Full wwPDB NMR Structure Validation Report (i)

Jun 11, 2024 – 07:45 PM EDT

PDB ID	:	2MSC
BMRB ID	:	25114
Title	:	NMR data-driven model of GTPase KRas-GDP tethered to a lipid-bilayer nanodisc
Authors	:	Mazhab-Jafari, M.; Stathopoulos, P.; Marshall, C.; Ikura, M.
Deposited on	:	2014-07-29

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
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:

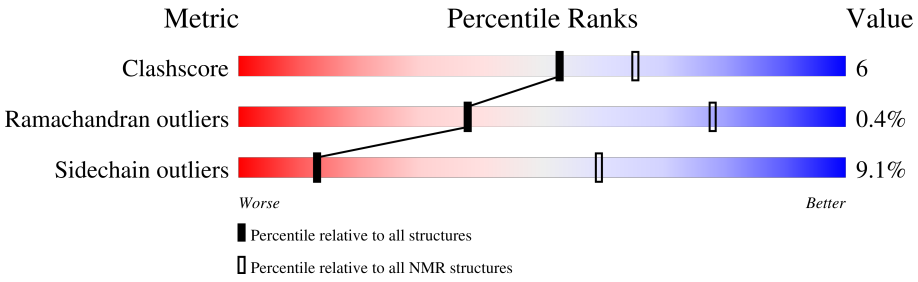
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 1%.

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)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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	200	84% 12% • •
1	C	200	82% 13% • •
2	B	187	68% 9% 22% •

2 Ensemble composition and analysis

This entry contains 10 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:201-A:395, C:402-C:593 (387)	0.45	4
2	B:3-B:146 (144)	0.57	8

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 3 single-model clusters were found.

Cluster number	Models
1	5, 6, 7, 10
2	1, 2, 4
Single-model clusters	3; 8; 9

3 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9134 atoms, of which 62 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Apolipoprotein A-I.

Mol	Chain	Residues	Atoms						Trace
1	A	198	Total	C	H	N	O	S	0
			1645	1019	22	287	314	3	
1	C	198	Total	C	H	N	O	S	0
			1646	1019	22	287	315	3	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	199	GLY	-	expression tag	UNP P02647
A	200	PRO	-	expression tag	UNP P02647
C	397	GLY	-	expression tag	UNP P02647
C	398	PRO	-	expression tag	UNP P02647

- Molecule 2 is a protein called GTPase KRas.

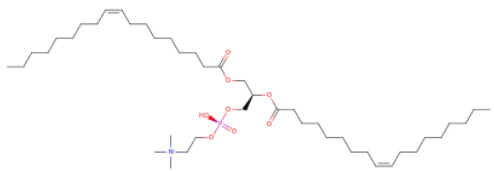
Mol	Chain	Residues	Atoms						Trace
2	B	185	Total	C	H	N	O	S	0
			1494	923	18	257	287	9	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP P01116
B	0	SER	-	expression tag	UNP P01116

- Molecule 3 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: $C_{44}H_{85}NO_8P$).

PCW



Mol	Chain	Residues	Atoms
3	A	1	Total C N O P 54 44 1 8 1
3	A	1	Total C N O P 54 44 1 8 1
3	A	1	Total C N O P 54 44 1 8 1
3	A	1	Total C N O P 54 44 1 8 1
3	A	1	Total C N O P 54 44 1 8 1
3	A	1	Total C N O P 54 44 1 8 1
3	A	1	Total C N O P 54 44 1 8 1
3	A	1	Total C N O P 54 44 1 8 1
3	A	1	Total C N O P 54 44 1 8 1
3	A	1	Total C N O P 54 44 1 8 1
3	A	1	Total C N O P 54 44 1 8 1
3	A	1	Total C N O P 54 44 1 8 1
3	A	1	Total C N O P 54 44 1 8 1
3	A	1	Total C N O P 54 44 1 8 1

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Mol	Chain	Residues	Atoms				
			Total	C	N	O	P
3	A	1	54	44	1	8	1
3	A	1	54	44	1	8	1
3	A	1	54	44	1	8	1
3	A	1	54	44	1	8	1
3	A	1	54	44	1	8	1
3	A	1	54	44	1	8	1
3	A	1	54	44	1	8	1
3	A	1	54	44	1	8	1
3	A	1	54	44	1	8	1
3	A	1	54	44	1	8	1
3	A	1	54	44	1	8	1
3	A	1	54	44	1	8	1
3	A	1	54	44	1	8	1
3	A	1	54	44	1	8	1
3	A	1	54	44	1	8	1
3	A	1	54	44	1	8	1
3	A	1	54	44	1	8	1
3	A	1	54	44	1	8	1
3	A	1	54	44	1	8	1
3	A	1	54	44	1	8	1
3	A	1	54	44	1	8	1

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Mol	Chain	Residues	Atoms				
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1

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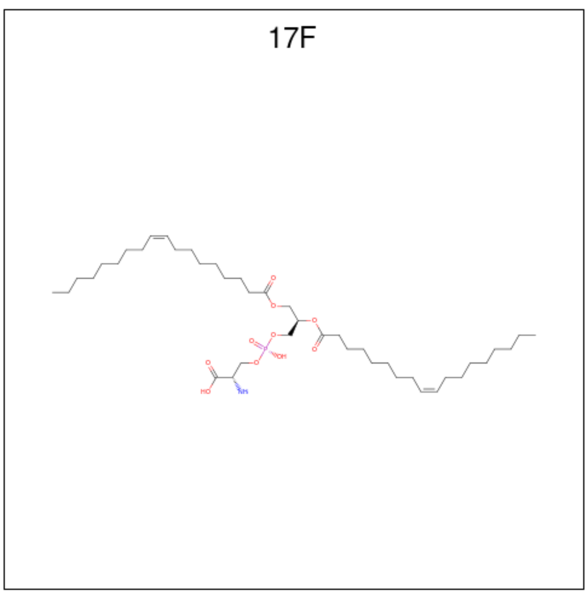
Mol	Chain	Residues	Atoms
3	A	1	Total C N O P 54 44 1 8 1
3	A	1	Total C N O P 54 44 1 8 1
3	A	1	Total C N O P 54 44 1 8 1
3	A	1	Total C N O P 54 44 1 8 1
3	A	1	Total C N O P 54 44 1 8 1
3	A	1	Total C N O P 54 44 1 8 1
3	A	1	Total C N O P 54 44 1 8 1
3	A	1	Total C N O P 54 44 1 8 1

- Molecule 4 is O-[(S)-({(2R)-2,3-bis[(9Z)-octadec-9-enoyloxy]propyl}oxy)(hydroxy)phosphoryl]-L-serine (three-letter code: 17F) (formula: $C_{42}H_{78}NO_{10}P$).



Mol	Chain	Residues	Atoms
4	A	1	Total C N O P 54 42 1 10 1
4	A	1	Total C N O P 54 42 1 10 1
4	A	1	Total C N O P 54 42 1 10 1

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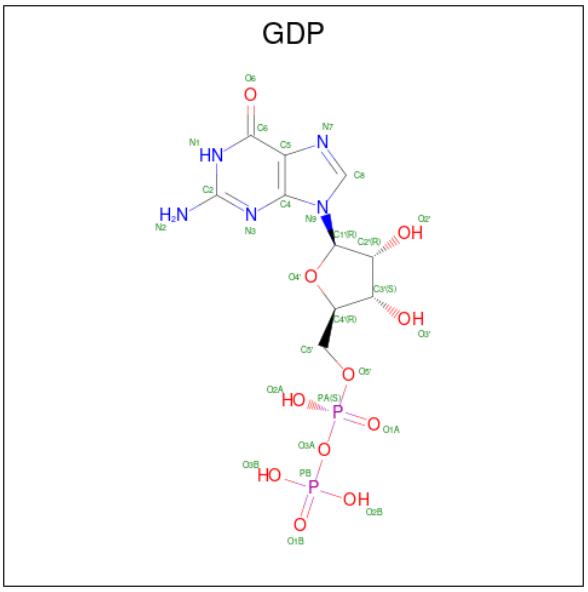
Mol	Chain	Residues	Atoms				
4	A	1	Total 54	C 42	N 1	O 10	P 1
4	A	1	Total 54	C 42	N 1	O 10	P 1
4	A	1	Total 54	C 42	N 1	O 10	P 1
4	A	1	Total 54	C 42	N 1	O 10	P 1
4	A	1	Total 54	C 42	N 1	O 10	P 1
4	A	1	Total 54	C 42	N 1	O 10	P 1
4	A	1	Total 54	C 42	N 1	O 10	P 1
4	A	1	Total 54	C 42	N 1	O 10	P 1
4	A	1	Total 54	C 42	N 1	O 10	P 1
4	A	1	Total 54	C 42	N 1	O 10	P 1
4	A	1	Total 54	C 42	N 1	O 10	P 1
4	A	1	Total 54	C 42	N 1	O 10	P 1
4	A	1	Total 54	C 42	N 1	O 10	P 1

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms				
			Total	C	N	O	P
5	B	1	28	10	5	11	2

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

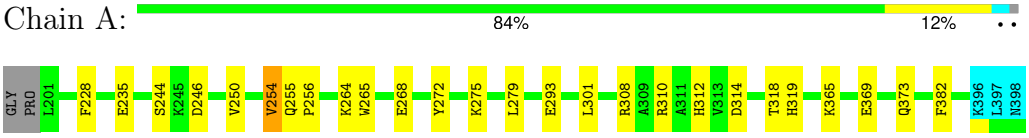
Mol	Chain	Residues	Atoms	
			Total	Mg
6	B	1	1	1

4 Residue-property plots

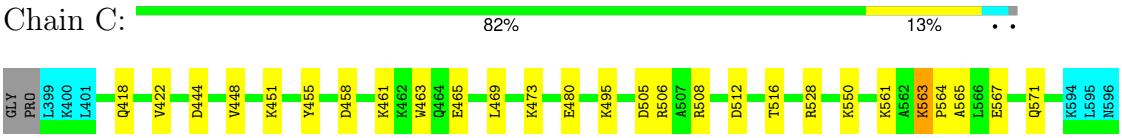
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

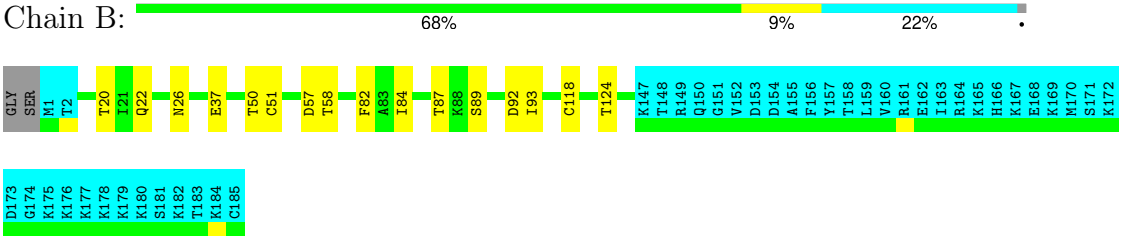
• Molecule 1: Apolipoprotein A-I



• Molecule 1: Apolipoprotein A-I



• Molecule 2: GTPase KRas

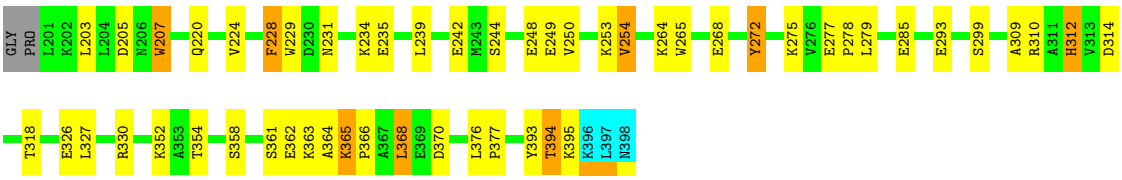


4.2 Scores per residue for each member of the ensemble

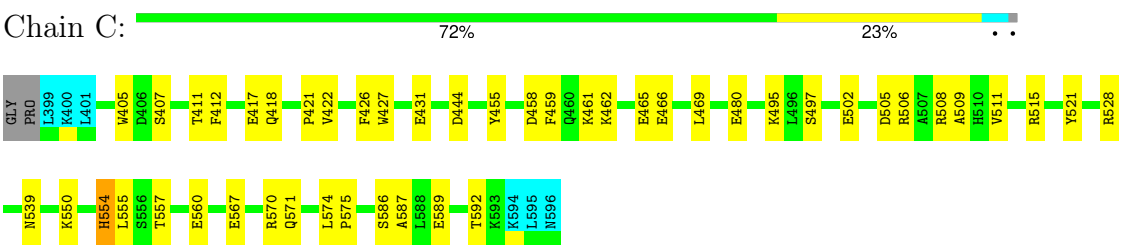
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

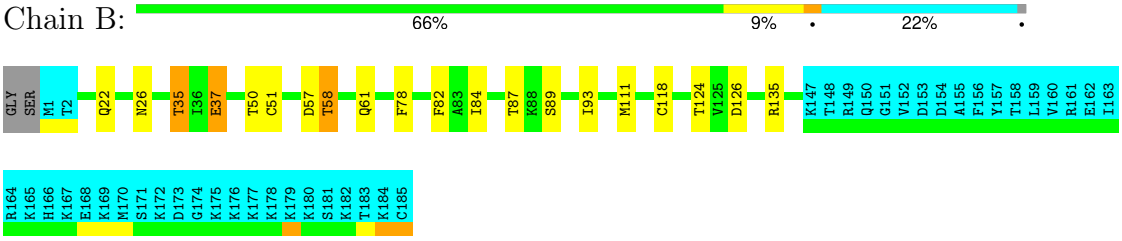
• Molecule 1: Apolipoprotein A-I



• Molecule 1: Apolipoprotein A-I

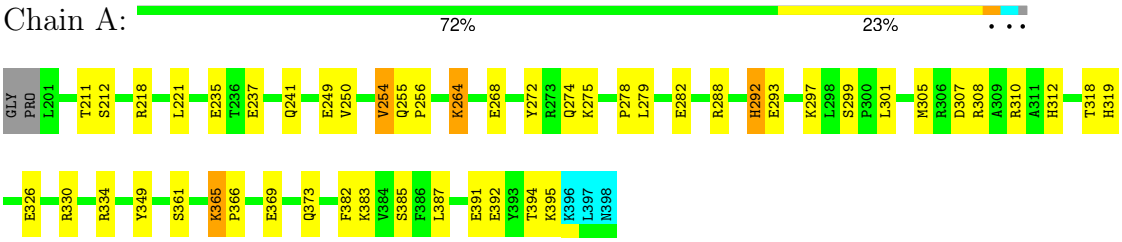


• Molecule 2: GTPase KRas

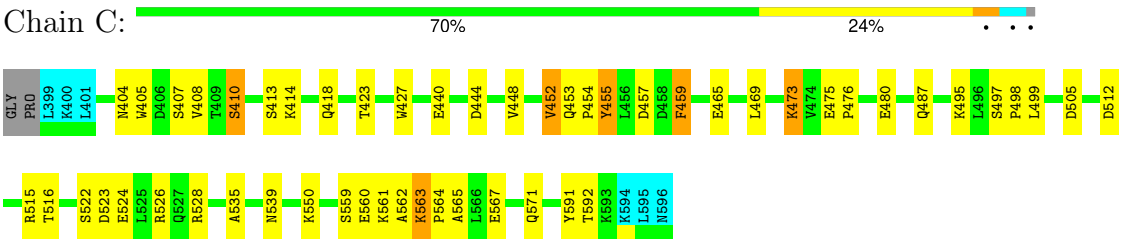


4.2.2 Score per residue for model 2

• Molecule 1: Apolipoprotein A-I

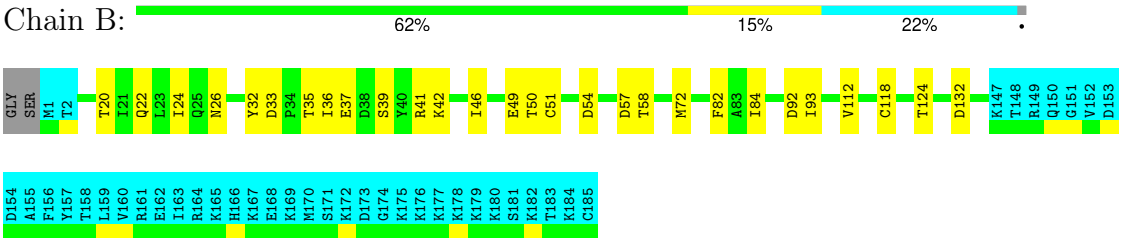


• Molecule 1: Apolipoprotein A-I



• Molecule 2: GTPase KRas

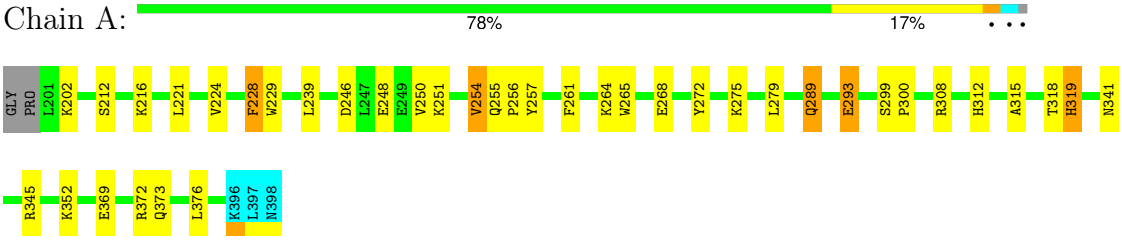
Chain B:



4.2.3 Score per residue for model 3

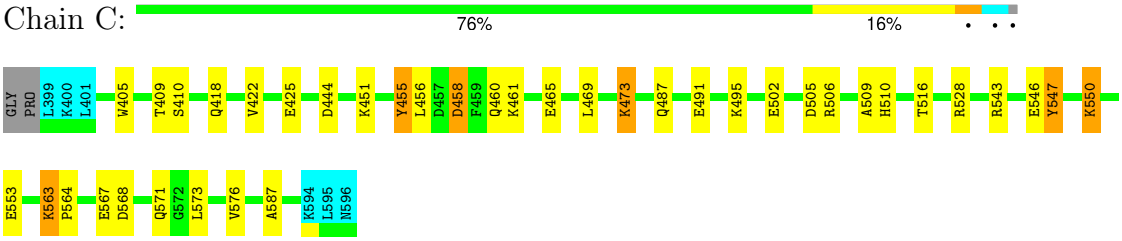
• Molecule 1: Apolipoprotein A-I

Chain A:



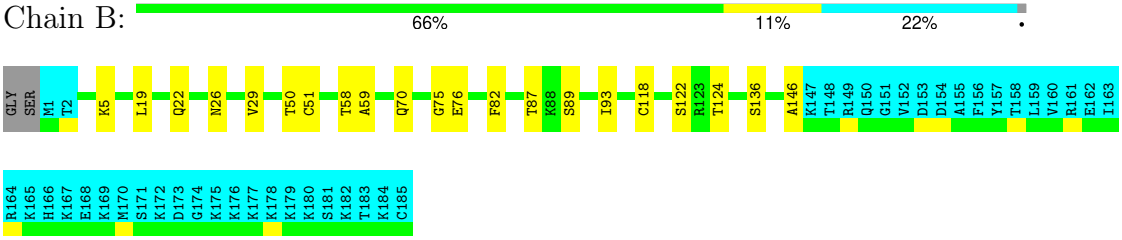
• Molecule 1: Apolipoprotein A-I

Chain C:



• Molecule 2: GTPase KRas

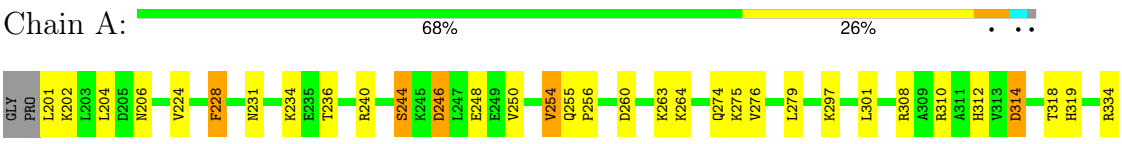
Chain B:



4.2.4 Score per residue for model 4 (medoid)

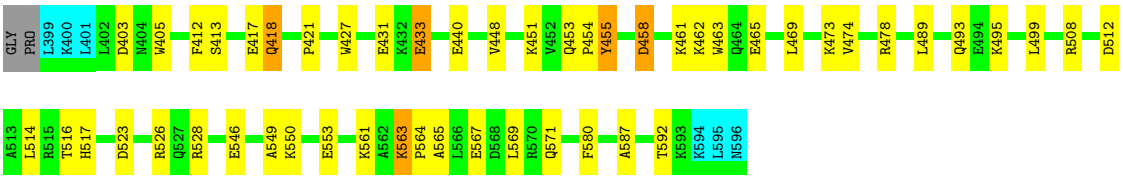
• Molecule 1: Apolipoprotein A-I

Chain A:



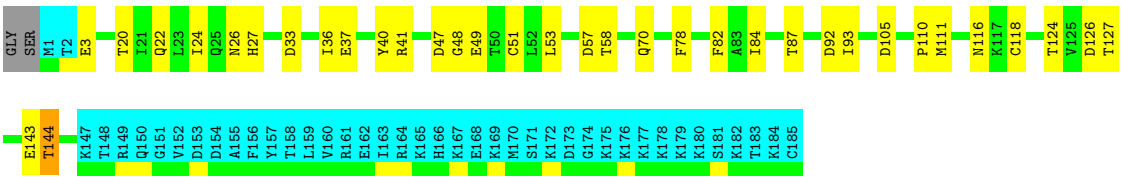
• Molecule 1: Apolipoprotein A-I

Chain C:



• Molecule 2: GTPase KRas

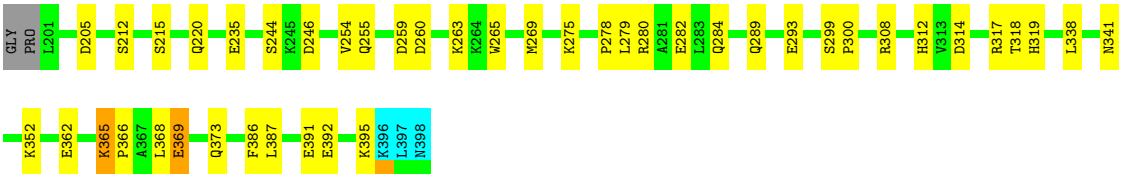
Chain B:



4.2.5 Score per residue for model 5

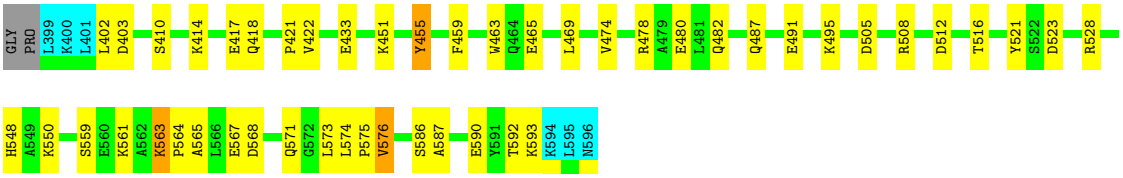
• Molecule 1: Apolipoprotein A-I

Chain A:



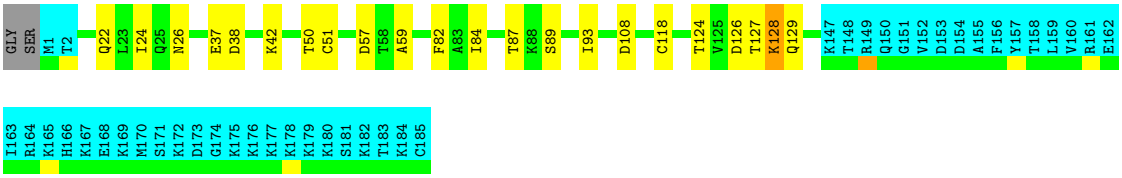
• Molecule 1: Apolipoprotein A-I

Chain C:



• Molecule 2: GTPase KRas

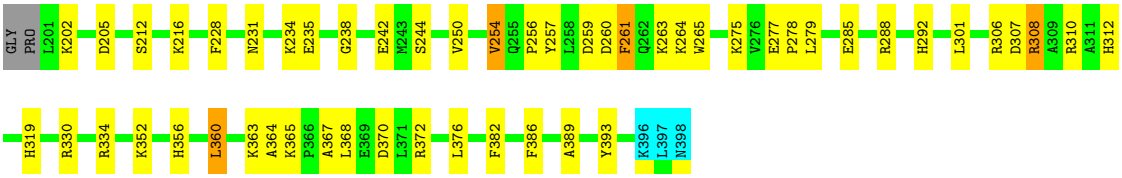
Chain B:



4.2.6 Score per residue for model 6

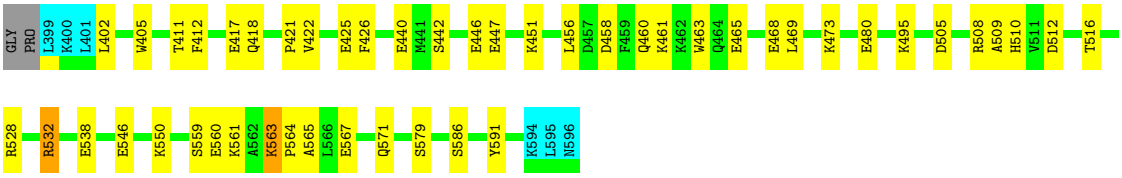
• Molecule 1: Apolipoprotein A-I

Chain A:



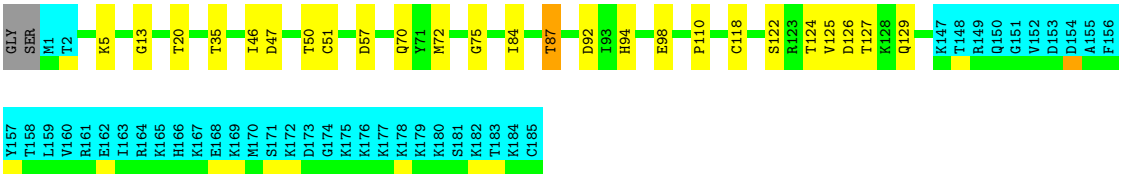
• Molecule 1: Apolipoprotein A-I

Chain C:



• Molecule 2: GTPase KRas

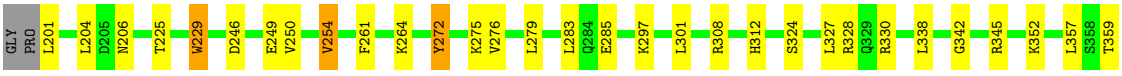
Chain B:



4.2.7 Score per residue for model 7

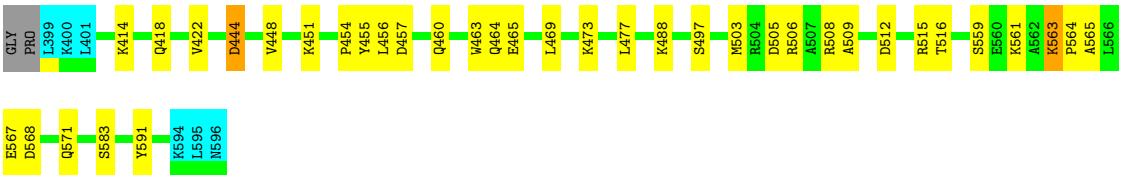
• Molecule 1: Apolipoprotein A-I

Chain A:



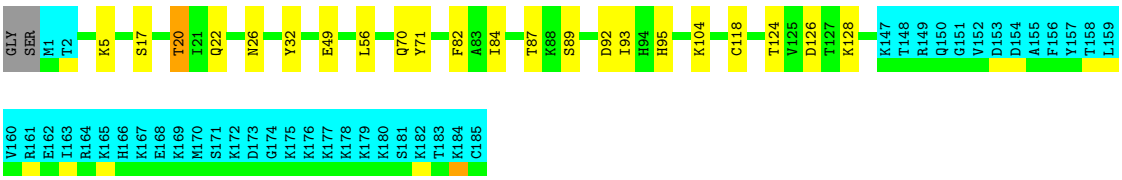
• Molecule 1: Apolipoprotein A-I

Chain C:



• Molecule 2: GTPase KRas

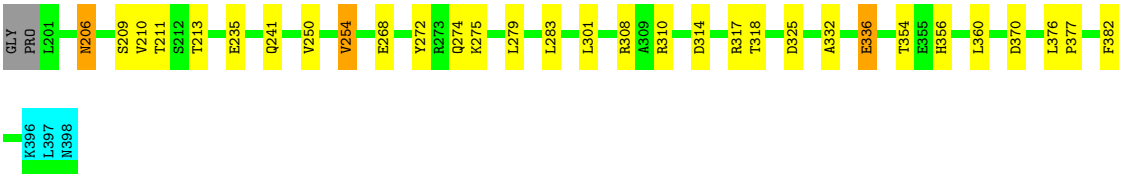
Chain B:



4.2.8 Score per residue for model 8

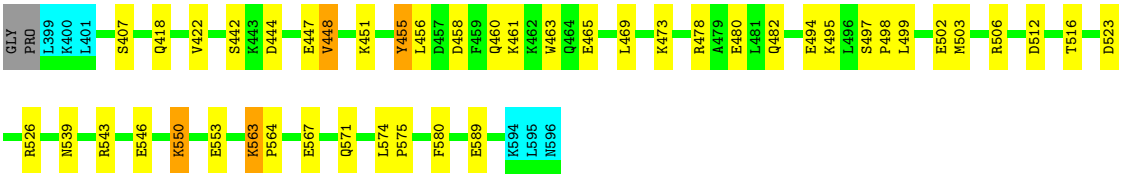
• Molecule 1: Apolipoprotein A-I

Chain A:



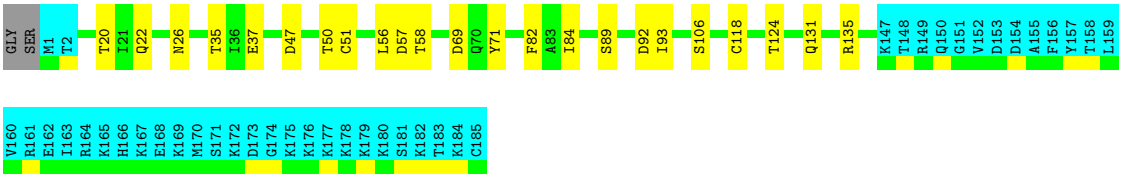
• Molecule 1: Apolipoprotein A-I

Chain C:



• Molecule 2: GTPase KRas

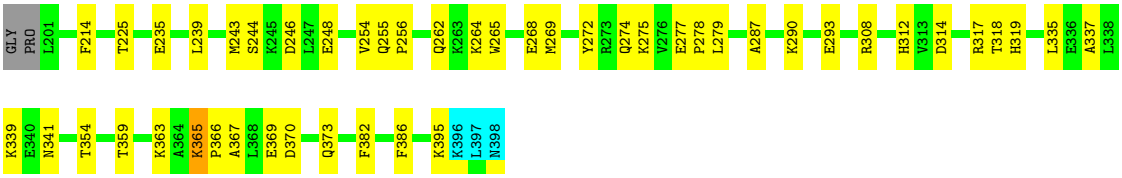
Chain B:



