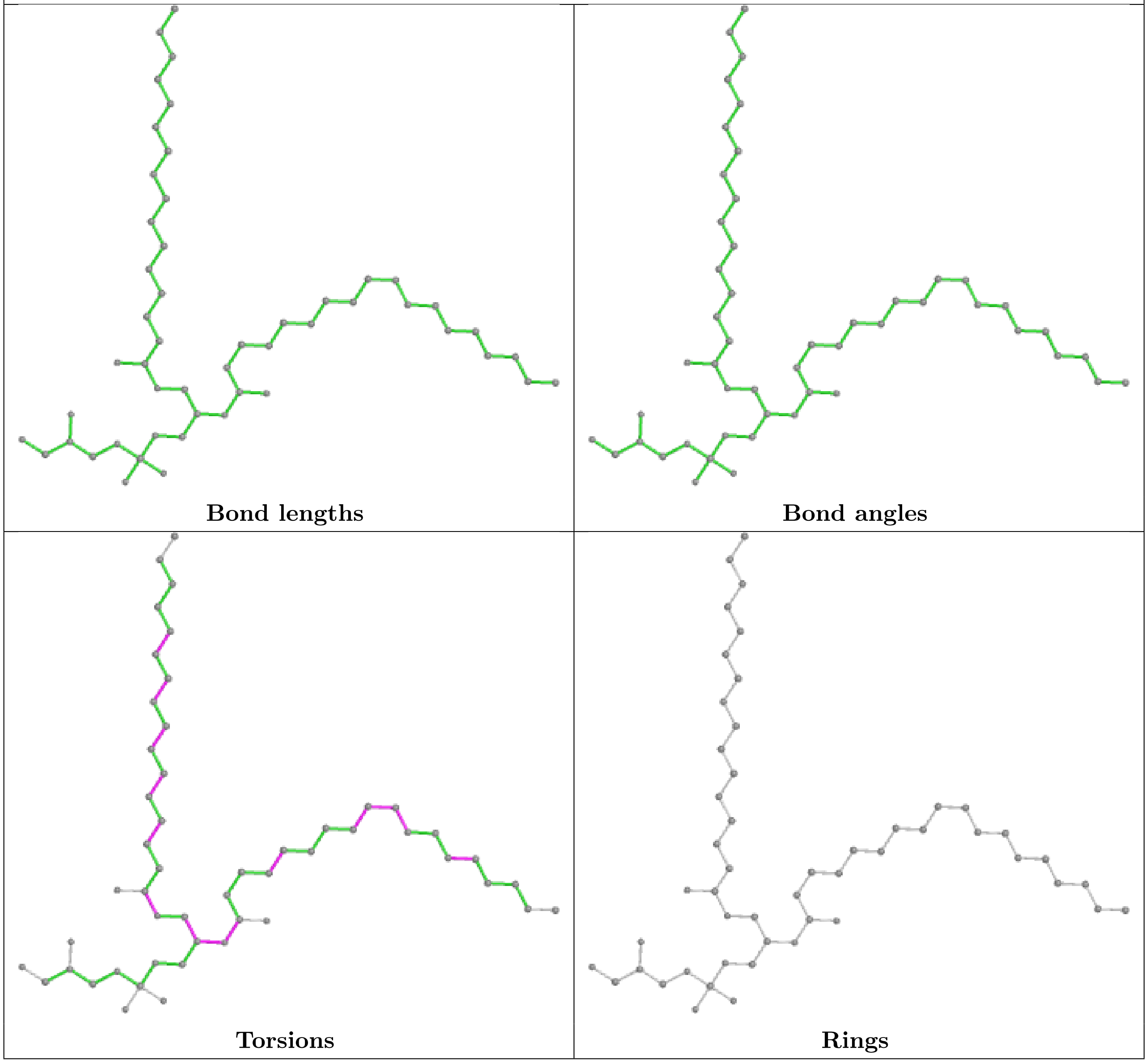


Bond lengths **Bond angles**



Torsions **Rings**

Ligand PGW 1D 101



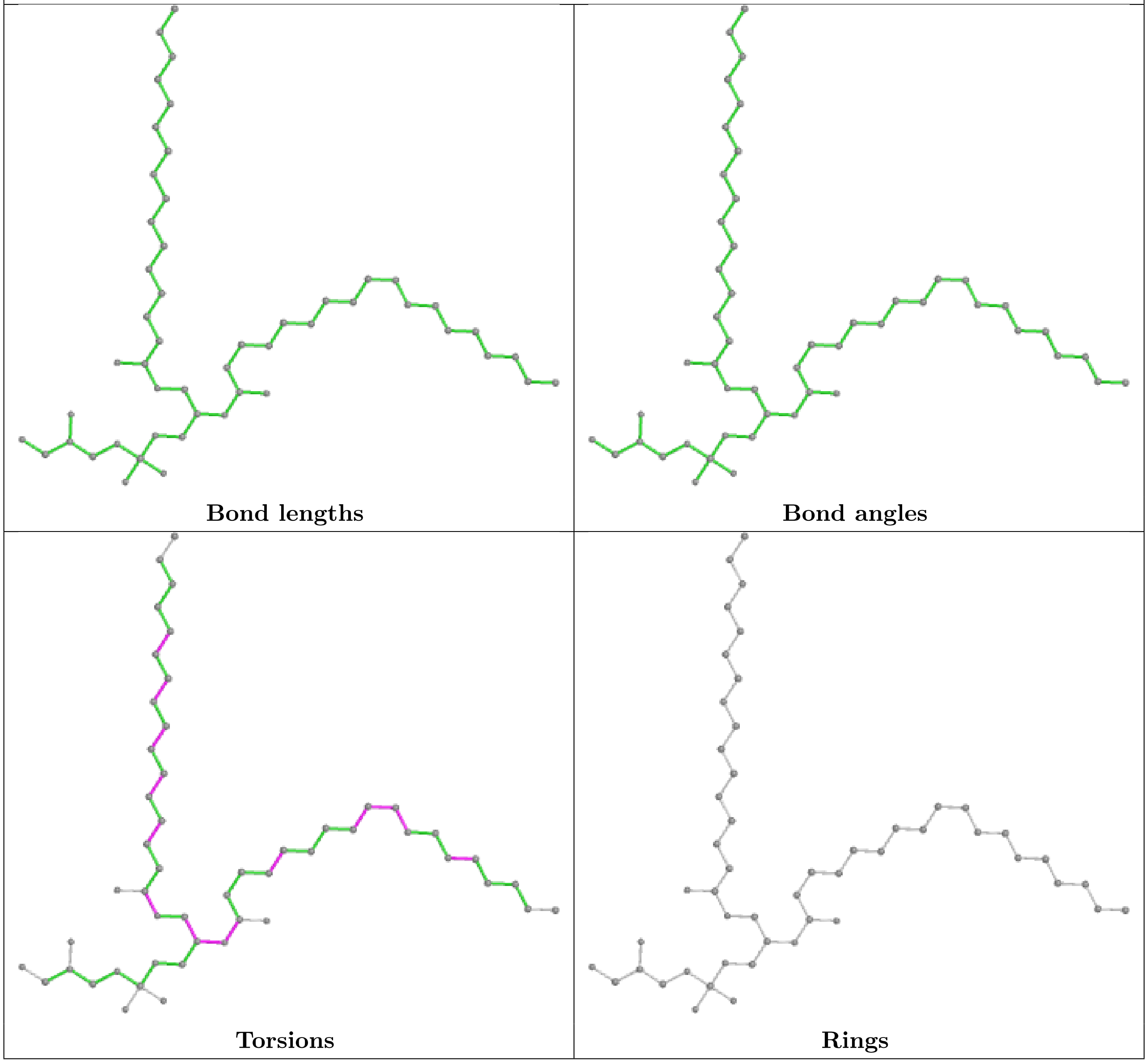
Bond lengths

Bond angles

Torsions

Rings

Ligand PGW 2J 101



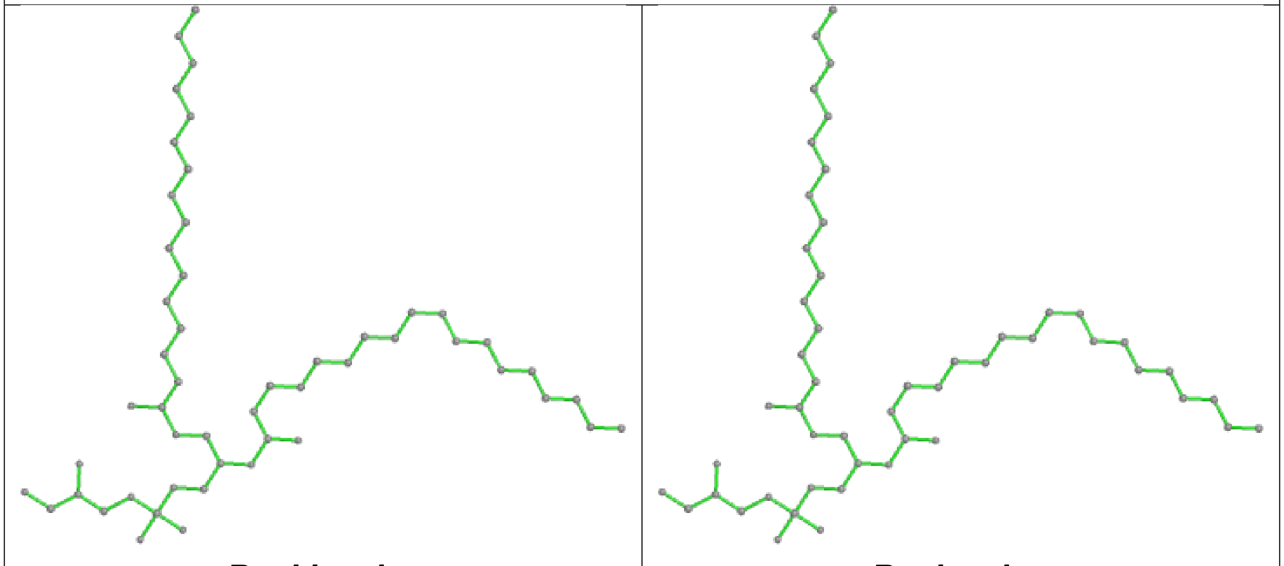
Bond lengths

Bond angles

Torsions

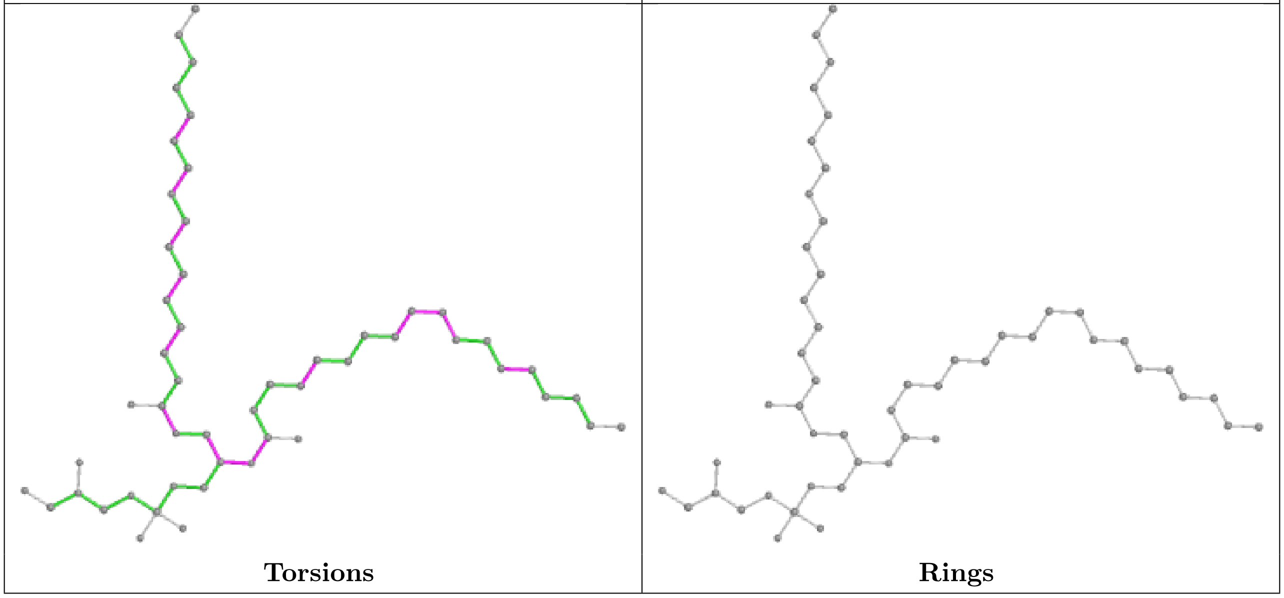
Rings

Ligand PGW 5E 101



Bond lengths

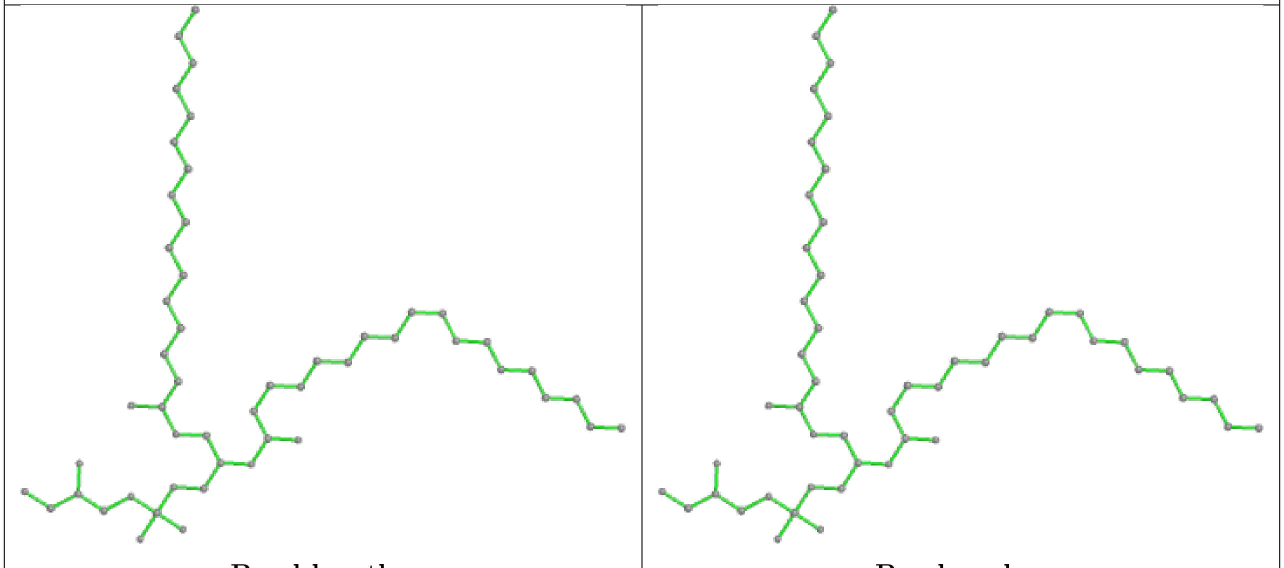
Bond angles



Torsions

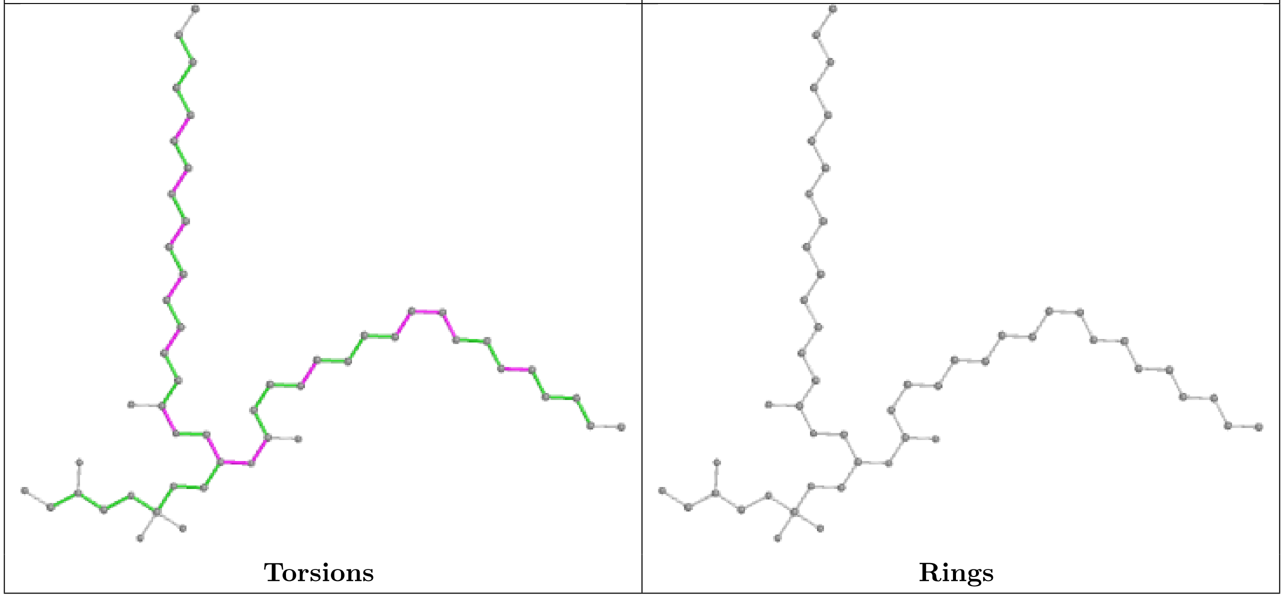
Rings

