wwPDB EM Validation Summary Report (i)

May 29, 2024 – 11:04 AM EDT

PDB ID	:	2BRD
Title	:	CRYSTAL STRUCTURE OF BACTERIORHODOPSIN IN PURPLE MEMBRANE
Authors	:	Henderson, R.; Grigorieff, N.
Deposited on	:	1995-12-27
Resolution	:	3.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

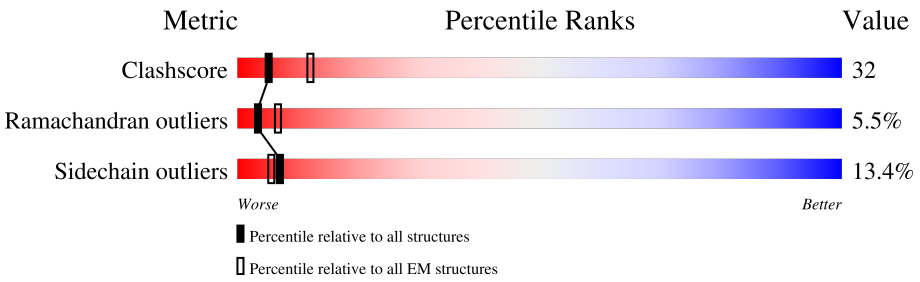
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 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%

Mol	Chain	Length	Quality of chain
1	A	248	39% 41% 9% • 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	RET	A	271	-	-	X	-

2 Entry composition (i)

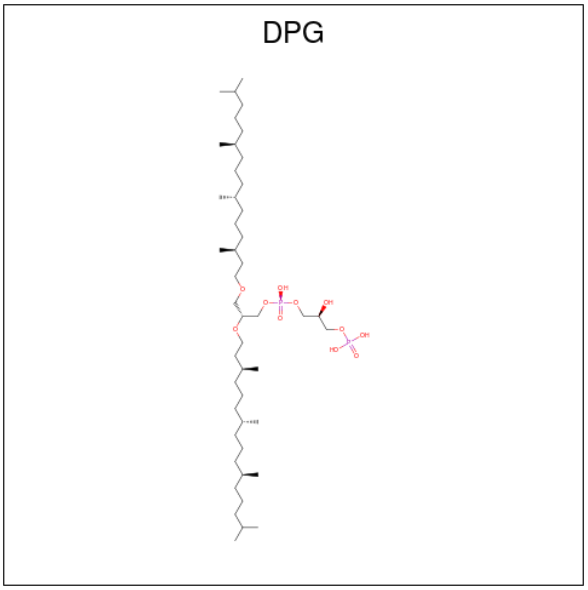
There are 3 unique types of molecules in this entry. The entry contains 2328 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called BACTERIORHODOPSIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	222	1718	1154	263	292	9	0	1

- Molecule 2 is PHOSPHORIC ACID 2,3-BIS-(3,7,11,15-TETRAMETHYL-HEXADECYLOXY)-PROPYL ESTER 2-HYDROXO-3-PHOSPHONOOXY-PROPYL ESTER (three-letter code: DPG) (formula: $C_{46}H_{96}O_{11}P_2$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
2	A	1	59	46	11	2	0
2	A	1	59	46	11	2	0
2	A	1	59	46	11	2	0
2	A	1	59	46	11	2	0
2	A	1	59	46	11	2	0

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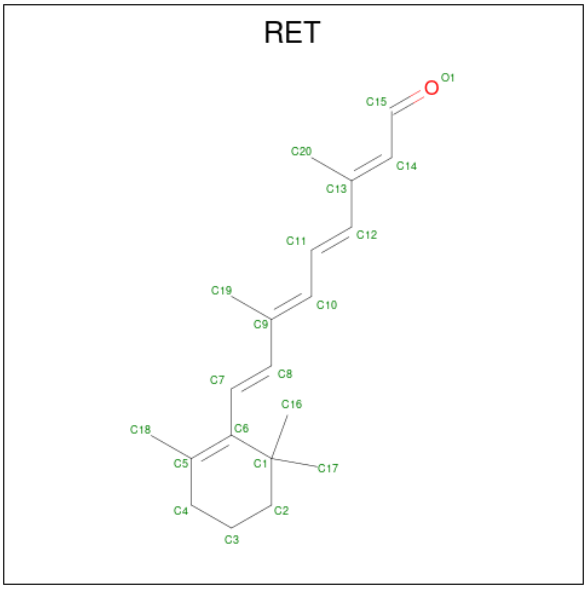
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
2	A	1	59	46	11	2	0
2	A	1	59	46	11	2	0
2	A	1	59	46	11	2	0
2	A	1	59	46	11	2	0
2	A	1	59	46	11	2	0

- Molecule 3 is RETINAL (three-letter code: RET) (formula: $C_{20}H_{28}O$).



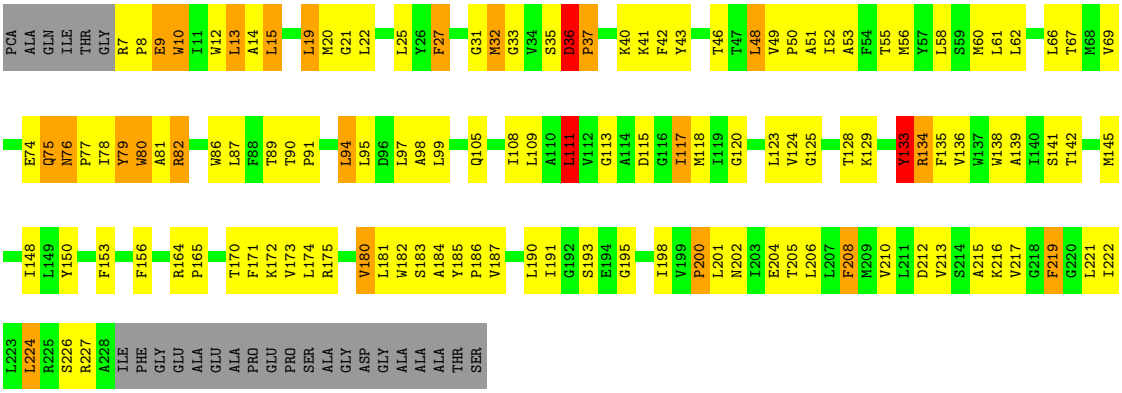
Mol	Chain	Residues	Atoms		AltConf
			Total	C	
3	A	1	20	20	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: BACTERIORHODOPSIN