4.2.9 Score per residue for model 9

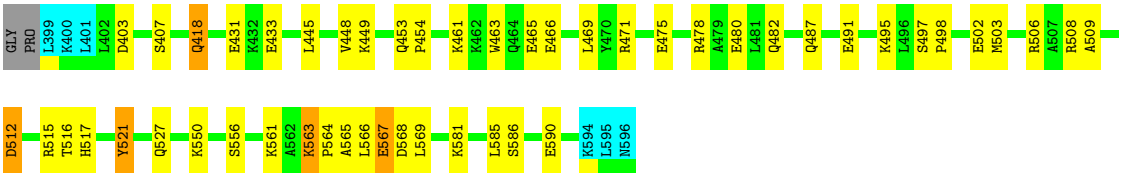
• Molecule 1: Apolipoprotein A-I

Chain A:



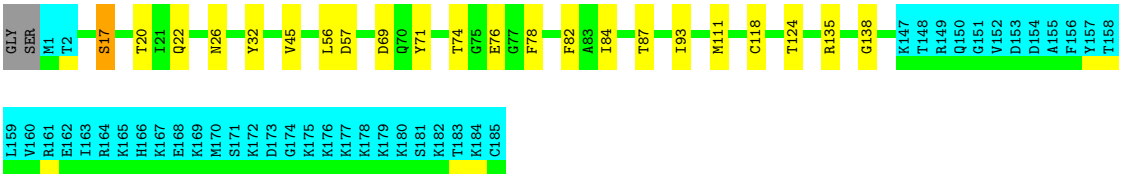
• Molecule 1: Apolipoprotein A-I

Chain C:



• Molecule 2: GTPase KRas

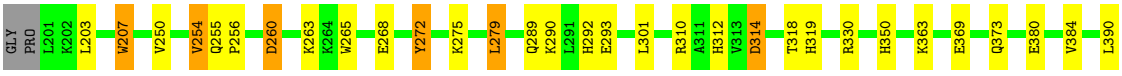
Chain B:



4.2.10 Score per residue for model 10

• Molecule 1: Apolipoprotein A-I

Chain A:

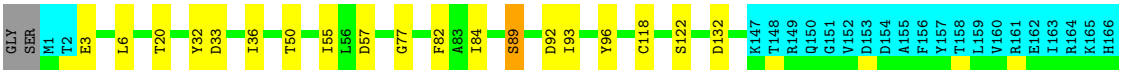


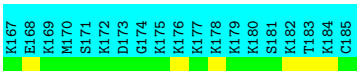
• Molecule 1: Apolipoprotein A-I

Chain C:

• Molecule 2: GTPase KRas

Chain B:





5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 3000 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CNS	structure solution	
HADDOCK	structure solution	
CHARMM-GUI	structure solution	
CNS	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	44
Number of shifts mapped to atoms	11
Number of unparsed shifts	0
Number of shifts with mapping errors	33
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	1%

6 Model quality

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 17F, PCW, MG, GDP

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1598	22	1596	25±7
1	C	1573	22	1562	27±7
2	B	1137	16	1109	8±2
3	A	3456	0	5376	54±5
4	A	864	0	1216	22±4
All	All	86570	600	108711	1101