Ligand PGW 1M 101



Bond lengths

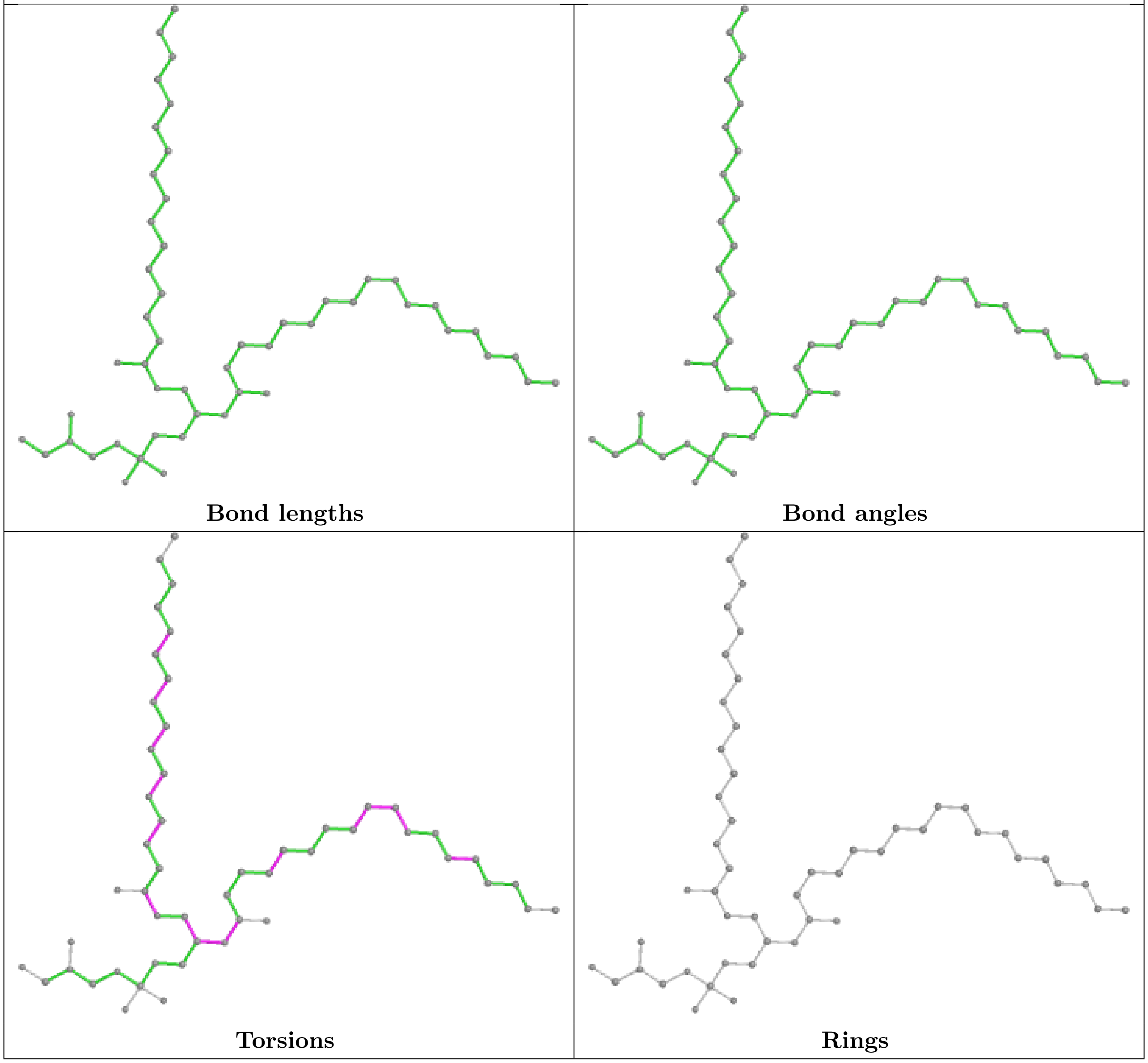
Bond angles



Torsions

Rings

Ligand PGW 5D 101



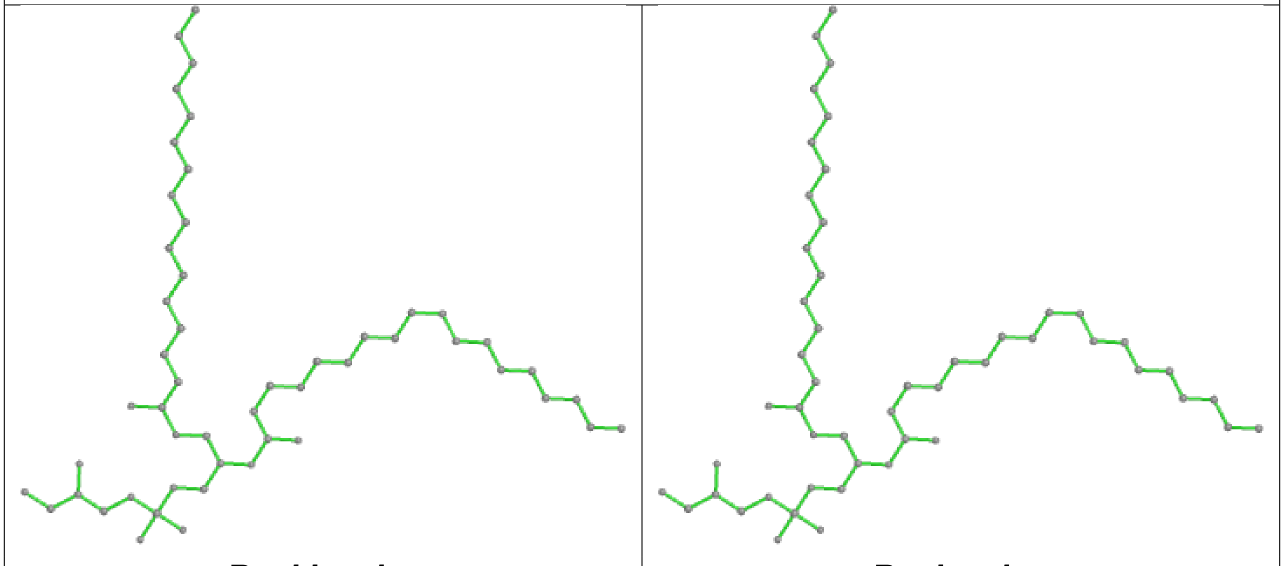
Bond lengths

Bond angles

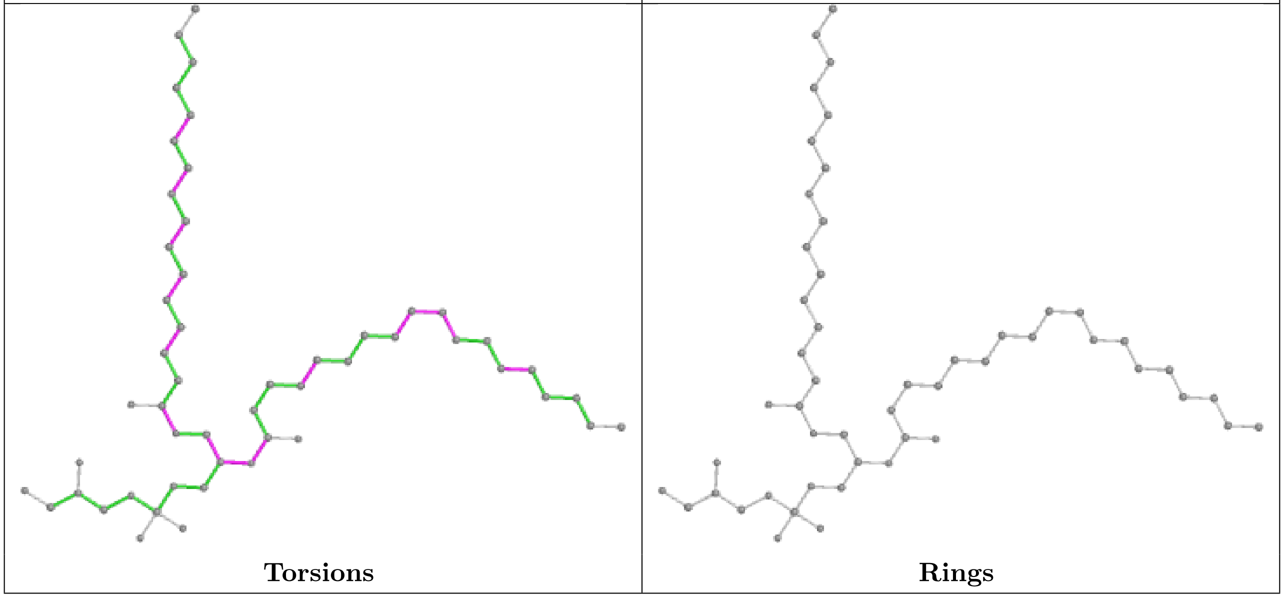
Torsions

Rings

Ligand PGW 3L 101

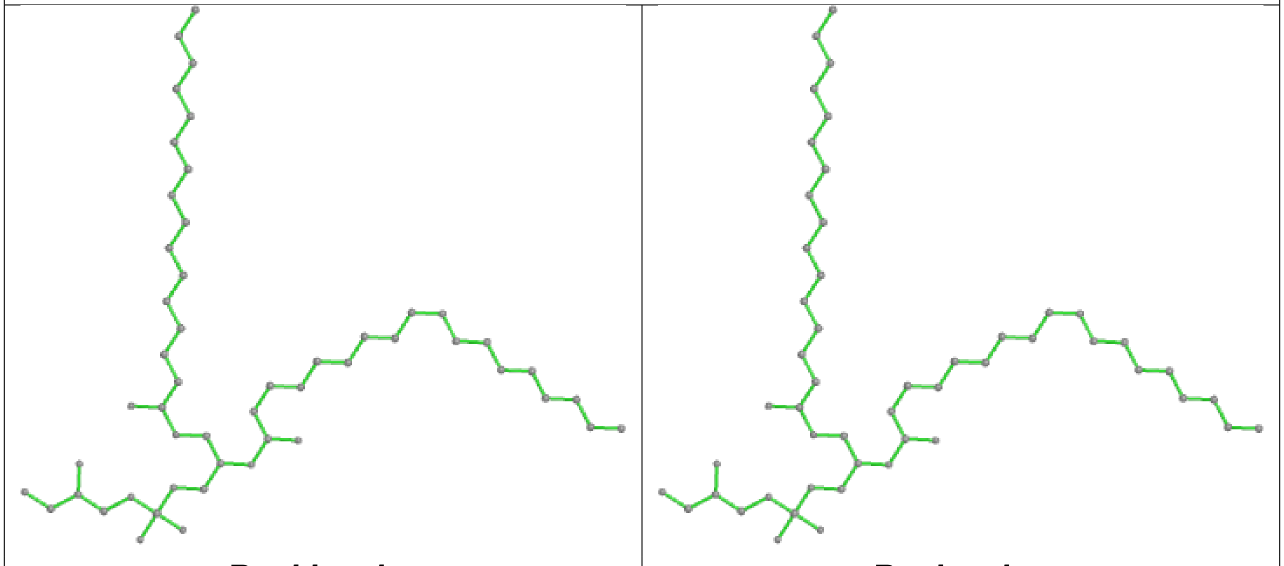


Bond lengths **Bond angles**



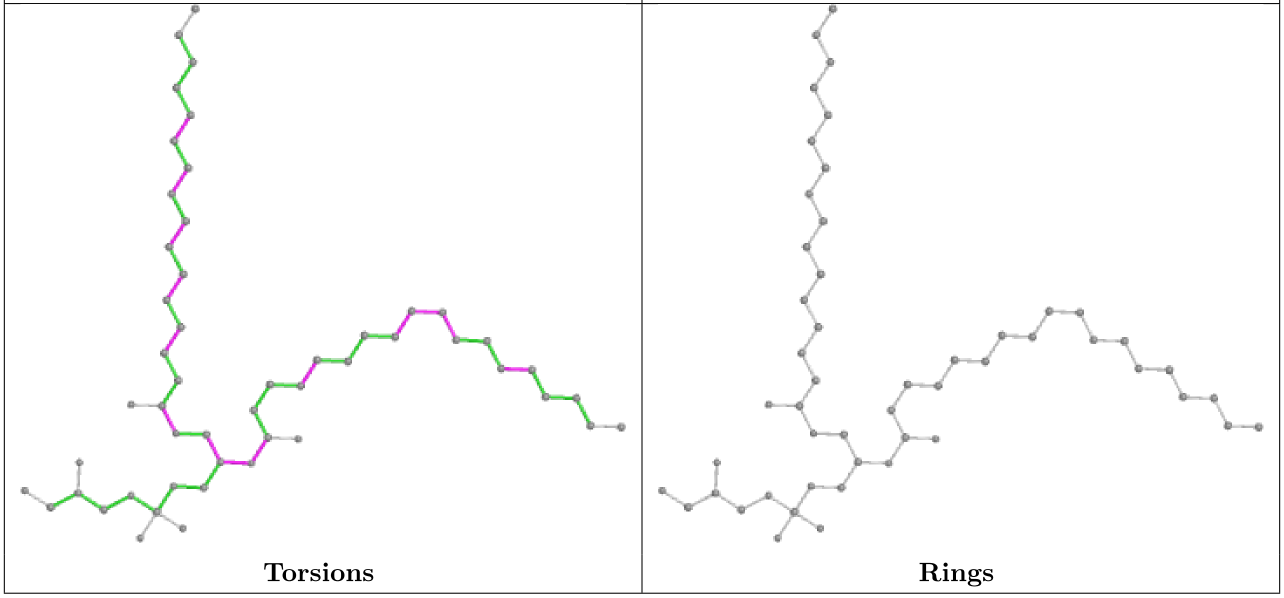
Torsions **Rings**

Ligand PGW 1L 101



Bond lengths

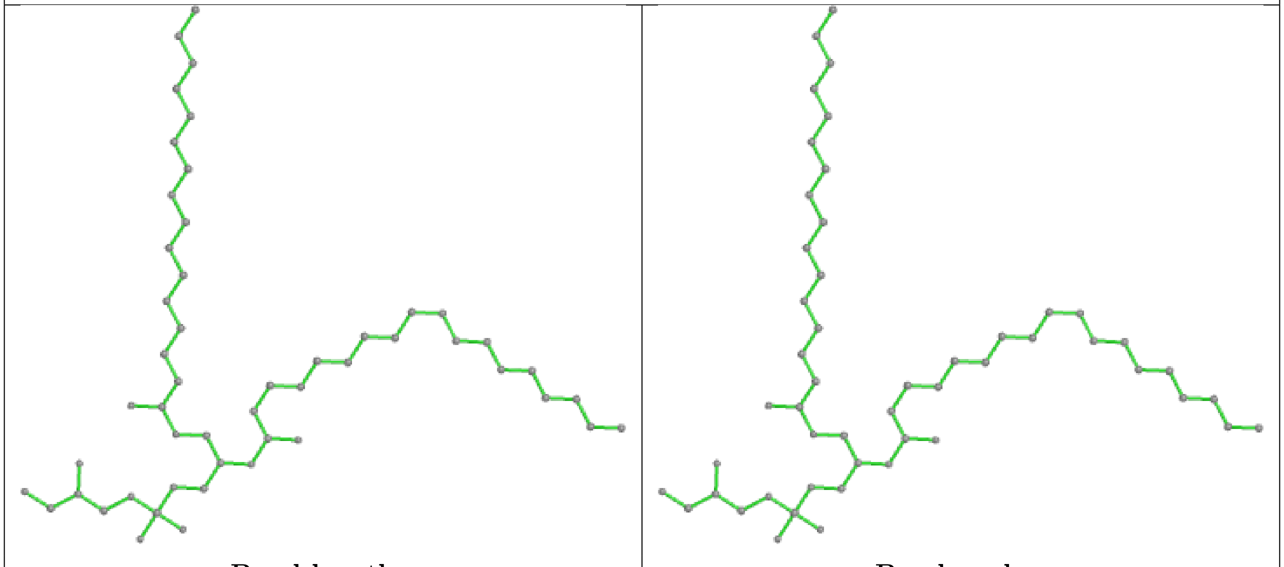
Bond angles