Chain A: 39% 41% 9% • 10%



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α, β, γ	62.45Å 62.45Å 100.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.50	Depositor
% Data completeness (in resolution range)	85.4 (30.00-3.50)	Depositor
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.280 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2328	wwPDB-VP
Average B, all atoms (Å^2)	114.0	wwPDB-VP

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: DPG, RET

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.67	0/1765	1.23	8/2412 (0.3%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	133	TYR	CA-CB-CG	7.68	128.00	113.40
1	A	80	TRP	CA-CB-CG	7.50	127.94	113.70
1	A	153	PHE	CA-CB-CG	5.87	128.00	113.90
1	A	111	LEU	CB-CA-C	5.47	120.58	110.20
1	A	134	ARG	NE-CZ-NH1	5.32	122.96	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1718	0	1774	118	0
2	A	590	0	930	68	0
3	A	20	0	27	11	0
All	All	2328	0	2731	163	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 32.

The worst 5 of 163 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)
2:A:265:DPG:H42	2:A:265:DPG:C3	1.60	1.32
2:A:265:DPG:C4	2:A:265:DPG:H31	1.63	1.26
2:A:263:DPG:H412	2:A:263:DPG:O3	1.36	1.09
3:A:271:RET:H8	3:A:271:RET:H161	1.20	1.09
3:A:271:RET:H161	3:A:271:RET:C8	1.97	0.93

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	220/248 (89%)	168 (76%)	40 (18%)	12 (6%)	2 17

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	32	MET
1	A	193	SER
1	A	200	PRO
1	A	9	GLU
1	A	33	GLY

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	179/193 (93%)	155 (87%)	24 (13%)	4 21

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	LYS
1	A	150	TYR
1	A	136	VAL
1	A	202	ASN
1	A	48	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

11 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	DPG	A	263	-	58,58,58	0.91	1 (1%)	67,73,73	1.03	5 (7%)
2	DPG	A	265	-	58,58,58	0.91	1 (1%)	67,73,73	1.04	3 (4%)
2	DPG	A	267	-	58,58,58	0.91	1 (1%)	67,73,73	1.08	4 (5%)
3	RET	A	271	1	20,20,21	1.39	3 (15%)	27,27,28	0.83	0
2	DPG	A	268	-	58,58,58	0.91	1 (1%)	67,73,73	1.07	5 (7%)
2	DPG	A	270	-	58,58,58	0.91	1 (1%)	67,73,73	1.05	4 (5%)
2	DPG	A	266	-	58,58,58	0.90	1 (1%)	67,73,73	0.95	2 (2%)
2	DPG	A	261	-	58,58,58	0.90	1 (1%)	67,73,73	1.02	3 (4%)
2	DPG	A	269	-	58,58,58	0.91	1 (1%)	67,73,73	0.96	3 (4%)
2	DPG	A	262	-	58,58,58	0.90	1 (1%)	67,73,73	1.02	5 (7%)
2	DPG	A	264	-	58,58,58	0.90	1 (1%)	67,73,73	1.04	3 (4%)

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	DPG	A	263	-	-	18/67/67/67	-
2	DPG	A	265	-	-	22/67/67/67	-
2	DPG	A	267	-	-	28/67/67/67	-
3	RET	A	271	1	-	0/13/30/31	0/1/1/1
2	DPG	A	268	-	-	25/67/67/67	-
2	DPG	A	270	-	-	28/67/67/67	-
2	DPG	A	266	-	-	28/67/67/67	-
2	DPG	A	261	-	-	28/67/67/67	-
2	DPG	A	269	-	-	29/67/67/67	-
2	DPG	A	262	-	-	23/67/67/67	-
2	DPG	A	264	-	-	29/67/67/67	-

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	271	RET	C14-C13	4.28	1.37	1.33
3	A	271	RET	C2-C3	-2.92	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	271	RET	C15-C14	-2.59	1.39	1.49
2	A	262	DPG	C4-C5	2.31	1.59	1.51
2	A	270	DPG	C4-C5	2.29	1.59	1.51

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	261	DPG	C21-C22-C23	3.42	126.98	115.92
2	A	264	DPG	C21-C22-C23	3.40	126.90	115.92
2	A	270	DPG	C21-C22-C23	2.88	125.23	115.92
2	A	262	DPG	C21-C22-C23	2.71	124.68	115.92
2	A	265	DPG	O2-C41-C42	-2.69	103.11	108.77

There are no chirality outliers.

5 of 258 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	261	DPG	O6-C4-C5-C6
2	A	261	DPG	C5-C4-O6-P1
2	A	261	DPG	C11-C12-C13-C14
2	A	261	DPG	C21-C22-C23-C24
2	A	261	DPG	C3-O3-P1-O4

There are no ring outliers.