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.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:308:ARG:HD2	1:C:469:LEU:CD2	1.30	1.57	9	1
1:C:465:GLU:O	1:C:469:LEU:CG	1.29	1.78	9	9
1:C:567:GLU:O	1:C:571:GLN:HG3	1.25	1.23	2	9
1:C:465:GLU:O	1:C:469:LEU:HG	1.25	1.26	7	9
1:A:308:ARG:CD	1:C:469:LEU:HD11	1.21	1.66	9	1
1:A:308:ARG:CD	1:C:469:LEU:HD21	1.15	1.71	9	1
1:A:308:ARG:HD3	1:C:469:LEU:HD11	1.04	1.06	9	1
1:C:567:GLU:O	1:C:571:GLN:CG	1.01	2.09	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:369:GLU:O	1:A:373:GLN:HG3	0.98	1.58	7	7
1:A:308:ARG:CD	1:C:469:LEU:CD1	0.95	2.43	9	1
3:A:30:PCW:H71	4:A:37:17F:HN1A	0.91	1.24	10	1
4:A:38:17F:HN1	2:B:131:GLN:HE21	0.89	1.05	8	1
1:A:308:ARG:HG3	1:C:469:LEU:HD11	0.89	1.43	5	3
3:A:70:PCW:H31	3:A:71:PCW:H32	0.86	1.43	9	1
1:A:260:ASP:HA	1:A:263:LYS:HE2	0.86	1.45	6	3
4:A:40:17F:H4	4:A:40:17F:HN1	0.85	1.30	4	1
1:C:563:LYS:HB2	1:C:564:PRO:HD3	0.85	1.46	2	8
1:A:389:ALA:O	1:A:393:TYR:CD2	0.84	2.30	6	1
1:A:308:ARG:HG3	1:C:469:LEU:HD21	0.84	1.47	7	7
1:C:465:GLU:O	1:C:469:LEU:CD1	0.83	2.26	1	3
1:C:458:ASP:HA	1:C:461:LYS:HE2	0.83	1.50	4	1
3:A:15:PCW:H71	4:A:39:17F:H2	0.82	1.49	3	1
1:A:308:ARG:CD	1:C:469:LEU:CD2	0.82	2.47	9	1
1:A:308:ARG:HD2	1:C:469:LEU:HD21	0.82	0.83	9	1
1:A:308:ARG:HD2	1:C:469:LEU:CG	0.80	2.05	9	1
1:A:365:LYS:HB2	1:A:366:PRO:HD3	0.80	1.50	9	5
3:A:63:PCW:P	4:A:75:17F:HN1A	0.80	2.00	3	1
3:A:32:PCW:H331	4:A:35:17F:H11	0.79	1.52	7	1
3:A:45:PCW:H71	3:A:71:PCW:H20	0.79	1.54	8	1
1:A:369:GLU:O	1:A:373:GLN:CG	0.79	2.30	7	3
1:A:308:ARG:HD3	1:C:469:LEU:CD1	0.79	2.00	9	1
3:A:32:PCW:H61	4:A:38:17F:HN1A	0.79	1.38	8	1
1:C:465:GLU:O	1:C:469:LEU:CB	0.78	2.31	1	4
1:A:389:ALA:O	1:A:393:TYR:HD2	0.78	1.60	6	1
3:A:51:PCW:H41	3:A:71:PCW:H382	0.75	1.56	3	1
3:A:42:PCW:H341	3:A:52:PCW:H331	0.75	1.59	1	1
3:A:57:PCW:H82	4:A:80:17F:HN1A	0.74	1.42	5	1
1:A:352:LYS:HG2	1:C:422:VAL:HG13	0.73	1.60	5	3
3:A:16:PCW:H19	4:A:39:17F:H5	0.73	1.59	6	1
1:A:308:ARG:CG	1:C:469:LEU:HD11	0.72	2.12	5	4
3:A:10:PCW:H62	4:A:36:17F:H2	0.72	1.61	6	1
3:A:17:PCW:H332	3:A:17:PCW:H132	0.70	1.63	7	1
1:A:250:VAL:O	1:A:254:VAL:HB	0.70	1.85	1	8
3:A:19:PCW:H41	3:A:23:PCW:H411	0.70	1.64	2	1
3:A:7:PCW:H73	4:A:35:17F:HN1A	0.69	1.46	1	1
4:A:33:17F:H8	4:A:35:17F:H9A	0.68	1.65	1	1
1:C:497:SER:HB2	1:C:498:PRO:HD3	0.67	1.64	8	3
1:C:453:GLN:HB2	1:C:454:PRO:HD3	0.67	1.65	2	4
4:A:38:17F:HN1	2:B:131:GLN:NE2	0.67	1.84	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:279:LEU:HD22	1:C:495:LYS:HG2	0.67	1.66	3	6
3:A:20:PCW:H32	3:A:24:PCW:H352	0.67	1.66	6	2
3:A:59:PCW:H61	4:A:77:17F:H6A	0.67	1.65	4	1
4:A:74:17F:H34	4:A:79:17F:H6A	0.67	1.67	7	1
3:A:70:PCW:H39	3:A:71:PCW:H152	0.66	1.66	10	1
1:A:275:LYS:O	1:A:279:LEU:HG	0.66	1.90	4	9
3:A:47:PCW:H12	4:A:73:17F:H1	0.66	1.68	8	1
3:A:5:PCW:H31	3:A:17:PCW:H382	0.66	1.67	9	1
1:C:418:GLN:O	1:C:422:VAL:HB	0.65	1.91	6	6
4:A:33:17F:P1	4:A:33:17F:HN1	0.65	2.14	9	7
2:B:82:PHE:HB3	2:B:93:ILE:HD11	0.65	1.69	7	9
3:A:51:PCW:H51	3:A:71:PCW:H382	0.65	1.69	4	1
3:A:14:PCW:H51	2:B:48:GLY:HA2	0.65	1.68	4	1
4:A:38:17F:O2	2:B:135:ARG:HD3	0.65	1.90	8	1
3:A:47:PCW:H231	4:A:76:17F:H5	0.65	1.67	9	1
1:A:231:ASN:HA	1:A:234:LYS:HE2	0.65	1.69	1	2
3:A:13:PCW:H62	4:A:34:17F:HN1	0.65	1.52	10	1
3:A:57:PCW:H19	4:A:76:17F:H40	0.65	1.68	5	1
2:B:84:ILE:HD11	2:B:118:CYS:HA	0.65	1.67	1	7
3:A:58:PCW:H372	3:A:60:PCW:H141	0.65	1.67	10	1
3:A:11:PCW:H81	3:A:25:PCW:H31	0.64	1.69	4	1
1:A:308:ARG:HG3	1:C:469:LEU:CD1	0.64	2.20	5	3
1:A:299:SER:HB2	1:A:300:PRO:HD3	0.64	1.67	3	2
1:C:465:GLU:O	1:C:469:LEU:HD12	0.64	1.92	1	1
3:A:14:PCW:H121	4:A:34:17F:H20	0.64	1.69	8	2
3:A:46:PCW:H322	3:A:71:PCW:H352	0.64	1.69	5	1
1:A:352:LYS:HZ2	1:C:425:GLU:HB3	0.64	1.52	3	2
3:A:9:PCW:H51	4:A:34:17F:H4	0.64	1.69	4	1
1:C:508:ARG:O	1:C:512:ASP:HB2	0.63	1.94	6	2
1:C:590:GLU:HA	1:C:593:LYS:HE3	0.63	1.70	5	1
1:C:505:ASP:HA	1:C:508:ARG:HD2	0.63	1.71	7	2
3:A:6:PCW:H341	3:A:16:PCW:H342	0.63	1.70	3	1
3:A:41:PCW:H131	3:A:52:PCW:H39	0.63	1.70	7	1
3:A:32:PCW:H332	4:A:35:17F:H62	0.63	1.70	9	1
1:A:301:LEU:HB3	1:C:473:LYS:HD2	0.63	1.68	2	1
1:A:301:LEU:HD22	1:C:473:LYS:HG2	0.63	1.68	10	2
3:A:27:PCW:H41	4:A:37:17F:O1	0.63	1.94	3	1
1:C:557:THR:HA	1:C:560:GLU:HG2	0.62	1.71	1	1
3:A:70:PCW:H73	3:A:70:PCW:H19	0.62	1.72	2	1
3:A:48:PCW:H61	3:A:61:PCW:H39	0.62	1.71	9	1
3:A:30:PCW:H61	4:A:37:17F:N1	0.62	2.10	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:376:LEU:HB2	1:A:377:PRO:HD3	0.62	1.72	1	2
1:C:512:ASP:HA	1:C:515:ARG:HD2	0.62	1.69	2	3
3:A:66:PCW:H212	3:A:67:PCW:H61	0.61	1.70	8	1
1:C:474:VAL:O	1:C:478:ARG:HB2	0.61	1.96	4	2
3:A:46:PCW:H31	3:A:71:PCW:H382	0.61	1.72	8	1
3:A:3:PCW:H142	3:A:3:PCW:H372	0.61	1.72	5	1
3:A:27:PCW:H73	4:A:37:17F:HN1	0.61	1.56	1	1
2:B:24:ILE:HA	2:B:42:LYS:HD2	0.61	1.73	5	2
3:A:4:PCW:H321	3:A:7:PCW:H12	0.61	1.71	3	1
3:A:49:PCW:H322	3:A:57:PCW:H2	0.61	1.71	7	1
1:C:574:LEU:HB2	1:C:575:PRO:HD3	0.60	1.71	5	2
3:A:25:PCW:H131	3:A:31:PCW:H31	0.60	1.71	3	1
3:A:14:PCW:H452	3:A:14:PCW:H232	0.60	1.73	7	1
3:A:13:PCW:H431	3:A:18:PCW:H172	0.60	1.72	2	1
1:C:458:ASP:HA	1:C:461:LYS:HE3	0.60	1.72	1	1
3:A:47:PCW:H232	4:A:76:17F:H33	0.60	1.74	3	1
3:A:59:PCW:H121	4:A:77:17F:H10A	0.60	1.73	3	1
3:A:1:PCW:H283	3:A:5:PCW:H241	0.60	1.73	2	1
3:A:48:PCW:H20	3:A:58:PCW:H151	0.60	1.74	2	1
1:C:563:LYS:HB2	1:C:564:PRO:CD	0.60	2.27	7	5
3:A:20:PCW:H42	3:A:31:PCW:O2P	0.59	1.97	2	1
4:A:73:17F:H58	4:A:76:17F:H19	0.59	1.73	3	1
1:A:352:LYS:NZ	1:C:425:GLU:HB3	0.59	2.12	6	2
3:A:48:PCW:H322	3:A:54:PCW:H152	0.59	1.73	2	1
1:C:503:MET:HA	1:C:506:ARG:HD2	0.59	1.74	9	4
1:A:341:ASN:HD21	1:C:433:GLU:HA	0.59	1.56	4	1
1:A:314:ASP:HA	1:A:317:ARG:HD2	0.59	1.74	9	3
1:A:256:PRO:HA	1:A:259:ASP:HB3	0.59	1.74	6	1
3:A:26:PCW:H132	3:A:26:PCW:H352	0.58	1.73	2	1
1:C:451:LYS:O	1:C:455:TYR:HB2	0.58	1.98	4	4
2:B:5:LYS:HB3	2:B:75:GLY:HA2	0.58	1.75	3	1
3:A:42:PCW:H162	3:A:52:PCW:H331	0.58	1.76	6	1
3:A:9:PCW:H351	3:A:14:PCW:H122	0.58	1.74	2	1
3:A:43:PCW:H181	3:A:43:PCW:H422	0.58	1.76	2	1
1:A:301:LEU:HB3	1:C:473:LYS:HE3	0.58	1.76	6	1
1:A:264:LYS:HE2	1:C:509:ALA:HB1	0.58	1.75	9	3
1:A:301:LEU:HD13	1:C:473:LYS:HG2	0.58	1.76	7	2
3:A:44:PCW:H122	4:A:77:17F:H1A	0.58	1.74	9	1
3:A:16:PCW:H182	4:A:39:17F:H33	0.58	1.76	7	1
3:A:13:PCW:H41	4:A:34:17F:O1	0.58	1.99	8	1
3:A:11:PCW:H142	3:A:28:PCW:H341	0.57	1.74	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:264:LYS:HG2	1:C:509:ALA:HB1	0.57	1.76	6	2
1:A:342:GLY:HA2	1:A:345:ARG:HD2	0.57	1.76	7	1
3:A:66:PCW:H451	4:A:79:17F:H10	0.57	1.76	10	1
1:C:448:VAL:O	1:C:452:VAL:HB	0.57	1.99	2	1
3:A:47:PCW:H73	3:A:71:PCW:H19	0.57	1.75	4	1
4:A:40:17F:H4	4:A:40:17F:N1	0.57	2.10	4	1
3:A:25:PCW:H11	3:A:31:PCW:H41	0.57	1.76	6	2
1:A:277:GLU:HB2	1:A:278:PRO:HD3	0.57	1.76	9	2
3:A:60:PCW:H421	3:A:63:PCW:H371	0.57	1.76	7	1
3:A:51:PCW:H132	3:A:71:PCW:H431	0.57	1.74	8	1
3:A:51:PCW:H62	3:A:71:PCW:H39	0.57	1.75	10	1
1:A:288:ARG:O	1:A:292:HIS:HB2	0.57	2.00	6	2
3:A:45:PCW:H412	3:A:57:PCW:H61	0.57	1.77	6	1
3:A:30:PCW:H71	4:A:34:17F:N1	0.57	2.15	8	1
2:B:22:GLN:O	2:B:26:ASN:HA	0.57	2.00	5	8
3:A:68:PCW:O2P	3:A:69:PCW:H41	0.57	2.00	9	1
3:A:43:PCW:H83	3:A:68:PCW:O1P	0.57	1.99	3	1
3:A:46:PCW:H322	3:A:71:PCW:H372	0.56	1.77	2	1
3:A:6:PCW:H39	3:A:16:PCW:H11	0.56	1.76	7	1
2:B:84:ILE:CD1	2:B:118:CYS:HA	0.56	2.30	10	7
1:A:279:LEU:HD13	1:C:495:LYS:HG2	0.56	1.76	4	1
3:A:57:PCW:H72	4:A:80:17F:HN1A	0.56	1.59	4	1
4:A:79:17F:H9	4:A:79:17F:H18A	0.56	1.76	9	1
3:A:30:PCW:H71	4:A:37:17F:N1	0.56	2.07	10	1
3:A:2:PCW:H62	4:A:36:17F:H1A	0.56	1.77	6	1
3:A:1:PCW:H39	4:A:33:17F:H39	0.56	1.77	6	1
1:C:502:GLU:HG2	1:C:506:ARG:HE	0.56	1.61	9	2
3:A:10:PCW:H331	3:A:21:PCW:H321	0.56	1.78	10	1
3:A:53:PCW:H321	3:A:68:PCW:H372	0.56	1.76	10	1
3:A:15:PCW:H41	3:A:16:PCW:H131	0.56	1.77	1	1
3:A:19:PCW:H322	3:A:23:PCW:H332	0.56	1.77	6	1
1:C:454:PRO:HA	1:C:457:ASP:HB3	0.56	1.78	7	1
2:B:37:GLU:HG3	2:B:58:THR:HA	0.56	1.78	4	4
3:A:62:PCW:H351	3:A:72:PCW:H332	0.56	1.77	5	1
1:C:465:GLU:O	1:C:469:LEU:HB2	0.56	2.01	1	1
3:A:6:PCW:O1P	3:A:16:PCW:H11	0.56	2.01	9	1
3:A:57:PCW:H142	4:A:80:17F:H8A	0.56	1.76	9	1
3:A:49:PCW:H62	4:A:80:17F:HN1	0.55	1.60	8	1
4:A:39:17F:H33	4:A:39:17F:H8	0.55	1.77	2	2
3:A:63:PCW:P	4:A:75:17F:N1	0.55	2.76	3	1
3:A:9:PCW:O2P	3:A:14:PCW:H11	0.55	2.01	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:14:PCW:H131	3:A:23:PCW:H41	0.55	1.78	7	2
3:A:66:PCW:H20	3:A:67:PCW:H71	0.55	1.77	10	1
3:A:3:PCW:H361	3:A:18:PCW:H12	0.55	1.78	4	1
3:A:65:PCW:H121	4:A:80:17F:H62	0.55	1.78	5	1
3:A:6:PCW:H332	3:A:28:PCW:H41	0.55	1.77	3	1
1:A:308:ARG:CD	1:C:469:LEU:CG	0.55	2.76	9	1
3:A:10:PCW:H81	4:A:36:17F:N1	0.55	2.17	9	1
4:A:74:17F:H5	4:A:74:17F:H20A	0.55	1.78	9	1
1:A:244:SER:O	1:A:248:GLU:HB2	0.55	2.02	4	3
4:A:36:17F:H44	4:A:40:17F:H38	0.55	1.78	1	1
3:A:49:PCW:H151	3:A:57:PCW:H322	0.55	1.78	1	1
1:C:495:LYS:O	1:C:499:LEU:HB2	0.55	2.01	2	3
3:A:9:PCW:H142	3:A:11:PCW:H132	0.55	1.78	3	1
2:B:118:CYS:HB3	2:B:143:GLU:HG2	0.55	1.77	4	1
2:B:19:LEU:HD23	2:B:146:ALA:HB2	0.54	1.77	3	1
3:A:25:PCW:H2	3:A:31:PCW:H41	0.54	1.79	2	1
3:A:23:PCW:H39	3:A:29:PCW:H372	0.54	1.79	2	1
1:A:307:ASP:HA	1:A:310:ARG:HD2	0.54	1.80	6	2
3:A:58:PCW:H31	3:A:61:PCW:H432	0.54	1.79	2	1
4:A:75:17F:H8	4:A:75:17F:H20A	0.54	1.79	9	1
1:A:231:ASN:HA	1:A:234:LYS:CE	0.54	2.33	1	1
1:C:466:GLU:HA	1:C:469:LEU:HD12	0.54	1.80	9	2
1:A:364:ALA:O	1:A:368:LEU:HB2	0.54	2.03	1	3
3:A:53:PCW:H352	3:A:64:PCW:H141	0.54	1.79	1	1
3:A:9:PCW:O4P	3:A:14:PCW:H322	0.54	2.03	2	1
3:A:9:PCW:H252	3:A:11:PCW:H421	0.54	1.80	9	1
3:A:5:PCW:H381	3:A:17:PCW:H81	0.53	1.80	1	1
3:A:42:PCW:H41	3:A:42:PCW:O31	0.53	2.03	4	2
1:C:528:ARG:HB3	1:C:532:ARG:NH2	0.53	2.17	6	1
3:A:26:PCW:H372	3:A:26:PCW:H131	0.53	1.78	9	1
3:A:63:PCW:H322	3:A:63:PCW:H51	0.53	1.80	4	1
3:A:4:PCW:H11	3:A:16:PCW:H62	0.53	1.79	9	1
3:A:53:PCW:H321	3:A:68:PCW:H332	0.53	1.80	9	1
3:A:58:PCW:H171	3:A:61:PCW:H381	0.53	1.78	9	1
3:A:16:PCW:H382	4:A:39:17F:H8A	0.53	1.80	10	1
1:A:212:SER:O	1:A:216:LYS:HG2	0.53	2.03	6	2
3:A:12:PCW:O2P	3:A:22:PCW:H32	0.53	2.03	9	1
3:A:6:PCW:H322	3:A:28:PCW:H2	0.53	1.78	1	1
3:A:54:PCW:H332	3:A:72:PCW:H132	0.53	1.80	3	1
1:C:517:HIS:O	1:C:521:TYR:HB2	0.53	2.04	9	1
1:C:447:GLU:OE1	1:C:451:LYS:HE2	0.53	2.03	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:43:PCW:H131	3:A:69:PCW:H332	0.53	1.79	6	1
4:A:33:17F:H39	4:A:35:17F:H32	0.53	1.81	7	1
3:A:10:PCW:H121	3:A:10:PCW:H371	0.53	1.79	2	1
4:A:36:17F:H4	4:A:36:17F:H1A	0.53	1.78	10	1
3:A:42:PCW:H31	3:A:69:PCW:H132	0.53	1.81	1	1
3:A:53:PCW:H382	3:A:64:PCW:H461	0.53	1.80	2	1
3:A:66:PCW:H352	4:A:79:17F:H9A	0.53	1.80	1	1
4:A:36:17F:H70	3:A:46:PCW:H451	0.53	1.81	6	1
2:B:33:ASP:HB3	2:B:36:ILE:HG13	0.52	1.81	4	3
3:A:1:PCW:H241	4:A:38:17F:H59	0.52	1.80	4	1
3:A:58:PCW:H352	3:A:61:PCW:H382	0.52	1.80	5	1
3:A:6:PCW:H31	3:A:16:PCW:H371	0.52	1.81	1	1
3:A:15:PCW:H63	4:A:39:17F:O2	0.52	2.04	1	1
3:A:1:PCW:H222	4:A:38:17F:H33	0.52	1.81	4	1
3:A:45:PCW:H381	3:A:57:PCW:H71	0.52	1.80	6	1
3:A:54:PCW:H142	3:A:72:PCW:H151	0.52	1.81	8	1
4:A:33:17F:H35	4:A:35:17F:H30	0.52	1.82	10	1
3:A:53:PCW:H121	3:A:56:PCW:H321	0.52	1.81	6	1
3:A:18:PCW:H42	3:A:23:PCW:O2P	0.52	2.05	5	1
3:A:13:PCW:H61	4:A:34:17F:O1	0.52	2.04	7	1
1:A:268:GLU:O	1:A:272:TYR:HB2	0.52	2.04	10	3
3:A:48:PCW:H121	3:A:54:PCW:H182	0.52	1.81	2	1
3:A:41:PCW:H121	3:A:61:PCW:H322	0.52	1.81	7	1
3:A:68:PCW:H63	3:A:70:PCW:H122	0.52	1.81	8	1
3:A:58:PCW:H11	3:A:61:PCW:H412	0.52	1.81	2	1
3:A:58:PCW:H362	3:A:61:PCW:H382	0.52	1.81	7	1
1:A:308:ARG:CG	1:C:469:LEU:CD1	0.52	2.87	9	1
1:A:326:GLU:O	1:A:330:ARG:HG3	0.52	2.05	1	2
3:A:20:PCW:H412	3:A:31:PCW:H20	0.52	1.81	3	1
1:A:236:THR:O	1:A:240:ARG:HB2	0.52	2.04	4	1
1:A:334:ARG:HD3	1:C:440:GLU:HB3	0.52	1.82	6	1
4:A:80:17F:H32	4:A:80:17F:H8	0.52	1.82	10	1
3:A:47:PCW:H61	3:A:57:PCW:O1P	0.52	2.04	8	1
1:C:561:LYS:HA	1:C:565:ALA:HB3	0.52	1.81	5	5
1:A:310:ARG:O	1:A:314:ASP:HB2	0.52	2.05	10	3
3:A:44:PCW:H321	3:A:68:PCW:H332	0.52	1.80	6	1
1:A:334:ARG:HA	1:C:440:GLU:HG2	0.51	1.80	2	1
3:A:22:PCW:H42	3:A:27:PCW:H41	0.51	1.82	8	1
3:A:2:PCW:H51	3:A:5:PCW:H11	0.51	1.81	10	1
2:B:82:PHE:HB2	2:B:89:SER:HB2	0.51	1.82	10	1
3:A:17:PCW:H142	3:A:21:PCW:H32	0.51	1.83	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:25:PCW:H32	3:A:31:PCW:H321	0.51	1.82	1	1
3:A:26:PCW:H322	3:A:28:PCW:H32	0.51	1.81	5	1
3:A:24:PCW:H121	4:A:39:17F:H31	0.51	1.83	6	1
3:A:14:PCW:H382	4:A:34:17F:H10	0.51	1.82	7	1
3:A:28:PCW:H72	2:B:47:ASP:HB3	0.51	1.82	8	1
1:A:249:GLU:O	1:A:253:LYS:HB2	0.51	2.04	1	1
3:A:27:PCW:H412	3:A:27:PCW:H142	0.51	1.81	2	1
1:A:315:ALA:O	1:A:319:HIS:HB2	0.51	2.06	3	1
3:A:60:PCW:H40	3:A:72:PCW:H261	0.51	1.82	3	1
3:A:25:PCW:H2	3:A:31:PCW:H73	0.51	1.80	8	1
3:A:49:PCW:H321	4:A:80:17F:H31	0.51	1.80	2	1
3:A:27:PCW:H73	4:A:37:17F:N1	0.51	2.21	1	1
3:A:21:PCW:O1P	4:A:36:17F:H1	0.51	2.06	6	1
1:A:279:LEU:HB3	1:C:495:LYS:HE3	0.51	1.83	8	2
3:A:45:PCW:H162	4:A:74:17F:H11A	0.51	1.83	2	1
3:A:1:PCW:H61	3:A:26:PCW:O2P	0.51	2.05	5	1
3:A:11:PCW:H371	3:A:16:PCW:H39	0.51	1.82	3	1
1:A:249:GLU:HB2	1:C:528:ARG:NH2	0.51	2.21	1	1
3:A:29:PCW:H122	3:A:31:PCW:H342	0.51	1.82	3	1
3:A:26:PCW:H121	4:A:40:17F:H33	0.51	1.83	5	1
3:A:49:PCW:H342	3:A:57:PCW:H382	0.51	1.82	6	1
3:A:27:PCW:H321	4:A:37:17F:H33	0.51	1.81	7	1
1:A:224:VAL:O	1:A:228:PHE:HB2	0.51	2.05	3	3
4:A:74:17F:H12	4:A:79:17F:H49	0.51	1.82	1	1
3:A:15:PCW:H412	3:A:20:PCW:H232	0.51	1.83	2	1
1:C:410:SER:O	1:C:414:LYS:HG2	0.51	2.05	2	1
1:A:308:ARG:CB	1:C:469:LEU:HD11	0.51	2.36	5	2
3:A:4:PCW:H381	3:A:7:PCW:H262	0.51	1.83	4	1
1:C:508:ARG:O	1:C:512:ASP:HB3	0.51	2.06	4	2
3:A:55:PCW:H11	3:A:64:PCW:H2	0.51	1.83	9	1
3:A:72:PCW:H412	4:A:78:17F:H51	0.50	1.83	1	1
3:A:13:PCW:H141	3:A:18:PCW:H141	0.50	1.82	5	1
3:A:46:PCW:H82	4:A:73:17F:O1	0.50	2.07	6	1
3:A:15:PCW:H321	3:A:16:PCW:H211	0.50	1.84	2	1
1:A:362:GLU:HB3	1:C:414:LYS:HD3	0.50	1.83	5	1
3:A:68:PCW:H2	3:A:69:PCW:H321	0.50	1.81	5	1
1:A:231:ASN:HA	1:A:234:LYS:HD2	0.50	1.84	6	1
3:A:10:PCW:H83	4:A:36:17F:N1	0.50	2.21	7	1
3:A:20:PCW:H19	3:A:31:PCW:H241	0.50	1.83	9	1
3:A:42:PCW:H72	3:A:63:PCW:O1P	0.50	2.06	2	1
3:A:58:PCW:H381	3:A:60:PCW:H122	0.50	1.84	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:9:PCW:H63	3:A:30:PCW:O2P	0.50	2.07	5	1
2:B:5:LYS:HD2	2:B:75:GLY:HA2	0.50	1.82	6	1
3:A:25:PCW:H2	3:A:31:PCW:H42	0.50	1.82	7	1
3:A:72:PCW:O31	3:A:72:PCW:H42	0.50	2.07	8	1
1:A:255:GLN:HB2	1:A:256:PRO:CD	0.50	2.37	2	5
1:C:469:LEU:O	1:C:473:LYS:HB2	0.50	2.06	2	2
4:A:39:17F:O4	2:B:136:SER:HA	0.50	2.06	3	1
3:A:63:PCW:H83	4:A:75:17F:O4	0.50	2.07	3	1
3:A:55:PCW:H63	3:A:64:PCW:O1P	0.50	2.07	6	1
3:A:17:PCW:H41	3:A:17:PCW:H322	0.50	1.81	10	1
3:A:7:PCW:H82	4:A:35:17F:N1	0.50	2.22	1	1
1:A:360:LEU:HA	1:A:363:LYS:HD2	0.50	1.82	6	1
1:A:372:ARG:O	1:A:376:LEU:HG	0.50	2.05	4	3
3:A:9:PCW:H81	4:A:34:17F:O5	0.50	2.06	3	1
3:A:12:PCW:H82	3:A:22:PCW:O2P	0.50	2.07	5	1
3:A:12:PCW:H62	3:A:22:PCW:O2P	0.50	2.06	9	1
3:A:54:PCW:H2	3:A:60:PCW:H11	0.50	1.83	10	1
3:A:49:PCW:H2	3:A:57:PCW:H62	0.50	1.83	5	1
4:A:33:17F:C4	4:A:33:17F:H1	0.50	2.37	9	4
1:A:289:GLN:O	1:A:293:GLU:HG2	0.50	2.07	5	1
1:A:330:ARG:HH22	1:C:448:VAL:HG23	0.50	1.66	10	1
3:A:18:PCW:O1P	3:A:23:PCW:H61	0.49	2.07	2	1
4:A:35:17F:H11A	4:A:35:17F:H33	0.49	1.83	2	1
3:A:3:PCW:H361	3:A:18:PCW:H342	0.49	1.82	6	1
3:A:1:PCW:H472	3:A:43:PCW:H262	0.49	1.83	7	1
3:A:14:PCW:H252	4:A:37:17F:H48	0.49	1.85	8	1
1:A:363:LYS:HD2	1:C:411:THR:HG23	0.49	1.82	10	1
3:A:6:PCW:P	3:A:16:PCW:O1P	0.49	2.70	10	1
4:A:33:17F:P1	4:A:33:17F:N1	0.49	2.84	9	5
3:A:25:PCW:H51	3:A:25:PCW:H321	0.49	1.84	2	1
3:A:48:PCW:H372	3:A:54:PCW:H231	0.49	1.84	4	1
2:B:37:GLU:HB2	2:B:59:ALA:HB2	0.49	1.84	5	1
3:A:14:PCW:O11	3:A:23:PCW:H42	0.49	2.06	8	2
4:A:33:17F:H35	4:A:35:17F:H34	0.49	1.84	6	1
3:A:62:PCW:O1P	3:A:72:PCW:H83	0.49	2.08	7	1
3:A:58:PCW:H12	3:A:61:PCW:H351	0.49	1.85	2	1
4:A:76:17F:H20A	4:A:76:17F:H11A	0.49	1.83	10	1
1:C:421:PRO:O	1:C:425:GLU:HG2	0.49	2.06	10	1
3:A:55:PCW:H2	4:A:77:17F:H2	0.49	1.85	3	1
2:B:126:ASP:OD2	2:B:128:LYS:HG3	0.49	2.07	5	1
3:A:24:PCW:H121	3:A:25:PCW:H141	0.49	1.84	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:32:PCW:H61	4:A:38:17F:N1	0.49	2.14	8	1
3:A:25:PCW:H222	3:A:67:PCW:H472	0.49	1.84	10	1
3:A:7:PCW:H82	4:A:35:17F:HN1A	0.49	1.67	1	1
3:A:5:PCW:H411	3:A:17:PCW:H331	0.49	1.83	3	1
3:A:50:PCW:H39	3:A:72:PCW:H81	0.49	1.83	5	1
3:A:41:PCW:H81	3:A:59:PCW:O1P	0.49	2.07	7	1
1:C:461:LYS:O	1:C:465:GLU:HG3	0.49	2.07	8	1
3:A:53:PCW:H81	3:A:69:PCW:O1P	0.49	2.08	3	1
3:A:17:PCW:H72	4:A:38:17F:O2	0.49	2.08	2	1
3:A:49:PCW:H472	4:A:80:17F:H47	0.49	1.85	2	1
3:A:48:PCW:H71	3:A:61:PCW:H411	0.49	1.82	7	1
1:A:365:LYS:HB2	1:A:366:PRO:CD	0.49	2.31	9	1
1:C:523:ASP:HA	1:C:526:ARG:HD2	0.49	1.85	8	3
3:A:50:PCW:H121	4:A:78:17F:H4A	0.49	1.85	5	1
3:A:70:PCW:H421	3:A:71:PCW:H472	0.49	1.84	6	1
3:A:50:PCW:H352	4:A:78:17F:H62	0.49	1.84	7	1
3:A:17:PCW:H81	4:A:38:17F:O1	0.49	2.07	9	1
2:B:17:SER:HB3	2:B:32:TYR:CE1	0.49	2.43	9	1
3:A:7:PCW:H42	4:A:33:17F:H4	0.49	1.85	10	1
1:A:309:ALA:HA	1:A:312:HIS:HB2	0.48	1.85	1	1
1:C:573:LEU:HA	1:C:576:VAL:HG12	0.48	1.84	5	2
3:A:8:PCW:H81	3:A:22:PCW:O1P	0.48	2.07	4	1
3:A:66:PCW:H32	4:A:79:17F:O1	0.48	2.08	2	1
4:A:38:17F:H10	4:A:38:17F:H60	0.48	1.85	3	1
3:A:25:PCW:H152	3:A:31:PCW:H322	0.48	1.83	4	1
3:A:46:PCW:H361	3:A:70:PCW:H40	0.48	1.84	4	1
1:A:359:THR:HA	1:A:362:GLU:HB2	0.48	1.84	7	1
1:C:458:ASP:O	1:C:462:LYS:HG2	0.48	2.08	1	2
3:A:10:PCW:H332	3:A:21:PCW:H341	0.48	1.85	4	1
3:A:49:PCW:H332	3:A:57:PCW:H371	0.48	1.84	5	1
1:C:465:GLU:HB3	1:C:469:LEU:HD11	0.48	1.84	10	1
3:A:53:PCW:H82	3:A:68:PCW:H332	0.48	1.85	2	1
3:A:22:PCW:H182	3:A:27:PCW:H431	0.48	1.85	4	1
3:A:6:PCW:H132	3:A:11:PCW:H322	0.48	1.85	1	1
3:A:4:PCW:H242	3:A:32:PCW:H252	0.48	1.86	4	1
1:A:234:LYS:HE3	1:C:539:ASN:OD1	0.48	2.09	1	1
3:A:55:PCW:H71	3:A:64:PCW:O1P	0.48	2.09	3	1
3:A:67:PCW:H172	4:A:75:17F:H56	0.48	1.86	3	1
1:C:514:LEU:HA	1:C:517:HIS:HB2	0.48	1.85	4	1
3:A:3:PCW:H352	3:A:3:PCW:H122	0.48	1.85	5	1
4:A:74:17F:H12	4:A:79:17F:H8	0.48	1.84	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:586:SER:O	1:C:590:GLU:HG3	0.48	2.07	5	2
3:A:20:PCW:H332	3:A:31:PCW:H132	0.48	1.85	10	1
1:A:327:LEU:HD23	1:A:330:ARG:HD3	0.48	1.86	1	1
3:A:14:PCW:H211	4:A:34:17F:H19	0.48	1.85	4	1
3:A:5:PCW:H2	3:A:5:PCW:H51	0.48	1.84	8	1
4:A:74:17F:H18A	4:A:74:17F:H9	0.48	1.86	9	1
1:C:455:TYR:O	1:C:459:PHE:HB2	0.48	2.08	2	2
3:A:29:PCW:H182	3:A:31:PCW:H71	0.48	1.86	2	1
3:A:12:PCW:H73	3:A:22:PCW:O2P	0.48	2.09	5	1
3:A:3:PCW:H61	3:A:19:PCW:O2P	0.48	2.08	7	1
3:A:12:PCW:H32	3:A:22:PCW:H12	0.48	1.85	8	1
3:A:24:PCW:O1P	3:A:25:PCW:H31	0.48	2.09	8	1
3:A:47:PCW:H411	4:A:73:17F:H9	0.48	1.86	8	1
1:A:335:LEU:O	1:A:339:LYS:HB2	0.48	2.08	9	1
3:A:30:PCW:H321	4:A:40:17F:H20A	0.48	1.85	2	1
3:A:7:PCW:O2P	3:A:16:PCW:H42	0.48	2.08	4	1
1:A:341:ASN:HD21	1:C:433:GLU:HG2	0.48	1.69	5	1
1:C:491:GLU:O	1:C:495:LYS:HG3	0.48	2.09	5	2
1:A:242:GLU:HB3	1:C:532:ARG:NH2	0.48	2.24	6	1
3:A:55:PCW:H381	3:A:55:PCW:H142	0.48	1.84	6	2
3:A:13:PCW:H141	3:A:18:PCW:H122	0.48	1.86	7	1
3:A:21:PCW:H361	3:A:21:PCW:H122	0.48	1.86	9	1
3:A:17:PCW:H252	4:A:36:17F:H63	0.47	1.85	1	1
3:A:10:PCW:H362	3:A:22:PCW:H432	0.47	1.85	2	1
3:A:68:PCW:H2	3:A:69:PCW:H342	0.47	1.85	6	1
1:A:301:LEU:HB3	1:C:473:LYS:HE2	0.47	1.86	8	1
4:A:77:17F:H9	4:A:77:17F:O10	0.47	2.09	8	1
3:A:13:PCW:H62	4:A:34:17F:O9	0.47	2.08	2	1
1:C:458:ASP:HA	1:C:461:LYS:HD2	0.47	1.85	6	2
3:A:25:PCW:H132	3:A:31:PCW:H321	0.47	1.85	8	1
3:A:9:PCW:H81	3:A:30:PCW:O2P	0.47	2.10	1	1
3:A:48:PCW:H362	3:A:54:PCW:H382	0.47	1.86	5	1
3:A:48:PCW:H162	3:A:54:PCW:H182	0.47	1.86	1	1
3:A:5:PCW:H132	3:A:17:PCW:H342	0.47	1.84	5	1
3:A:11:PCW:H83	3:A:24:PCW:O2P	0.47	2.09	5	1
3:A:45:PCW:H211	3:A:49:PCW:H162	0.47	1.86	7	1
3:A:8:PCW:H171	3:A:27:PCW:H241	0.47	1.85	9	1
3:A:42:PCW:H52	4:A:75:17F:H2	0.47	1.85	9	1
1:C:483:GLU:O	1:C:487:GLN:HG3	0.47	2.09	10	1
3:A:58:PCW:H12	3:A:61:PCW:H412	0.47	1.87	3	1
3:A:51:PCW:H361	3:A:70:PCW:H182	0.47	1.85	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:70:PCW:H2	3:A:70:PCW:O4P	0.47	2.09	5	1
1:C:444:ASP:O	1:C:448:VAL:HB	0.47	2.09	7	2
3:A:65:PCW:H221	4:A:80:17F:H37	0.47	1.85	1	1
3:A:15:PCW:H81	4:A:39:17F:N1	0.47	2.25	3	1
3:A:17:PCW:H162	4:A:36:17F:H32	0.47	1.86	3	1
3:A:57:PCW:H121	4:A:80:17F:H6	0.47	1.87	5	1
3:A:15:PCW:H31	3:A:16:PCW:H181	0.47	1.86	7	1
3:A:13:PCW:H19	3:A:18:PCW:H262	0.47	1.86	10	1
3:A:17:PCW:O1P	4:A:36:17F:H6	0.47	2.10	10	1
3:A:27:PCW:H41	4:A:37:17F:P1	0.47	2.49	1	1
3:A:12:PCW:H371	3:A:21:PCW:H321	0.47	1.84	2	1
3:A:6:PCW:H73	3:A:28:PCW:H73	0.47	1.86	3	1
3:A:10:PCW:H61	3:A:12:PCW:O31	0.47	2.08	3	1
3:A:20:PCW:H452	3:A:31:PCW:H261	0.47	1.86	3	1
3:A:50:PCW:H12	4:A:78:17F:H4	0.47	1.86	3	1
2:B:41:ARG:HA	2:B:53:LEU:O	0.47	2.09	4	1
1:A:356:HIS:O	1:A:360:LEU:HB2	0.47	2.09	6	2
3:A:41:PCW:H71	4:A:77:17F:HN1A	0.47	1.70	9	1
1:A:387:LEU:O	1:A:391:GLU:HG3	0.47	2.09	2	2
1:C:563:LYS:O	1:C:567:GLU:HG2	0.47	2.09	7	2
2:B:126:ASP:HB3	2:B:129:GLN:HG3	0.47	1.85	6	1
1:A:287:ALA:HA	1:A:290:LYS:HD2	0.47	1.86	9	1
3:A:9:PCW:H41	2:B:49:GLU:HG3	0.47	1.86	2	1
3:A:9:PCW:H152	4:A:34:17F:H37	0.47	1.85	4	1
3:A:27:PCW:H82	4:A:37:17F:O2	0.47	2.10	6	1
3:A:48:PCW:H142	3:A:54:PCW:H181	0.47	1.85	7	1
3:A:16:PCW:H152	4:A:39:17F:H58	0.47	1.87	9	1
4:A:75:17F:H11	4:A:75:17F:H20	0.47	1.85	3	1
3:A:30:PCW:H83	4:A:34:17F:HN1	0.47	1.70	4	1
3:A:49:PCW:H351	4:A:80:17F:H31	0.47	1.86	4	1
3:A:68:PCW:O31	3:A:69:PCW:H61	0.47	2.09	6	1
3:A:60:PCW:H472	3:A:63:PCW:H422	0.47	1.87	9	1
3:A:59:PCW:H82	3:A:59:PCW:O31	0.46	2.10	4	1
4:A:74:17F:H46	4:A:75:17F:H36	0.46	1.86	6	1
1:C:442:SER:O	1:C:446:GLU:HG3	0.46	2.09	6	1
3:A:1:PCW:H322	3:A:5:PCW:H371	0.46	1.88	7	1
1:C:473:LYS:O	1:C:477:LEU:HB2	0.46	2.11	10	2
3:A:24:PCW:H62	4:A:39:17F:O1	0.46	2.11	1	1
3:A:31:PCW:H52	3:A:31:PCW:O31	0.46	2.10	2	2
3:A:9:PCW:H31	3:A:14:PCW:H361	0.46	1.87	5	1
3:A:32:PCW:H342	4:A:33:17F:H60	0.46	1.87	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:30:PCW:H382	3:A:30:PCW:H142	0.46	1.87	9	1
3:A:72:PCW:H431	4:A:78:17F:H47	0.46	1.87	10	1
1:A:310:ARG:O	1:A:314:ASP:HB3	0.46	2.11	1	1
1:A:308:ARG:HG3	1:C:469:LEU:CD2	0.46	2.39	2	2
3:A:9:PCW:H72	3:A:30:PCW:O2P	0.46	2.11	3	2
3:A:45:PCW:H241	4:A:74:17F:H40	0.46	1.87	3	1
1:A:260:ASP:HA	1:A:263:LYS:HE3	0.46	1.87	5	1
3:A:48:PCW:H321	3:A:54:PCW:H132	0.46	1.87	10	1
2:B:78:PHE:O	2:B:111:MET:HA	0.46	2.10	9	3
3:A:16:PCW:H121	4:A:39:17F:H9A	0.46	1.87	6	1
3:A:13:PCW:H182	3:A:23:PCW:H162	0.46	1.88	8	1
1:A:337:ALA:O	1:A:341:ASN:HB2	0.46	2.10	9	1
3:A:13:PCW:H121	3:A:23:PCW:H142	0.46	1.87	9	1
4:A:39:17F:H58	4:A:39:17F:H10	0.46	1.86	2	1
3:A:67:PCW:H41	3:A:67:PCW:C31	0.46	2.41	2	1
3:A:59:PCW:H2	4:A:77:17F:H8	0.46	1.88	5	1
1:C:478:ARG:O	1:C:482:GLN:HB2	0.46	2.10	5	3
3:A:15:PCW:H51	4:A:39:17F:N1	0.46	2.26	6	1
3:A:26:PCW:H441	4:A:33:17F:H46	0.46	1.86	7	1
2:B:17:SER:HA	2:B:20:THR:OG1	0.46	2.11	7	1
4:A:74:17F:H38	4:A:75:17F:H10	0.46	1.88	8	1
1:A:203:LEU:O	1:A:207:TRP:HB2	0.46	2.11	10	2
1:A:255:GLN:HB2	1:A:256:PRO:HD3	0.46	1.88	4	4
3:A:48:PCW:H371	3:A:54:PCW:H382	0.46	1.88	3	1
2:B:94:HIS:O	2:B:98:GLU:HG2	0.46	2.11	6	1
3:A:5:PCW:H12	3:A:17:PCW:H321	0.46	1.88	3	2
3:A:10:PCW:N	4:A:36:17F:N1	0.46	2.61	3	1
3:A:49:PCW:O2P	3:A:57:PCW:H62	0.46	2.10	3	1
3:A:14:PCW:H162	4:A:34:17F:H18A	0.46	1.88	9	1
4:A:37:17F:O5	2:B:135:ARG:HD3	0.46	2.10	9	1
1:A:312:HIS:HE1	1:C:465:GLU:HB2	0.46	1.71	1	2
3:A:60:PCW:H411	3:A:62:PCW:H481	0.46	1.87	6	1
3:A:52:PCW:H441	3:A:69:PCW:H442	0.46	1.88	7	1
3:A:47:PCW:H61	4:A:74:17F:O1	0.46	2.10	9	1
1:C:560:GLU:O	1:C:564:PRO:HD2	0.45	2.10	2	1
3:A:3:PCW:H342	3:A:23:PCW:H322	0.45	1.86	4	1
2:B:24:ILE:HG13	2:B:40:TYR:HB3	0.45	1.87	4	1
3:A:7:PCW:H41	4:A:33:17F:H8	0.45	1.88	5	1
3:A:6:PCW:H342	3:A:16:PCW:H321	0.45	1.87	6	1
3:A:10:PCW:H83	4:A:36:17F:HN1	0.45	1.69	7	1
2:B:92:ASP:O	2:B:95:HIS:HB3	0.45	2.11	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:56:PCW:O1P	3:A:70:PCW:H41	0.45	2.11	8	1
3:A:30:PCW:H332	4:A:40:17F:H57	0.45	1.88	10	1
3:A:16:PCW:H271	3:A:24:PCW:H452	0.45	1.88	1	1
3:A:57:PCW:H19	4:A:80:17F:H12	0.45	1.88	1	1
1:C:559:SER:HA	1:C:562:ALA:HB3	0.45	1.88	2	1
3:A:22:PCW:H2	3:A:22:PCW:H52	0.45	1.88	4	1
3:A:1:PCW:H71	3:A:26:PCW:O2P	0.45	2.11	5	1
3:A:4:PCW:H51	3:A:7:PCW:O1P	0.45	2.11	6	1
3:A:41:PCW:H71	4:A:77:17F:H1A	0.45	1.87	6	1
3:A:5:PCW:H332	4:A:38:17F:O9	0.45	2.11	8	1
3:A:51:PCW:H2	3:A:71:PCW:H422	0.45	1.87	1	1
1:A:246:ASP:HA	1:C:528:ARG:CZ	0.45	2.41	3	1
3:A:15:PCW:H81	4:A:39:17F:HN1A	0.45	1.71	3	1
3:A:2:PCW:H342	3:A:5:PCW:H151	0.45	1.87	6	1
3:A:46:PCW:H62	4:A:73:17F:N1	0.45	2.27	8	1
3:A:17:PCW:H42	2:B:45:VAL:HB	0.45	1.88	9	1
3:A:49:PCW:H321	3:A:57:PCW:H322	0.45	1.88	9	1
3:A:55:PCW:H71	3:A:64:PCW:H12	0.45	1.87	3	1
3:A:16:PCW:H122	4:A:39:17F:H9A	0.45	1.88	5	1
1:A:272:TYR:O	1:A:276:VAL:HB	0.45	2.11	7	1
3:A:45:PCW:H152	4:A:74:17F:H11A	0.45	1.87	10	1
3:A:41:PCW:H242	3:A:58:PCW:H422	0.45	1.88	1	1
3:A:47:PCW:H171	4:A:73:17F:H32	0.45	1.87	2	1
3:A:16:PCW:O31	3:A:16:PCW:H41	0.45	2.11	5	1
1:A:330:ARG:NH2	1:C:444:ASP:HA	0.45	2.27	1	1
3:A:43:PCW:H482	3:A:70:PCW:H152	0.45	1.87	2	1
1:C:565:ALA:O	1:C:569:LEU:HG	0.45	2.10	4	1
2:B:56:LEU:HB2	2:B:71:TYR:CD2	0.45	2.46	7	3
3:A:67:PCW:H181	4:A:75:17F:H58	0.45	1.88	1	1
3:A:17:PCW:H232	4:A:36:17F:H33	0.45	1.87	5	1
3:A:48:PCW:H81	3:A:61:PCW:H411	0.45	1.89	6	1
3:A:62:PCW:H451	3:A:72:PCW:H231	0.45	1.88	6	1
3:A:2:PCW:O1P	3:A:17:PCW:H11	0.45	2.11	7	1
3:A:66:PCW:H20	3:A:67:PCW:H81	0.45	1.88	7	1
3:A:11:PCW:H251	3:A:67:PCW:H442	0.45	1.89	9	1
3:A:25:PCW:O31	3:A:31:PCW:H82	0.45	2.11	10	1
1:C:554:HIS:HA	1:C:557:THR:OG1	0.45	2.12	1	1
3:A:4:PCW:H52	3:A:7:PCW:O1P	0.45	2.12	3	1
1:C:491:GLU:HB3	1:C:495:LYS:HE2	0.45	1.87	3	1
3:A:10:PCW:H71	4:A:36:17F:HN1A	0.45	1.71	9	1
3:A:26:PCW:H142	3:A:28:PCW:H122	0.45	1.89	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:32:PCW:H122	4:A:33:17F:H20	0.45	1.86	1	1
1:C:535:ALA:O	1:C:539:ASN:HB2	0.45	2.12	2	1
1:A:257:TYR:O	1:A:261:PHE:HB2	0.45	2.12	6	1
3:A:3:PCW:H181	3:A:19:PCW:H251	0.45	1.89	3	1
3:A:5:PCW:H52	3:A:5:PCW:O31	0.45	2.12	3	1
3:A:69:PCW:O11	3:A:69:PCW:H82	0.45	2.12	3	1
3:A:48:PCW:H42	3:A:58:PCW:O2P	0.45	2.12	4	1
3:A:3:PCW:H81	3:A:19:PCW:O11	0.45	2.11	6	1
3:A:42:PCW:N	4:A:75:17F:N1	0.45	2.64	6	1
1:A:277:GLU:HB2	1:A:278:PRO:CD	0.44	2.42	6	2
3:A:43:PCW:O11	3:A:43:PCW:H82	0.44	2.12	1	1
1:C:427:TRP:O	1:C:431:GLU:HG2	0.44	2.12	1	2
3:A:42:PCW:H462	3:A:52:PCW:H421	0.44	1.89	3	1
3:A:64:PCW:H161	3:A:64:PCW:H412	0.44	1.89	4	1
3:A:6:PCW:H31	3:A:11:PCW:O2P	0.44	2.12	7	1
3:A:7:PCW:H483	3:A:52:PCW:H40	0.44	1.89	8	1
3:A:2:PCW:H51	3:A:5:PCW:C1	0.44	2.41	10	1
1:C:475:GLU:HB2	1:C:476:PRO:HD3	0.44	1.89	2	1
3:A:3:PCW:O2P	3:A:23:PCW:H51	0.44	2.12	4	1
1:A:378:VAL:O	1:A:382:PHE:HB2	0.44	2.12	4	1
3:A:49:PCW:H322	3:A:57:PCW:H352	0.44	1.88	4	1
1:A:330:ARG:NH2	1:C:451:LYS:HD2	0.44	2.27	7	1
2:B:6:LEU:O	2:B:55:ILE:HA	0.44	2.12	10	1
3:A:6:PCW:O2P	3:A:6:PCW:N	0.44	2.50	4	2
3:A:57:PCW:H152	4:A:76:17F:H29	0.44	1.90	1	1
1:C:570:ARG:O	1:C:574:LEU:HG	0.44	2.11	1	1
3:A:1:PCW:N	4:A:35:17F:N1	0.44	2.64	6	1
3:A:42:PCW:H421	3:A:52:PCW:H471	0.44	1.88	9	1
3:A:55:PCW:H72	3:A:64:PCW:O11	0.44	2.12	9	1
3:A:46:PCW:H121	3:A:71:PCW:H39	0.44	1.88	2	1
3:A:8:PCW:H332	3:A:27:PCW:H172	0.44	1.90	3	1
1:C:456:LEU:O	1:C:460:GLN:HB2	0.44	2.11	8	4
1:C:550:LYS:HA	1:C:553:GLU:OE1	0.44	2.13	8	2
4:A:39:17F:H12	4:A:39:17F:H65	0.44	1.89	5	1
3:A:43:PCW:O11	3:A:43:PCW:H41	0.44	2.13	6	1
3:A:11:PCW:H82	3:A:24:PCW:O2P	0.44	2.12	10	1
3:A:30:PCW:H63	4:A:34:17F:O2	0.44	2.13	10	1
3:A:67:PCW:O31	3:A:67:PCW:H42	0.44	2.12	10	1
1:A:363:LYS:HD3	1:C:411:THR:HG23	0.44	1.87	1	1
3:A:5:PCW:H83	4:A:38:17F:H6	0.44	1.88	2	1
3:A:6:PCW:P	4:A:39:17F:O2	0.44	2.75	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:18:PCW:H441	3:A:23:PCW:H221	0.44	1.89	3	1
3:A:42:PCW:H122	3:A:67:PCW:H212	0.44	1.89	5	1
3:A:52:PCW:H232	3:A:58:PCW:H461	0.44	1.89	5	1
3:A:16:PCW:H151	4:A:39:17F:H11A	0.44	1.88	8	1
3:A:1:PCW:H281	3:A:17:PCW:H441	0.44	1.88	2	1
1:A:363:LYS:O	1:A:367:ALA:HB3	0.44	2.11	4	3
1:A:260:ASP:HA	1:A:263:LYS:CE	0.44	2.30	6	1
3:A:3:PCW:H321	3:A:23:PCW:H12	0.44	1.90	6	1
3:A:14:PCW:H152	4:A:34:17F:H1A	0.44	1.90	9	1
3:A:29:PCW:H232	3:A:31:PCW:H382	0.44	1.90	9	1
3:A:10:PCW:H122	3:A:10:PCW:H372	0.44	1.89	1	1
3:A:12:PCW:O1P	3:A:22:PCW:H11	0.44	2.13	2	1
2:B:116:ASN:HA	2:B:144:THR:O	0.44	2.13	4	1
3:A:53:PCW:O2P	3:A:55:PCW:H62	0.43	2.13	2	1
3:A:13:PCW:H81	4:A:37:17F:H1	0.43	1.89	3	1
1:A:336:GLU:O	1:A:340:GLU:HG2	0.43	2.12	4	1
3:A:4:PCW:H83	4:A:33:17F:HN1A	0.43	1.73	4	1
1:A:268:GLU:OE1	1:C:506:ARG:HD3	0.43	2.13	8	1
3:A:6:PCW:P	3:A:11:PCW:O2P	0.43	2.76	2	1
3:A:2:PCW:H73	3:A:21:PCW:O1P	0.43	2.13	5	1
3:A:52:PCW:O1P	3:A:60:PCW:H73	0.43	2.12	5	1
3:A:50:PCW:H82	4:A:78:17F:O1	0.43	2.13	6	1
3:A:52:PCW:H131	3:A:60:PCW:H11	0.43	1.89	7	1
1:C:539:ASN:HB3	1:C:543:ARG:HH21	0.43	1.73	8	1
3:A:7:PCW:H362	4:A:33:17F:H11	0.43	1.89	9	1
3:A:12:PCW:H121	3:A:30:PCW:H211	0.43	1.89	9	1
3:A:68:PCW:O2P	3:A:69:PCW:H73	0.43	2.12	9	1
3:A:42:PCW:O11	3:A:42:PCW:H51	0.43	2.14	10	1
3:A:14:PCW:H121	4:A:34:17F:H34	0.43	1.90	1	1
3:A:48:PCW:H361	3:A:54:PCW:H431	0.43	1.90	2	1
3:A:68:PCW:H331	3:A:69:PCW:H342	0.43	1.89	2	1
3:A:41:PCW:H242	3:A:61:PCW:H481	0.43	1.89	5	1
3:A:5:PCW:H381	3:A:17:PCW:H61	0.43	1.89	7	1
3:A:51:PCW:H11	3:A:71:PCW:H421	0.43	1.90	7	1
3:A:7:PCW:H73	4:A:35:17F:N1	0.43	2.24	1	1
1:A:278:PRO:O	1:A:282:GLU:HG3	0.43	2.13	2	2
3:A:16:PCW:H51	3:A:16:PCW:O11	0.43	2.14	4	1
3:A:70:PCW:H332	3:A:70:PCW:H181	0.43	1.90	4	1
3:A:3:PCW:H382	3:A:3:PCW:H161	0.43	1.90	6	1
1:C:560:GLU:O	1:C:564:PRO:HG2	0.43	2.13	6	1
1:A:338:LEU:HA	1:A:345:ARG:HH12	0.43	1.72	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:58:PCW:H362	3:A:61:PCW:H351	0.43	1.91	9	1
1:A:275:LYS:O	1:A:279:LEU:HB2	0.43	2.12	10	1
3:A:43:PCW:H83	4:A:74:17F:HN1A	0.43	1.73	10	1
1:C:417:GLU:O	1:C:421:PRO:HD2	0.43	2.12	6	4
1:A:254:VAL:HA	1:A:257:TYR:HB2	0.43	1.89	3	1
3:A:17:PCW:O1P	3:A:17:PCW:H31	0.43	2.12	4	1
3:A:12:PCW:H73	3:A:30:PCW:O11	0.43	2.14	8	1
3:A:21:PCW:H331	3:A:22:PCW:H441	0.43	1.91	9	1
1:A:349:TYR:HB3	3:A:2:PCW:H252	0.43	1.90	2	1
3:A:3:PCW:C7	3:A:19:PCW:H2	0.43	2.43	5	1
1:A:264:LYS:CG	1:C:509:ALA:HB1	0.43	2.43	6	1
3:A:62:PCW:H122	3:A:72:PCW:H131	0.43	1.91	7	1
1:C:561:LYS:O	1:C:565:ALA:HB3	0.43	2.14	7	1
3:A:31:PCW:O31	3:A:31:PCW:H62	0.43	2.14	8	1
3:A:25:PCW:O2P	3:A:31:PCW:H51	0.43	2.14	9	1
3:A:20:PCW:H31	3:A:31:PCW:H12	0.43	1.90	2	1
1:A:359:THR:HG21	1:C:418:GLN:HB2	0.43	1.89	9	2
3:A:27:PCW:H371	3:A:27:PCW:H161	0.43	1.90	4	1
3:A:18:PCW:H371	3:A:19:PCW:H172	0.43	1.89	5	1
3:A:25:PCW:O31	3:A:31:PCW:H12	0.43	2.13	9	1
3:A:63:PCW:H32	4:A:75:17F:N1	0.43	2.29	10	1
3:A:20:PCW:H172	3:A:20:PCW:H411	0.43	1.90	1	1
3:A:26:PCW:H342	4:A:40:17F:H56	0.43	1.91	1	1
2:B:41:ARG:HG2	2:B:54:ASP:HA	0.43	1.91	2	1
3:A:71:PCW:H342	3:A:71:PCW:H131	0.43	1.91	4	1
3:A:57:PCW:H452	4:A:79:17F:H38	0.43	1.90	6	1
3:A:7:PCW:O2P	3:A:16:PCW:H83	0.43	2.13	8	1
3:A:13:PCW:H122	3:A:23:PCW:C3	0.43	2.44	8	1
3:A:30:PCW:H71	2:B:138:GLY:O	0.43	2.13	9	1
1:C:426:PHE:O	1:C:430:LEU:HG	0.43	2.14	10	1
1:C:502:GLU:O	1:C:506:ARG:HG3	0.43	2.14	3	2
1:A:202:LYS:NZ	1:C:576:VAL:HG21	0.43	2.29	3	1
1:A:289:GLN:O	1:A:293:GLU:HB2	0.43	2.14	3	1
3:A:68:PCW:O1P	3:A:69:PCW:H41	0.43	2.14	6	1
3:A:53:PCW:H371	3:A:68:PCW:H422	0.43	1.89	7	1
1:A:280:ARG:O	1:A:284:GLN:HB2	0.43	2.13	5	1
3:A:43:PCW:H411	3:A:47:PCW:H71	0.43	1.89	7	1
4:A:38:17F:H18	4:A:38:17F:H9A	0.43	1.91	8	1
2:B:35:THR:HG22	2:B:61:GLN:HG2	0.42	1.90	1	1
1:C:489:LEU:O	1:C:493:GLN:HG3	0.42	2.14	4	1
3:A:3:PCW:H251	3:A:19:PCW:H211	0.42	1.91	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:14:PCW:H121	4:A:34:17F:O10	0.42	2.14	7	1
1:A:308:ARG:HD3	1:C:465:GLU:HB3	0.42	1.90	9	1
1:C:445:LEU:O	1:C:449:LYS:HG3	0.42	2.13	9	1
1:C:524:GLU:HB3	1:C:528:ARG:NH2	0.42	2.29	2	1
1:C:543:ARG:O	1:C:547:TYR:HB2	0.42	2.13	3	1
3:A:41:PCW:H31	3:A:52:PCW:H352	0.42	1.90	4	1
3:A:32:PCW:H63	4:A:35:17F:O1	0.42	2.14	8	1
3:A:54:PCW:H72	3:A:62:PCW:O2P	0.42	2.13	8	1
3:A:5:PCW:H481	4:A:36:17F:H45	0.42	1.91	1	1
1:A:293:GLU:O	1:A:297:LYS:HG2	0.42	2.15	2	1
3:A:48:PCW:H422	3:A:54:PCW:H261	0.42	1.91	1	1
1:A:383:LYS:O	1:A:387:LEU:HB2	0.42	2.14	2	1
3:A:54:PCW:H352	3:A:72:PCW:H132	0.42	1.90	2	1
4:A:79:17F:H31	4:A:79:17F:H11A	0.42	1.91	2	1
3:A:5:PCW:H451	3:A:17:PCW:H141	0.42	1.92	5	1
3:A:42:PCW:H121	3:A:67:PCW:H283	0.42	1.90	5	1
3:A:50:PCW:H31	4:A:78:17F:H4	0.42	1.92	10	1
1:C:574:LEU:HB2	1:C:575:PRO:CD	0.42	2.44	1	1
3:A:32:PCW:H332	4:A:35:17F:H10A	0.42	1.91	2	1
4:A:36:17F:H73	3:A:51:PCW:H232	0.42	1.91	4	1
3:A:4:PCW:H51	3:A:7:PCW:O11	0.42	2.14	7	1
2:B:56:LEU:HB2	2:B:71:TYR:HD2	0.42	1.74	7	1
3:A:32:PCW:H63	4:A:38:17F:O4	0.42	2.14	9	1
1:C:563:LYS:O	1:C:567:GLU:HB2	0.42	2.14	9	1
3:A:48:PCW:H362	3:A:54:PCW:H172	0.42	1.91	10	1
2:B:6:LEU:HA	2:B:77:GLY:O	0.42	2.14	10	1
1:A:380:GLU:O	1:A:384:VAL:HG23	0.42	2.15	4	3
3:A:5:PCW:H12	3:A:17:PCW:O2P	0.42	2.15	5	1
3:A:23:PCW:N	4:A:34:17F:N1	0.42	2.67	9	1
3:A:41:PCW:H372	3:A:59:PCW:H351	0.42	1.91	1	1
3:A:30:PCW:H142	4:A:40:17F:H4	0.42	1.91	2	1
1:A:251:LYS:O	1:A:254:VAL:HG12	0.42	2.15	3	1
3:A:9:PCW:H462	4:A:34:17F:H67	0.42	1.92	6	1
3:A:49:PCW:H131	4:A:79:17F:H50	0.42	1.91	7	1
1:A:221:LEU:HA	1:A:224:VAL:HB	0.42	1.92	3	1
3:A:53:PCW:O11	3:A:64:PCW:H51	0.42	2.14	3	1
1:A:306:ARG:O	1:A:310:ARG:HG3	0.42	2.14	6	1
3:A:7:PCW:H72	4:A:33:17F:H4	0.42	1.92	10	1
4:A:37:17F:H11	4:A:37:17F:H32	0.42	1.90	10	1
1:A:341:ASN:O	1:A:345:ARG:HB2	0.42	2.15	3	1
3:A:42:PCW:H222	3:A:52:PCW:H162	0.42	1.91	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:13:PCW:H41	4:A:34:17F:HN1A	0.42	1.74	5	1
3:A:10:PCW:H452	3:A:21:PCW:H432	0.42	1.92	6	1
3:A:16:PCW:H31	3:A:16:PCW:H51	0.42	1.92	6	1
3:A:45:PCW:H381	3:A:57:PCW:C7	0.42	2.45	6	1
1:C:469:LEU:O	1:C:473:LYS:HD3	0.42	2.15	6	1
3:A:51:PCW:H51	3:A:71:PCW:H39	0.42	1.92	7	1
3:A:65:PCW:O2P	3:A:66:PCW:H62	0.42	2.15	10	1
4:A:38:17F:H11A	4:A:38:17F:H34	0.42	1.92	4	1
3:A:10:PCW:H181	3:A:12:PCW:H222	0.42	1.91	6	1
3:A:45:PCW:H211	4:A:79:17F:H48	0.42	1.91	6	1
3:A:19:PCW:O1P	3:A:29:PCW:H62	0.42	2.14	7	1
3:A:28:PCW:H122	3:A:28:PCW:H361	0.42	1.91	7	1
3:A:62:PCW:H341	4:A:78:17F:H38	0.42	1.92	7	1
3:A:65:PCW:H281	1:C:488:LYS:HG2	0.42	1.90	7	1
3:A:4:PCW:H331	3:A:4:PCW:H131	0.42	1.92	8	1
3:A:22:PCW:H51	3:A:22:PCW:H2	0.42	1.91	8	1
3:A:22:PCW:H52	4:A:37:17F:H4A	0.42	1.91	8	1
3:A:60:PCW:H41	3:A:63:PCW:H42	0.42	1.92	8	1
3:A:6:PCW:H331	3:A:28:PCW:H61	0.42	1.90	10	1
3:A:6:PCW:H362	3:A:28:PCW:H132	0.41	1.93	2	1
3:A:60:PCW:H162	3:A:62:PCW:H271	0.41	1.92	2	1
3:A:25:PCW:H272	3:A:25:PCW:H441	0.41	1.91	4	1
3:A:65:PCW:H432	3:A:65:PCW:H272	0.41	1.91	4	1
3:A:68:PCW:H42	3:A:69:PCW:O1P	0.41	2.14	5	1
1:A:264:LYS:O	1:A:268:GLU:HG3	0.41	2.15	9	2
4:A:77:17F:HN1	4:A:77:17F:P1	0.41	2.38	2	1
1:A:279:LEU:O	1:A:283:LEU:HG	0.41	2.15	8	2
3:A:31:PCW:H2	3:A:31:PCW:O4P	0.41	2.15	8	1
3:A:51:PCW:H32	3:A:71:PCW:H40	0.41	1.91	8	1
3:A:4:PCW:C1	3:A:16:PCW:H62	0.41	2.46	9	1
3:A:47:PCW:H262	4:A:76:17F:H58	0.41	1.91	4	1
1:A:238:GLY:O	1:A:242:GLU:HG2	0.41	2.15	6	1
3:A:24:PCW:H81	3:A:31:PCW:O1P	0.41	2.16	6	1
4:A:74:17F:H12	4:A:79:17F:H45	0.41	1.93	6	1
3:A:6:PCW:H351	3:A:16:PCW:H12	0.41	1.92	8	1
3:A:43:PCW:H321	3:A:71:PCW:H283	0.41	1.92	8	1
3:A:1:PCW:H151	4:A:38:17F:H18	0.41	1.92	9	1
3:A:9:PCW:H282	3:A:28:PCW:H251	0.41	1.92	9	1
1:A:239:LEU:HA	1:A:242:GLU:HB2	0.41	1.92	1	1
1:C:404:ASN:O	1:C:408:VAL:HG23	0.41	2.15	2	1
3:A:6:PCW:O11	3:A:24:PCW:H11	0.41	2.15	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:6:PCW:H162	3:A:11:PCW:H331	0.41	1.92	5	1
1:A:308:ARG:HH12	1:C:468:GLU:HB2	0.41	1.76	6	1
3:A:15:PCW:H431	3:A:24:PCW:H451	0.41	1.93	7	1
2:B:126:ASP:OD2	2:B:128:LYS:HB2	0.41	2.15	7	1
1:A:239:LEU:O	1:A:243:MET:HG2	0.41	2.15	9	1
3:A:13:PCW:H11	3:A:14:PCW:H19	0.41	1.93	9	1
3:A:30:PCW:H81	4:A:37:17F:N1	0.41	2.31	10	1
1:A:365:LYS:CB	1:A:366:PRO:HD3	0.41	2.42	2	1
3:A:41:PCW:H462	3:A:61:PCW:H211	0.41	1.92	2	1
1:A:202:LYS:O	1:A:206:ASN:HB2	0.41	2.16	4	1
3:A:21:PCW:H122	4:A:36:17F:H31	0.41	1.93	4	1
3:A:12:PCW:H42	3:A:22:PCW:O2P	0.41	2.15	5	1
1:A:332:ALA:O	1:A:336:GLU:HB2	0.41	2.14	8	1
3:A:10:PCW:C7	4:A:36:17F:HN1A	0.41	2.28	9	1
3:A:3:PCW:H42	3:A:23:PCW:O2P	0.41	2.15	6	1
3:A:17:PCW:H52	2:B:135:ARG:HD2	0.41	1.92	8	1
3:A:63:PCW:H142	3:A:67:PCW:H182	0.41	1.91	10	1
3:A:30:PCW:H372	4:A:34:17F:H10A	0.41	1.93	5	1
3:A:51:PCW:H121	3:A:56:PCW:H271	0.41	1.93	5	1
1:C:563:LYS:CB	1:C:564:PRO:HD3	0.41	2.38	5	1
1:A:330:ARG:HH12	1:C:448:VAL:HG23	0.41	1.75	7	1
1:A:308:ARG:CG	1:C:469:LEU:CD2	0.41	2.98	9	1
3:A:16:PCW:H12	3:A:16:PCW:H73	0.41	1.92	9	1
3:A:14:PCW:H42	3:A:23:PCW:O1P	0.41	2.14	10	1
3:A:67:PCW:H121	4:A:74:17F:H57	0.41	1.91	10	1
3:A:57:PCW:H132	3:A:57:PCW:H332	0.41	1.92	1	1
2:B:37:GLU:HA	2:B:57:ASP:O	0.41	2.16	1	1
3:A:20:PCW:H371	3:A:20:PCW:H142	0.41	1.91	2	1
1:A:201:LEU:HA	1:A:204:LEU:HD12	0.41	1.92	4	2
3:A:41:PCW:H162	3:A:59:PCW:H412	0.41	1.91	4	1
3:A:43:PCW:H341	3:A:45:PCW:H132	0.41	1.91	4	1
1:C:567:GLU:OE1	1:C:567:GLU:HA	0.41	2.16	5	1
3:A:50:PCW:H41	4:A:78:17F:C6	0.41	2.46	8	1
3:A:57:PCW:H2	3:A:57:PCW:C4	0.41	2.46	10	1
1:A:358:SER:O	1:A:362:GLU:HG3	0.41	2.15	1	1
4:A:33:17F:H1	4:A:33:17F:C4	0.41	2.46	1	1
1:C:511:VAL:O	1:C:515:ARG:HG3	0.41	2.16	1	1
3:A:42:PCW:H83	3:A:63:PCW:O1P	0.41	2.15	2	1
3:A:46:PCW:O11	3:A:51:PCW:H51	0.41	2.16	2	1
3:A:53:PCW:O2P	3:A:55:PCW:H83	0.41	2.16	2	1
3:A:5:PCW:H31	3:A:17:PCW:H342	0.41	1.93	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:32:PCW:H121	4:A:33:17F:H20	0.41	1.93	3	1
3:A:43:PCW:O11	3:A:43:PCW:H62	0.41	2.14	4	1
1:A:246:ASP:OD2	1:C:528:ARG:HD3	0.41	2.16	5	1
1:A:255:GLN:O	1:A:259:ASP:HB3	0.41	2.16	5	1
1:A:391:GLU:O	1:A:395:LYS:HB2	0.41	2.16	5	1
3:A:9:PCW:H51	3:A:14:PCW:O31	0.41	2.15	9	1
3:A:30:PCW:H72	4:A:34:17F:O2	0.41	2.15	10	1
4:A:33:17F:H37	4:A:35:17F:H31	0.41	1.94	3	1
3:A:41:PCW:H431	3:A:41:PCW:H211	0.41	1.93	3	1
3:A:11:PCW:H62	3:A:24:PCW:O2P	0.41	2.16	4	1
3:A:16:PCW:H251	3:A:24:PCW:H362	0.41	1.92	4	1
1:A:299:SER:HB2	1:A:300:PRO:CD	0.41	2.46	5	1
3:A:54:PCW:N	3:A:62:PCW:O1P	0.41	2.54	5	1
3:A:9:PCW:H332	3:A:14:PCW:H351	0.41	1.92	7	1
3:A:54:PCW:H41	3:A:54:PCW:H322	0.41	1.93	7	1
3:A:50:PCW:H41	4:A:78:17F:H6A	0.41	1.93	8	1
3:A:59:PCW:O31	3:A:59:PCW:H41	0.41	2.16	8	1
1:C:423:THR:HG22	1:C:427:TRP:HD1	0.40	1.76	2	1
1:A:268:GLU:OE2	1:C:510:HIS:NE2	0.40	2.55	3	1
3:A:16:PCW:O31	3:A:16:PCW:H73	0.40	2.15	5	1
3:A:43:PCW:O31	3:A:45:PCW:H83	0.40	2.16	8	1
1:A:243:MET:HA	1:A:246:ASP:HB3	0.40	1.93	9	1
3:A:59:PCW:O2P	3:A:61:PCW:H63	0.40	2.17	10	1
1:A:305:MET:SD	1:C:469:LEU:HD13	0.40	2.56	2	1
3:A:56:PCW:H211	3:A:56:PCW:H472	0.40	1.93	2	1
1:C:523:ASP:O	1:C:526:ARG:HB2	0.40	2.16	2	1
1:A:246:ASP:CG	1:C:528:ARG:HD3	0.40	2.37	4	1
1:A:334:ARG:HD3	1:C:440:GLU:CD	0.40	2.37	4	1
1:C:549:ALA:O	1:C:553:GLU:HG3	0.40	2.17	4	1
3:A:72:PCW:H431	4:A:78:17F:H50	0.40	1.92	5	1
1:A:324:SER:O	1:A:328:ARG:HG3	0.40	2.16	7	1
1:A:206:ASN:O	1:A:210:VAL:HG23	0.40	2.17	8	1
3:A:23:PCW:H71	4:A:34:17F:H1	0.40	1.93	8	1
3:A:42:PCW:H431	3:A:69:PCW:H19	0.40	1.93	8	1
3:A:43:PCW:H41	3:A:68:PCW:O1P	0.40	2.17	9	1
4:A:36:17F:H1A	4:A:36:17F:C4	0.40	2.46	10	1
3:A:1:PCW:H122	4:A:35:17F:H19	0.40	1.91	2	1
1:A:371:LEU:O	1:A:375:LEU:HG	0.40	2.16	4	1
3:A:69:PCW:H52	3:A:69:PCW:O31	0.40	2.16	4	1
3:A:6:PCW:H122	3:A:16:PCW:H341	0.40	1.93	5	1
3:A:9:PCW:H382	3:A:14:PCW:H82	0.40	1.92	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:25:PCW:O31	3:A:31:PCW:H42	0.40	2.17	7	1
1:C:566:LEU:HD23	1:C:569:LEU:HD12	0.40	1.93	9	1
1:A:218:ARG:HA	1:A:221:LEU:HB2	0.40	1.93	2	1
3:A:3:PCW:H83	3:A:3:PCW:H322	0.40	1.92	6	1
2:B:87:THR:HG23	2:B:125:VAL:HG22	0.40	1.91	6	1
1:A:225:THR:O	1:A:229:TRP:HB2	0.40	2.17	7	1
4:A:74:17F:H49	4:A:75:17F:H44	0.40	1.92	9	1
1:C:581:LYS:O	1:C:585:LEU:HG	0.40	2.17	9	1
3:A:71:PCW:O11	3:A:71:PCW:H51	0.40	2.16	10	1
3:A:1:PCW:H412	4:A:36:17F:H35	0.40	1.92	1	1
3:A:23:PCW:H411	4:A:34:17F:H70	0.40	1.92	7	1
3:A:28:PCW:H2	3:A:28:PCW:H41	0.40	1.93	7	1
1:C:471:ARG:O	1:C:475:GLU:HB2	0.40	2.16	9	1