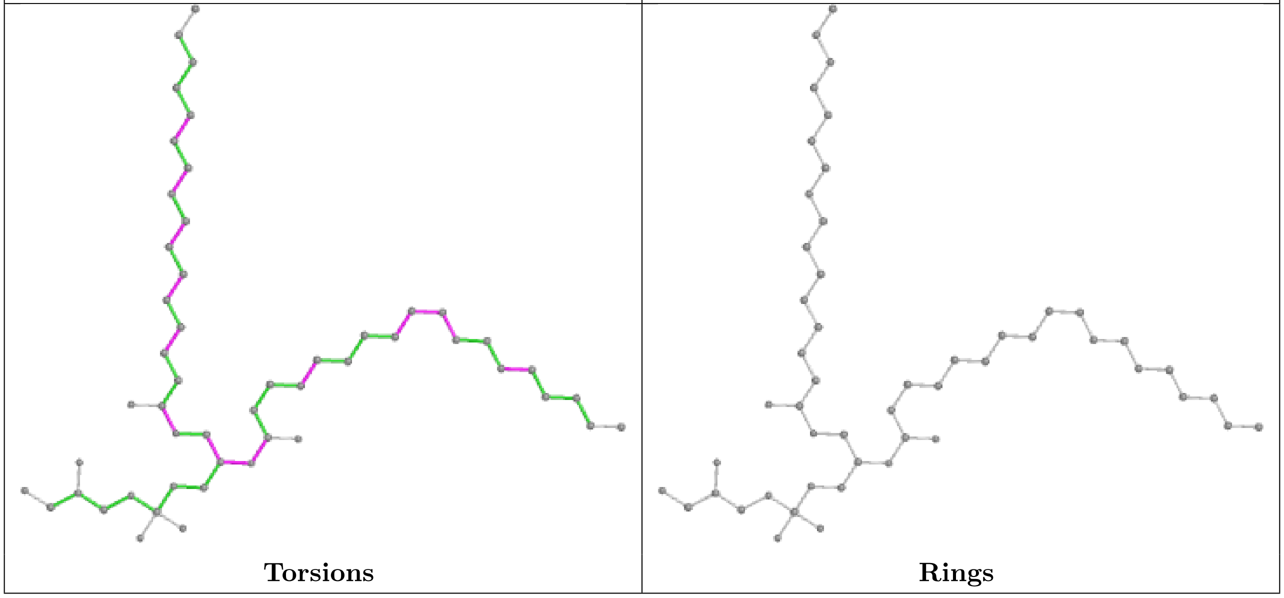
Torsions

Rings

Ligand PGW 3F 101

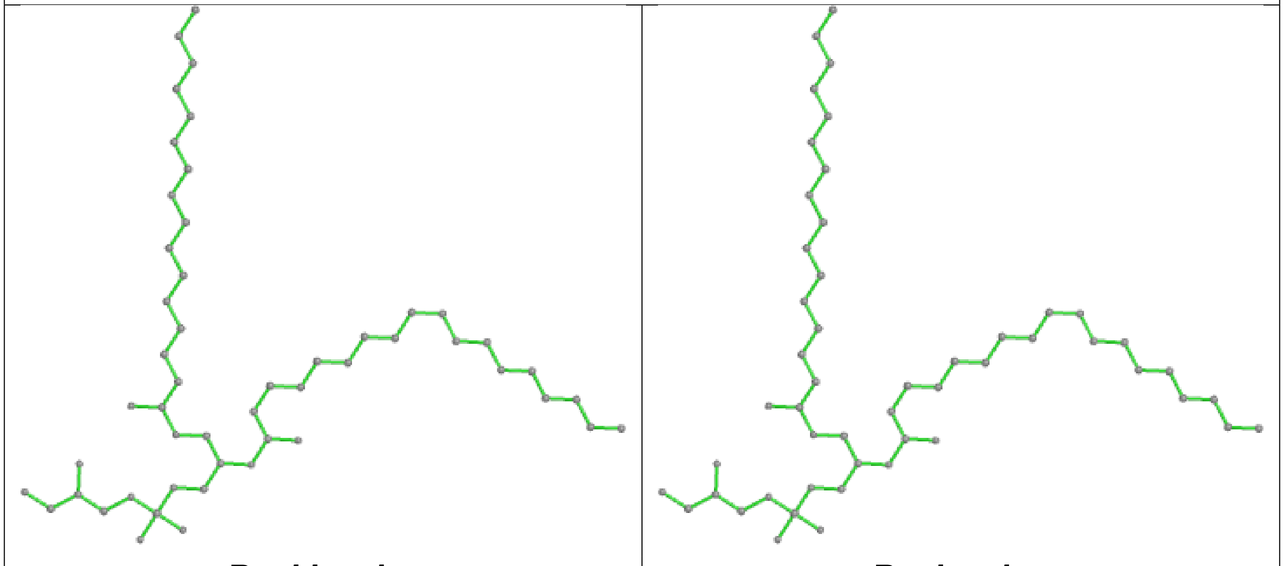


Bond lengths **Bond angles**



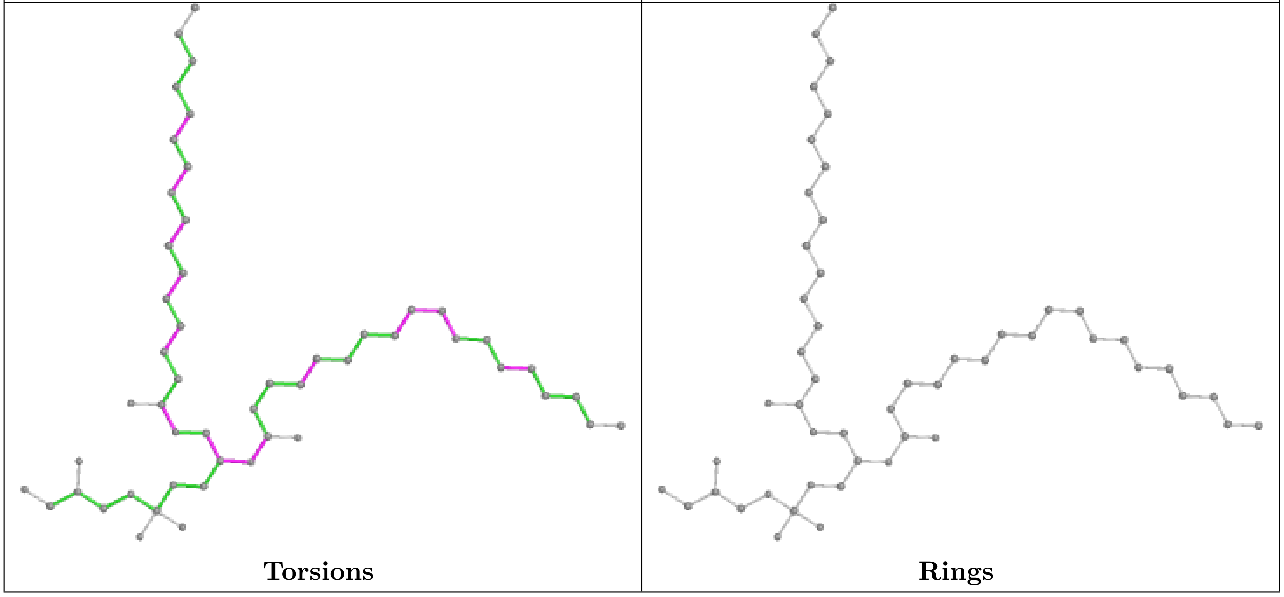
Torsions **Rings**

Ligand PGW 1G 101



Bond lengths

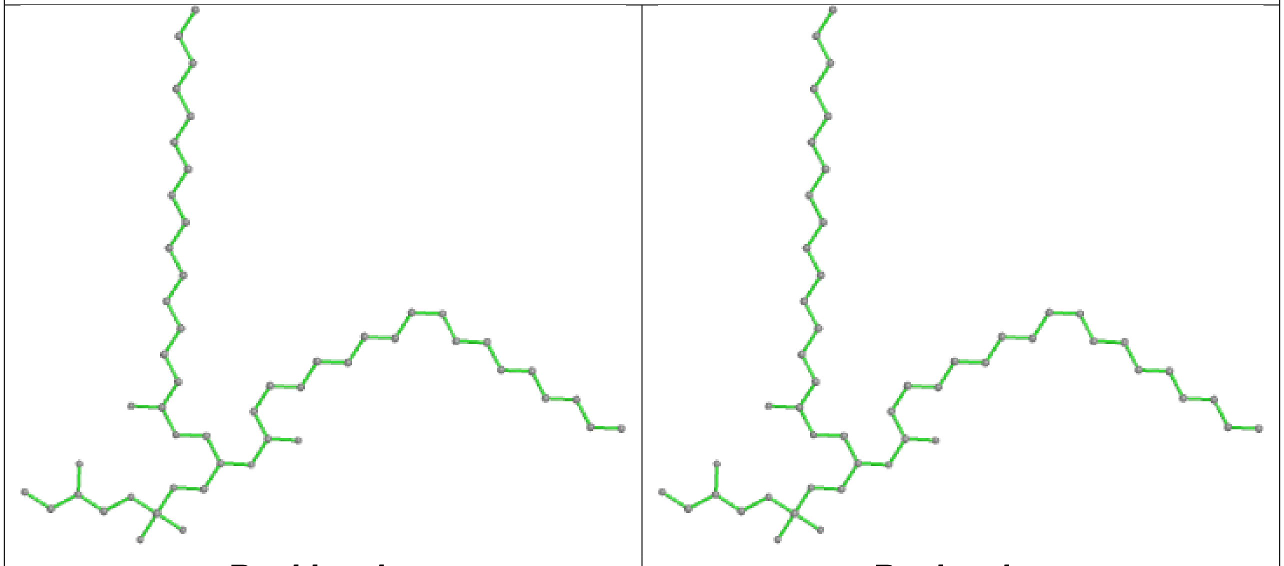
Bond angles



Torsions

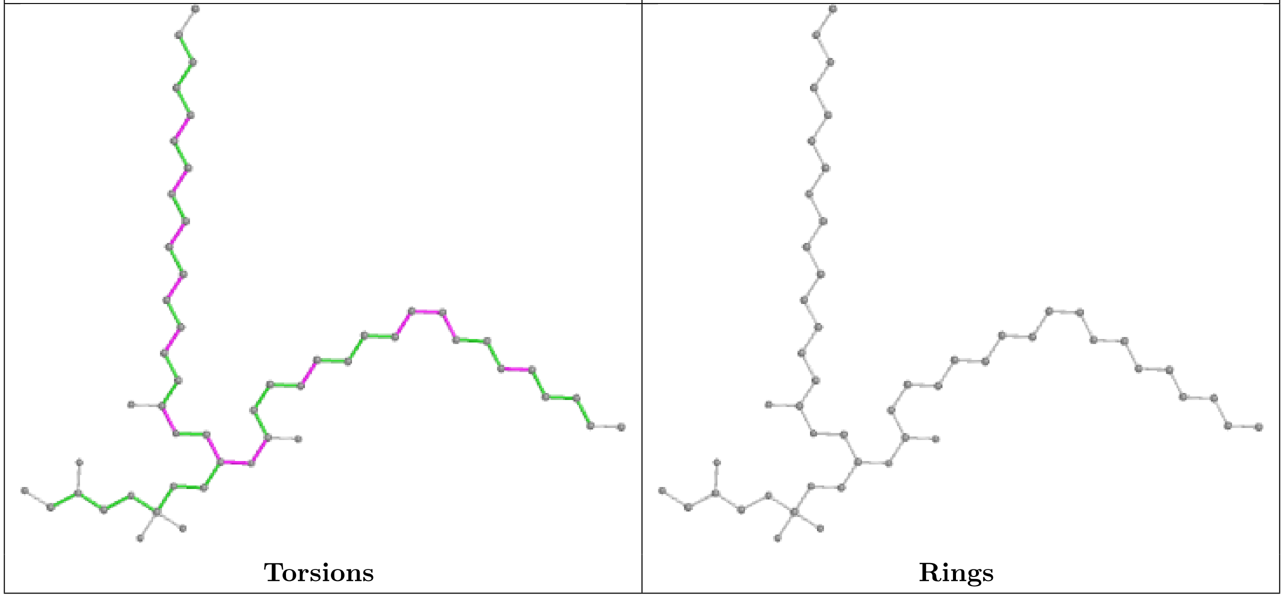
Rings

Ligand PGW 4H 101



Bond lengths

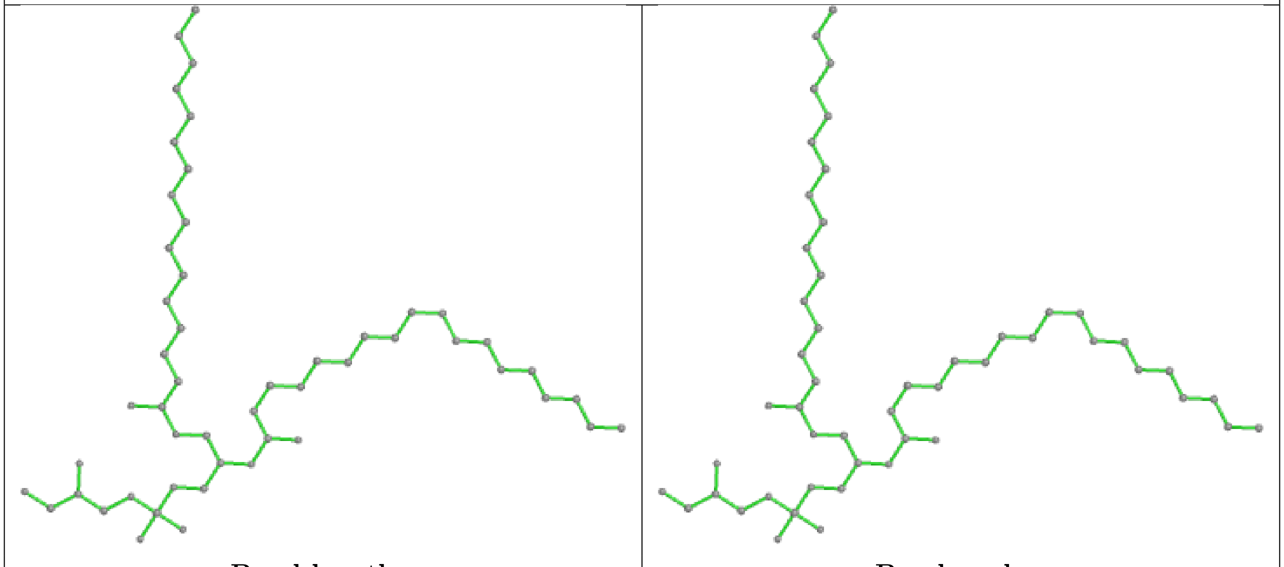
Bond angles



Torsions

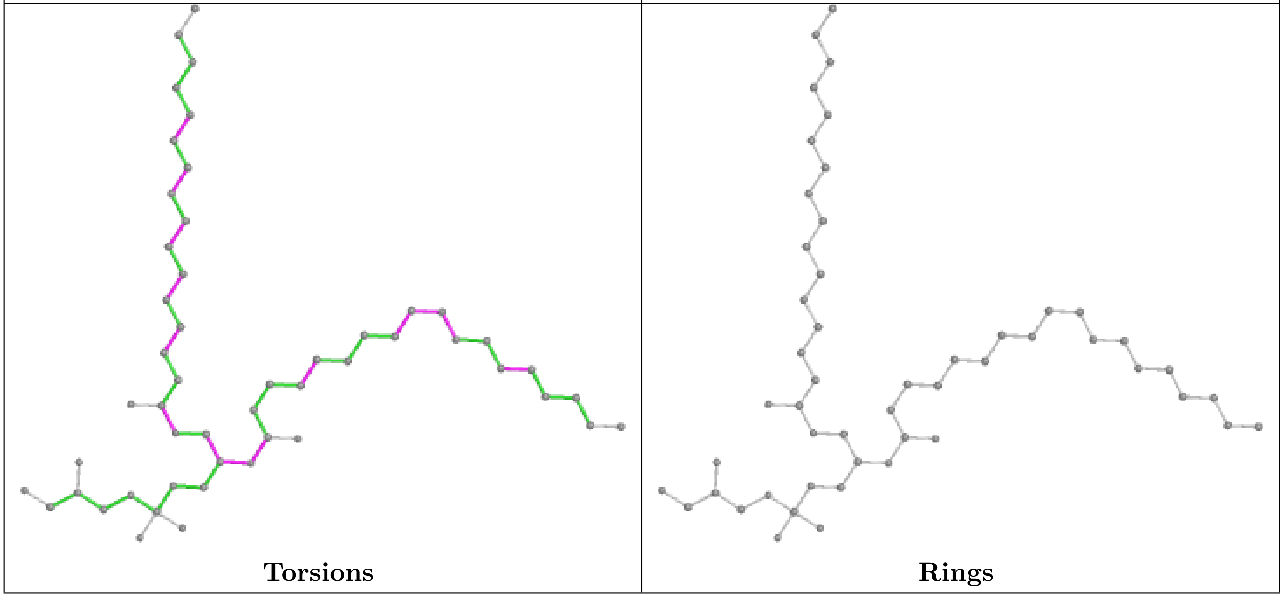
Rings