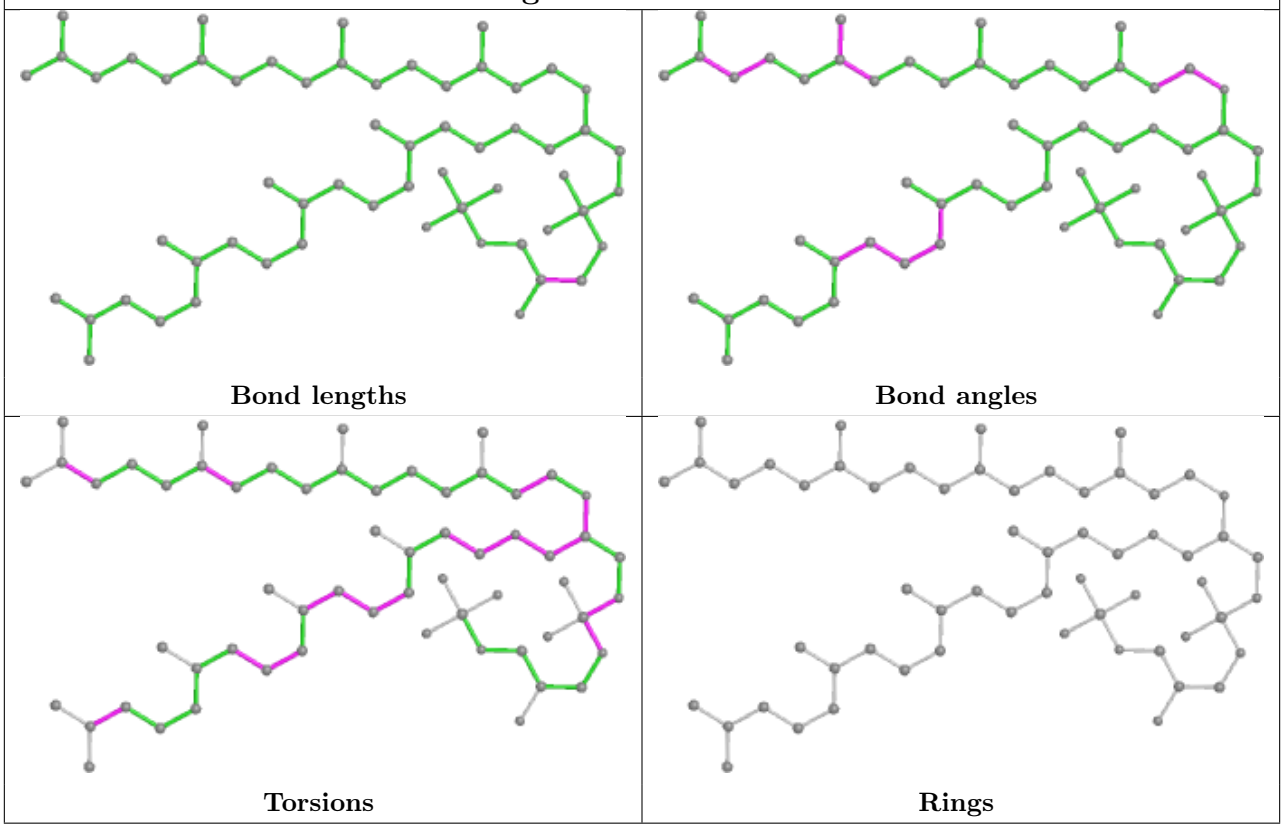
11 monomers are involved in 79 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	263	DPG	11	0
2	A	265	DPG	11	0
2	A	267	DPG	13	0
3	A	271	RET	11	0
2	A	268	DPG	11	0
2	A	270	DPG	1	0
2	A	266	DPG	12	0
2	A	261	DPG	5	0
2	A	269	DPG	6	0
2	A	262	DPG	11	0
2	A	264	DPG	5	0

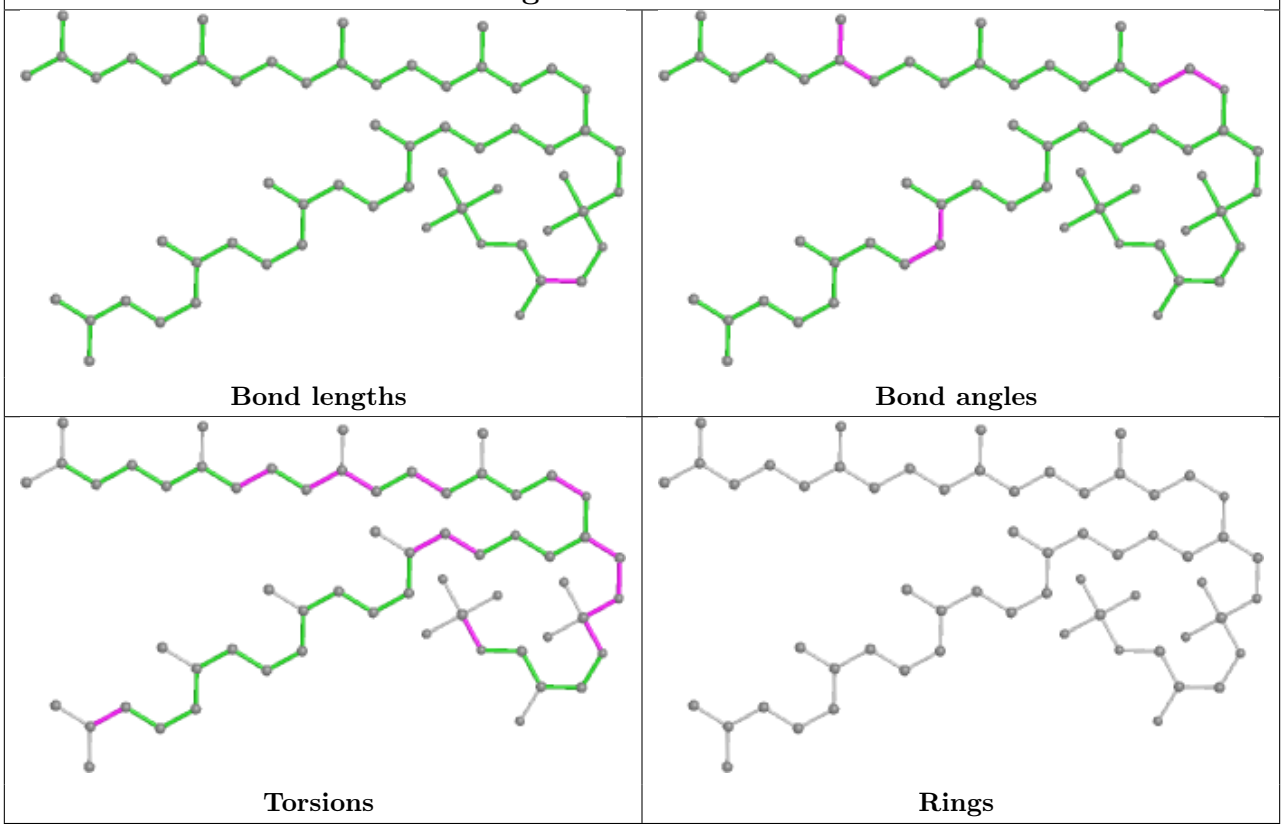
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