6.3 Torsion angles (i)

6.3.1 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 NMR 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	194/200 (97%)	190±2 (98±1%)	4±1 (2±1%)	1±0 (0±0%)	44	80
1	C	192/200 (96%)	188±2 (98±1%)	3±1 (2±1%)	1±0 (0±0%)	38	78
2	B	144/187 (77%)	138±2 (96±1%)	6±2 (4±2%)	1±1 (0±1%)	32	76
All	All	5300/5870 (90%)	5155 (97%)	124 (2%)	21 (0%)	38	78

All 7 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	C	563	LYS	8
1	A	365	LYS	6
2	B	58	THR	2
2	B	110	PRO	2
2	B	59	ALA	1
2	B	47	ASP	1
2	B	13	GLY	1

6.3.2 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 NMR 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	171/175 (98%)	154±2 (90±1%)	17±2 (10±1%)	11	57
1	C	168/175 (96%)	153±2 (91±1%)	15±2 (9±1%)	13	60
2	B	126/165 (76%)	116±2 (92±1%)	10±2 (8±1%)	15	62
All	All	4650/5150 (90%)	4227 (91%)	423 (9%)	13	59

All 171 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	254	VAL	10
1	C	550	LYS	9
2	B	124	THR	9
1	C	516	THR	9
1	A	312	HIS	8
1	A	318	THR	8
2	B	50	THR	7
2	B	51	CYS	7
2	B	87	THR	7
1	A	319	HIS	7
2	B	20	THR	7
2	B	57	ASP	7
1	C	463	TRP	7
1	A	235	GLU	6
1	A	265	TRP	6
1	A	272	TYR	6
1	C	480	GLU	6
2	B	89	SER	6
1	A	382	PHE	6
1	C	455	TYR	6
1	A	370	ASP	5
1	C	405	TRP	5
2	B	92	ASP	5
1	C	546	GLU	5
1	C	568	ASP	5
1	A	228	PHE	4

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Mol	Chain	Res	Type	Models (Total)
1	A	293	GLU	4
1	A	361	SER	4
1	C	407	SER	4
1	C	592	THR	4
2	B	35	THR	4
1	A	274	GLN	4
1	C	487	GLN	4
1	C	505	ASP	4
2	B	70	GLN	4
1	A	386	PHE	4
1	C	448	VAL	4
1	A	205	ASP	3
1	A	229	TRP	3
1	A	285	GLU	3
1	A	354	THR	3
1	A	394	THR	3
1	C	412	PHE	3
1	C	521	TYR	3
1	C	410	SER	3
1	C	418	GLN	3
1	C	444	ASP	3
2	B	32	TYR	3
1	A	261	PHE	3
1	C	458	ASP	3
2	B	122	SER	3
1	A	244	SER	3
1	A	369	GLU	3
1	C	403	ASP	3
2	B	127	THR	3
1	C	559	SER	3
1	A	207	TRP	2
1	A	220	GLN	2
1	A	299	SER	2
1	A	368	LEU	2
1	C	426	PHE	2
1	C	497	SER	2
1	C	589	GLU	2
2	B	126	ASP	2
1	A	211	THR	2
1	A	212	SER	2
1	A	241	GLN	2
1	A	249	GLU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	264	LYS	2
1	A	292	HIS	2
1	C	413	SER	2
1	C	457	ASP	2
1	C	459	PHE	2
1	C	473	LYS	2
2	B	72	MET	2
2	B	132	ASP	2
1	A	289	GLN	2
2	B	76	GLU	2
1	A	246	ASP	2
1	A	297	LYS	2
1	A	314	ASP	2
1	C	433	GLU	2
1	C	580	PHE	2
2	B	3	GLU	2
1	A	269	MET	2
1	C	402	LEU	2
1	C	591	TYR	2
1	A	206	ASN	2
1	C	512	ASP	2
2	B	69	ASP	2
1	A	393	TYR	1
1	C	466	GLU	1
1	C	554	HIS	1
1	C	555	LEU	1
2	B	37	GLU	1
2	B	135	ARG	1
1	A	237	GLU	1
1	A	385	SER	1
1	A	395	LYS	1
1	C	452	VAL	1
1	C	522	SER	1
2	B	39	SER	1
1	A	239	LEU	1
1	A	248	GLU	1
1	C	409	THR	1
1	C	547	TYR	1
2	B	29	VAL	1
2	B	118	CYS	1
1	A	276	VAL	1
1	A	345	ARG	1

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Mol	Chain	Res	Type	Models (Total)
1	A	356	HIS	1
2	B	27	HIS	1
2	B	105	ASP	1
2	B	144	THR	1
1	A	215	SER	1
1	A	338	LEU	1
1	A	392	GLU	1
1	C	523	ASP	1
1	C	548	HIS	1
1	C	576	VAL	1
2	B	38	ASP	1
2	B	108	ASP	1
2	B	128	LYS	1
2	B	129	GLN	1
1	A	202	LYS	1
1	A	308	ARG	1
1	A	330	ARG	1
1	A	360	LEU	1
1	C	411	THR	1
1	C	510	HIS	1
1	C	532	ARG	1
1	C	538	GLU	1
1	C	579	SER	1
1	C	586	SER	1
2	B	47	ASP	1
1	A	327	LEU	1
1	A	357	LEU	1
1	C	414	LYS	1
1	C	464	GLN	1
1	C	583	SER	1
2	B	5	LYS	1
2	B	49	GLU	1
2	B	104	LYS	1
1	A	209	SER	1
1	A	213	THR	1
1	A	325	ASP	1
1	A	336	GLU	1
1	C	442	SER	1
1	C	494	GLU	1
2	B	106	SER	1
1	A	214	PHE	1
1	A	225	THR	1

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Mol	Chain	Res	Type	Models (Total)
1	A	262	GLN	1
1	C	431	GLU	1
1	C	461	LYS	1
1	C	527	GLN	1
1	C	556	SER	1
1	C	567	GLU	1
2	B	17	SER	1
2	B	74	THR	1
1	A	260	ASP	1
1	A	279	LEU	1
1	A	290	LYS	1
1	A	350	HIS	1
1	A	390	LEU	1
1	C	447	GLU	1
1	C	451	LYS	1
1	C	467	MET	1
1	C	488	LYS	1
1	C	552	THR	1
2	B	96	TYR	1

6.3.3 RNA

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains

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

6.5 Carbohydrates

There are no monosaccharides in this entry.

6.6 Ligand geometry

Of 82 ligands modelled in this entry, 1 is monoatomic - leaving 81 for Mogul analysis.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds 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 is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is

considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	17F	A	75	-	52,53,53	1.03±0.00	3±0 (5±0%)
3	PCW	A	25	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	A	70	-	53,53,53	1.04±0.01	4±0 (7±0%)
3	PCW	A	62	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	A	13	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	A	52	-	53,53,53	1.04±0.01	4±0 (6±0%)
3	PCW	A	50	-	53,53,53	1.04±0.01	5±0 (9±0%)
3	PCW	A	59	-	53,53,53	1.05±0.01	4±0 (6±0%)
3	PCW	A	68	-	53,53,53	1.05±0.00	4±0 (6±0%)
4	17F	A	38	-	52,53,53	1.03±0.01	3±0 (5±0%)
4	17F	A	78	-	52,53,53	1.03±0.01	3±0 (5±0%)
3	PCW	A	58	-	53,53,53	1.04±0.01	4±0 (7±0%)
3	PCW	A	71	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	A	42	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	A	22	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	A	18	-	53,53,53	1.04±0.01	4±0 (7±0%)
4	17F	A	33	-	52,53,53	1.03±0.01	3±0 (5±0%)
4	17F	A	35	-	52,53,53	1.03±0.01	3±0 (5±0%)
3	PCW	A	29	-	53,53,53	1.04±0.00	4±0 (7±0%)
3	PCW	A	12	-	53,53,53	1.05±0.01	5±0 (8±0%)
4	17F	A	79	-	52,53,53	1.03±0.01	3±0 (5±0%)
3	PCW	A	44	-	53,53,53	1.05±0.00	4±0 (6±0%)
3	PCW	A	64	-	53,53,53	1.05±0.01	4±0 (7±0%)
4	17F	A	37	-	52,53,53	1.03±0.00	3±0 (5±0%)
3	PCW	A	45	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	A	53	-	53,53,53	1.04±0.01	4±0 (6±0%)
3	PCW	A	55	-	53,53,53	1.07±0.01	5±0 (9±0%)
5	GDP	B	201	-	25,30,30	1.03±0.03	2±1 (8±2%)
3	PCW	A	69	-	53,53,53	1.05±0.00	4±0 (7±0%)
3	PCW	A	57	-	53,53,53	1.04±0.01	4±0 (7±0%)
4	17F	A	74	-	52,53,53	1.03±0.01	3±0 (5±0%)
4	17F	A	34	-	52,53,53	1.03±0.01	3±0 (5±0%)
3	PCW	A	26	-	53,53,53	1.05±0.01	4±0 (7±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	17F	A	36	-	52,53,53	1.03±0.00	3±0 (5±0%)
3	PCW	A	14	-	53,53,53	1.04±0.01	4±0 (6±0%)
3	PCW	A	24	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	A	11	-	53,53,53	1.05±0.01	5±0 (9±0%)
4	17F	A	80	-	52,53,53	1.03±0.01	3±0 (5±0%)
3	PCW	A	46	-	53,53,53	1.04±0.01	4±0 (6±0%)
3	PCW	A	1	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	A	16	-	53,53,53	1.05±0.01	5±0 (9±0%)
3	PCW	A	32	-	53,53,53	1.05±0.01	5±0 (9±0%)
3	PCW	A	30	-	53,53,53	1.05±0.01	5±0 (8±0%)
3	PCW	A	9	-	53,53,53	1.05±0.01	5±0 (8±0%)
3	PCW	A	54	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	A	48	-	53,53,53	1.04±0.01	5±0 (9±0%)
3	PCW	A	10	-	53,53,53	1.04±0.01	4±0 (6±0%)
3	PCW	A	49	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	A	6	-	53,53,53	1.04±0.01	4±0 (7±0%)
3	PCW	A	41	-	53,53,53	1.04±0.01	4±0 (6±0%)
3	PCW	A	20	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	A	61	-	53,53,53	1.04±0.00	4±0 (7±0%)
3	PCW	A	31	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	A	8	-	53,53,53	1.05±0.01	5±0 (9±0%)
3	PCW	A	28	-	53,53,53	1.04±0.01	4±0 (7±0%)
3	PCW	A	72	-	53,53,53	1.04±0.01	5±0 (8±0%)
3	PCW	A	60	-	53,53,53	1.05±0.01	4±0 (6±0%)
3	PCW	A	43	-	53,53,53	1.04±0.01	4±0 (6±0%)
3	PCW	A	23	-	53,53,53	1.04±0.01	4±0 (7±0%)
3	PCW	A	15	-	53,53,53	1.05±0.01	5±0 (9±0%)
4	17F	A	76	-	52,53,53	1.03±0.01	3±0 (5±0%)
3	PCW	A	56	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	A	65	-	53,53,53	1.04±0.01	5±0 (9±0%)
3	PCW	A	66	-	53,53,53	1.04±0.01	5±0 (9±0%)
3	PCW	A	47	-	53,53,53	1.04±0.01	5±0 (9±0%)
3	PCW	A	5	-	53,53,53	1.04±0.01	4±0 (7±0%)
3	PCW	A	2	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	A	7	-	53,53,53	1.05±0.01	5±0 (9±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	PCW	A	3	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	A	17	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	A	4	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	A	27	-	53,53,53	1.06±0.01	5±0 (9±0%)
4	17F	A	77	-	52,53,53	1.04±0.01	3±0 (5±0%)
3	PCW	A	63	-	53,53,53	1.04±0.01	4±0 (6±0%)
3	PCW	A	21	-	53,53,53	1.05±0.01	4±0 (7±0%)
4	17F	A	73	-	52,53,53	1.03±0.01	3±0 (5±0%)
3	PCW	A	19	-	53,53,53	1.05±0.01	5±0 (9±0%)
4	17F	A	39	-	52,53,53	1.03±0.01	3±0 (5±0%)
4	17F	A	40	-	52,53,53	1.03±0.01	3±0 (5±0%)
3	PCW	A	67	-	53,53,53	1.05±0.00	4±0 (7±0%)
3	PCW	A	51	-	53,53,53	1.04±0.01	4±0 (6±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of 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 angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	17F	A	75	-	54,60,60	1.04±0.02	5±0 (9±0%)
3	PCW	A	25	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	70	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	62	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	13	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	A	52	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	50	-	59,61,61	0.84±0.00	1±0 (1±0%)
3	PCW	A	59	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	68	-	59,61,61	2.32±0.00	5±0 (8±0%)
4	17F	A	38	-	54,60,60	1.03±0.01	5±0 (9±0%)
4	17F	A	78	-	54,60,60	1.05±0.02	5±0 (9±0%)
3	PCW	A	58	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	71	-	59,61,61	2.32±0.00	5±0 (8±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	PCW	A	42	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	A	22	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	18	-	59,61,61	2.32±0.00	5±0 (8±0%)
4	17F	A	33	-	54,60,60	1.79±0.02	10±0 (18±0%)
4	17F	A	35	-	54,60,60	1.05±0.02	5±0 (9±0%)
3	PCW	A	29	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	12	-	59,61,61	0.84±0.01	1±0 (1±0%)
4	17F	A	79	-	54,60,60	1.05±0.01	5±0 (9±0%)
3	PCW	A	44	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	64	-	59,61,61	2.32±0.00	5±0 (8±0%)
4	17F	A	37	-	54,60,60	1.05±0.02	5±0 (9±0%)
3	PCW	A	45	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	53	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	55	-	59,61,61	0.83±0.01	1±0 (1±0%)
5	GDP	B	201	-	30,47,47	1.10±0.02	2±0 (6±0%)
3	PCW	A	69	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	57	-	59,61,61	2.32±0.00	5±0 (8±0%)
4	17F	A	74	-	54,60,60	1.06±0.02	5±0 (9±0%)
4	17F	A	34	-	54,60,60	1.05±0.02	5±0 (9±0%)
3	PCW	A	26	-	59,61,61	2.32±0.01	5±0 (8±0%)
4	17F	A	36	-	54,60,60	1.05±0.02	5±0 (9±0%)
3	PCW	A	14	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	24	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	11	-	59,61,61	0.84±0.01	1±0 (1±0%)
4	17F	A	80	-	54,60,60	1.02±0.01	4±0 (7±0%)
3	PCW	A	46	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	1	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	16	-	59,61,61	0.84±0.01	1±0 (1±0%)
3	PCW	A	32	-	59,61,61	0.84±0.00	1±0 (1±0%)
3	PCW	A	30	-	59,61,61	0.84±0.01	1±0 (1±0%)
3	PCW	A	9	-	59,61,61	0.84±0.01	1±0 (1±0%)
3	PCW	A	54	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	48	-	59,61,61	0.84±0.01	1±0 (1±0%)
3	PCW	A	10	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	49	-	59,61,61	2.32±0.00	5±0 (8±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	PCW	A	6	-	59,61,61	2.76±0.01	9±0 (15±0%)
3	PCW	A	41	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	20	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	61	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	31	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	8	-	59,61,61	0.84±0.01	1±0 (1±0%)
3	PCW	A	28	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	72	-	59,61,61	0.84±0.01	1±0 (1±0%)
3	PCW	A	60	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	A	43	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	23	-	59,61,61	2.33±0.01	5±0 (8±0%)
3	PCW	A	15	-	59,61,61	0.84±0.01	1±0 (1±0%)
4	17F	A	76	-	54,60,60	1.04±0.02	5±0 (9±0%)
3	PCW	A	56	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	65	-	59,61,61	0.85±0.01	1±0 (1±0%)
3	PCW	A	66	-	59,61,61	0.84±0.00	1±0 (1±0%)
3	PCW	A	47	-	59,61,61	0.85±0.01	1±0 (1±0%)
3	PCW	A	5	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	2	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	7	-	59,61,61	0.85±0.01	1±0 (1±0%)
3	PCW	A	3	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	A	17	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	A	4	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	A	27	-	59,61,61	0.83±0.01	1±0 (1±0%)
4	17F	A	77	-	54,60,60	1.76±0.02	10±0 (18±0%)
3	PCW	A	63	-	59,61,61	2.76±0.00	9±0 (15±0%)
3	PCW	A	21	-	59,61,61	2.32±0.00	5±0 (8±0%)
4	17F	A	73	-	54,60,60	1.04±0.01	5±0 (9±0%)
3	PCW	A	19	-	59,61,61	0.84±0.00	1±0 (1±0%)
4	17F	A	39	-	54,60,60	1.06±0.02	5±0 (9±0%)
4	17F	A	40	-	54,60,60	1.04±0.02	5±0 (8±0%)
3	PCW	A	67	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	51	-	59,61,61	2.32±0.00	5±0 (8±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
3	PCW	A	59	-	-	0±0,57,57,57	-
4	17F	A	38	-	-	0±0,59,59,59	-
3	PCW	A	64	-	-	0±0,57,57,57	-
3	PCW	A	70	-	-	0±0,57,57,57	-
3	PCW	A	42	-	-	0±0,57,57,57	-
3	PCW	A	68	-	-	0±0,57,57,57	-
3	PCW	A	20	-	-	0±0,57,57,57	-
3	PCW	A	72	-	-	0±0,57,57,57	-
3	PCW	A	43	-	-	0±0,57,57,57	-
3	PCW	A	25	-	-	0±0,57,57,57	-
3	PCW	A	57	-	-	0±0,57,57,57	-
3	PCW	A	31	-	-	0±0,57,57,57	-
3	PCW	A	13	-	-	0±0,57,57,57	-
4	17F	A	74	-	-	0±0,59,59,59	-
3	PCW	A	22	-	-	0±0,57,57,57	-
3	PCW	A	1	-	-	0±0,57,57,57	-
3	PCW	A	29	-	-	0±0,57,57,57	-
3	PCW	A	48	-	-	0±0,57,57,57	-
4	17F	A	35	-	-	0±0,59,59,59	-
3	PCW	A	60	-	-	0±0,57,57,57	-
3	PCW	A	16	-	-	0±0,57,57,57	-
3	PCW	A	53	-	-	0±0,57,57,57	-
3	PCW	A	67	-	-	0±0,57,57,57	-
4	17F	A	37	-	-	0±0,59,59,59	-
3	PCW	A	54	-	-	0±0,57,57,57	-
4	17F	A	77	-	-	0±0,59,59,59	-
3	PCW	A	26	-	-	0±0,57,57,57	-
3	PCW	A	18	-	-	0±0,57,57,57	-
3	PCW	A	49	-	-	0±0,57,57,57	-
3	PCW	A	15	-	-	0±0,57,57,57	-
4	17F	A	39	-	-	0±0,59,59,59	-
3	PCW	A	65	-	-	0±0,57,57,57	-
5	GDP	B	201	-	-	0±0,12,32,32	0±0,3,3,3
4	17F	A	79	-	-	0±0,59,59,59	-
3	PCW	A	30	-	-	0±0,57,57,57	-
3	PCW	A	14	-	-	0±0,57,57,57	-
3	PCW	A	63	-	-	0±0,57,57,57	-
4	17F	A	36	-	-	0±0,59,59,59	-
4	17F	A	34	-	-	0±0,59,59,59	-
3	PCW	A	62	-	-	0±0,57,57,57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	17F	A	76	-	-	0±0,59,59,59	-
3	PCW	A	50	-	-	0±0,57,57,57	-
3	PCW	A	24	-	-	0±0,57,57,57	-
3	PCW	A	69	-	-	0±0,57,57,57	-
4	17F	A	78	-	-	0±0,59,59,59	-
3	PCW	A	19	-	-	0±0,57,57,57	-
3	PCW	A	6	-	-	0±0,57,57,57	-
4	17F	A	75	-	-	0±0,59,59,59	-
3	PCW	A	47	-	-	0±0,57,57,57	-
3	PCW	A	8	-	-	0±0,57,57,57	-
3	PCW	A	61	-	-	0±0,57,57,57	-
4	17F	A	73	-	-	0±0,59,59,59	-
3	PCW	A	51	-	-	0±0,57,57,57	-
3	PCW	A	46	-	-	0±0,57,57,57	-
3	PCW	A	11	-	-	0±0,57,57,57	-
3	PCW	A	71	-	-	0±0,57,57,57	-
3	PCW	A	44	-	-	0±0,57,57,57	-
3	PCW	A	23	-	-	0±0,57,57,57	-
4	17F	A	80	-	-	0±0,59,59,59	-
3	PCW	A	10	-	-	0±0,57,57,57	-
3	PCW	A	28	-	-	0±0,57,57,57	-
3	PCW	A	17	-	-	0±0,57,57,57	-
3	PCW	A	55	-	-	0±0,57,57,57	-
3	PCW	A	4	-	-	0±0,57,57,57	-
3	PCW	A	7	-	-	0±0,57,57,57	-
3	PCW	A	32	-	-	0±0,57,57,57	-
3	PCW	A	5	-	-	0±0,57,57,57	-
3	PCW	A	21	-	-	0±0,57,57,57	-
3	PCW	A	41	-	-	0±0,57,57,57	-
4	17F	A	40	-	-	0±0,59,59,59	-
3	PCW	A	2	-	-	0±0,57,57,57	-
3	PCW	A	3	-	-	0±0,57,57,57	-
3	PCW	A	56	-	-	0±0,57,57,57	-
3	PCW	A	45	-	-	0±0,57,57,57	-
3	PCW	A	52	-	-	0±0,57,57,57	-
4	17F	A	33	-	-	0±0,59,59,59	-
3	PCW	A	27	-	-	0±0,57,57,57	-
3	PCW	A	9	-	-	0±0,57,57,57	-
3	PCW	A	66	-	-	0±0,57,57,57	-
3	PCW	A	12	-	-	0±0,57,57,57	-
3	PCW	A	58	-	-	0±0,57,57,57	-