Ligand PGW 2N 101



Bond lengths

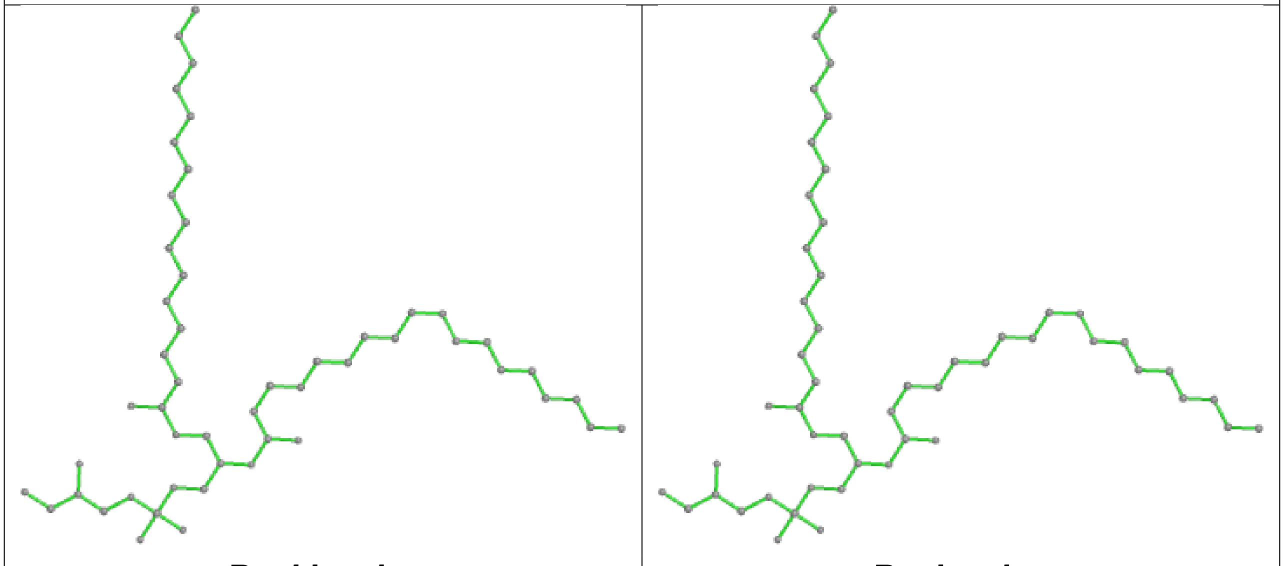
Bond angles



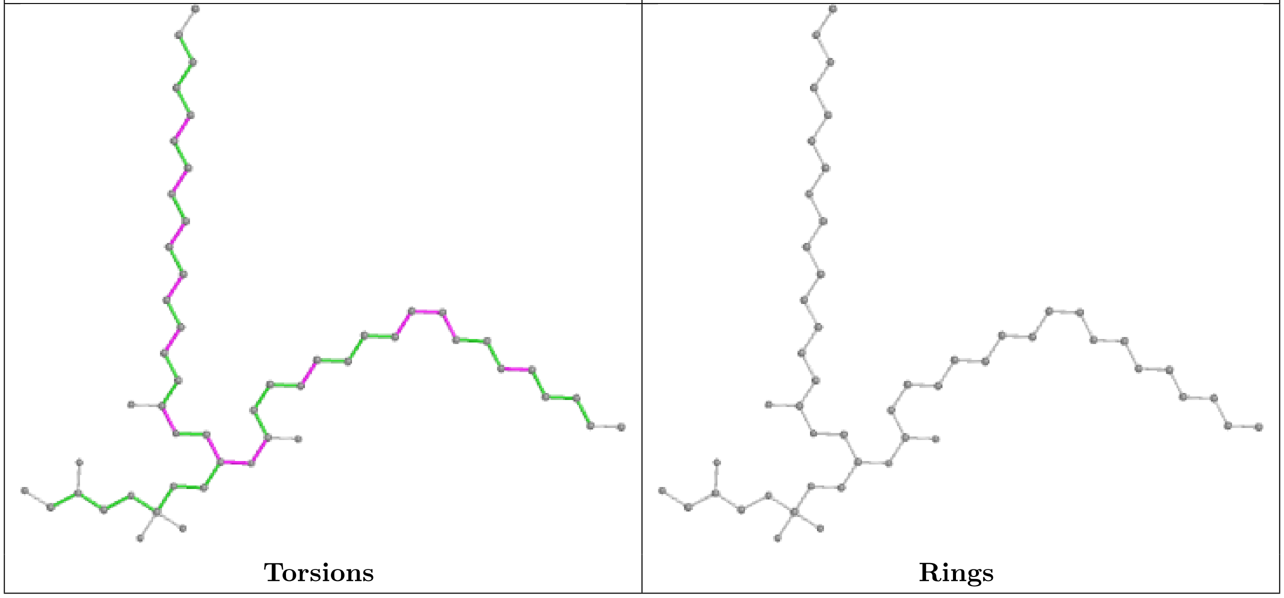
Torsions

Rings

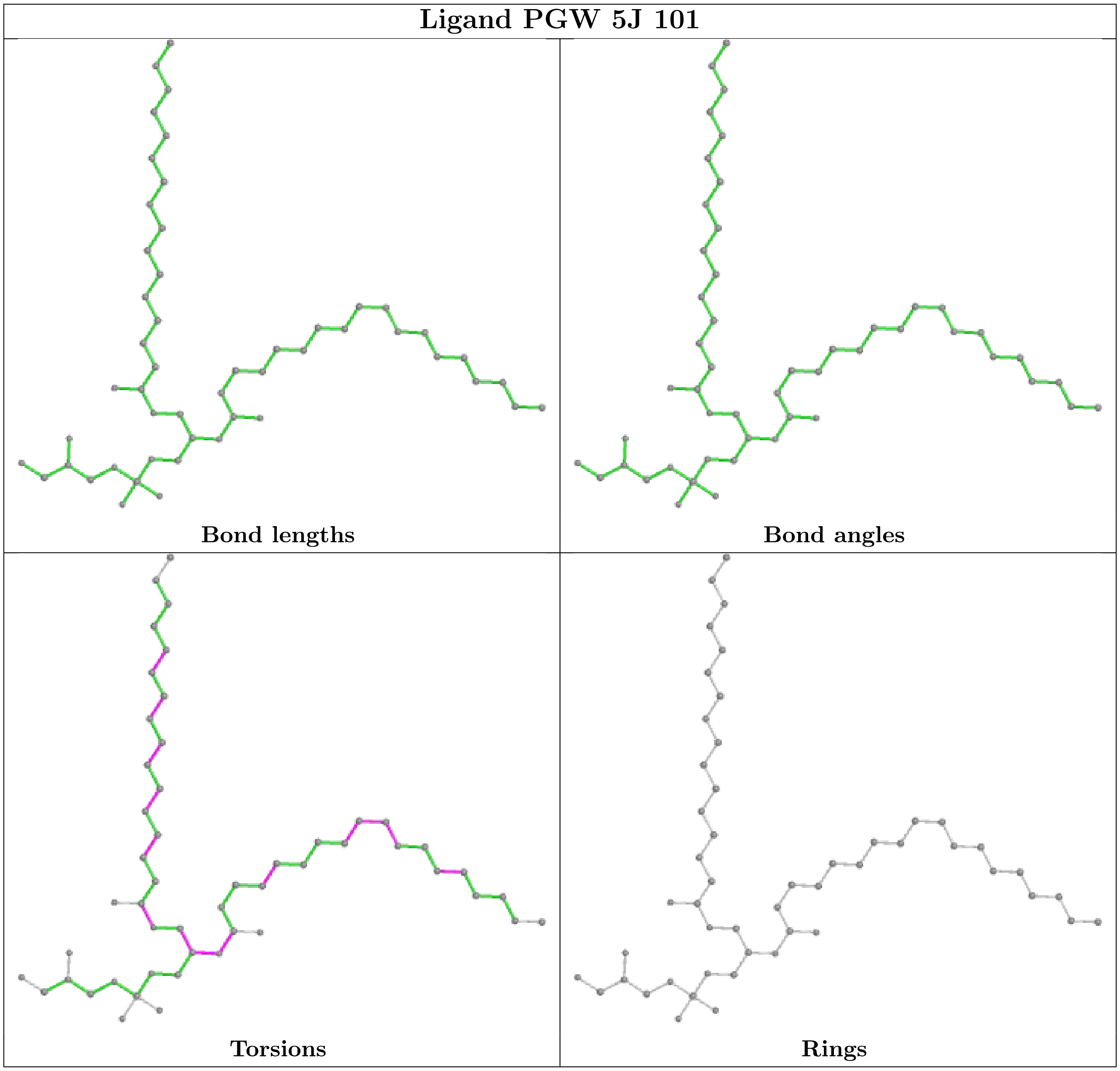
Ligand PGW 4K 101



Bond lengths **Bond angles**



Torsions **Rings**



Ligand PGW 5J 101

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

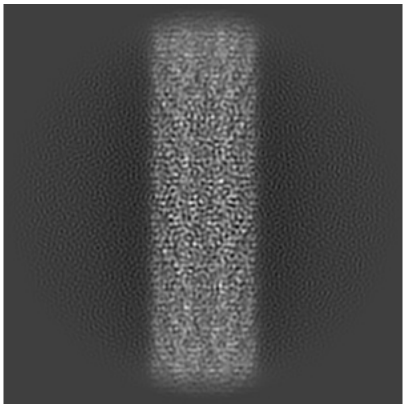
6 Map visualisation

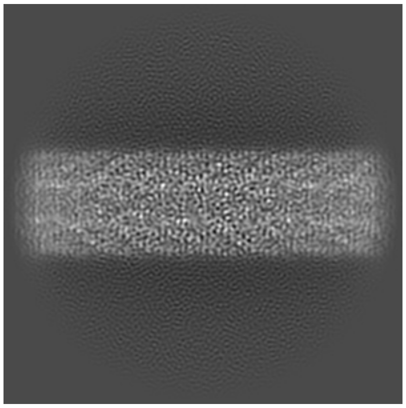