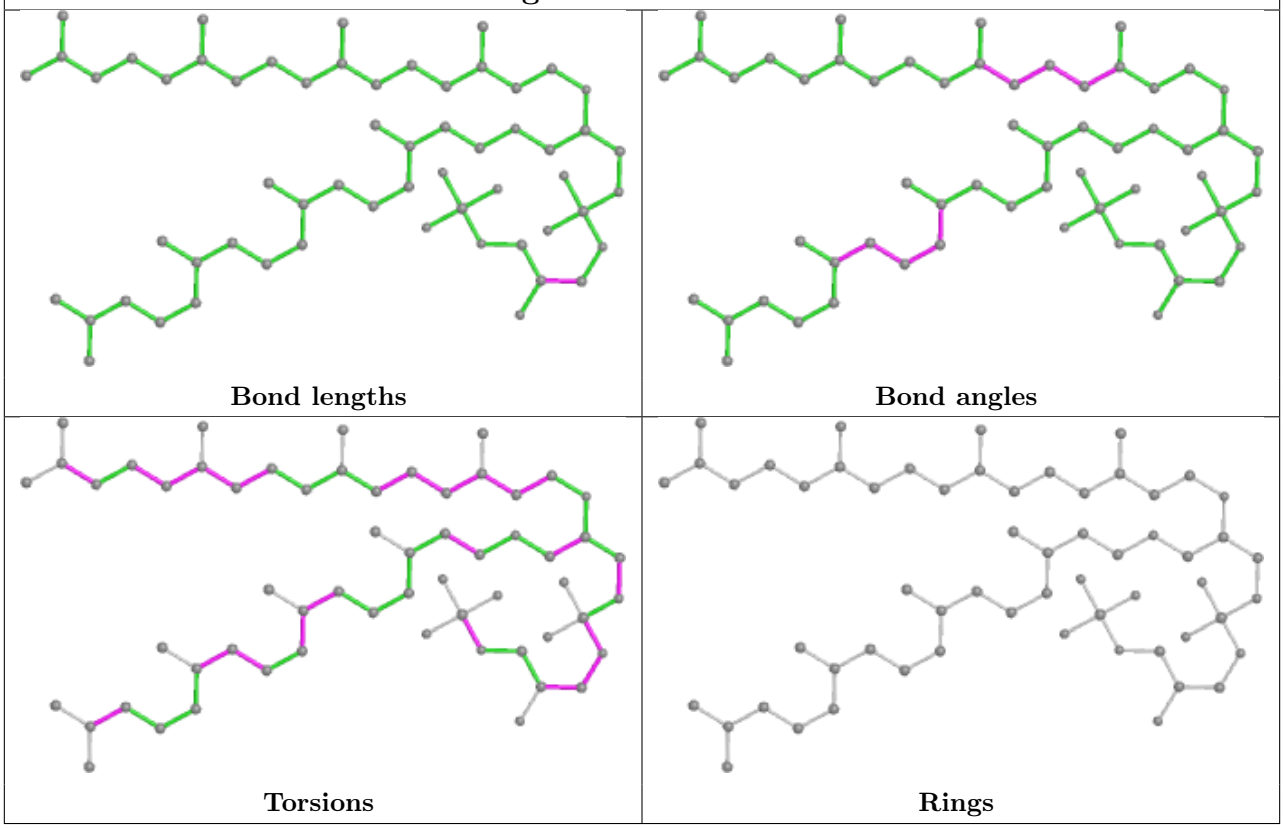
Ligand DPG A 263



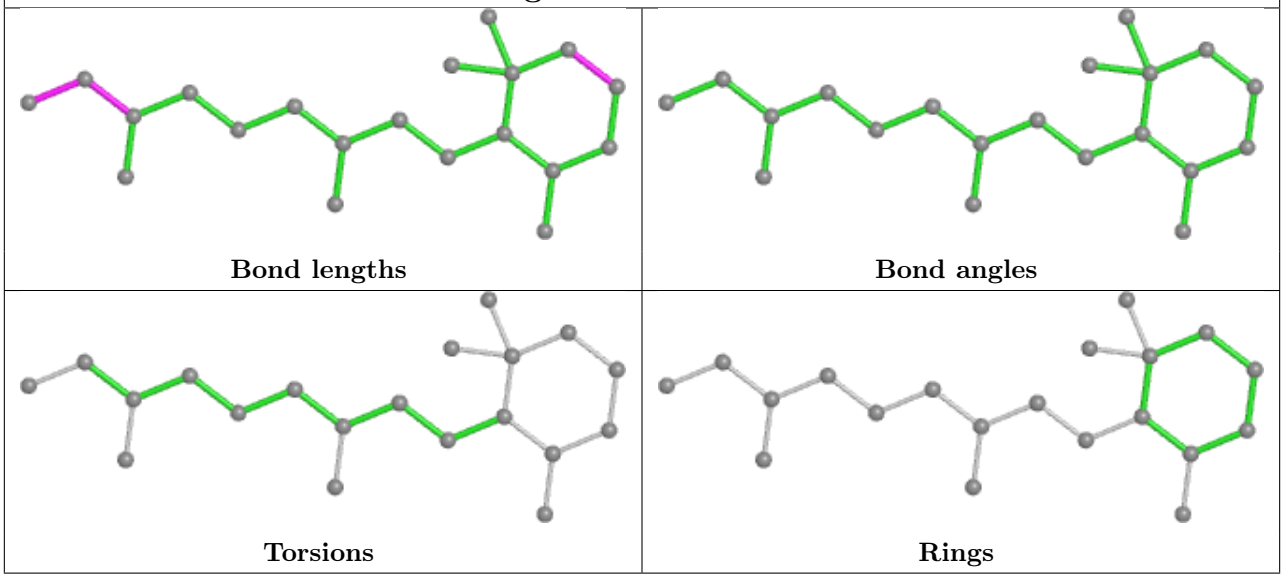
Ligand DPG A 265