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst

occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	41	PCW	C5-N	2.81	1.42	1.51	8	10
3	A	59	PCW	C5-N	2.79	1.43	1.51	6	10
3	A	69	PCW	C5-N	2.78	1.43	1.51	7	10
3	A	53	PCW	C5-N	2.77	1.43	1.51	4	10
3	A	58	PCW	C5-N	2.77	1.43	1.51	4	10
3	A	22	PCW	C5-N	2.77	1.43	1.51	3	10
3	A	13	PCW	C5-N	2.77	1.43	1.51	3	10
3	A	31	PCW	C5-N	2.77	1.43	1.51	6	10
3	A	45	PCW	C5-N	2.76	1.43	1.51	8	10
3	A	63	PCW	C5-N	2.75	1.43	1.51	7	10
3	A	64	PCW	C5-N	2.75	1.43	1.51	7	10
3	A	43	PCW	C5-N	2.75	1.43	1.51	9	10
3	A	68	PCW	C5-N	2.75	1.43	1.51	10	10
3	A	70	PCW	C5-N	2.74	1.43	1.51	1	10
3	A	25	PCW	C5-N	2.74	1.43	1.51	5	10
3	A	46	PCW	C1-C2	2.74	1.59	1.50	3	10
3	A	57	PCW	C5-N	2.74	1.43	1.51	7	10
3	A	5	PCW	C5-N	2.73	1.43	1.51	4	10
3	A	3	PCW	C5-N	2.73	1.43	1.51	7	10
3	A	60	PCW	C5-N	2.73	1.43	1.51	7	10
3	A	2	PCW	C5-N	2.73	1.43	1.51	10	10
3	A	20	PCW	C5-N	2.73	1.43	1.51	8	10
3	A	49	PCW	C5-N	2.73	1.43	1.51	5	10
3	A	54	PCW	C5-N	2.73	1.43	1.51	10	10
3	A	62	PCW	C5-N	2.73	1.43	1.51	6	10
3	A	17	PCW	C5-N	2.73	1.43	1.51	7	10
3	A	42	PCW	C5-N	2.73	1.43	1.51	5	10
3	A	44	PCW	C5-N	2.72	1.43	1.51	1	10
3	A	52	PCW	C5-N	2.72	1.43	1.51	5	10
3	A	26	PCW	C5-N	2.72	1.43	1.51	6	10
3	A	1	PCW	C5-N	2.71	1.43	1.51	1	10
3	A	56	PCW	C5-N	2.71	1.43	1.51	3	10
3	A	23	PCW	C5-N	2.71	1.43	1.51	2	10
3	A	71	PCW	C5-N	2.71	1.43	1.51	1	10
3	A	29	PCW	C5-N	2.71	1.43	1.51	9	10
3	A	6	PCW	C5-N	2.70	1.43	1.51	7	10
3	A	67	PCW	C5-N	2.70	1.43	1.51	1	10
3	A	51	PCW	C5-N	2.70	1.43	1.51	10	10
3	A	61	PCW	C5-N	2.70	1.43	1.51	10	10
3	A	4	PCW	C5-N	2.70	1.43	1.51	7	10
3	A	24	PCW	C5-N	2.69	1.43	1.51	1	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	21	PCW	C5-N	2.68	1.43	1.51	6	10
3	A	46	PCW	C5-N	2.68	1.43	1.51	2	10
3	A	14	PCW	C5-N	2.68	1.43	1.51	10	10
3	A	10	PCW	C5-N	2.68	1.43	1.51	2	10
3	A	42	PCW	C1-C2	2.67	1.59	1.50	10	10
3	A	28	PCW	C5-N	2.66	1.43	1.51	6	10
3	A	16	PCW	C1-C2	2.65	1.59	1.50	3	10
3	A	18	PCW	C5-N	2.64	1.43	1.51	2	10
3	A	28	PCW	C1-C2	2.63	1.59	1.50	9	10
3	A	6	PCW	C1-C2	2.62	1.59	1.50	1	10
3	A	15	PCW	C1-C2	2.61	1.59	1.50	2	10
3	A	4	PCW	C1-C2	2.60	1.58	1.50	2	10
3	A	71	PCW	C1-C2	2.60	1.58	1.50	1	10
5	B	201	GDP	PA-O3A	2.60	1.62	1.59	8	9
3	A	30	PCW	C1-C2	2.59	1.58	1.50	4	10
3	A	63	PCW	C1-C2	2.59	1.58	1.50	4	10
3	A	3	PCW	C1-C2	2.59	1.58	1.50	4	10
3	A	9	PCW	C1-C2	2.59	1.58	1.50	1	10
3	A	14	PCW	C1-C2	2.58	1.58	1.50	7	10
3	A	27	PCW	C1-C2	2.57	1.58	1.50	2	10
3	A	67	PCW	C1-C2	2.57	1.58	1.50	7	10
4	A	35	17F	O4-C3	2.57	1.29	1.22	7	10
3	A	7	PCW	C1-C2	2.56	1.58	1.50	8	10
4	A	38	17F	O4-C3	2.56	1.29	1.22	8	10
3	A	8	PCW	C1-C2	2.56	1.58	1.50	9	10
3	A	56	PCW	C1-C2	2.56	1.58	1.50	8	10
3	A	26	PCW	C1-C2	2.55	1.58	1.50	5	10
3	A	55	PCW	C1-C2	2.55	1.58	1.50	5	10
3	A	64	PCW	C1-C2	2.55	1.58	1.50	4	10
3	A	69	PCW	C1-C2	2.55	1.58	1.50	2	10
3	A	70	PCW	C1-C2	2.55	1.58	1.50	3	10
3	A	25	PCW	C1-C2	2.54	1.58	1.50	3	10
3	A	32	PCW	C1-C2	2.54	1.58	1.50	3	10
4	A	80	17F	O4-C3	2.54	1.29	1.22	7	10
3	A	48	PCW	C1-C2	2.54	1.58	1.50	4	10
4	A	34	17F	O4-C3	2.54	1.29	1.22	10	10
4	A	37	17F	O4-C3	2.54	1.29	1.22	8	10
4	A	39	17F	O4-C3	2.54	1.29	1.22	2	10
3	A	11	PCW	C1-C2	2.53	1.58	1.50	4	10
3	A	17	PCW	C1-C2	2.54	1.58	1.50	2	10
3	A	19	PCW	C1-C2	2.54	1.58	1.50	4	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	49	PCW	C1-C2	2.54	1.58	1.50	6	10
3	A	58	PCW	C1-C2	2.54	1.58	1.50	5	10
3	A	60	PCW	C1-C2	2.54	1.58	1.50	4	10
3	A	66	PCW	C1-C2	2.53	1.58	1.50	1	10
5	B	201	GDP	O4'-C1'	2.53	1.44	1.40	3	10
3	A	5	PCW	C1-C2	2.53	1.58	1.50	3	10
3	A	20	PCW	C1-C2	2.53	1.58	1.50	1	10
3	A	61	PCW	C1-C2	2.53	1.58	1.50	6	10
4	A	74	17F	O4-C3	2.53	1.29	1.22	10	10
4	A	76	17F	O4-C3	2.53	1.29	1.22	9	10
3	A	1	PCW	C1-C2	2.53	1.58	1.50	2	10
3	A	12	PCW	C1-C2	2.53	1.58	1.50	2	10
3	A	23	PCW	C1-C2	2.53	1.58	1.50	3	10
3	A	24	PCW	C1-C2	2.53	1.58	1.50	6	10
4	A	36	17F	O4-C3	2.53	1.29	1.22	9	10
3	A	2	PCW	C1-C2	2.53	1.58	1.50	2	10
3	A	10	PCW	C1-C2	2.52	1.58	1.50	9	10
3	A	45	PCW	C1-C2	2.52	1.58	1.50	4	10
3	A	47	PCW	C1-C2	2.52	1.58	1.50	1	10
3	A	54	PCW	C1-C2	2.52	1.58	1.50	5	10
3	A	21	PCW	C1-C2	2.52	1.58	1.50	9	10
3	A	22	PCW	C1-C2	2.52	1.58	1.50	3	10
3	A	65	PCW	C1-C2	2.52	1.58	1.50	2	10
4	A	77	17F	O4-C3	2.52	1.29	1.22	9	10
3	A	52	PCW	C1-C2	2.52	1.58	1.50	8	10
3	A	57	PCW	C1-C2	2.52	1.58	1.50	1	10
3	A	16	PCW	C5-N	2.52	1.43	1.51	4	10
3	A	68	PCW	C1-C2	2.52	1.58	1.50	9	10
3	A	43	PCW	C1-C2	2.51	1.58	1.50	10	10
3	A	59	PCW	C1-C2	2.51	1.58	1.50	9	10
3	A	51	PCW	C1-C2	2.51	1.58	1.50	9	10
4	A	73	17F	O4-C3	2.51	1.29	1.22	10	10
4	A	78	17F	O4-C3	2.51	1.29	1.22	6	10
3	A	29	PCW	C1-C2	2.51	1.58	1.50	5	10
3	A	18	PCW	C1-C2	2.50	1.58	1.50	4	10
4	A	79	17F	O4-C3	2.50	1.29	1.22	10	10
3	A	41	PCW	C1-C2	2.50	1.58	1.50	2	10
3	A	44	PCW	C1-C2	2.50	1.58	1.50	8	10
4	A	40	17F	O4-C3	2.50	1.29	1.22	1	10
3	A	13	PCW	C1-C2	2.49	1.58	1.50	2	10
3	A	55	PCW	C5-N	2.49	1.43	1.51	2	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	31	PCW	C1-C2	2.49	1.58	1.50	8	10
4	A	33	17F	O4-C3	2.49	1.29	1.22	6	10
3	A	62	PCW	C1-C2	2.48	1.58	1.50	10	10
3	A	72	PCW	C5-N	2.49	1.43	1.51	9	10
4	A	75	17F	O4-C3	2.48	1.29	1.22	3	10
3	A	53	PCW	C1-C2	2.48	1.58	1.50	6	10
3	A	8	PCW	C5-N	2.48	1.43	1.51	2	10
3	A	9	PCW	C5-N	2.48	1.43	1.51	1	10
3	A	72	PCW	C1-C2	2.47	1.58	1.50	3	10
3	A	71	PCW	C33-C32	2.46	1.61	1.52	2	10
3	A	50	PCW	C1-C2	2.46	1.58	1.50	1	10
3	A	27	PCW	C5-N	2.46	1.44	1.51	10	10
3	A	7	PCW	C5-N	2.45	1.44	1.51	3	10
3	A	50	PCW	C5-N	2.45	1.44	1.51	1	10
3	A	30	PCW	C5-N	2.44	1.44	1.51	2	10
3	A	12	PCW	C5-N	2.44	1.44	1.51	4	10
3	A	48	PCW	C5-N	2.44	1.44	1.51	9	10
3	A	32	PCW	C33-C32	2.43	1.61	1.52	5	10
3	A	65	PCW	C5-N	2.43	1.44	1.51	2	10
3	A	10	PCW	C33-C32	2.43	1.61	1.52	3	10
3	A	44	PCW	C33-C32	2.43	1.61	1.52	4	10
3	A	47	PCW	C5-N	2.43	1.44	1.51	8	10
3	A	32	PCW	C5-N	2.43	1.44	1.51	3	10
3	A	41	PCW	C33-C32	2.42	1.61	1.52	5	10
3	A	67	PCW	C33-C32	2.42	1.61	1.52	4	10
3	A	30	PCW	C33-C32	2.42	1.61	1.52	9	10
3	A	66	PCW	C5-N	2.42	1.44	1.51	1	10
3	A	64	PCW	C33-C32	2.42	1.61	1.52	9	10
3	A	29	PCW	C33-C32	2.42	1.61	1.52	4	10
3	A	18	PCW	C33-C32	2.42	1.61	1.52	5	10
3	A	2	PCW	C33-C32	2.41	1.61	1.52	5	10
3	A	47	PCW	C33-C32	2.42	1.61	1.52	5	10
3	A	49	PCW	C33-C32	2.41	1.61	1.52	1	10
4	A	37	17F	O5-C3	2.41	1.23	1.30	9	10
3	A	11	PCW	C5-N	2.41	1.44	1.51	8	10
3	A	50	PCW	C33-C32	2.41	1.61	1.52	8	10
4	A	77	17F	O5-C3	2.41	1.23	1.30	1	10
3	A	5	PCW	C33-C32	2.41	1.61	1.52	6	10
3	A	28	PCW	C33-C32	2.41	1.61	1.52	3	10
3	A	59	PCW	C33-C32	2.41	1.61	1.52	5	10
4	A	33	17F	O5-C3	2.41	1.23	1.30	5	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	15	PCW	C5-N	2.40	1.44	1.51	4	10
3	A	15	PCW	C33-C32	2.40	1.61	1.52	6	10
3	A	62	PCW	C33-C32	2.40	1.61	1.52	4	10
3	A	19	PCW	C33-C32	2.40	1.61	1.52	4	10
3	A	69	PCW	C33-C32	2.40	1.61	1.52	6	10
4	A	76	17F	O5-C3	2.40	1.23	1.30	8	10
3	A	19	PCW	C5-N	2.40	1.44	1.51	7	10
3	A	60	PCW	C33-C32	2.39	1.61	1.52	7	10
4	A	38	17F	O5-C3	2.40	1.23	1.30	7	10
3	A	48	PCW	C33-C32	2.39	1.61	1.52	3	10
3	A	31	PCW	C33-C32	2.39	1.61	1.52	9	10
3	A	16	PCW	C33-C32	2.39	1.60	1.52	4	10
3	A	54	PCW	C33-C32	2.39	1.60	1.52	4	10
3	A	72	PCW	C33-C32	2.39	1.60	1.52	3	10
3	A	11	PCW	C33-C32	2.38	1.60	1.52	10	10
3	A	27	PCW	C33-C32	2.38	1.60	1.52	2	10
3	A	26	PCW	C33-C32	2.38	1.60	1.52	8	10
3	A	45	PCW	C33-C32	2.38	1.60	1.52	7	10
3	A	52	PCW	C33-C32	2.38	1.60	1.52	7	10
3	A	1	PCW	C33-C32	2.38	1.60	1.52	8	10
3	A	51	PCW	C33-C32	2.38	1.60	1.52	3	10
3	A	55	PCW	C33-C32	2.38	1.60	1.52	1	10
3	A	63	PCW	C33-C32	2.38	1.60	1.52	5	10
3	A	4	PCW	C33-C32	2.38	1.60	1.52	10	10
3	A	21	PCW	C33-C32	2.38	1.60	1.52	6	10
4	A	79	17F	O5-C3	2.38	1.23	1.30	6	10
3	A	8	PCW	C33-C32	2.38	1.60	1.52	6	10
3	A	6	PCW	C33-C32	2.38	1.60	1.52	6	10
3	A	17	PCW	C33-C32	2.38	1.60	1.52	3	10
4	A	78	17F	O5-C3	2.38	1.23	1.30	7	10
3	A	7	PCW	C33-C32	2.37	1.60	1.52	5	10
3	A	66	PCW	C33-C32	2.37	1.60	1.52	10	10
3	A	58	PCW	C33-C32	2.37	1.60	1.52	7	10
4	A	36	17F	O5-C3	2.37	1.23	1.30	6	10
3	A	9	PCW	C33-C32	2.37	1.60	1.52	6	10
3	A	24	PCW	C33-C32	2.37	1.60	1.52	10	10
3	A	43	PCW	C33-C32	2.37	1.60	1.52	5	10
3	A	46	PCW	C33-C32	2.37	1.60	1.52	10	10
3	A	56	PCW	C33-C32	2.37	1.60	1.52	5	10
3	A	61	PCW	C33-C32	2.37	1.60	1.52	5	10
4	A	74	17F	O5-C3	2.37	1.23	1.30	1	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
4	A	40	17F	O5-C3	2.37	1.23	1.30	7	10
3	A	22	PCW	C33-C32	2.36	1.60	1.52	10	10
3	A	68	PCW	C33-C32	2.36	1.60	1.52	9	10
3	A	57	PCW	C33-C32	2.36	1.60	1.52	10	10
3	A	20	PCW	C33-C32	2.36	1.60	1.52	3	10
3	A	3	PCW	C33-C32	2.36	1.60	1.52	1	10
3	A	42	PCW	C33-C32	2.36	1.60	1.52	6	10
3	A	53	PCW	C33-C32	2.36	1.60	1.52	3	10
4	A	39	17F	O5-C3	2.36	1.23	1.30	4	10
4	A	73	17F	O5-C3	2.36	1.23	1.30	5	10
3	A	12	PCW	C33-C32	2.35	1.60	1.52	1	10
3	A	14	PCW	C33-C32	2.35	1.60	1.52	3	10
3	A	25	PCW	C33-C32	2.35	1.60	1.52	3	10
4	A	75	17F	O5-C3	2.35	1.23	1.30	10	10
3	A	65	PCW	C33-C32	2.35	1.60	1.52	3	10
3	A	23	PCW	C33-C32	2.35	1.60	1.52	1	10
4	A	34	17F	O5-C3	2.35	1.23	1.30	5	10
4	A	80	17F	O5-C3	2.35	1.23	1.30	9	10
3	A	70	PCW	C33-C32	2.35	1.60	1.52	9	10
3	A	13	PCW	C33-C32	2.34	1.60	1.52	6	10
4	A	35	17F	O5-C3	2.33	1.23	1.30	7	10
3	A	12	PCW	C7-N	2.32	1.43	1.50	6	10
3	A	27	PCW	C7-N	2.28	1.43	1.50	8	10
3	A	9	PCW	C7-N	2.28	1.43	1.50	8	10
3	A	11	PCW	C7-N	2.27	1.43	1.50	9	10
3	A	8	PCW	C7-N	2.27	1.43	1.50	10	10
3	A	65	PCW	C7-N	2.26	1.43	1.50	2	10
3	A	32	PCW	C7-N	2.26	1.43	1.50	10	10
3	A	66	PCW	C7-N	2.26	1.43	1.50	10	10
3	A	72	PCW	C7-N	2.26	1.43	1.50	8	10
3	A	15	PCW	C7-N	2.25	1.43	1.50	10	10
3	A	50	PCW	C7-N	2.25	1.43	1.50	1	10
3	A	30	PCW	C7-N	2.22	1.43	1.50	9	10
3	A	16	PCW	C7-N	2.22	1.43	1.50	6	10
3	A	19	PCW	C7-N	2.21	1.43	1.50	3	10
3	A	55	PCW	C7-N	2.21	1.43	1.50	5	10
3	A	69	PCW	C3-C2	2.21	1.57	1.50	2	9
3	A	48	PCW	C7-N	2.20	1.43	1.50	3	10
5	B	201	GDP	C6-N1	2.20	1.34	1.37	7	3
3	A	7	PCW	C7-N	2.20	1.43	1.50	10	10
3	A	17	PCW	C3-C2	2.19	1.57	1.50	7	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	16	PCW	C3-C2	2.19	1.57	1.50	3	8
3	A	22	PCW	C3-C2	2.19	1.57	1.50	5	9
3	A	55	PCW	C3-C2	2.18	1.57	1.50	6	10
3	A	50	PCW	C3-C2	2.18	1.57	1.50	5	8
3	A	70	PCW	C3-C2	2.18	1.57	1.50	7	9
3	A	71	PCW	C3-C2	2.18	1.57	1.50	5	8
3	A	27	PCW	C3-C2	2.17	1.57	1.50	2	10
3	A	47	PCW	C7-N	2.17	1.43	1.50	4	10
3	A	48	PCW	C3-C2	2.17	1.57	1.50	4	9
3	A	32	PCW	C3-C2	2.17	1.57	1.50	9	9
3	A	58	PCW	C3-C2	2.16	1.57	1.50	5	10
3	A	21	PCW	C3-C2	2.15	1.57	1.50	9	8
3	A	42	PCW	C3-C2	2.15	1.57	1.50	10	10
3	A	18	PCW	C3-C2	2.15	1.57	1.50	4	8
4	A	40	17F	C1X-C2X	2.15	1.61	1.52	2	10
3	A	11	PCW	C3-C2	2.15	1.57	1.50	7	10
3	A	25	PCW	C3-C2	2.15	1.57	1.50	10	9
3	A	49	PCW	C3-C2	2.15	1.57	1.50	1	8
3	A	56	PCW	C3-C2	2.15	1.57	1.50	6	9
3	A	57	PCW	C3-C2	2.14	1.57	1.50	4	9
3	A	29	PCW	C3-C2	2.14	1.57	1.50	4	9
4	A	76	17F	C1X-C2X	2.14	1.61	1.52	4	10
3	A	63	PCW	C3-C2	2.13	1.57	1.50	8	7
4	A	74	17F	C1X-C2X	2.13	1.61	1.52	5	8
3	A	31	PCW	C3-C2	2.13	1.57	1.50	4	8
3	A	2	PCW	C3-C2	2.13	1.57	1.50	3	9
3	A	64	PCW	C3-C2	2.13	1.57	1.50	3	8
3	A	7	PCW	C3-C2	2.13	1.57	1.50	4	8
3	A	13	PCW	C3-C2	2.12	1.57	1.50	2	8
3	A	20	PCW	C3-C2	2.12	1.57	1.50	8	10
3	A	51	PCW	C3-C2	2.12	1.57	1.50	5	7
3	A	1	PCW	C3-C2	2.12	1.57	1.50	1	10
3	A	19	PCW	C3-C2	2.12	1.57	1.50	3	10
4	A	34	17F	C1X-C2X	2.12	1.61	1.52	10	10
4	A	37	17F	C1X-C2X	2.12	1.61	1.52	4	10
3	A	26	PCW	C3-C2	2.12	1.57	1.50	9	9
3	A	30	PCW	C3-C2	2.12	1.57	1.50	4	7
3	A	45	PCW	C3-C2	2.12	1.57	1.50	3	9
4	A	78	17F	C1X-C2X	2.12	1.61	1.52	4	10
4	A	73	17F	C1X-C2X	2.12	1.61	1.52	9	9
3	A	5	PCW	C3-C2	2.11	1.57	1.50	10	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	10	PCW	C3-C2	2.11	1.57	1.50	1	7
3	A	41	PCW	C3-C2	2.11	1.57	1.50	6	6
3	A	59	PCW	C3-C2	2.11	1.57	1.50	8	7
4	A	79	17F	C1X-C2X	2.12	1.61	1.52	4	10
3	A	62	PCW	C3-C2	2.11	1.57	1.50	9	8
3	A	3	PCW	C3-C2	2.11	1.57	1.50	2	10
3	A	14	PCW	C3-C2	2.11	1.57	1.50	4	7
4	A	33	17F	C1X-C2X	2.11	1.61	1.52	1	8
4	A	38	17F	C1X-C2X	2.11	1.61	1.52	4	8
3	A	54	PCW	C3-C2	2.11	1.57	1.50	10	8
3	A	6	PCW	C3-C2	2.10	1.57	1.50	10	9
3	A	60	PCW	C3-C2	2.10	1.57	1.50	1	7
3	A	15	PCW	C3-C2	2.10	1.57	1.50	6	10
3	A	28	PCW	C3-C2	2.10	1.57	1.50	4	9
3	A	8	PCW	C3-C2	2.10	1.57	1.50	5	9
3	A	24	PCW	C3-C2	2.10	1.57	1.50	4	10
4	A	75	17F	C1X-C2X	2.10	1.61	1.52	10	10
3	A	9	PCW	C3-C2	2.10	1.57	1.50	7	6
3	A	47	PCW	C3-C2	2.09	1.57	1.50	6	8
3	A	66	PCW	C3-C2	2.09	1.57	1.50	3	9
3	A	68	PCW	C3-C2	2.09	1.57	1.50	3	6
3	A	44	PCW	C3-C2	2.09	1.57	1.50	3	6
4	A	36	17F	C1X-C2X	2.09	1.61	1.52	2	10
4	A	80	17F	C1X-C2X	2.09	1.61	1.52	8	10
3	A	4	PCW	C3-C2	2.08	1.57	1.50	5	10
3	A	23	PCW	C3-C2	2.08	1.57	1.50	5	8
4	A	39	17F	C1X-C2X	2.08	1.61	1.52	4	10
4	A	77	17F	C1X-C2X	2.08	1.61	1.52	2	10
3	A	43	PCW	C3-C2	2.08	1.57	1.50	9	5
4	A	35	17F	C1X-C2X	2.08	1.61	1.52	8	9
3	A	12	PCW	C3-C2	2.07	1.57	1.50	2	7
3	A	46	PCW	C3-C2	2.07	1.57	1.50	3	7
3	A	72	PCW	C3-C2	2.07	1.57	1.50	6	6
3	A	65	PCW	C3-C2	2.07	1.57	1.50	5	9
3	A	52	PCW	C3-C2	2.06	1.57	1.50	8	7
3	A	61	PCW	C3-C2	2.06	1.57	1.50	6	10
3	A	53	PCW	C3-C2	2.05	1.57	1.50	9	6
3	A	67	PCW	C3-C2	2.05	1.57	1.50	6	8