This section contains visualisations of the EMDB entry EMD-27023. These allow visual inspection of the internal detail of the map and identification of artifacts.

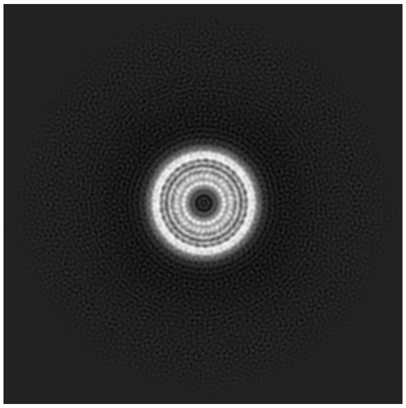
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

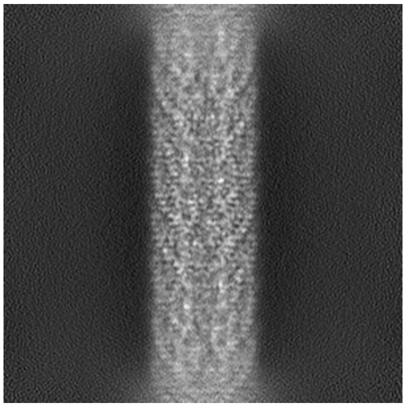
6.1.1 Primary map

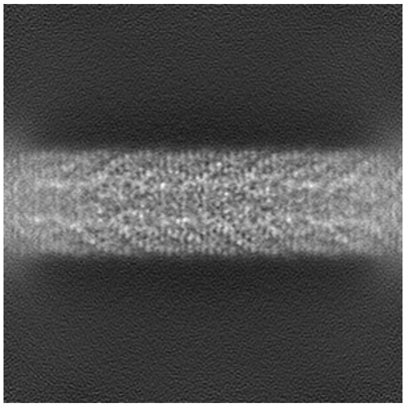

X

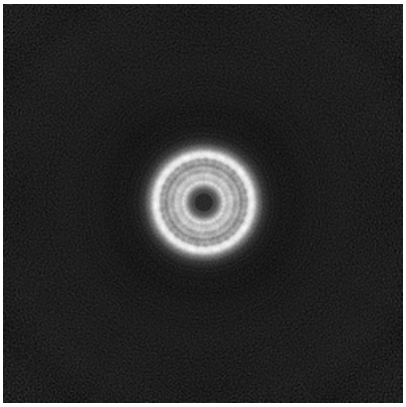

Y


Z

6.1.2 Raw map


X

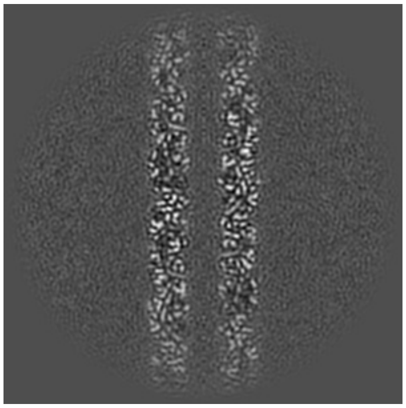

Y


Z

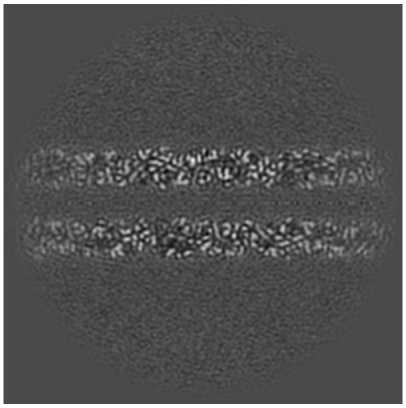
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