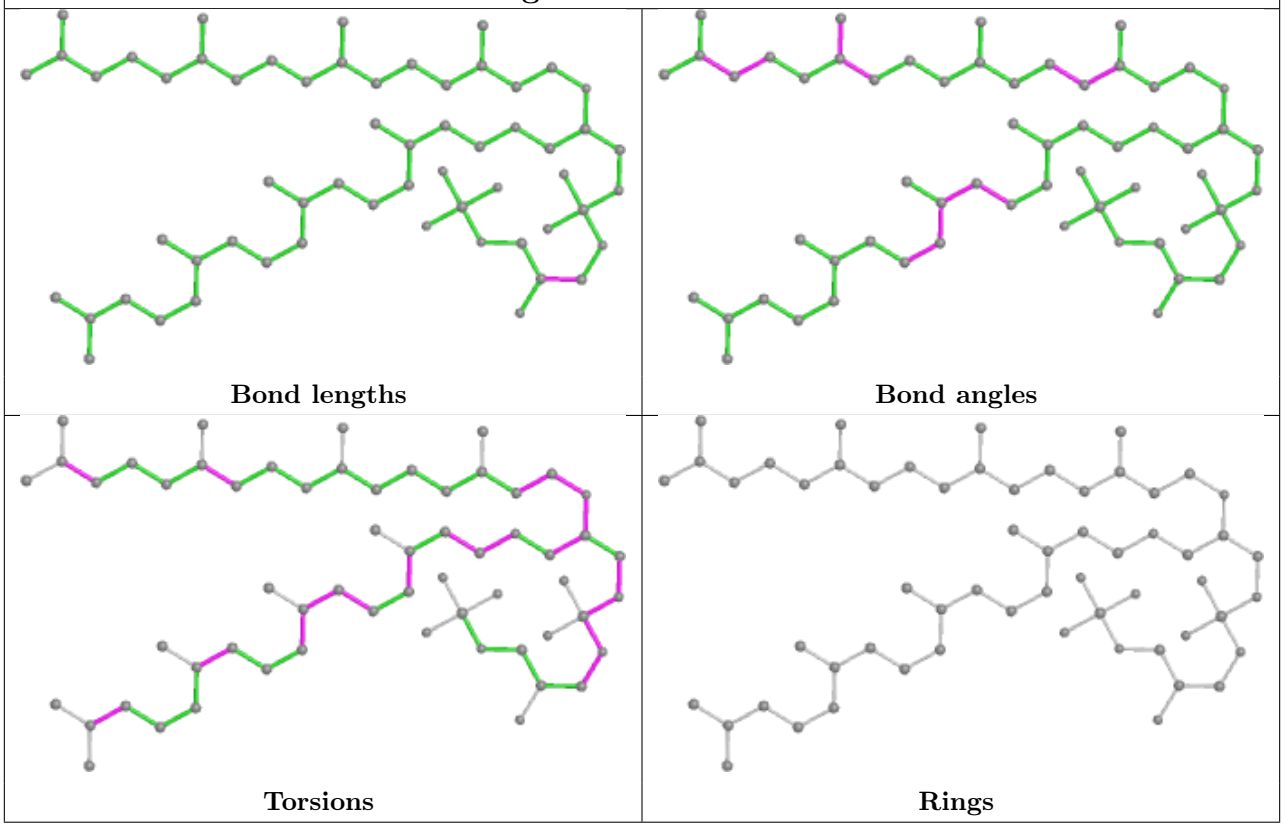
Ligand DPG A 267



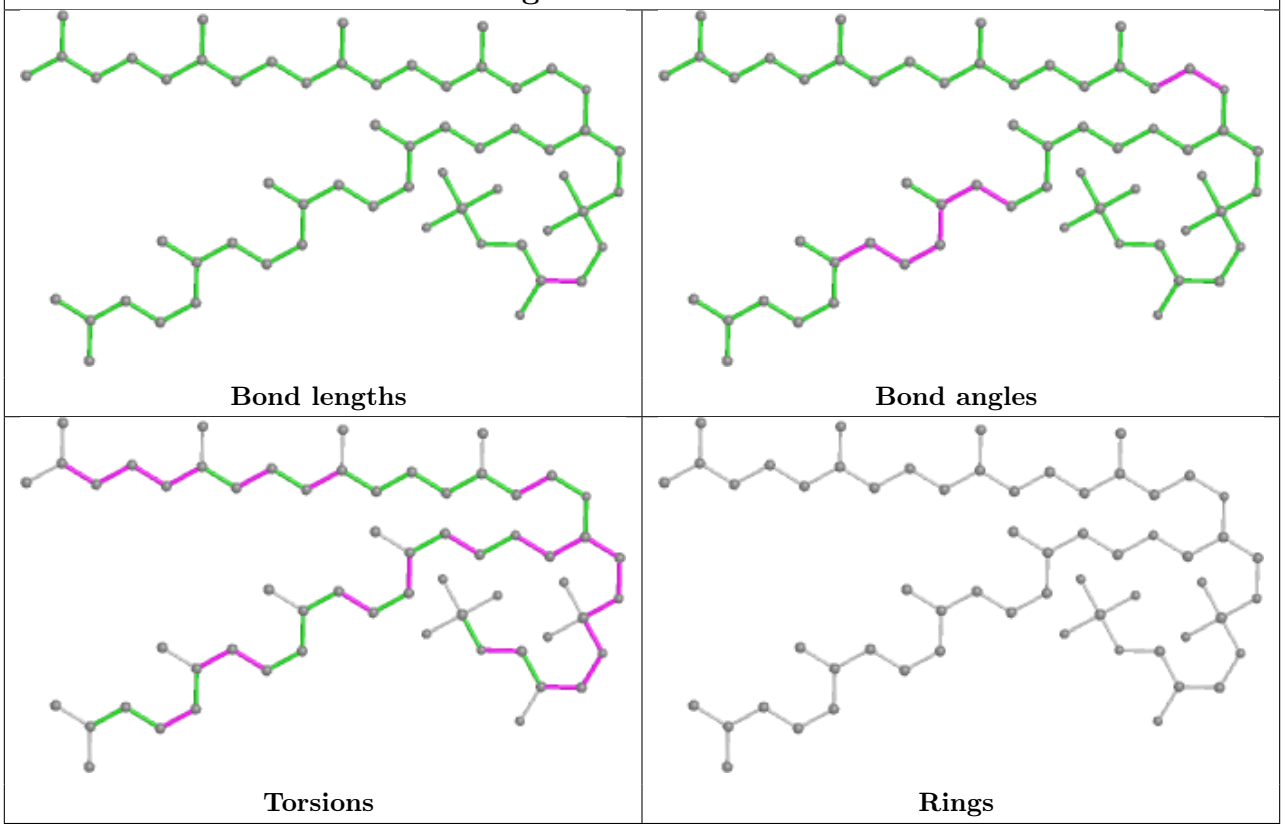
Ligand RET A 271



Ligand DPG A 268



Ligand DPG A 270