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	13	PCW	C8-N-C7	11.99	77.49	108.98	10	10
3	A	46	PCW	C8-N-C7	11.97	77.53	108.98	6	10
3	A	3	PCW	C8-N-C7	11.97	77.55	108.98	5	10
3	A	2	PCW	C8-N-C7	11.96	77.56	108.98	5	10
3	A	20	PCW	C8-N-C7	11.95	77.57	108.98	4	10
3	A	67	PCW	C8-N-C7	11.94	77.62	108.98	8	10
3	A	24	PCW	C8-N-C7	11.93	77.63	108.98	5	10
3	A	64	PCW	C8-N-C7	11.93	77.63	108.98	6	10
3	A	21	PCW	C8-N-C7	11.93	77.64	108.98	10	10
3	A	52	PCW	C8-N-C7	11.93	77.64	108.98	3	10
3	A	59	PCW	C8-N-C7	11.93	77.64	108.98	4	10
3	A	69	PCW	C8-N-C7	11.93	77.65	108.98	8	10
3	A	68	PCW	C8-N-C7	11.92	77.67	108.98	9	10
3	A	70	PCW	C8-N-C7	11.92	77.67	108.98	4	10
3	A	4	PCW	C8-N-C7	11.92	77.68	108.98	4	10
3	A	56	PCW	C8-N-C7	11.92	77.68	108.98	8	10
3	A	63	PCW	C8-N-C7	11.91	77.69	108.98	4	10
3	A	58	PCW	C8-N-C7	11.91	77.70	108.98	6	10
3	A	18	PCW	C8-N-C7	11.90	77.71	108.98	7	10
3	A	6	PCW	C8-N-C7	11.90	77.72	108.98	1	10
3	A	51	PCW	C8-N-C7	11.90	77.73	108.98	10	10
3	A	71	PCW	C8-N-C7	11.90	77.73	108.98	9	10
3	A	10	PCW	C8-N-C7	11.89	77.74	108.98	1	10
3	A	41	PCW	C8-N-C7	11.89	77.73	108.98	4	10
3	A	42	PCW	C8-N-C7	11.89	77.74	108.98	4	10
3	A	23	PCW	C8-N-C7	11.89	77.74	108.98	4	10
3	A	31	PCW	C8-N-C7	11.89	77.74	108.98	9	10
3	A	44	PCW	C8-N-C7	11.89	77.75	108.98	7	10
3	A	57	PCW	C8-N-C7	11.89	77.75	108.98	5	10
3	A	28	PCW	C8-N-C7	11.89	77.75	108.98	3	10
3	A	29	PCW	C8-N-C7	11.88	77.78	108.98	1	10
3	A	5	PCW	C8-N-C7	11.87	77.79	108.98	9	10
3	A	17	PCW	C8-N-C7	11.87	77.79	108.98	7	10
3	A	25	PCW	C8-N-C7	11.87	77.79	108.98	8	10
3	A	61	PCW	C8-N-C7	11.87	77.79	108.98	6	10
3	A	14	PCW	C8-N-C7	11.87	77.80	108.98	5	10
3	A	43	PCW	C8-N-C7	11.87	77.80	108.98	6	10
3	A	53	PCW	C8-N-C7	11.87	77.80	108.98	2	10
3	A	54	PCW	C8-N-C7	11.86	77.82	108.98	9	10
3	A	60	PCW	C8-N-C7	11.86	77.82	108.98	6	10
3	A	26	PCW	C8-N-C7	11.86	77.82	108.98	4	10
3	A	22	PCW	C8-N-C7	11.86	77.83	108.98	1	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	62	PCW	C8-N-C7	11.85	77.84	108.98	6	10
3	A	1	PCW	C8-N-C7	11.84	77.87	108.98	5	10
3	A	45	PCW	C8-N-C7	11.84	77.88	108.98	10	10
3	A	49	PCW	C8-N-C7	11.81	77.96	108.98	8	10
3	A	23	PCW	C8-N-C6	10.27	82.01	108.98	3	10
3	A	58	PCW	C8-N-C6	10.15	82.31	108.98	2	10
3	A	42	PCW	C8-N-C6	10.12	82.38	108.98	3	10
3	A	60	PCW	C8-N-C6	10.08	82.49	108.98	10	10
3	A	10	PCW	C8-N-C6	10.08	82.50	108.98	6	10
3	A	52	PCW	C8-N-C6	10.07	82.52	108.98	4	10
3	A	57	PCW	C8-N-C6	10.07	82.52	108.98	6	10
3	A	21	PCW	C8-N-C6	10.06	82.54	108.98	5	10
3	A	29	PCW	C8-N-C6	10.06	82.55	108.98	7	10
3	A	4	PCW	C8-N-C6	10.06	82.56	108.98	8	10
3	A	54	PCW	C8-N-C6	10.06	82.56	108.98	7	10
3	A	63	PCW	C8-N-C6	10.05	82.57	108.98	3	10
3	A	43	PCW	C8-N-C6	10.05	82.57	108.98	2	10
3	A	17	PCW	C8-N-C6	10.05	82.58	108.98	4	10
3	A	53	PCW	C8-N-C6	10.05	82.58	108.98	10	10
3	A	24	PCW	C8-N-C6	10.04	82.59	108.98	4	10
3	A	5	PCW	C8-N-C6	10.04	82.60	108.98	10	10
3	A	61	PCW	C8-N-C6	10.04	82.60	108.98	8	10
3	A	2	PCW	C8-N-C6	10.04	82.62	108.98	10	10
3	A	1	PCW	C8-N-C6	10.03	82.62	108.98	8	10
3	A	59	PCW	C8-N-C6	10.03	82.62	108.98	6	10
3	A	6	PCW	C8-N-C6	10.03	82.63	108.98	3	10
3	A	22	PCW	C8-N-C6	10.03	82.63	108.98	7	10
3	A	51	PCW	C8-N-C6	10.03	82.63	108.98	4	10
3	A	18	PCW	C8-N-C6	10.03	82.64	108.98	8	10
3	A	25	PCW	C8-N-C6	10.03	82.64	108.98	9	10
3	A	41	PCW	C8-N-C6	10.03	82.64	108.98	6	10
3	A	46	PCW	C8-N-C6	10.03	82.64	108.98	5	10
3	A	67	PCW	C8-N-C6	10.03	82.64	108.98	3	10
3	A	45	PCW	C8-N-C6	10.03	82.64	108.98	8	10
3	A	62	PCW	C8-N-C6	10.02	82.64	108.98	10	10
3	A	28	PCW	C8-N-C6	10.02	82.65	108.98	9	10
3	A	68	PCW	C8-N-C6	10.02	82.66	108.98	8	10
3	A	3	PCW	C8-N-C6	10.02	82.67	108.98	10	10
3	A	14	PCW	C8-N-C6	10.01	82.68	108.98	1	10
3	A	69	PCW	C8-N-C6	10.01	82.68	108.98	10	10
3	A	71	PCW	C8-N-C6	10.01	82.68	108.98	9	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	26	PCW	C8-N-C6	10.01	82.69	108.98	10	10
3	A	49	PCW	C8-N-C6	10.01	82.69	108.98	9	10
3	A	64	PCW	C8-N-C6	10.01	82.69	108.98	7	10
3	A	31	PCW	C8-N-C6	10.00	82.71	108.98	5	10
3	A	44	PCW	C8-N-C6	10.00	82.72	108.98	7	10
3	A	70	PCW	C8-N-C6	10.00	82.72	108.98	5	10
3	A	13	PCW	C8-N-C6	9.99	82.72	108.98	1	10
3	A	56	PCW	C8-N-C6	9.97	82.79	108.98	6	10
3	A	20	PCW	C8-N-C6	9.95	82.84	108.98	6	10
3	A	6	PCW	O4P-P-O2P	7.70	78.43	108.94	4	10
3	A	63	PCW	O4P-P-O2P	7.65	78.60	108.94	2	10
4	A	33	17F	O2-P1-O6	6.33	78.89	107.57	2	10
4	A	77	17F	O2-P1-O6	6.32	78.91	107.57	9	10
4	A	33	17F	O2-P1-O3	6.16	79.67	107.57	6	10
4	A	77	17F	O2-P1-O3	6.14	79.73	107.57	7	10
3	A	63	PCW	O1P-P-O2P	5.87	85.16	112.44	4	10
3	A	6	PCW	O1P-P-O2P	5.86	85.17	112.44	10	10
3	A	6	PCW	O3P-P-O2P	5.83	85.84	108.94	10	10
3	A	63	PCW	O3P-P-O2P	5.77	86.08	108.94	3	10
3	A	58	PCW	C8-N-C5	5.44	88.29	109.91	4	10
3	A	52	PCW	C8-N-C5	5.42	88.35	109.91	6	10
3	A	45	PCW	C8-N-C5	5.41	88.39	109.91	7	10
3	A	4	PCW	C8-N-C5	5.40	88.43	109.91	6	10
3	A	13	PCW	C8-N-C5	5.40	88.43	109.91	2	10
3	A	25	PCW	C8-N-C5	5.39	88.47	109.91	3	10
3	A	31	PCW	C8-N-C5	5.39	88.47	109.91	3	10
3	A	14	PCW	C8-N-C5	5.39	88.48	109.91	7	10
3	A	10	PCW	C8-N-C5	5.39	88.48	109.91	9	10
3	A	24	PCW	C8-N-C5	5.39	88.48	109.91	1	10
3	A	41	PCW	C8-N-C5	5.39	88.49	109.91	7	10
3	A	53	PCW	C8-N-C5	5.39	88.50	109.91	1	10
3	A	49	PCW	C8-N-C5	5.38	88.52	109.91	4	10
3	A	1	PCW	C8-N-C5	5.38	88.53	109.91	9	10
3	A	43	PCW	C8-N-C5	5.38	88.53	109.91	1	10
3	A	62	PCW	C8-N-C5	5.37	88.55	109.91	2	10
3	A	42	PCW	C8-N-C5	5.37	88.56	109.91	10	10
3	A	70	PCW	C8-N-C5	5.37	88.56	109.91	10	10
3	A	21	PCW	C8-N-C5	5.37	88.57	109.91	3	10
3	A	44	PCW	C8-N-C5	5.37	88.57	109.91	8	10
3	A	3	PCW	C8-N-C5	5.37	88.58	109.91	2	10
3	A	28	PCW	C8-N-C5	5.37	88.58	109.91	6	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	29	PCW	C8-N-C5	5.37	88.58	109.91	10	10
3	A	69	PCW	C8-N-C5	5.37	88.58	109.91	6	10
3	A	17	PCW	C8-N-C5	5.36	88.60	109.91	2	10
3	A	56	PCW	C8-N-C5	5.36	88.59	109.91	3	10
3	A	46	PCW	C8-N-C5	5.36	88.60	109.91	8	10
3	A	54	PCW	C8-N-C5	5.36	88.60	109.91	6	10
3	A	64	PCW	C8-N-C5	5.36	88.60	109.91	4	10
3	A	67	PCW	C8-N-C5	5.36	88.60	109.91	7	10
3	A	26	PCW	C8-N-C5	5.36	88.61	109.91	7	10
3	A	20	PCW	C8-N-C5	5.36	88.62	109.91	3	10
3	A	51	PCW	C8-N-C5	5.35	88.62	109.91	5	10
3	A	60	PCW	C8-N-C5	5.36	88.62	109.91	3	10
3	A	5	PCW	C8-N-C5	5.35	88.64	109.91	6	10
3	A	59	PCW	C8-N-C5	5.35	88.64	109.91	10	10
3	A	22	PCW	C8-N-C5	5.35	88.65	109.91	8	10
3	A	57	PCW	C8-N-C5	5.35	88.66	109.91	9	10
3	A	63	PCW	C8-N-C5	5.34	88.67	109.91	7	10
3	A	71	PCW	C8-N-C5	5.34	88.67	109.91	10	10
3	A	6	PCW	C8-N-C5	5.34	88.69	109.91	4	10
3	A	61	PCW	C8-N-C5	5.34	88.69	109.91	2	10
3	A	2	PCW	C8-N-C5	5.34	88.70	109.91	4	10
3	A	68	PCW	C8-N-C5	5.34	88.69	109.91	9	10
3	A	18	PCW	C8-N-C5	5.34	88.70	109.91	2	10
3	A	23	PCW	C8-N-C5	5.32	88.76	109.91	10	10
4	A	33	17F	O3-C1-C2	4.96	112.38	108.06	2	10
4	A	77	17F	O2-P1-O1	4.77	90.25	112.44	1	10
4	A	33	17F	O2-P1-O1	4.72	90.48	112.44	10	10
4	A	74	17F	O3-C1-C2	3.91	111.47	108.06	2	10
4	A	77	17F	O3-C1-C2	3.85	111.42	108.06	3	9
4	A	78	17F	O3-C1-C2	3.75	111.33	108.06	6	10
4	A	40	17F	O3-C1-C2	3.72	111.30	108.06	5	10
4	A	35	17F	O3-C1-C2	3.70	111.28	108.06	10	10
4	A	39	17F	O3-C1-C2	3.70	111.28	108.06	8	10
4	A	36	17F	O3-C1-C2	3.60	111.19	108.06	7	10
3	A	6	PCW	O1P-P-O4P	3.54	123.63	107.57	6	10
4	A	76	17F	O3-C1-C2	3.52	111.13	108.06	8	10
4	A	75	17F	O3-C1-C2	3.52	111.13	108.06	9	10
3	A	63	PCW	O1P-P-O4P	3.51	123.46	107.57	2	10
4	A	33	17F	O5-C3-O4	3.41	116.34	124.08	5	10
3	A	25	PCW	C6-N-C5	3.38	123.33	109.91	3	10
4	A	74	17F	O5-C3-O4	3.38	116.42	124.08	4	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	76	17F	O5-C3-O4	3.38	116.42	124.08	7	10
4	A	34	17F	O3-C1-C2	3.36	110.99	108.06	5	10
4	A	35	17F	O5-C3-O4	3.36	116.46	124.08	8	10
4	A	40	17F	O5-C3-O4	3.36	116.45	124.08	3	10
4	A	75	17F	O5-C3-O4	3.36	116.46	124.08	6	10
4	A	78	17F	O5-C3-O4	3.35	116.47	124.08	7	10
4	A	79	17F	O5-C3-O4	3.35	116.47	124.08	1	10
4	A	37	17F	O3-C1-C2	3.35	110.98	108.06	6	10
4	A	73	17F	O5-C3-O4	3.35	116.48	124.08	6	10
4	A	39	17F	O5-C3-O4	3.35	116.49	124.08	5	10
4	A	38	17F	O5-C3-O4	3.34	116.49	124.08	6	10
4	A	36	17F	O5-C3-O4	3.34	116.50	124.08	7	10
3	A	45	PCW	C6-N-C5	3.34	123.19	109.91	7	10
4	A	34	17F	O5-C3-O4	3.34	116.51	124.08	7	10
4	A	37	17F	O5-C3-O4	3.34	116.51	124.08	4	10
3	A	24	PCW	C6-N-C5	3.34	123.17	109.91	8	10
3	A	67	PCW	C6-N-C5	3.33	123.15	109.91	9	10
3	A	10	PCW	C6-N-C5	3.33	123.14	109.91	2	10
4	A	77	17F	O5-C3-O4	3.33	116.52	124.08	7	10
3	A	62	PCW	C6-N-C5	3.33	123.14	109.91	10	10
3	A	22	PCW	C6-N-C5	3.33	123.13	109.91	8	10
4	A	80	17F	O5-C3-O4	3.33	116.53	124.08	8	10
3	A	1	PCW	C6-N-C5	3.33	123.13	109.91	10	10
3	A	64	PCW	C6-N-C5	3.32	123.13	109.91	4	10
3	A	18	PCW	C6-N-C5	3.32	123.12	109.91	8	10
3	A	21	PCW	C6-N-C5	3.32	123.12	109.91	7	10
3	A	42	PCW	C6-N-C5	3.32	123.11	109.91	3	10
3	A	44	PCW	C6-N-C5	3.32	123.11	109.91	4	10
3	A	58	PCW	C6-N-C5	3.32	123.10	109.91	2	10
3	A	4	PCW	C6-N-C5	3.32	123.10	109.91	6	10
3	A	70	PCW	C6-N-C5	3.32	123.09	109.91	8	10
4	A	80	17F	O3-C1-C2	3.32	110.95	108.06	10	10
3	A	3	PCW	C6-N-C5	3.32	123.09	109.91	10	10
3	A	49	PCW	C6-N-C5	3.31	123.09	109.91	2	10
3	A	61	PCW	C6-N-C5	3.31	123.08	109.91	7	10
3	A	31	PCW	C6-N-C5	3.31	123.07	109.91	4	10
3	A	51	PCW	C6-N-C5	3.31	123.07	109.91	6	10
3	A	53	PCW	C6-N-C5	3.31	123.06	109.91	1	10
4	A	79	17F	O3-C1-C2	3.31	110.94	108.06	5	10
3	A	28	PCW	C6-N-C5	3.31	123.05	109.91	9	10
3	A	63	PCW	C6-N-C5	3.30	123.05	109.91	7	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	52	PCW	C6-N-C5	3.30	123.03	109.91	8	10
3	A	5	PCW	C6-N-C5	3.30	123.03	109.91	7	10
3	A	43	PCW	C6-N-C5	3.30	123.03	109.91	5	10
3	A	60	PCW	C6-N-C5	3.30	123.03	109.91	8	10
3	A	54	PCW	C6-N-C5	3.30	123.01	109.91	3	10
3	A	56	PCW	C6-N-C5	3.29	123.01	109.91	10	10
3	A	59	PCW	C6-N-C5	3.29	123.00	109.91	3	10
3	A	17	PCW	C6-N-C5	3.29	122.99	109.91	3	10
3	A	57	PCW	C6-N-C5	3.29	122.99	109.91	7	10
3	A	71	PCW	C6-N-C5	3.29	122.98	109.91	8	10
3	A	46	PCW	C6-N-C5	3.29	122.98	109.91	10	10
3	A	13	PCW	C6-N-C5	3.28	122.96	109.91	4	10
3	A	68	PCW	C6-N-C5	3.28	122.96	109.91	10	10
3	A	41	PCW	C6-N-C5	3.28	122.95	109.91	1	10
3	A	20	PCW	C6-N-C5	3.28	122.94	109.91	6	10
3	A	29	PCW	C6-N-C5	3.27	122.93	109.91	2	10
3	A	6	PCW	C6-N-C5	3.27	122.91	109.91	4	10
3	A	26	PCW	C6-N-C5	3.27	122.90	109.91	9	10
3	A	23	PCW	C6-N-C5	3.26	122.89	109.91	10	10
3	A	69	PCW	C6-N-C5	3.26	122.87	109.91	3	10
3	A	14	PCW	C6-N-C5	3.26	122.86	109.91	5	10
3	A	2	PCW	C6-N-C5	3.25	122.83	109.91	10	10
4	A	73	17F	O3-C1-C2	3.22	110.87	108.06	6	10
5	B	201	GDP	C8-N7-C5	3.19	107.99	102.55	4	10
4	A	38	17F	O3-C1-C2	3.16	110.81	108.06	7	10
4	A	74	17F	O7-C7-O8	2.97	131.06	123.63	3	10
4	A	39	17F	O7-C7-O8	2.92	130.93	123.63	9	10
4	A	40	17F	O7-C7-O8	2.91	130.91	123.63	7	10
4	A	79	17F	O7-C7-O8	2.91	130.91	123.63	9	10
4	A	38	17F	O7-C7-O8	2.91	130.90	123.63	8	10
4	A	76	17F	O7-C7-O8	2.90	130.88	123.63	8	10
4	A	77	17F	O7-C7-O8	2.90	130.88	123.63	6	10
4	A	78	17F	O7-C7-O8	2.88	130.83	123.63	8	10
4	A	36	17F	O7-C7-O8	2.87	130.81	123.63	10	10
4	A	80	17F	O7-C7-O8	2.87	130.80	123.63	6	10
4	A	35	17F	O7-C7-O8	2.87	130.80	123.63	4	10
4	A	37	17F	O7-C7-O8	2.87	130.80	123.63	2	10
4	A	33	17F	O7-C7-O8	2.86	130.79	123.63	2	10
4	A	34	17F	O7-C7-O8	2.86	130.79	123.63	1	10
4	A	73	17F	O7-C7-O8	2.86	130.79	123.63	4	10
4	A	75	17F	O7-C7-O8	2.86	130.78	123.63	4	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	9	PCW	C8-N-C7	2.78	101.67	108.98	10	10
4	A	77	17F	O3-P1-O1	2.77	119.91	108.94	8	10
4	A	33	17F	O3-P1-O1	2.75	119.84	108.94	8	10
3	A	30	PCW	C8-N-C7	2.71	101.86	108.98	7	10
3	A	19	PCW	C8-N-C7	2.70	101.89	108.98	9	10
3	A	72	PCW	C8-N-C7	2.69	101.91	108.98	7	10
3	A	66	PCW	C8-N-C7	2.68	101.93	108.98	5	10
3	A	32	PCW	C8-N-C7	2.68	101.95	108.98	10	10
3	A	11	PCW	C8-N-C7	2.67	101.95	108.98	4	10
3	A	12	PCW	C8-N-C7	2.67	101.97	108.98	7	10
3	A	16	PCW	C8-N-C7	2.66	101.98	108.98	10	10
3	A	65	PCW	C8-N-C7	2.67	101.97	108.98	10	10
3	A	55	PCW	C8-N-C7	2.66	101.98	108.98	4	10
3	A	7	PCW	C8-N-C7	2.66	101.98	108.98	10	10
3	A	15	PCW	C8-N-C7	2.66	101.98	108.98	4	10
3	A	8	PCW	C8-N-C7	2.65	102.01	108.98	9	10
3	A	48	PCW	C8-N-C7	2.65	102.02	108.98	9	10
3	A	50	PCW	C8-N-C7	2.64	102.03	108.98	2	10
3	A	27	PCW	C8-N-C7	2.64	102.05	108.98	8	10
3	A	47	PCW	C8-N-C7	2.63	102.06	108.98	6	10
4	A	73	17F	C5-O9-C17	2.57	111.65	117.80	9	10
4	A	33	17F	O9-C17-O10	2.54	129.65	123.70	2	10
4	A	39	17F	C5-O9-C17	2.52	111.75	117.80	1	10
4	A	79	17F	C5-O9-C17	2.52	111.77	117.80	1	10
3	A	44	PCW	C7-N-C5	2.50	119.87	109.91	3	10
3	A	13	PCW	C7-N-C5	2.50	119.86	109.91	8	10
4	A	74	17F	C5-O9-C17	2.50	111.81	117.80	10	10
3	A	63	PCW	C7-N-C5	2.48	119.79	109.91	4	10
4	A	77	17F	C5-O9-C17	2.48	111.86	117.80	7	10
4	A	80	17F	O9-C17-O10	2.48	129.50	123.70	7	10
3	A	6	PCW	C7-N-C5	2.48	119.75	109.91	10	10
3	A	20	PCW	C7-N-C5	2.47	119.74	109.91	9	10
4	A	77	17F	O6-P1-O1	2.47	118.74	108.94	4	10
4	A	33	17F	C5-O9-C17	2.47	111.88	117.80	3	8
4	A	75	17F	C5-O9-C17	2.47	111.88	117.80	6	10
4	A	76	17F	C5-O9-C17	2.47	111.88	117.80	4	10
3	A	43	PCW	C7-N-C5	2.47	119.72	109.91	2	10
3	A	45	PCW	C7-N-C5	2.47	119.72	109.91	4	10
3	A	2	PCW	C7-N-C5	2.47	119.71	109.91	7	10
3	A	21	PCW	C7-N-C5	2.46	119.70	109.91	10	10
3	A	42	PCW	C7-N-C5	2.46	119.69	109.91	4	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	57	PCW	C7-N-C5	2.45	119.67	109.91	5	10
4	A	36	17F	C5-O9-C17	2.46	111.92	117.80	4	10
3	A	41	PCW	C7-N-C5	2.45	119.66	109.91	2	10
3	A	23	PCW	C7-N-C5	2.45	119.64	109.91	4	10
3	A	29	PCW	C7-N-C5	2.45	119.64	109.91	10	10
3	A	58	PCW	C7-N-C5	2.45	119.64	109.91	6	10
4	A	40	17F	C5-O9-C17	2.45	111.94	117.80	4	7
3	A	64	PCW	C7-N-C5	2.44	119.62	109.91	8	10
3	A	69	PCW	C7-N-C5	2.44	119.62	109.91	9	10
3	A	56	PCW	C7-N-C5	2.44	119.61	109.91	5	10
3	A	67	PCW	C7-N-C5	2.44	119.61	109.91	8	10
3	A	14	PCW	C7-N-C5	2.44	119.60	109.91	7	10
3	A	26	PCW	C7-N-C5	2.44	119.60	109.91	5	10
3	A	62	PCW	C7-N-C5	2.44	119.60	109.91	4	10
3	A	24	PCW	C7-N-C5	2.44	119.59	109.91	5	10
3	A	17	PCW	C7-N-C5	2.44	119.59	109.91	9	10
3	A	54	PCW	C7-N-C5	2.43	119.58	109.91	8	10
3	A	28	PCW	C7-N-C5	2.43	119.57	109.91	2	10
4	A	34	17F	C5-O9-C17	2.43	111.98	117.80	5	10
3	A	18	PCW	C7-N-C5	2.42	119.54	109.91	3	10
3	A	46	PCW	C7-N-C5	2.42	119.55	109.91	2	10
3	A	59	PCW	C7-N-C5	2.42	119.54	109.91	4	10
3	A	1	PCW	C7-N-C5	2.42	119.54	109.91	6	10
3	A	49	PCW	C7-N-C5	2.42	119.54	109.91	6	10
3	A	52	PCW	C7-N-C5	2.42	119.53	109.91	3	10
4	A	78	17F	C5-O9-C17	2.42	112.00	117.80	6	10
3	A	60	PCW	C7-N-C5	2.42	119.52	109.91	2	10
3	A	25	PCW	C7-N-C5	2.42	119.52	109.91	2	10
3	A	3	PCW	C7-N-C5	2.41	119.51	109.91	7	10
3	A	31	PCW	C7-N-C5	2.41	119.51	109.91	3	10
3	A	68	PCW	C7-N-C5	2.41	119.51	109.91	1	10
4	A	33	17F	O6-P1-O1	2.41	118.50	108.94	8	10
4	A	37	17F	O9-C17-O10	2.41	129.34	123.70	4	10
3	A	4	PCW	C7-N-C5	2.41	119.49	109.91	6	10
4	A	35	17F	C5-O9-C17	2.41	112.03	117.80	7	10
3	A	70	PCW	C7-N-C5	2.41	119.48	109.91	6	10
3	A	10	PCW	C7-N-C5	2.40	119.46	109.91	5	10
3	A	53	PCW	C7-N-C5	2.40	119.46	109.91	3	10
3	A	61	PCW	C7-N-C5	2.40	119.46	109.91	6	10
3	A	71	PCW	C7-N-C5	2.40	119.45	109.91	3	10
4	A	40	17F	O9-C17-O10	2.40	129.31	123.70	3	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	5	PCW	C7-N-C5	2.39	119.42	109.91	3	10
3	A	51	PCW	C7-N-C5	2.39	119.42	109.91	9	10
4	A	79	17F	O9-C17-O10	2.39	129.30	123.70	3	10
4	A	78	17F	O9-C17-O10	2.39	129.29	123.70	2	10
4	A	37	17F	C5-O9-C17	2.38	112.09	117.80	3	10
4	A	38	17F	O9-C17-O10	2.38	129.28	123.70	4	10
3	A	22	PCW	C7-N-C5	2.38	119.38	109.91	2	10
4	A	38	17F	C5-O9-C17	2.38	112.10	117.80	7	9
4	A	73	17F	O9-C17-O10	2.38	129.26	123.70	7	10
5	B	201	GDP	C5-C6-N1	2.35	118.56	114.07	7	10
4	A	34	17F	O9-C17-O10	2.35	129.19	123.70	10	10
4	A	35	17F	O9-C17-O10	2.34	129.17	123.70	3	10
4	A	36	17F	O9-C17-O10	2.34	129.18	123.70	8	10
4	A	39	17F	O9-C17-O10	2.33	129.15	123.70	6	10
4	A	76	17F	O9-C17-O10	2.31	129.11	123.70	9	10
4	A	74	17F	O9-C17-O10	2.28	129.03	123.70	1	10
4	A	77	17F	O9-C17-O10	2.26	128.98	123.70	9	10
4	A	75	17F	O9-C17-O10	2.23	128.91	123.70	10	10
3	A	17	PCW	C7-N-C6	2.03	114.30	108.98	4	1
3	A	6	PCW	O1P-P-O3P	2.03	116.75	107.57	2	2
3	A	44	PCW	C7-N-C6	2.01	114.27	108.98	5	1

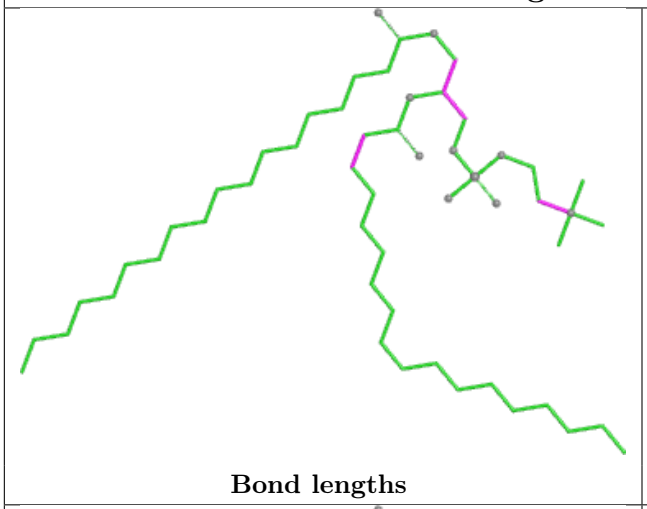
There are no chirality outliers.

There are no torsion outliers.

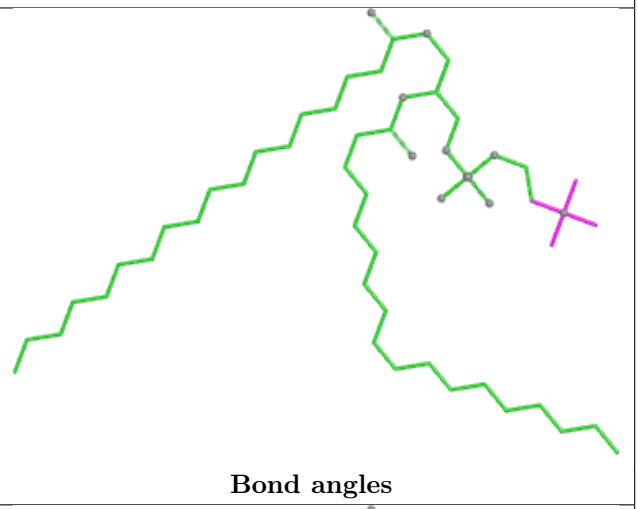
There are no ring outliers.

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.