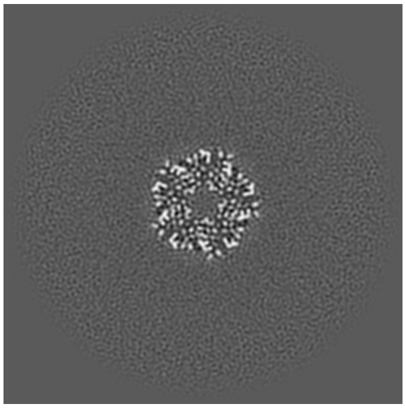
6.2.1 Primary map



X Index: 128

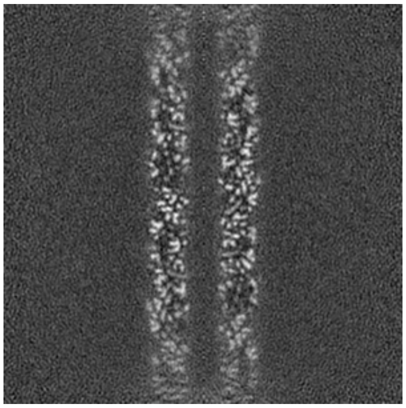


Y Index: 128

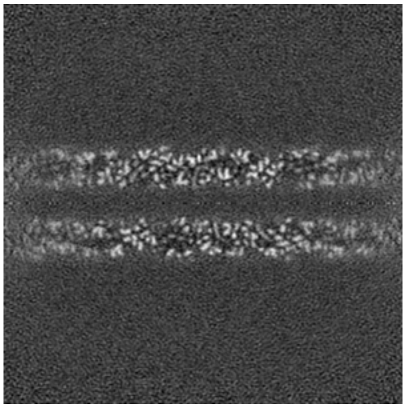


Z Index: 128

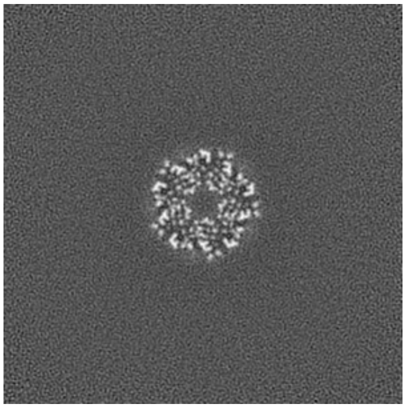
6.2.2 Raw map



X Index: 128



Y Index: 128

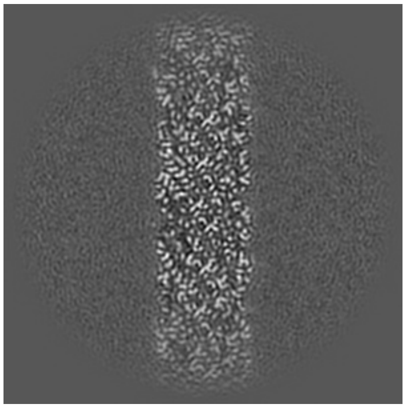


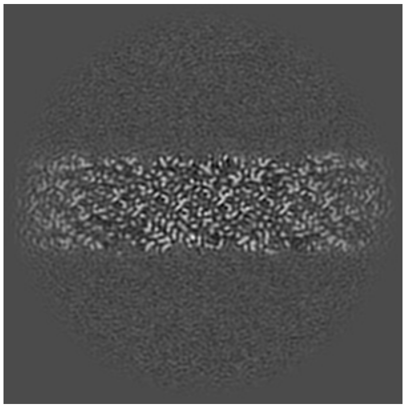
Z Index: 128

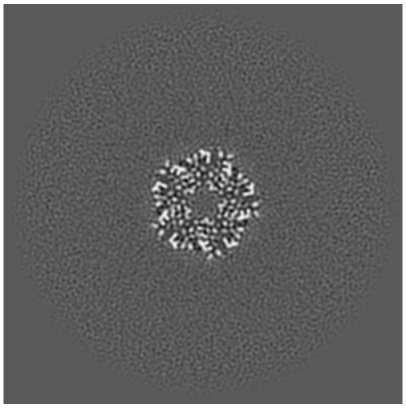
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

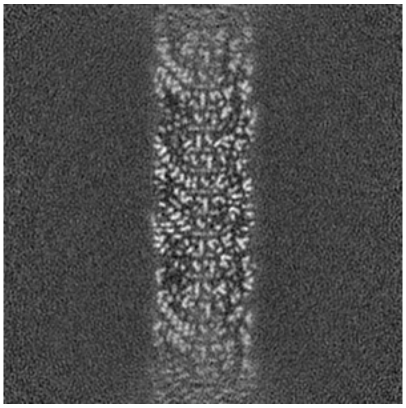
6.3.1 Primary map

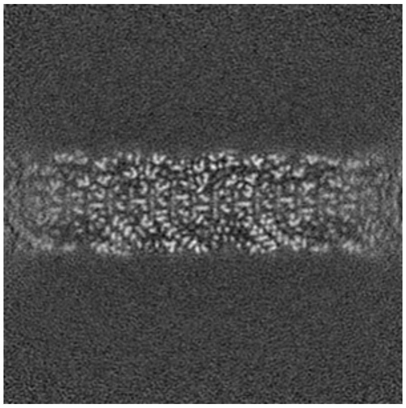

X Index: 112

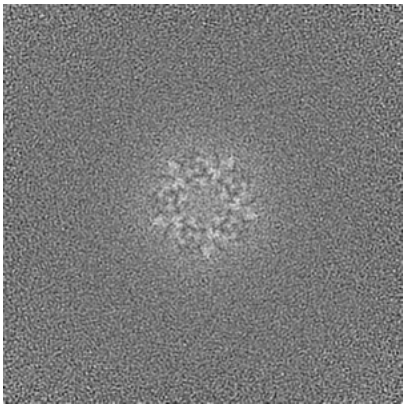

Y Index: 144


Z Index: 128

6.3.2 Raw map


X Index: 115

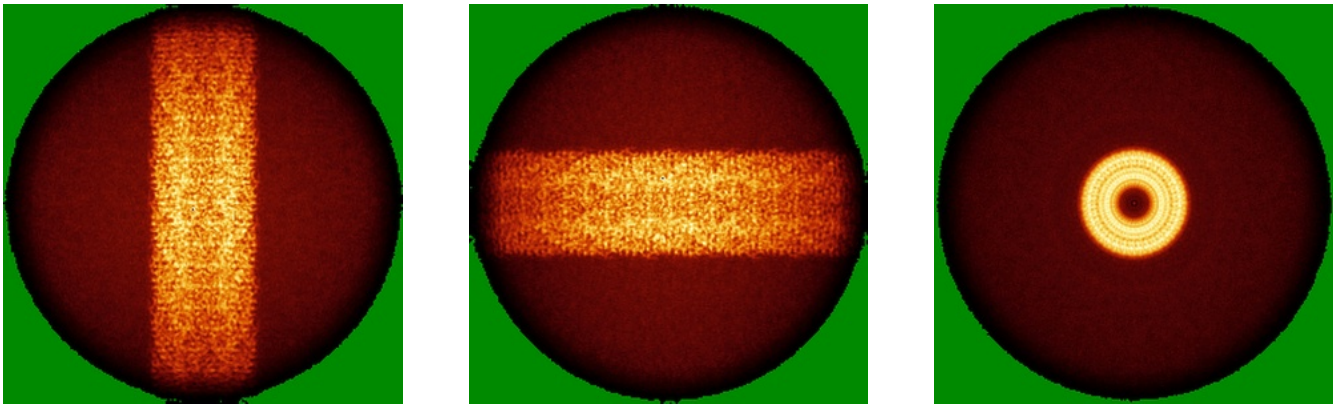

Y Index: 141


Z Index: 0

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

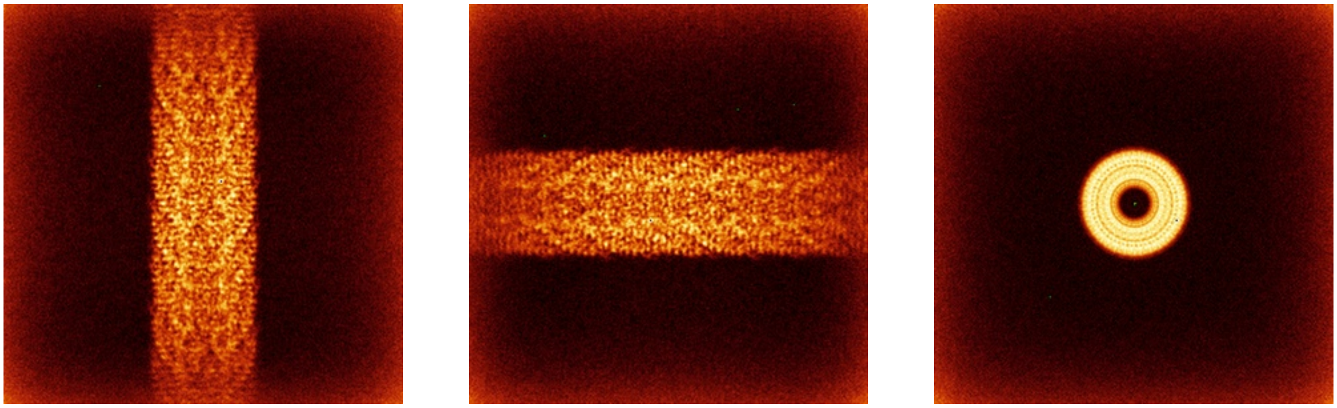
6.4 Orthogonal standard-deviation projections (False-color)

6.4.1 Primary map



X Y Z

6.4.2 Raw map



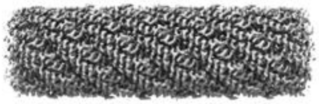
X Y Z

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

6.5 Orthogonal surface views ⓘ

6.5.1 Primary map

X

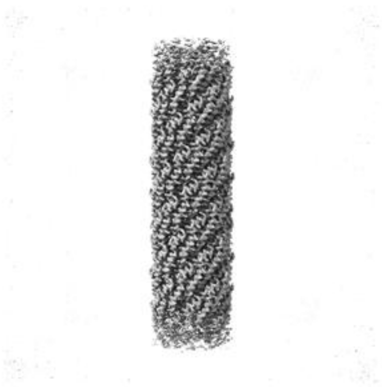


Y

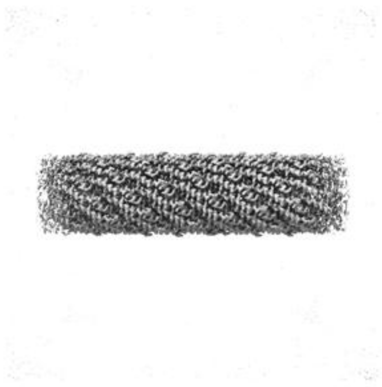
Z

The images above show the 3D surface view of the map at the recommended contour level 0.364. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y

Z

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

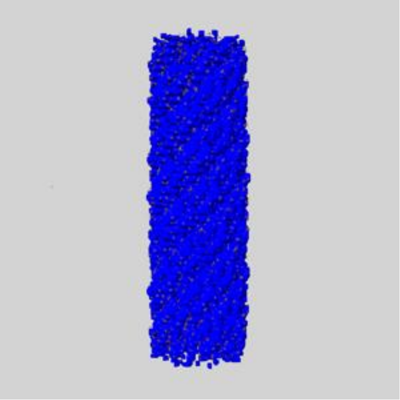
6.6 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

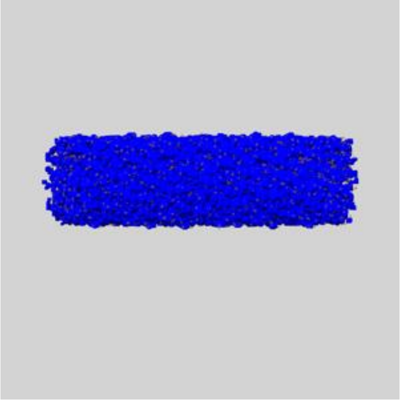
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