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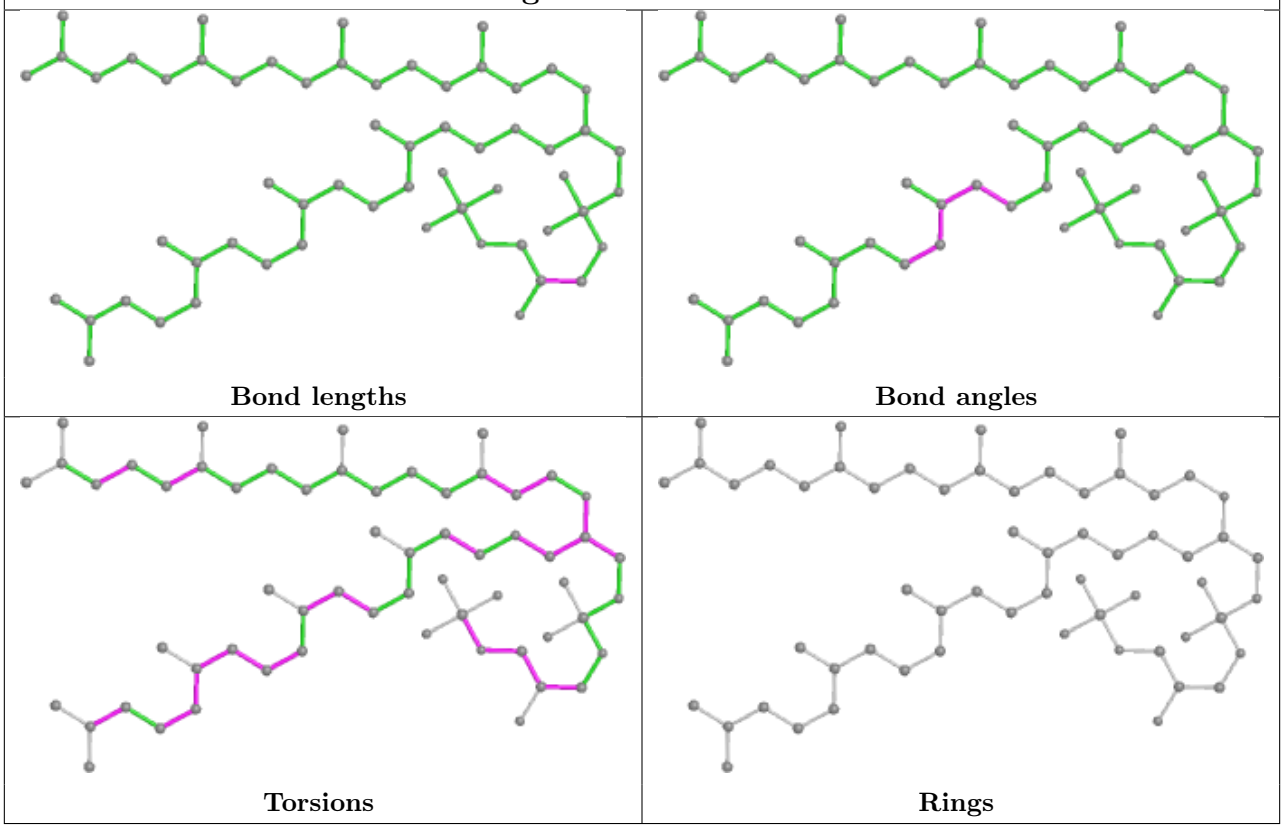
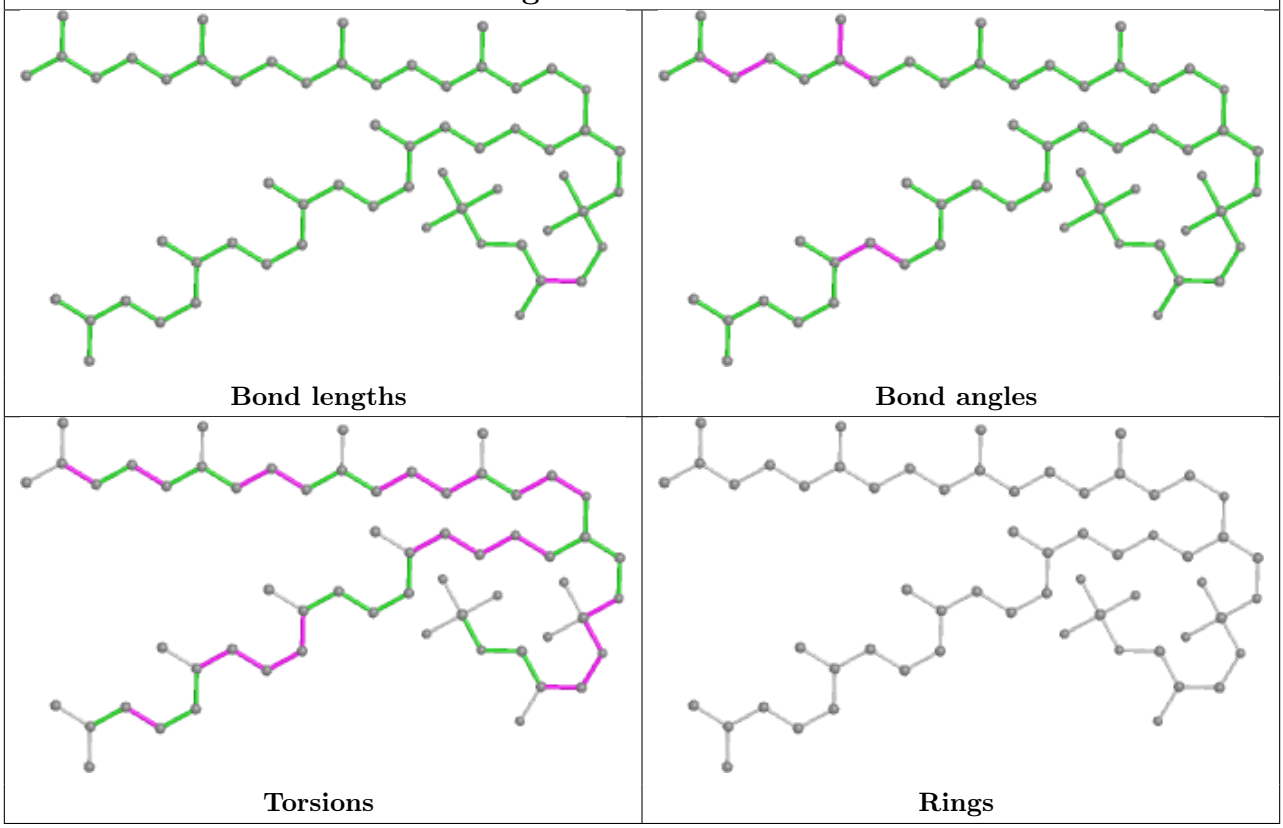