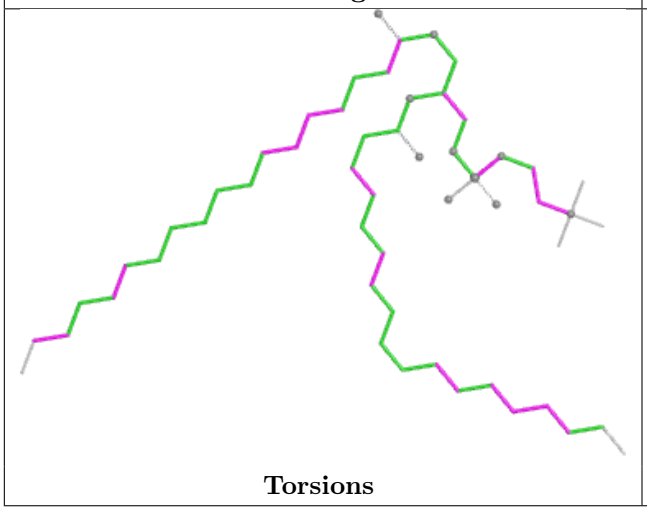
Ligand PCW A 59



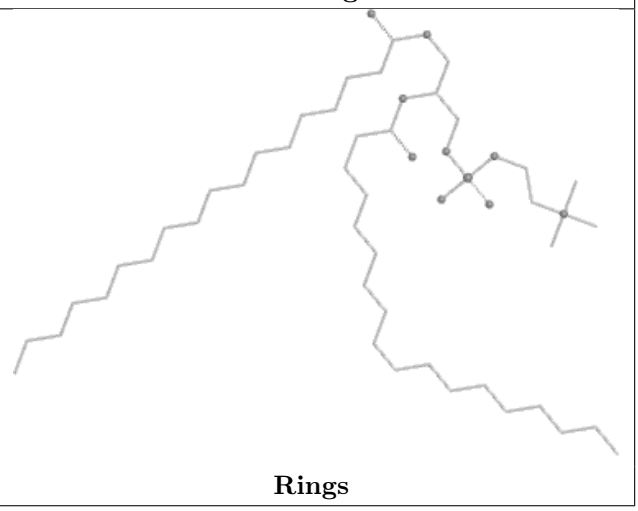
Bond lengths



Bond angles

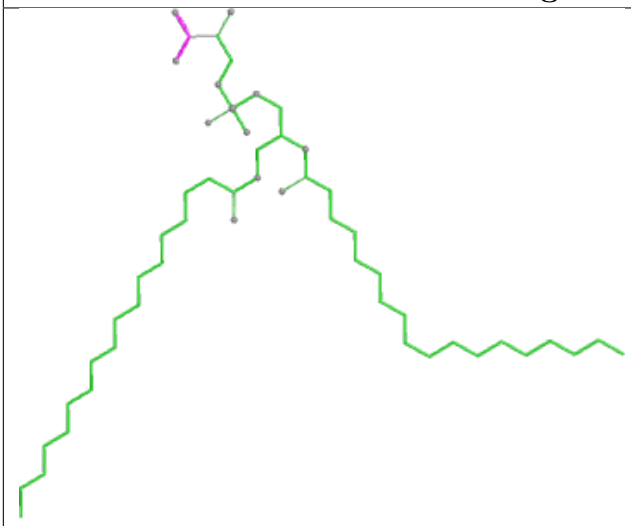


Torsions

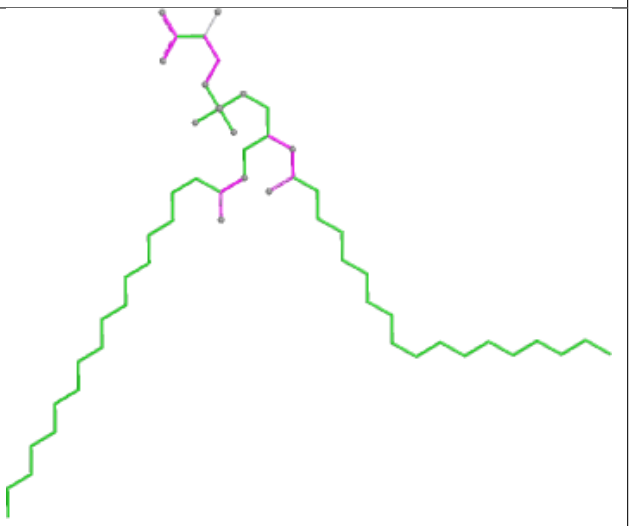


Rings

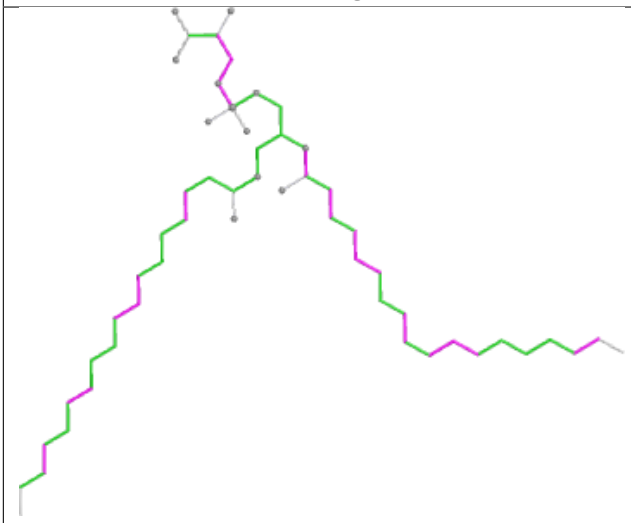
Ligand 17F A 38



Bond lengths



Bond angles



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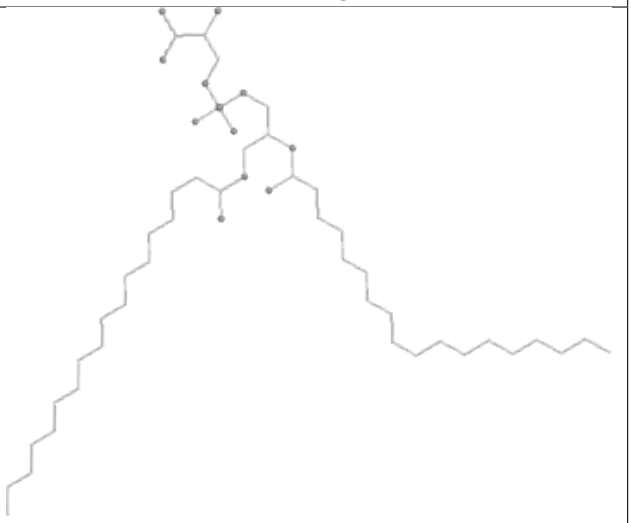
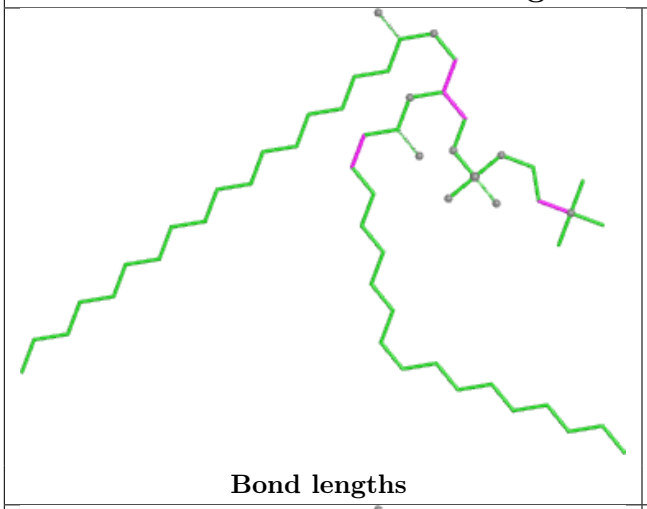
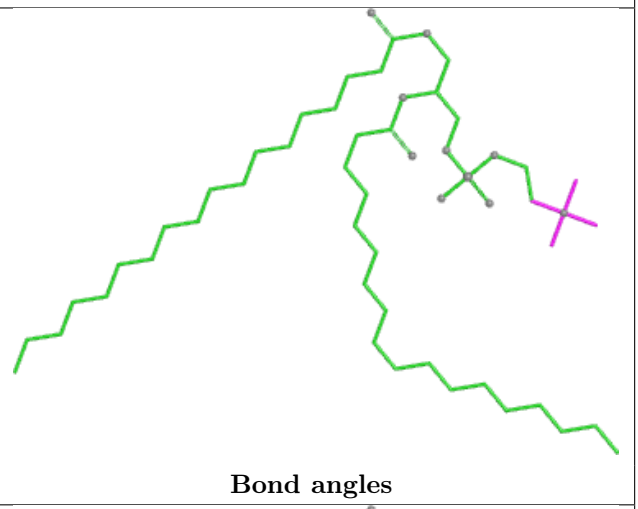


Rings

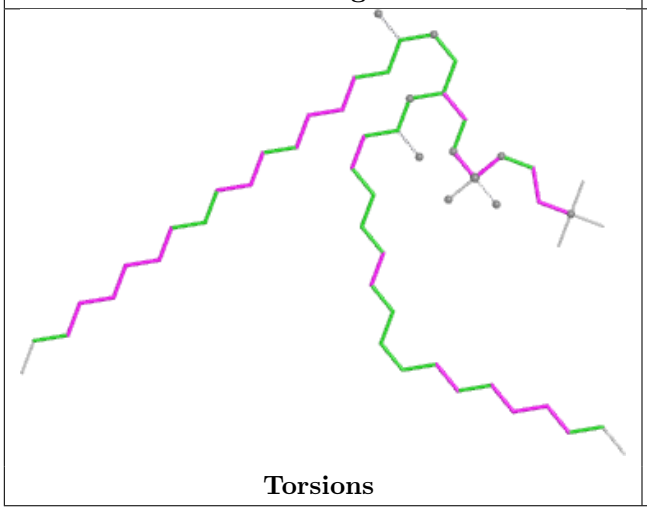
Ligand PCW A 64



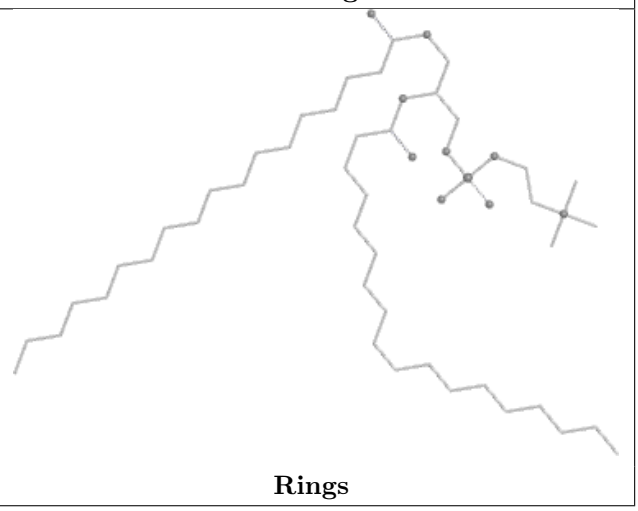
Bond lengths



Bond angles

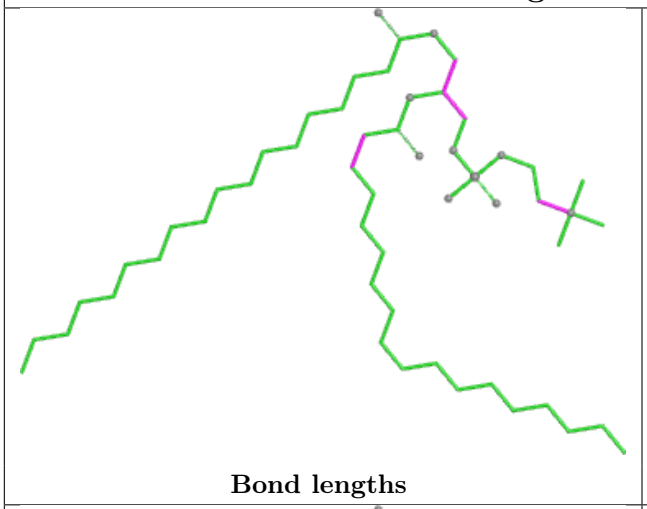


Torsions

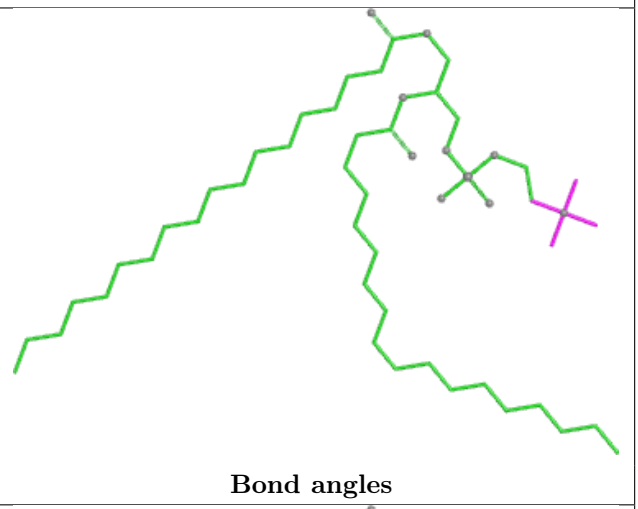


Rings

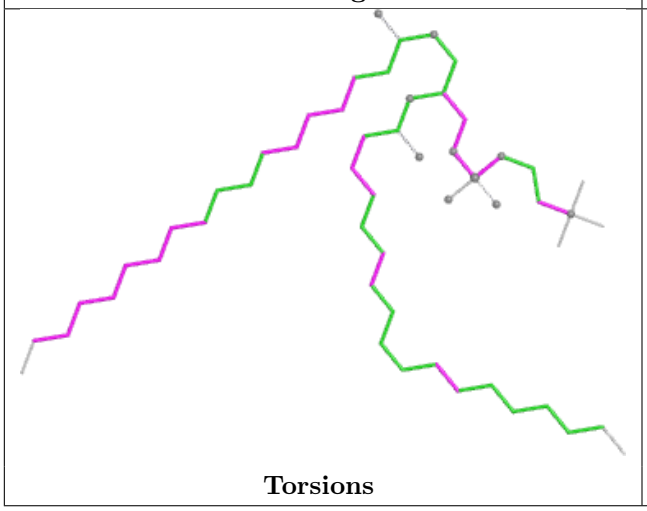
Ligand PCW A 70



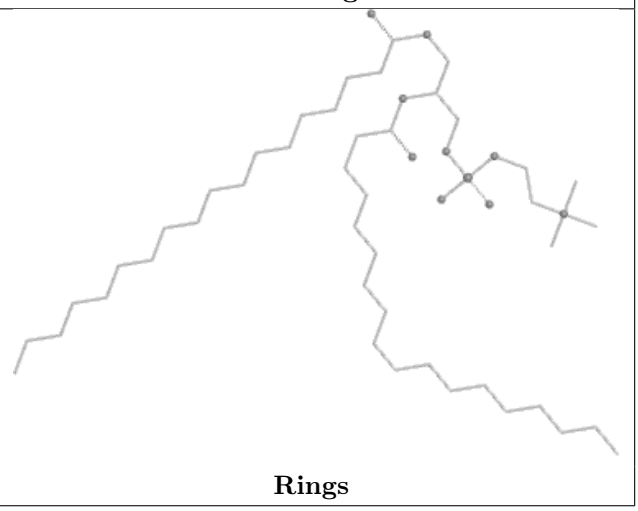
Bond lengths



Bond angles

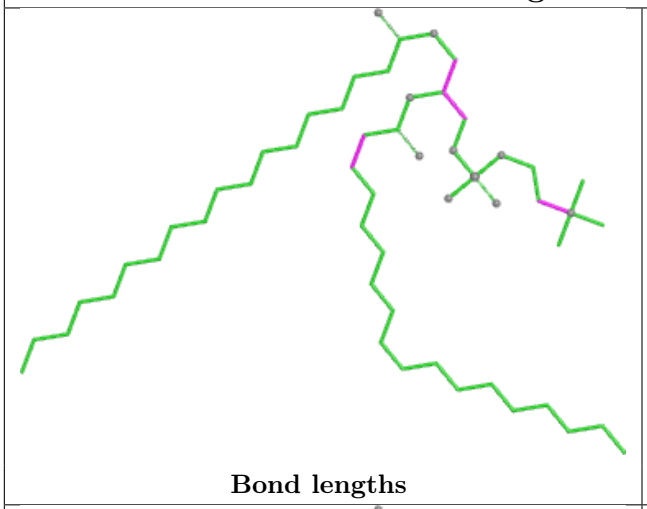


Torsions

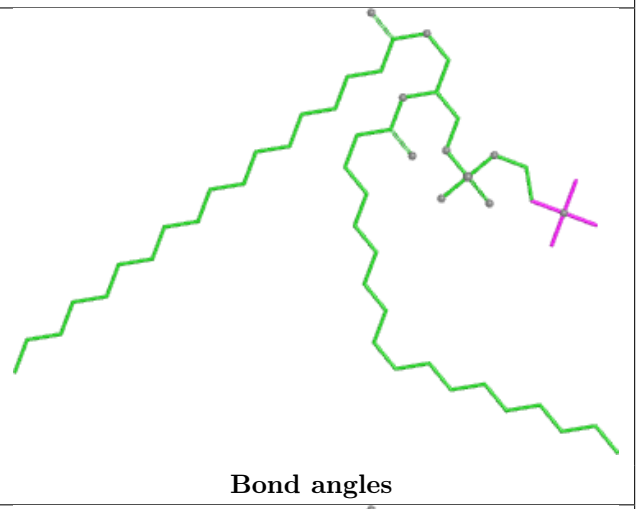


Rings

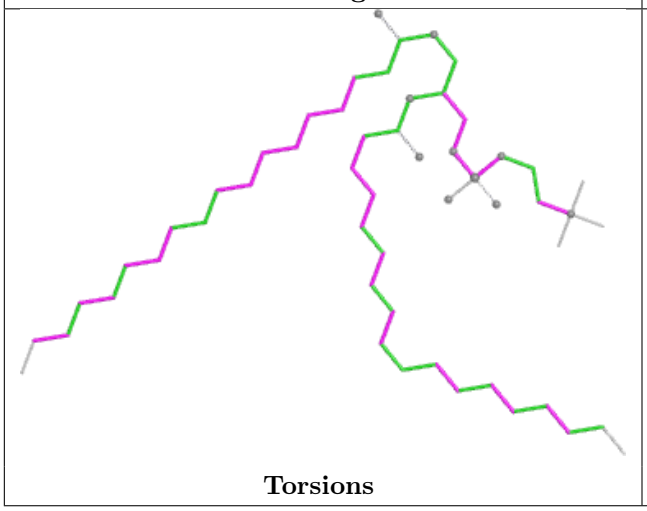
Ligand PCW A 42



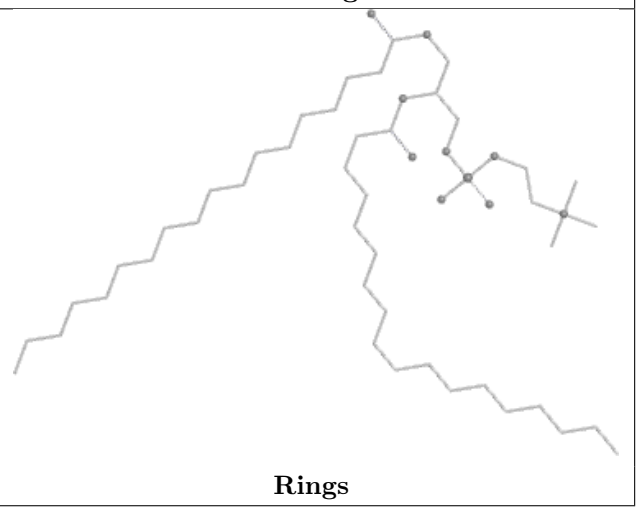
Bond lengths



Bond angles

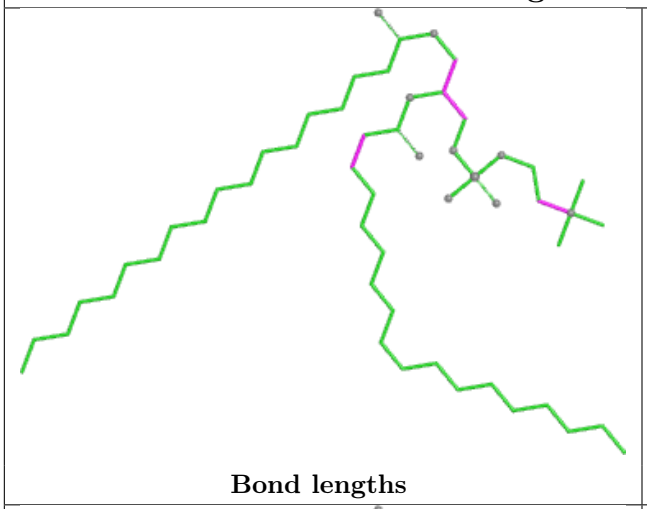


Torsions



Rings

Ligand PCW A 68



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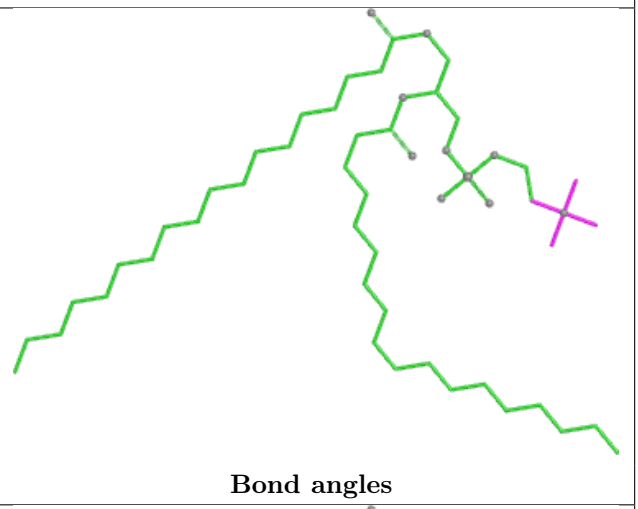
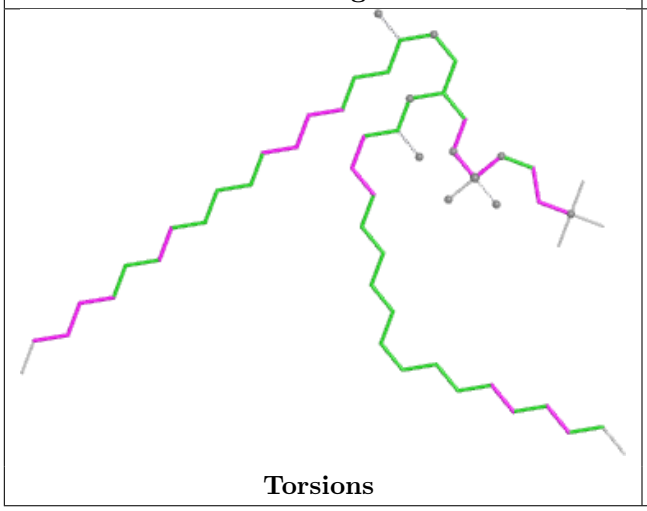


Bond angles



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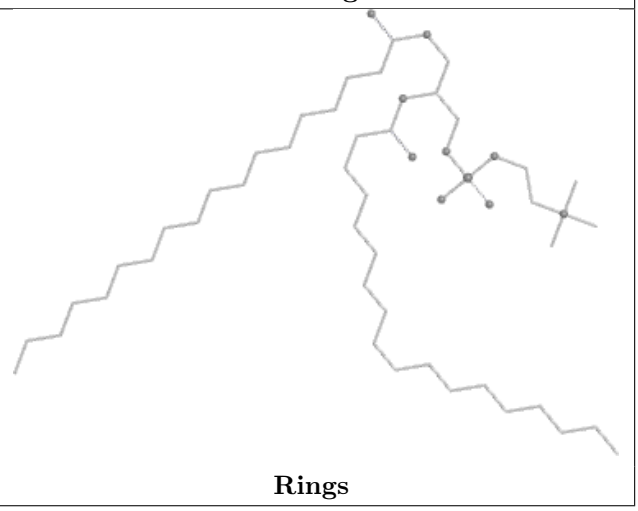
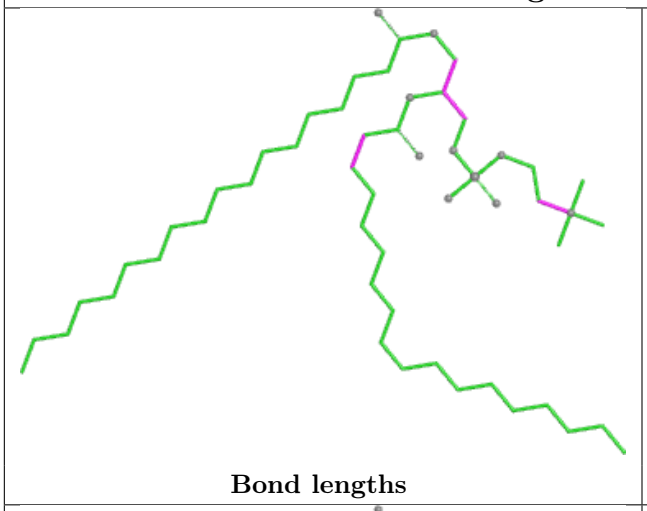
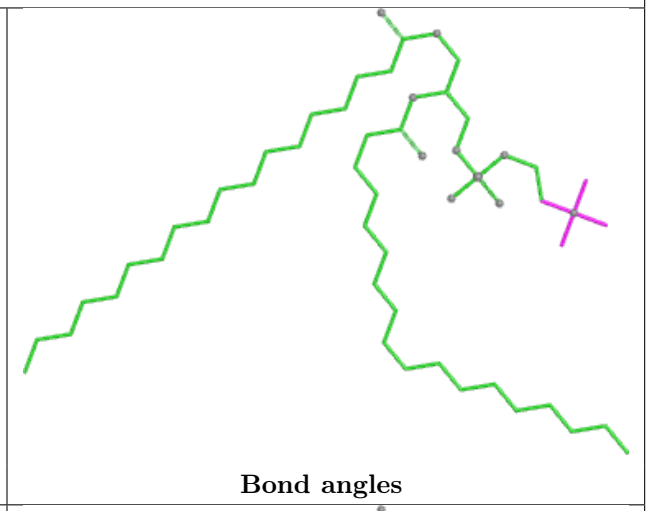


Rings

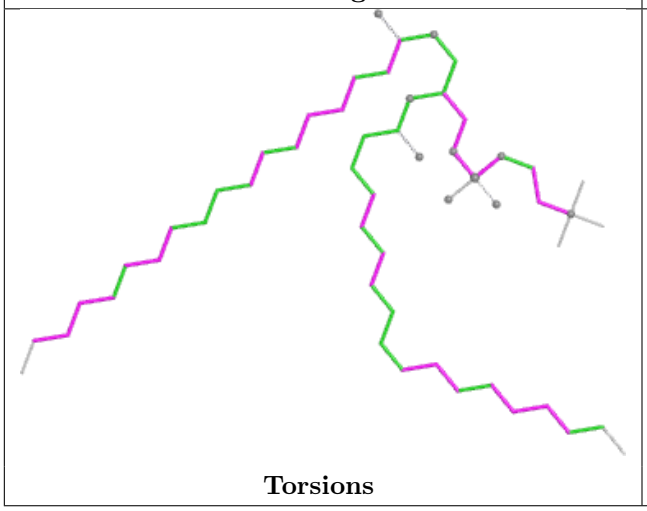
Ligand PCW A 20



Bond lengths



Bond angles



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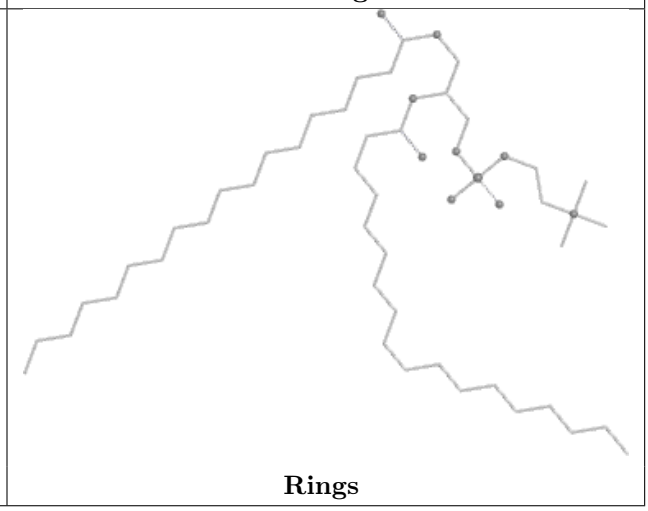
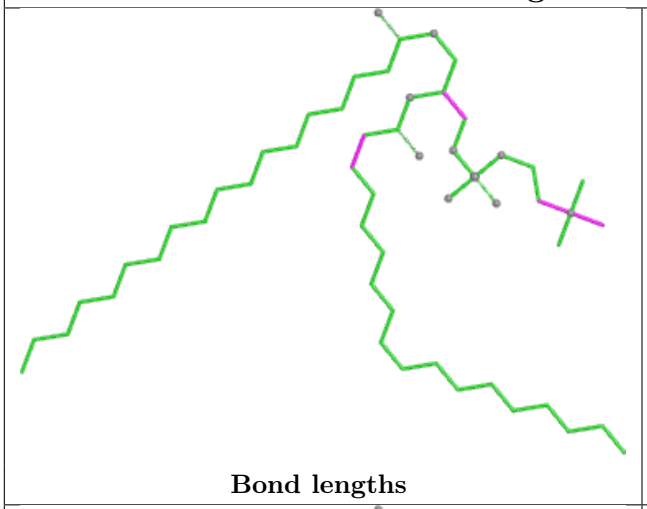
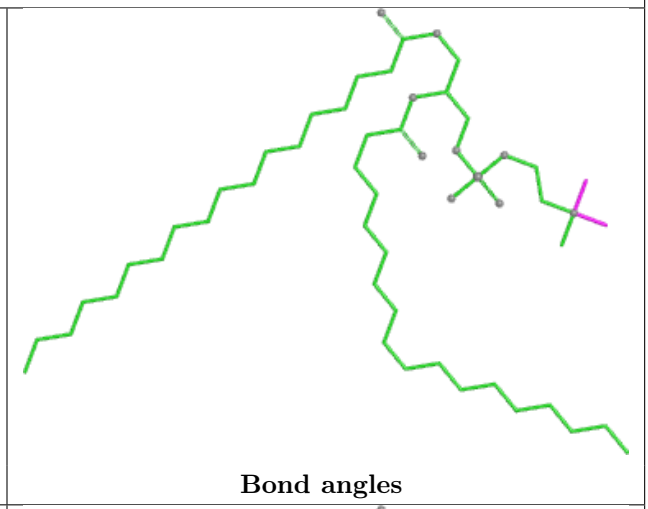