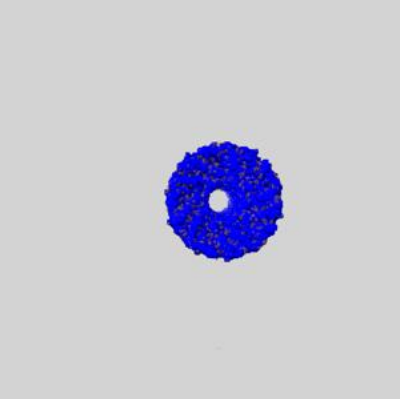
6.6.1 emd_27023_msk_1.map



X



Y

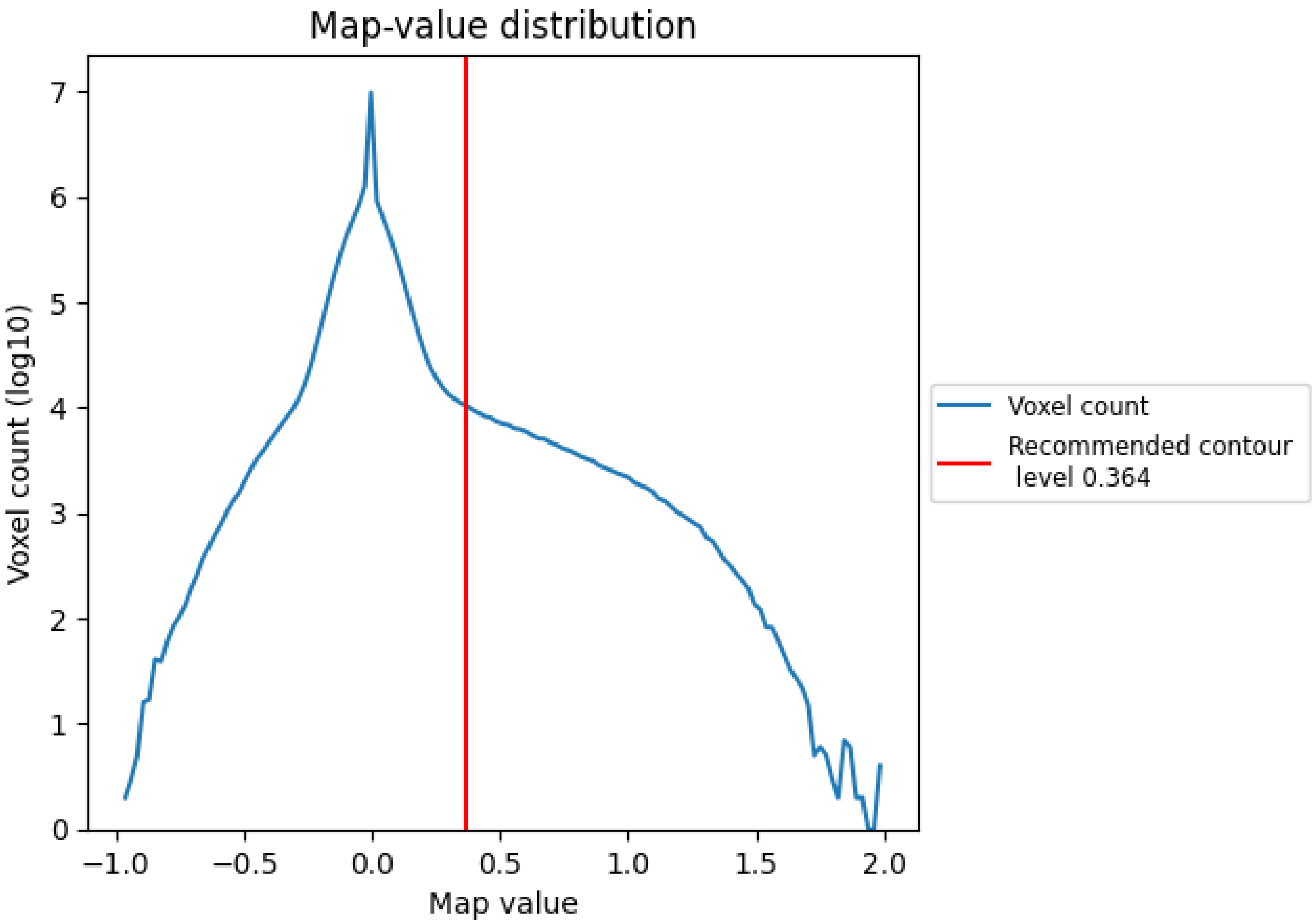


Z

7 Map analysis ⓘ

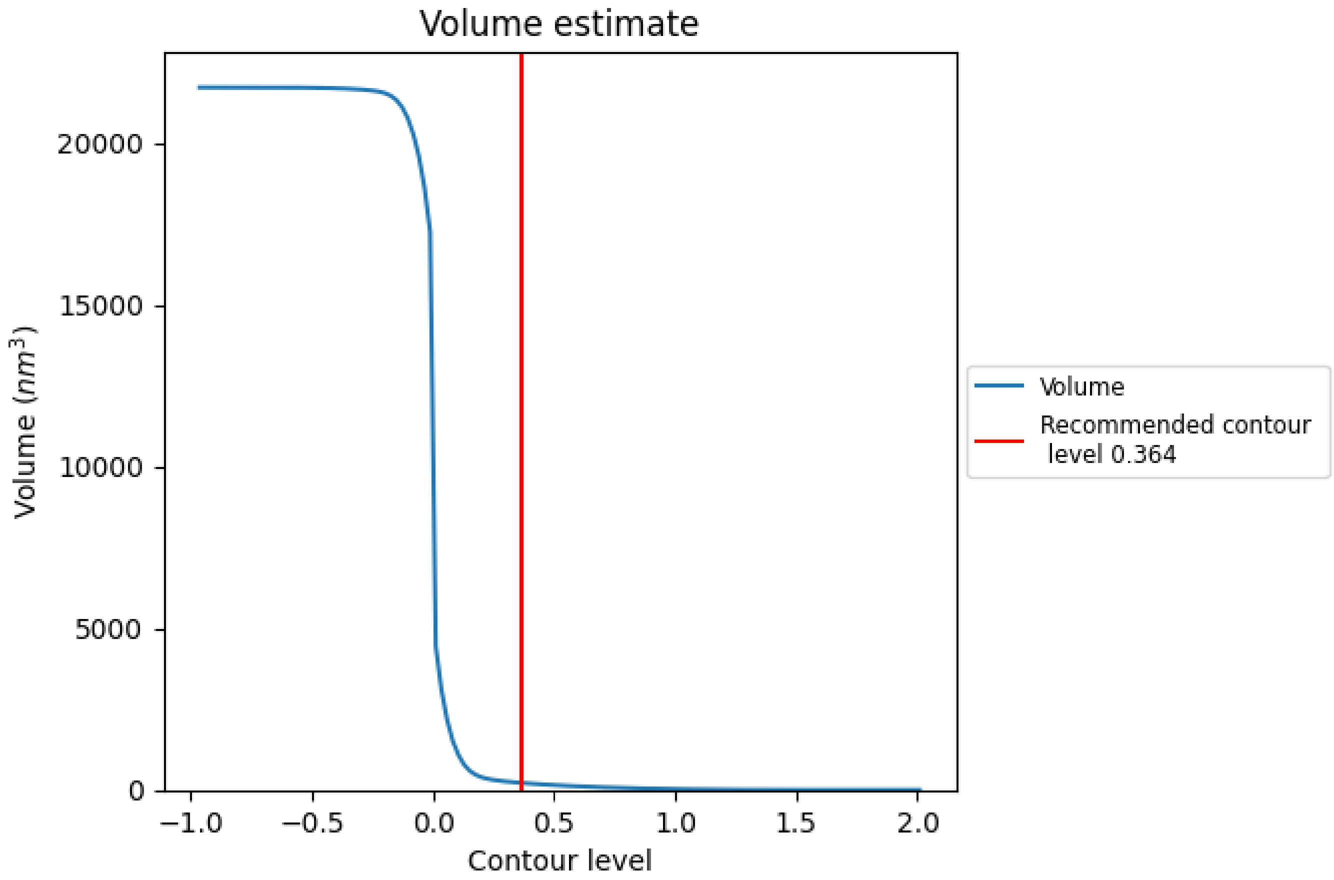
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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.

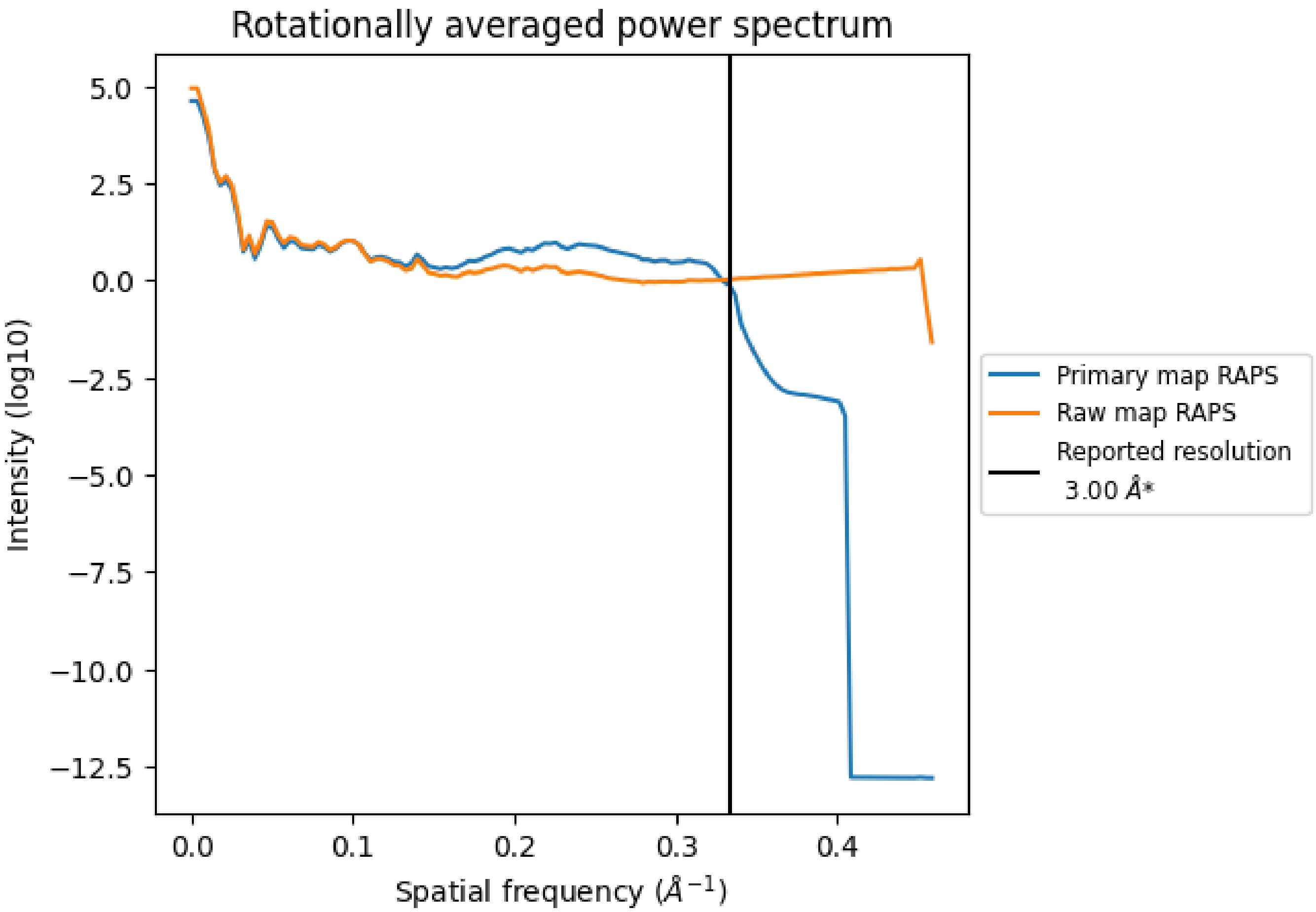
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 217 nm^3; this corresponds to an approximate mass of 196 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 ⓘ

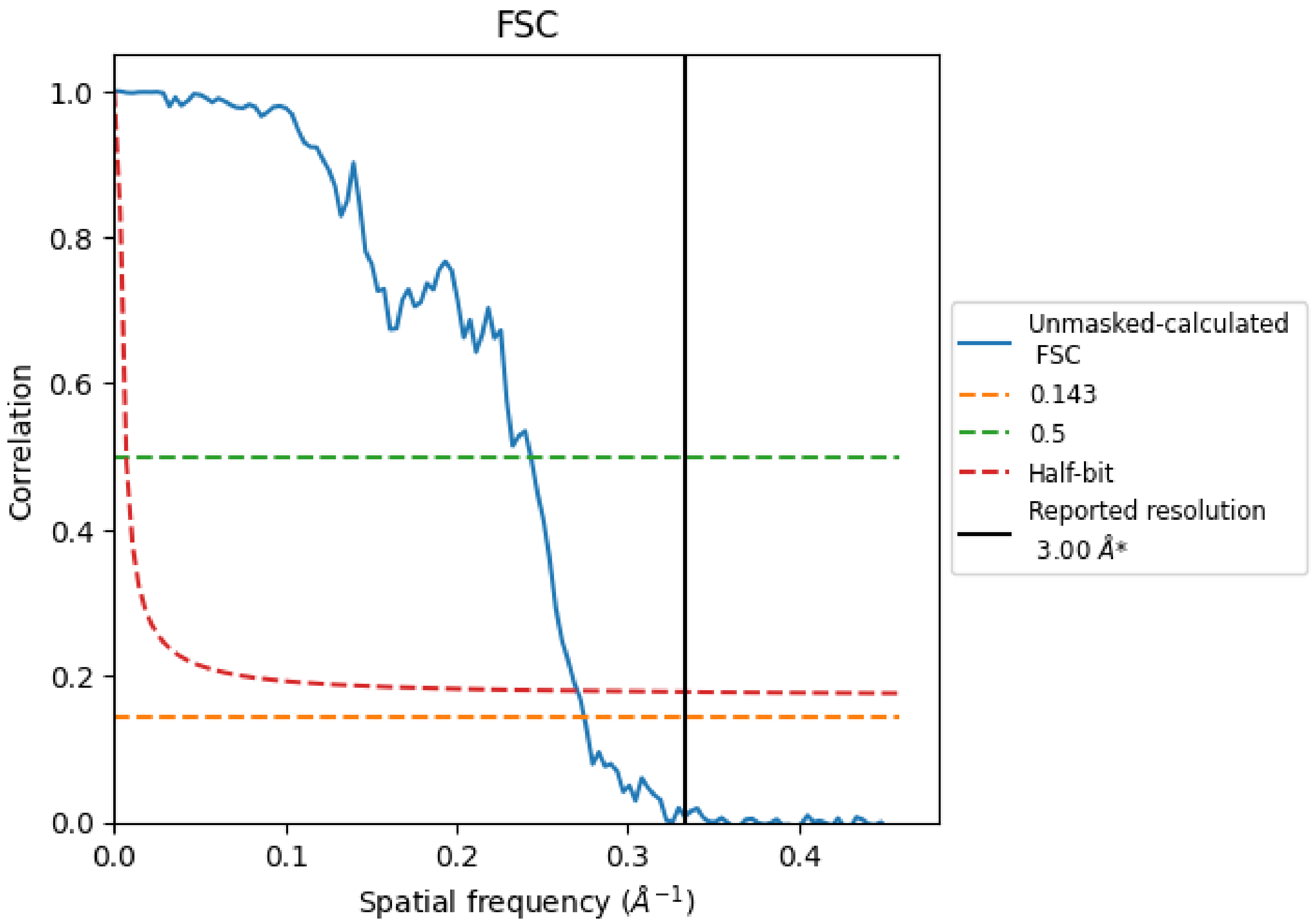


*Reported resolution corresponds to spatial frequency of 0.333 $Å^{-1}$

8 Fourier-Shell correlation ⓘ

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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8.2 Resolution estimates