Ligand DPG A 261



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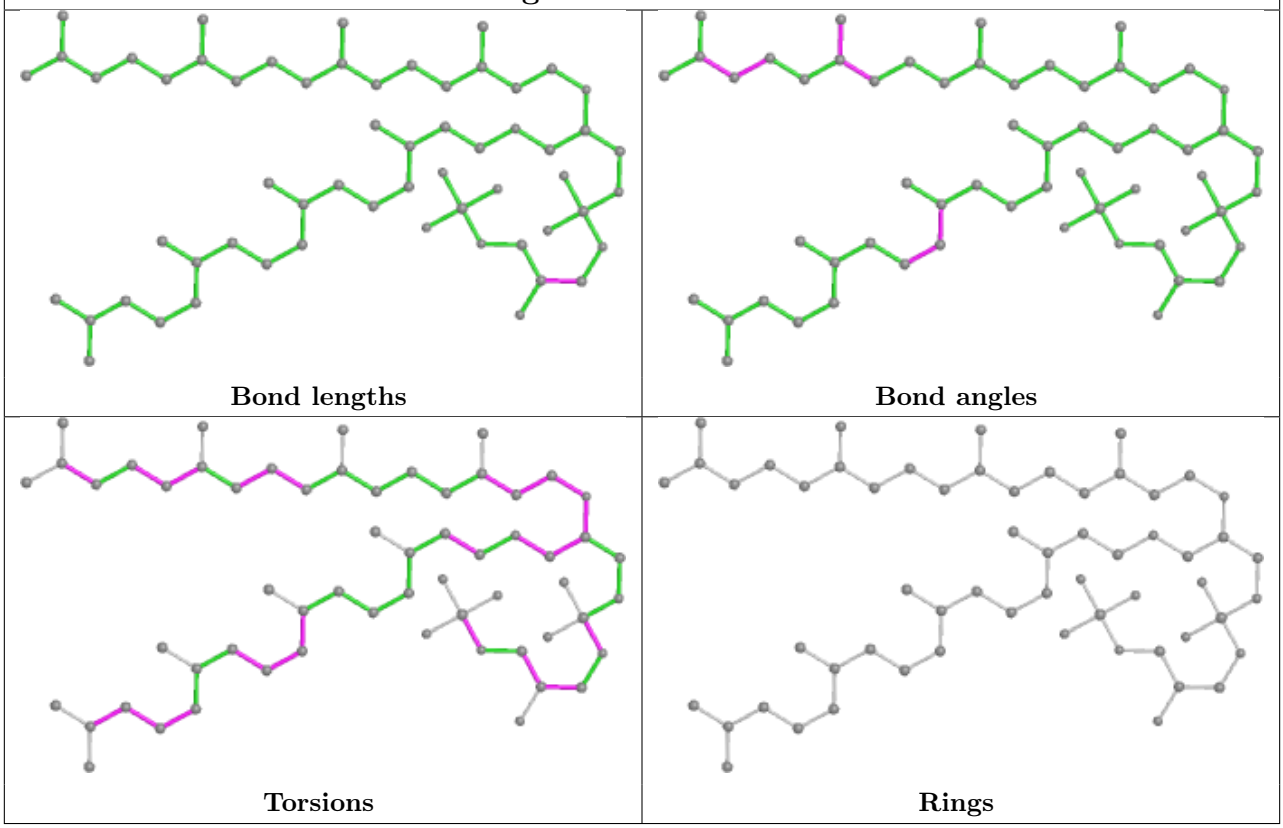