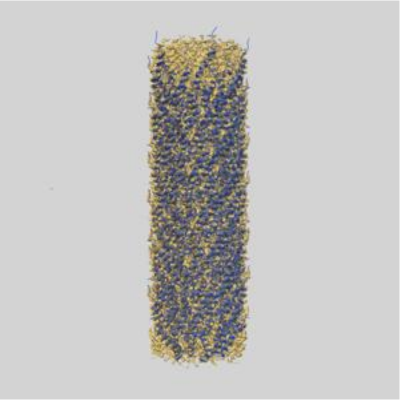
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.64	4.11	3.70

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.64 differs from the reported value 3.0 by more than 10 %

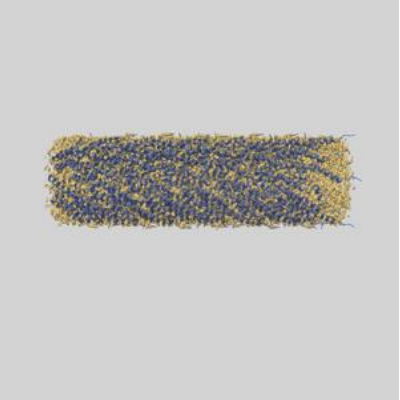
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-27023 and PDB model 8CW4. Per-residue inclusion information can be found in section 3 on page 14.

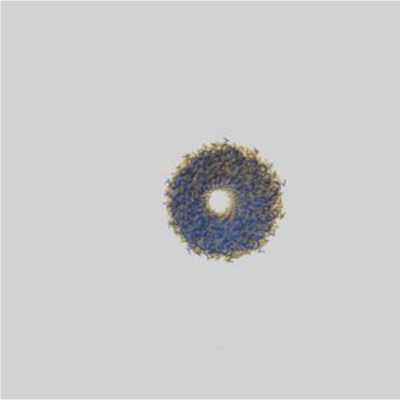
9.1 Map-model overlay (i)



X



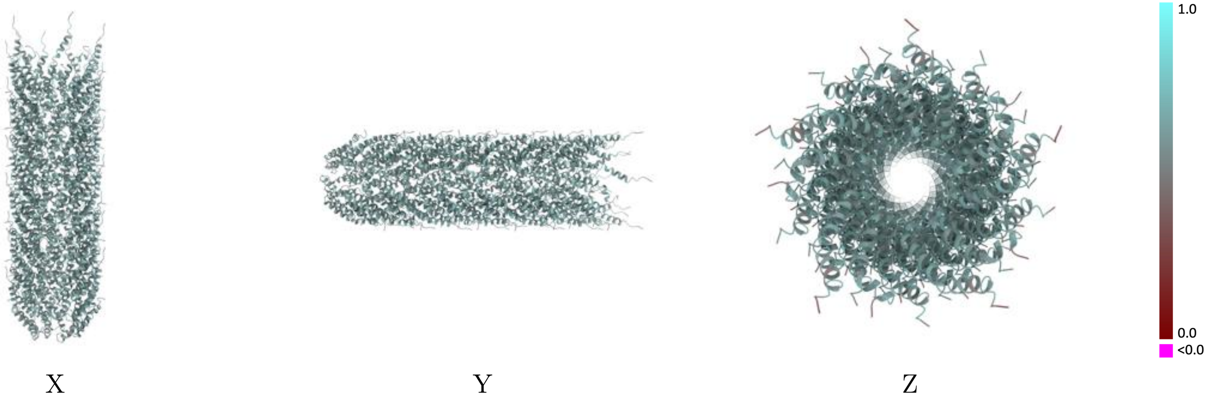
Y



Z

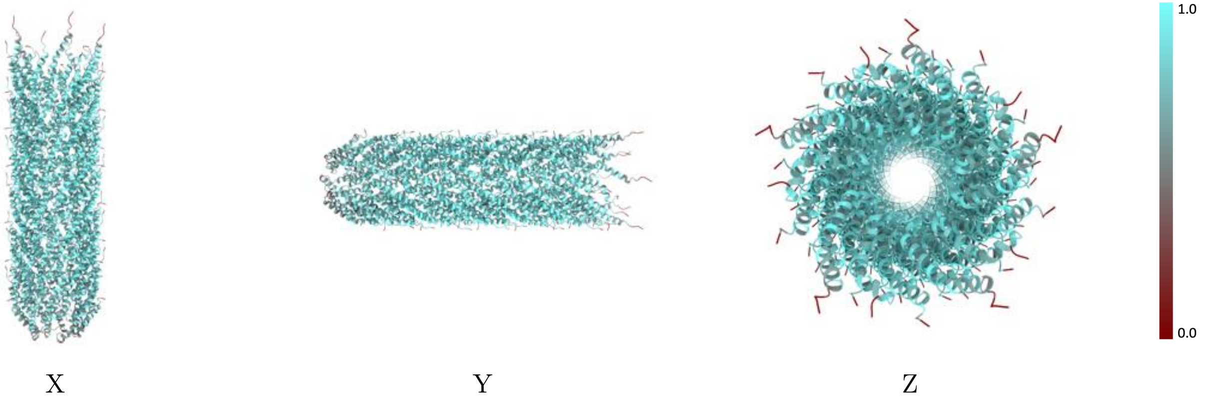
The images above show the 3D surface view of the map at the recommended contour level 0.364 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ



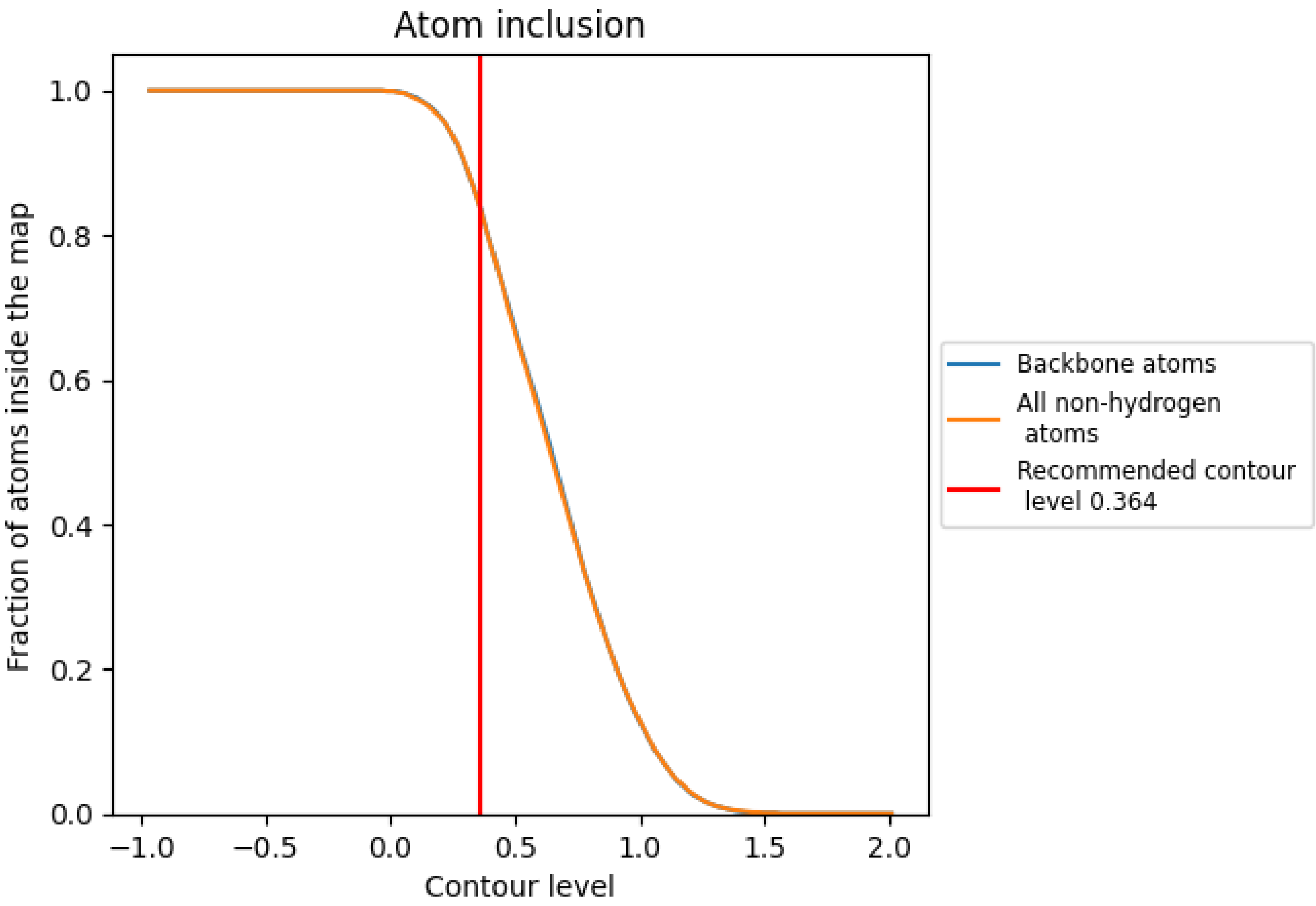
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model ⓘ



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 (0.364).

9.4 Atom inclusion ⓘ



At the recommended contour level, 84% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.364) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8340	0.5930
1A	0.6630	0.5640
1B	0.6910	0.5750
1C	0.8200	0.5930
1D	0.8580	0.5930
1E	0.8880	0.6010
1F	0.8880	0.5970
1G	0.8950	0.6050
1H	0.8990	0.5980
1I	0.8990	0.6030
1J	0.8740	0.5980
1K	0.8850	0.6020
1L	0.8580	0.5970
1M	0.8200	0.5980
1N	0.7550	0.5820
2A	0.6510	0.5630
2B	0.7230	0.5780
2C	0.8020	0.5900
2D	0.8380	0.5890
2E	0.8810	0.6010
2F	0.8880	0.5980
2G	0.9030	0.6060
2H	0.8850	0.5990
2I	0.8940	0.6050
2J	0.8850	0.5990
2K	0.8850	0.6040
2L	0.8540	0.5980
2M	0.8220	0.5960
2N	0.7440	0.5780
3A	0.6630	0.5620
3B	0.7100	0.5760
3C	0.7930	0.5930
3D	0.8370	0.5890
3E	0.8790	0.6010
3F	0.8940	0.6000

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Chain	Atom inclusion	Q-score
3G	0.9010	0.6110
3H	0.8950	0.6020
3I	0.8850	0.6040
3J	0.8850	0.5980
3K	0.8860	0.6020
3L	0.8470	0.5950
3M	0.8340	0.5920
3N	0.7510	0.5800
4A	0.6570	0.5610
4B	0.7100	0.5790
4C	0.7820	0.5890
4D	0.8600	0.5940
4E	0.8790	0.6050
4F	0.8830	0.6010
4G	0.8990	0.6080
4H	0.8950	0.6000
4I	0.8880	0.6040
4J	0.8830	0.5970
4K	0.8850	0.5980
4L	0.8580	0.5970
4M	0.8290	0.5960
4N	0.7410	0.5820
5A	0.6590	0.5640
5B	0.7150	0.5790
5C	0.7690	0.5880
5D	0.8600	0.5940
5E	0.8880	0.6030
5F	0.8880	0.6010
5G	0.9010	0.6060
5H	0.8950	0.5960
5I	0.8950	0.6040
5J	0.8810	0.5970
5K	0.8790	0.5990
5L	0.8450	0.5970
5M	0.8270	0.5970
5N	0.7510	0.5810