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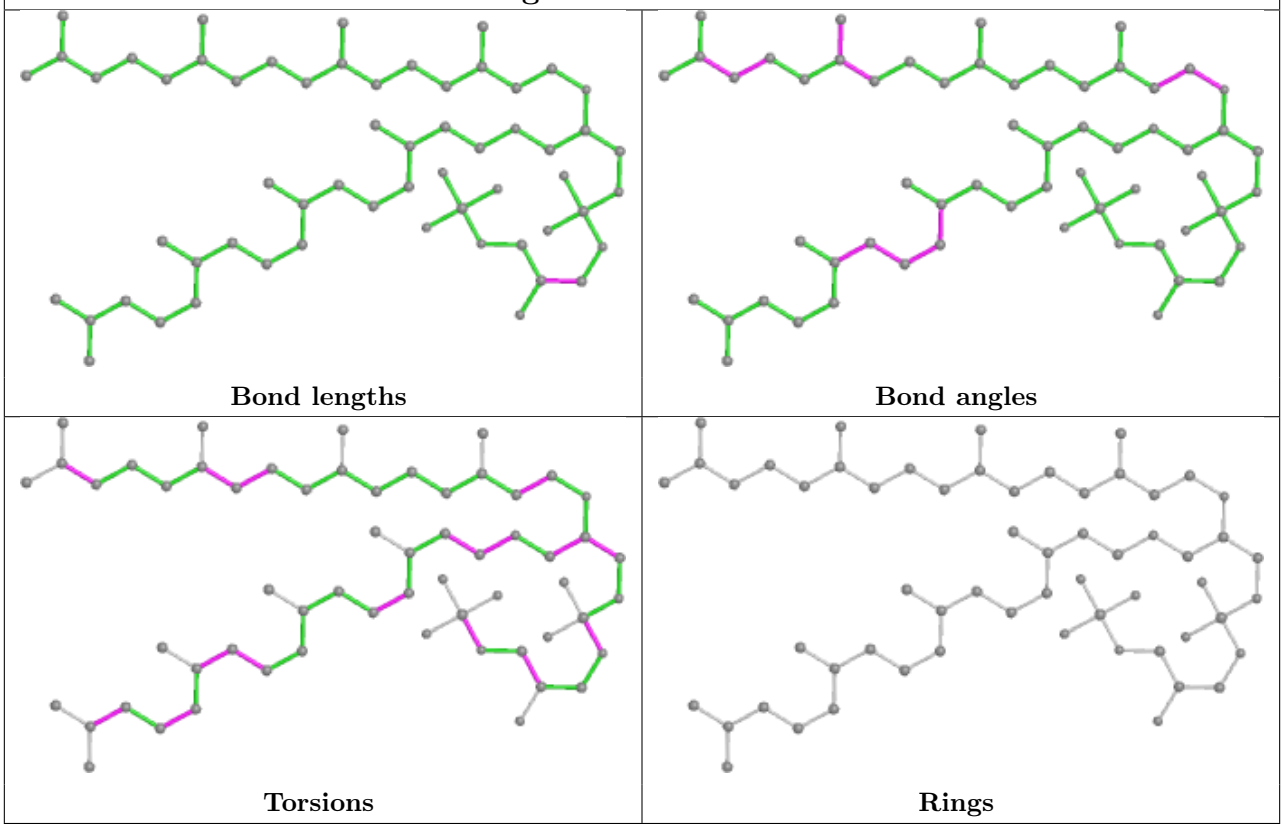

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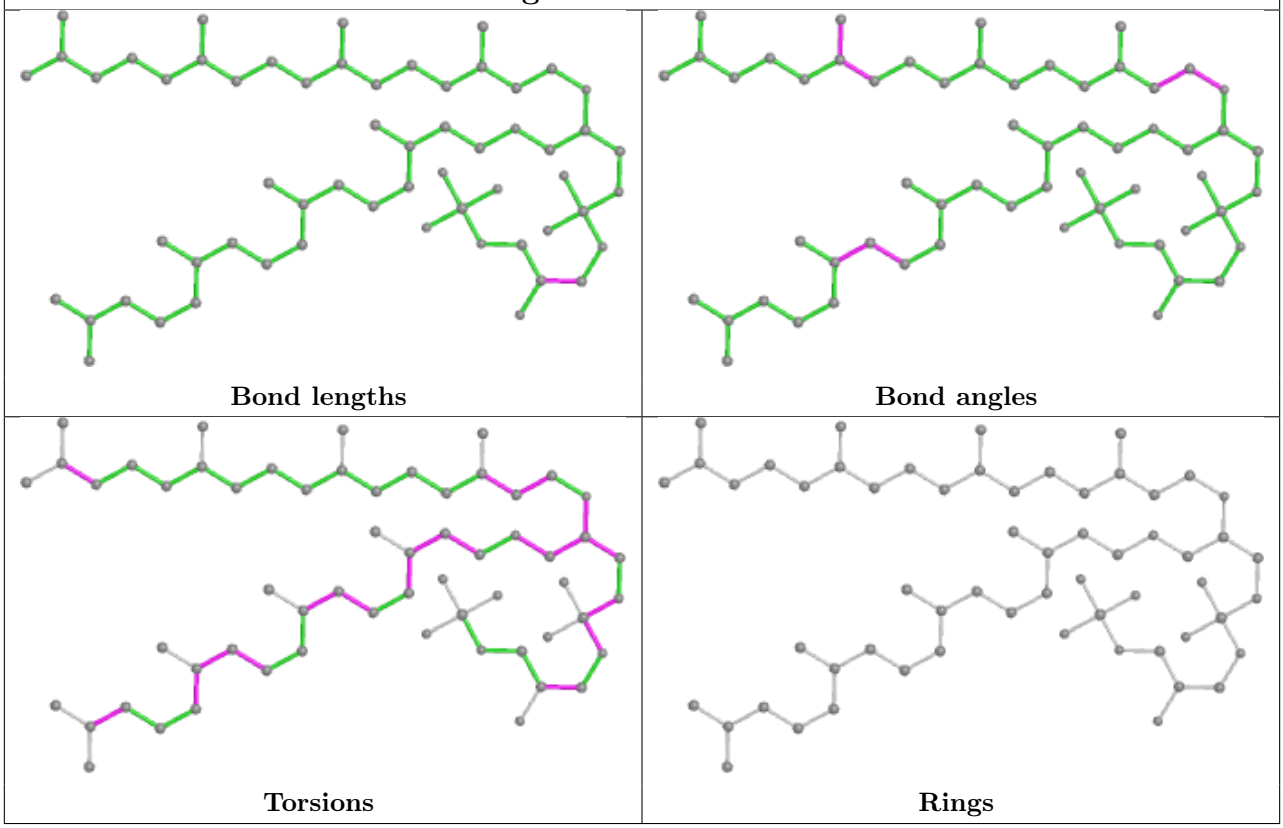

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.