Rings

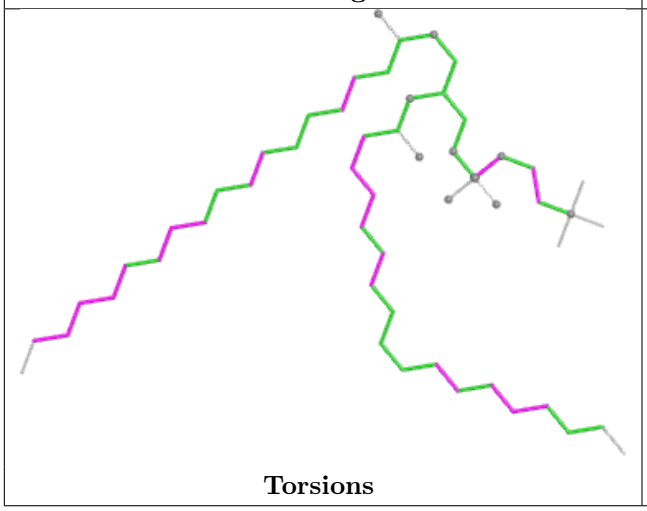
Ligand PCW A 72



Bond lengths



Bond angles



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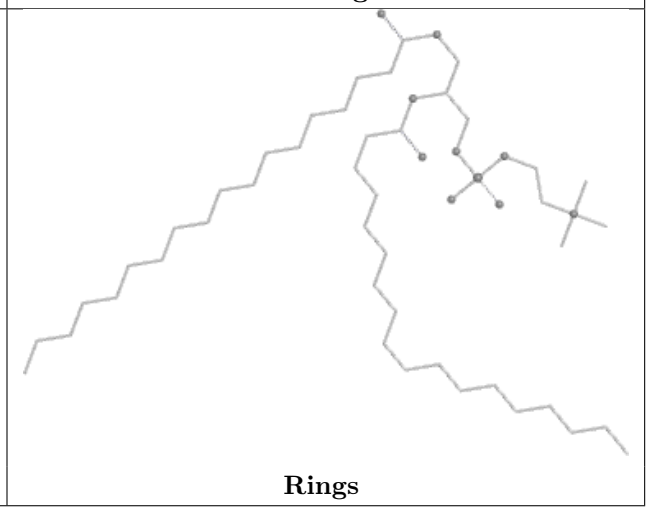
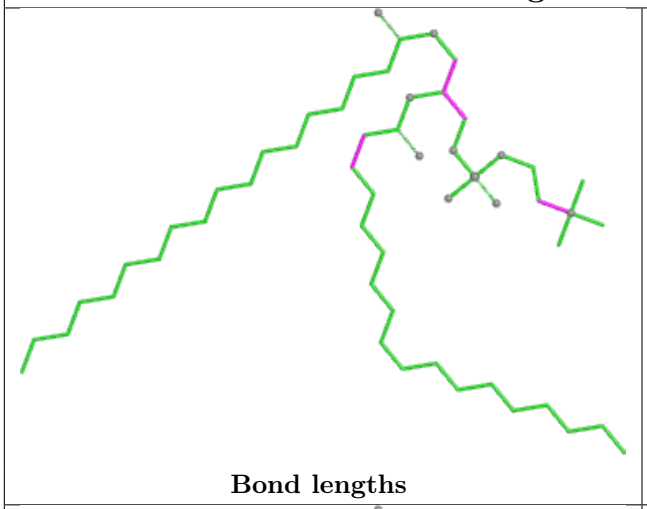


Rings

Ligand PCW A 43



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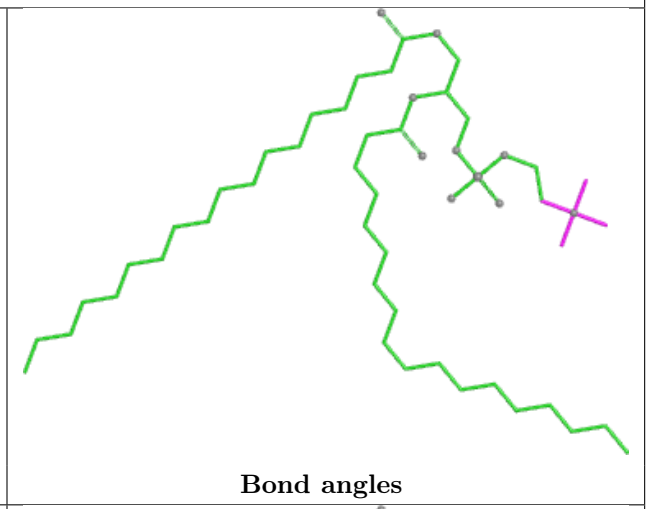
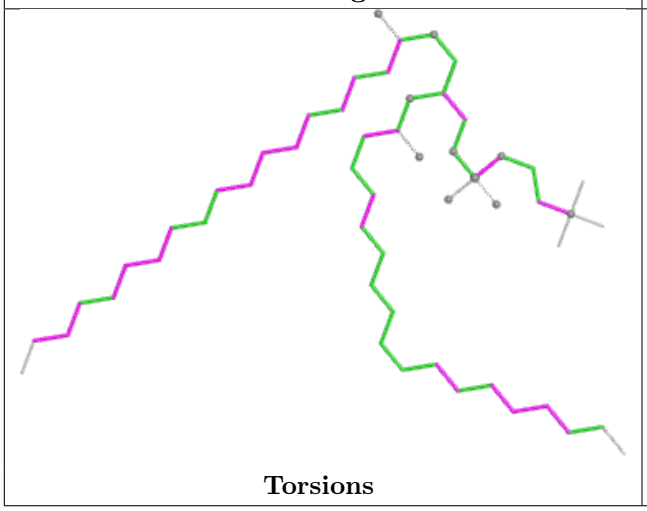
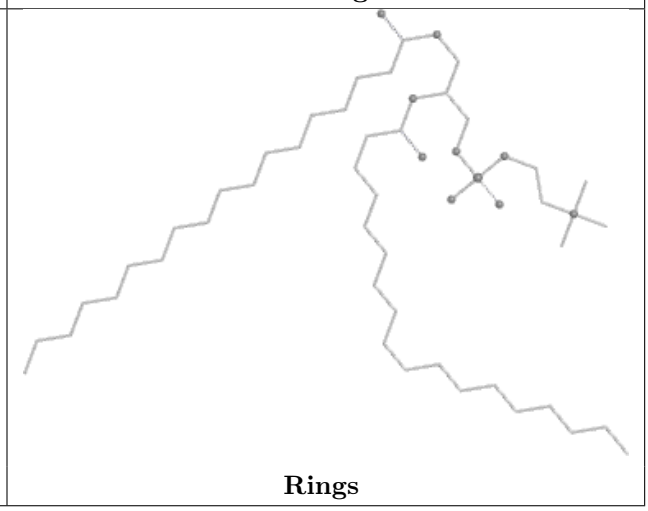


Bond angles

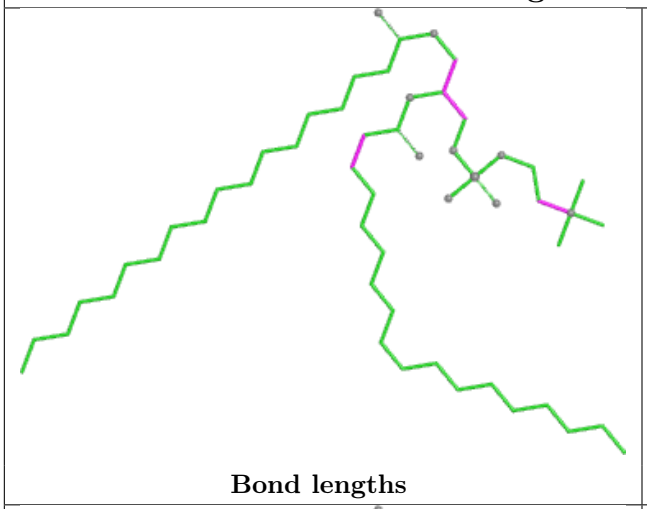


Torsions

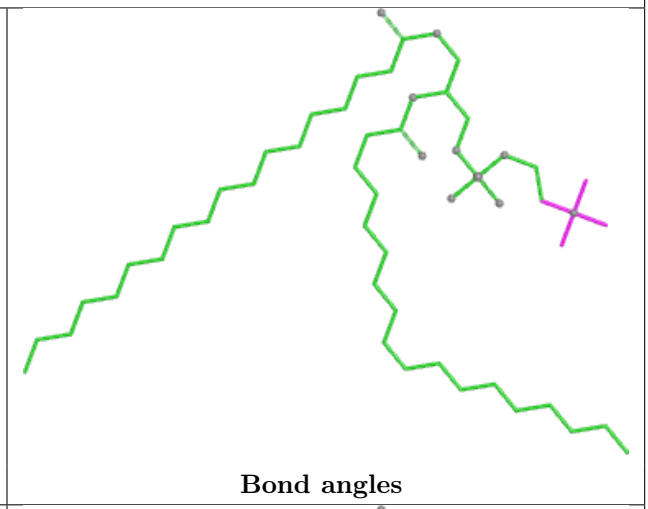


Rings

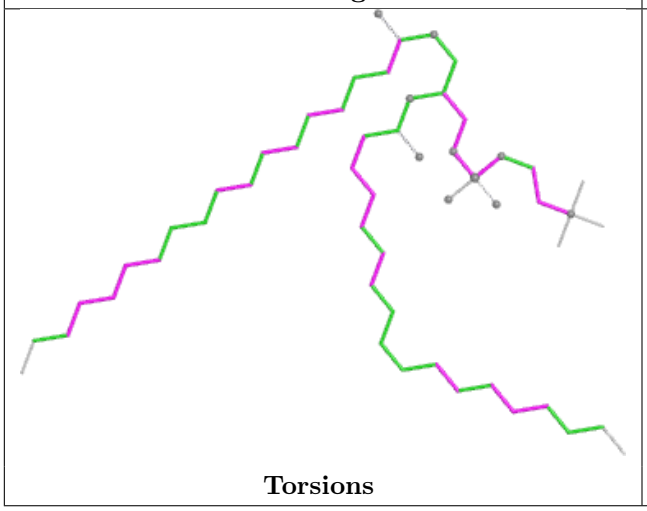
Ligand PCW A 25



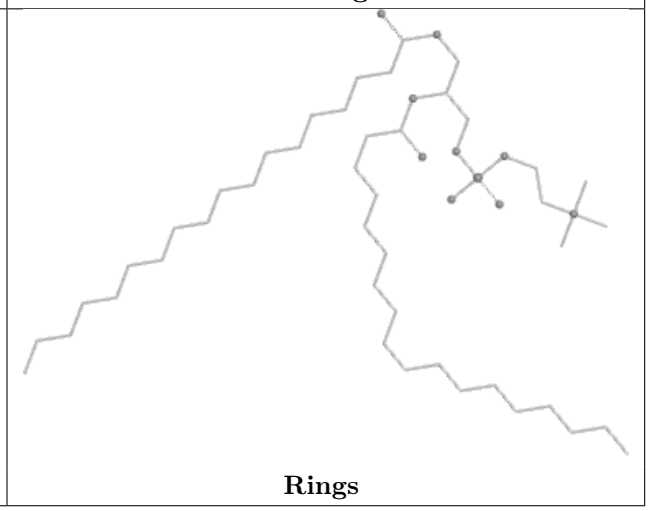
Bond lengths



Bond angles

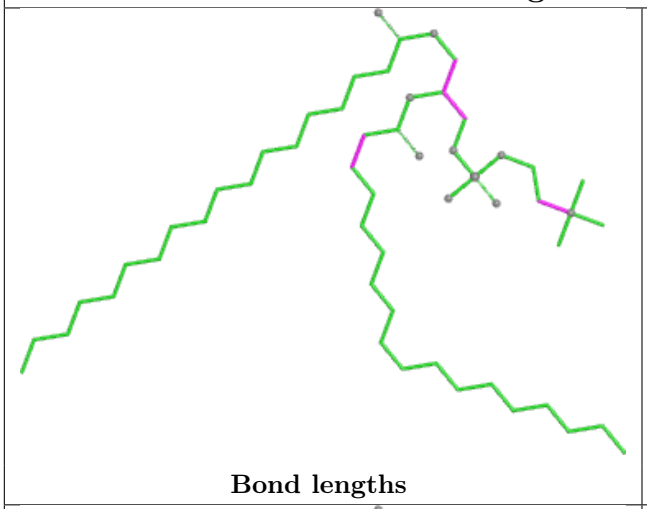


Torsions

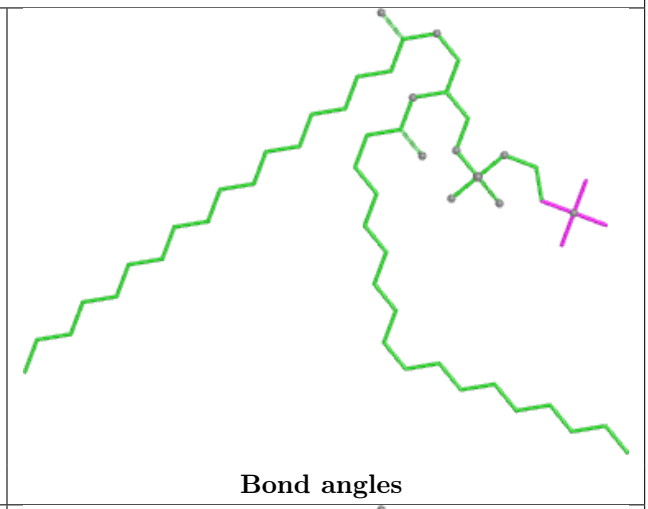


Rings

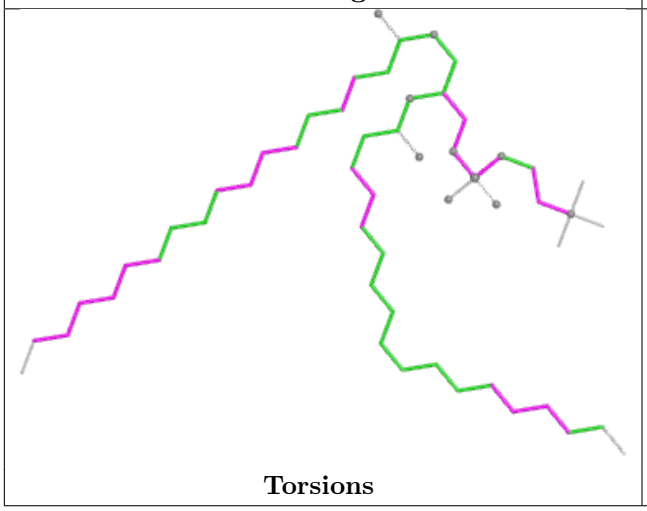
Ligand PCW A 57



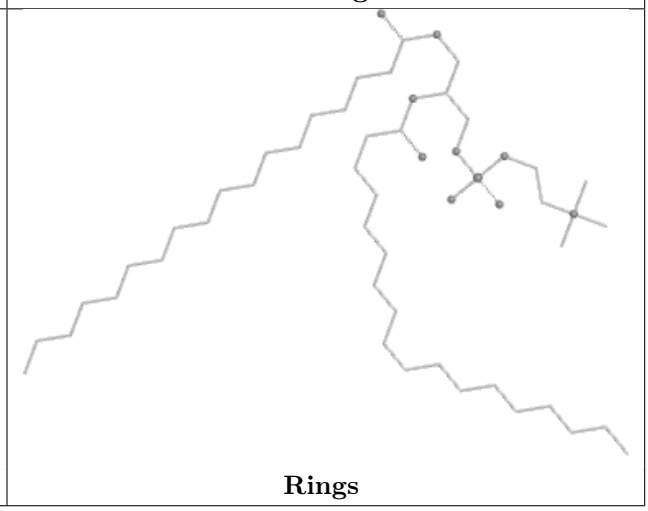
Bond lengths



Bond angles

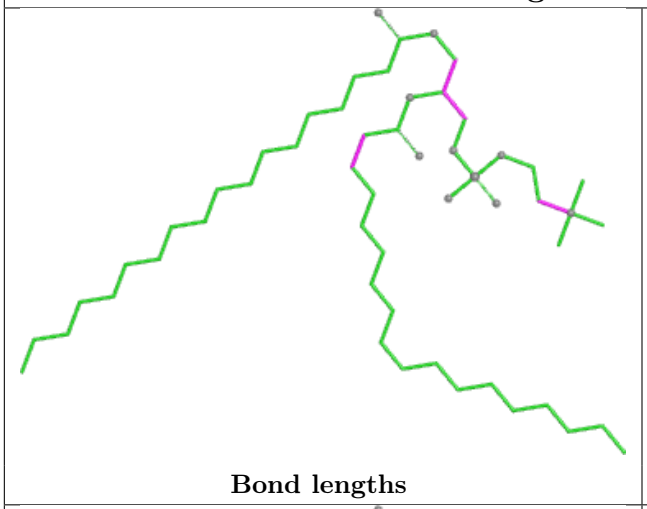


Torsions



Rings

Ligand PCW A 31



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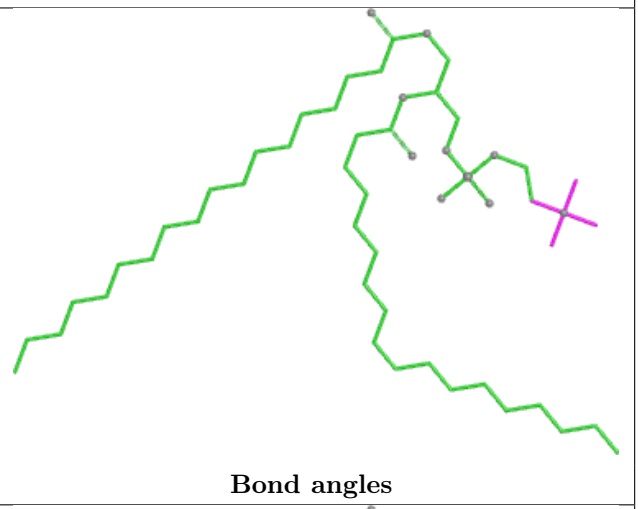
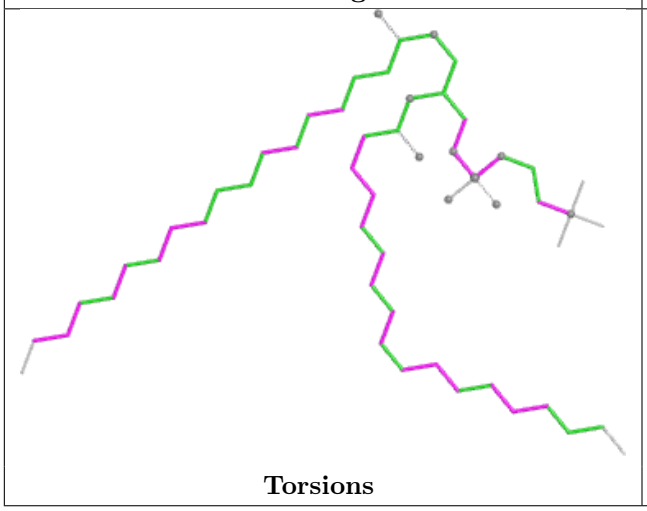
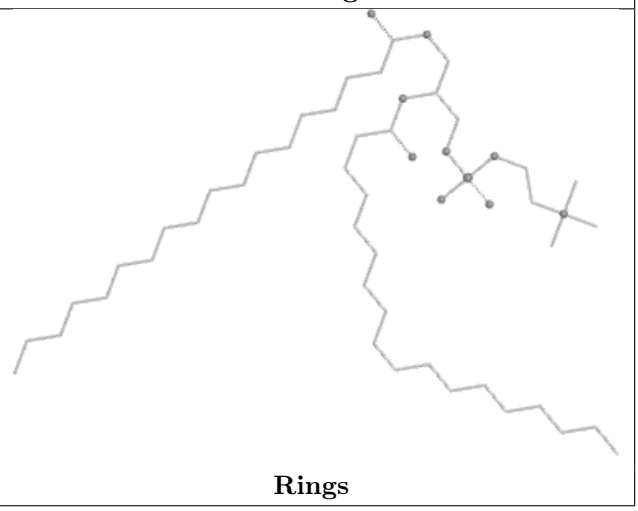


Bond angles

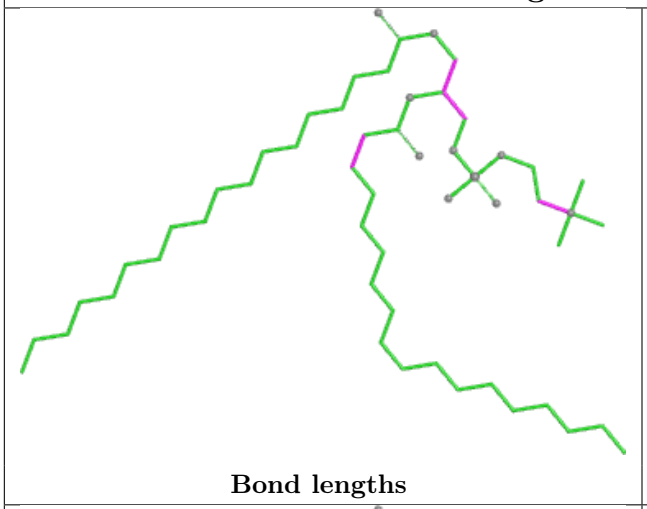


Torsions

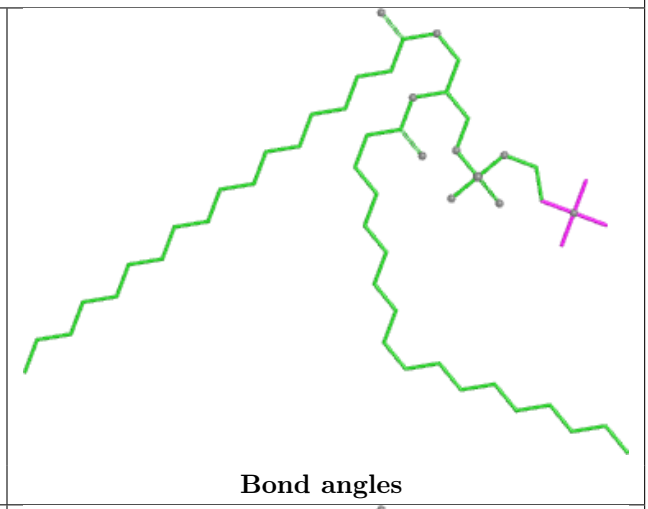


Rings

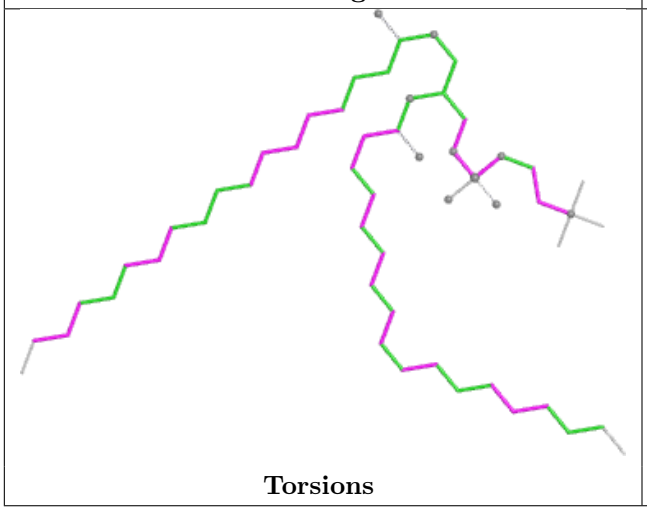
Ligand PCW A 13



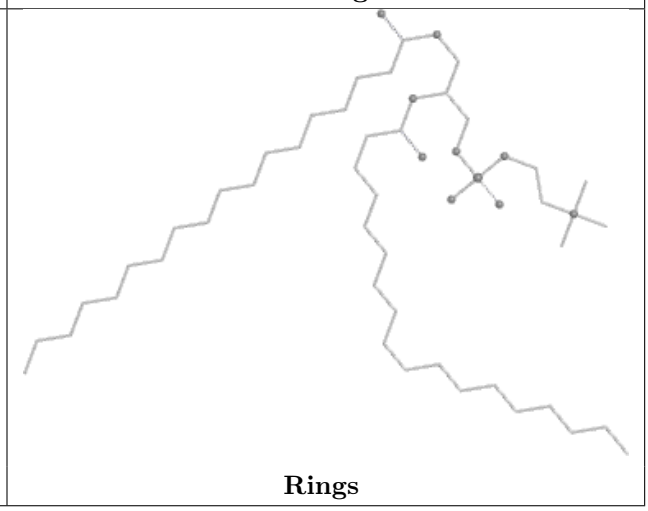
Bond lengths



Bond angles

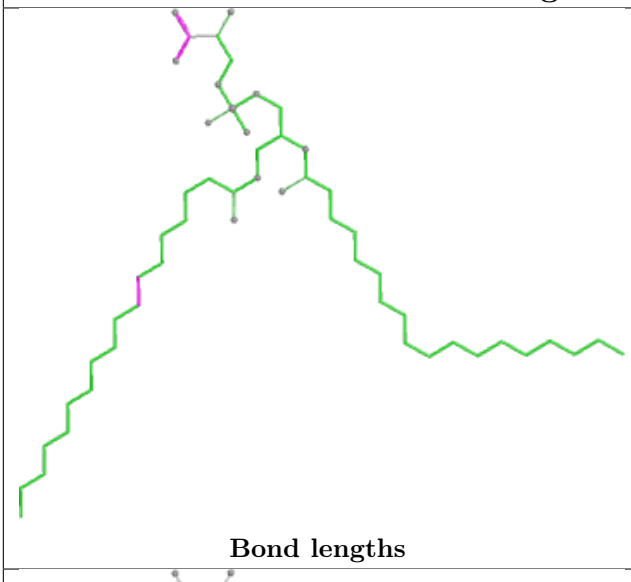


Torsions



Rings

Ligand 17F A 74



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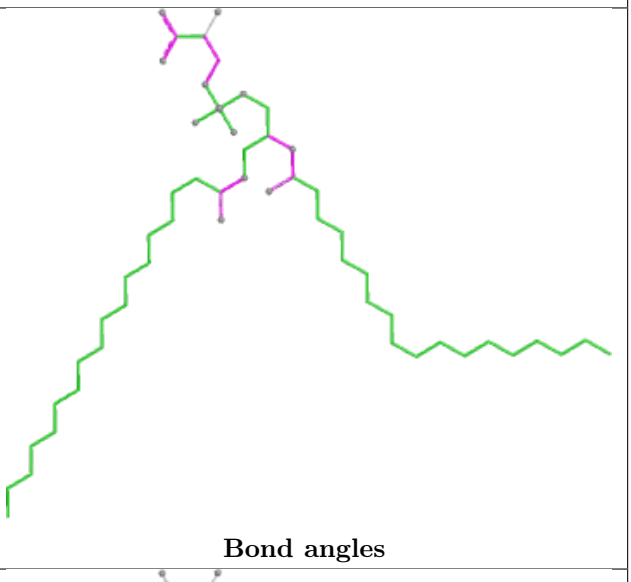
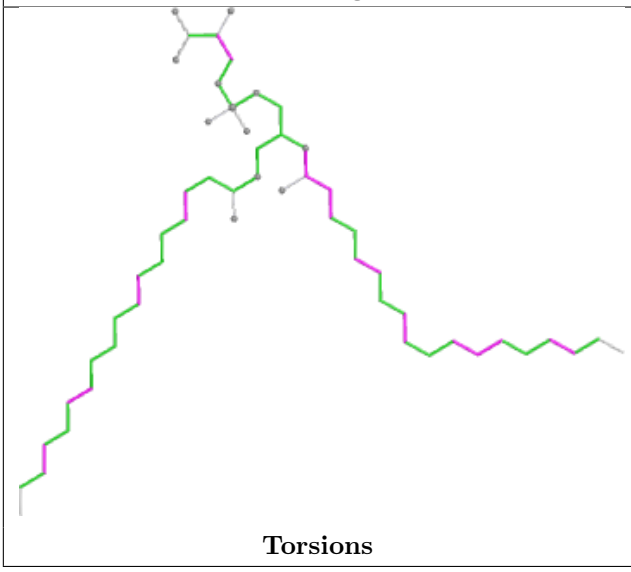


Bond angles



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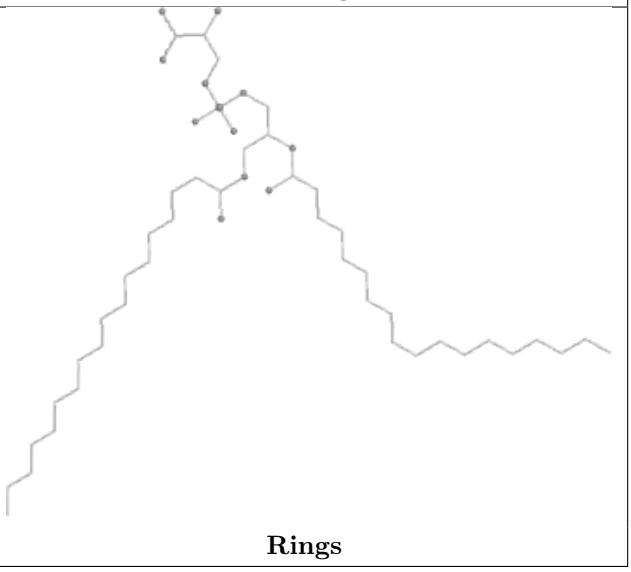
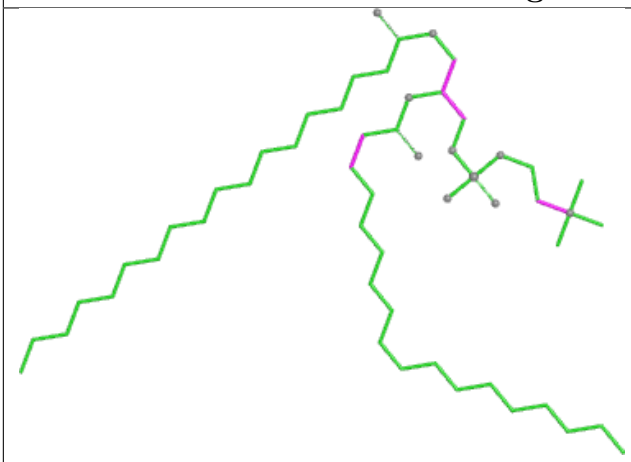


Rings

Ligand PCW A 22



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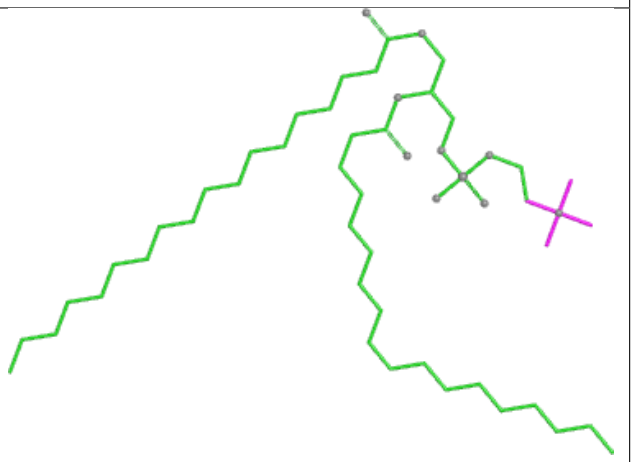
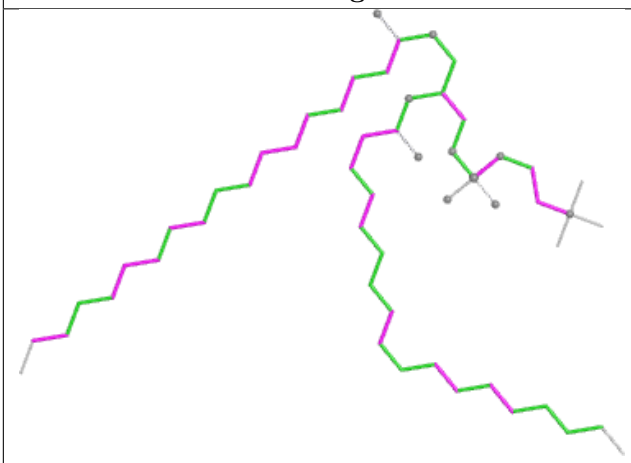


Bond angles



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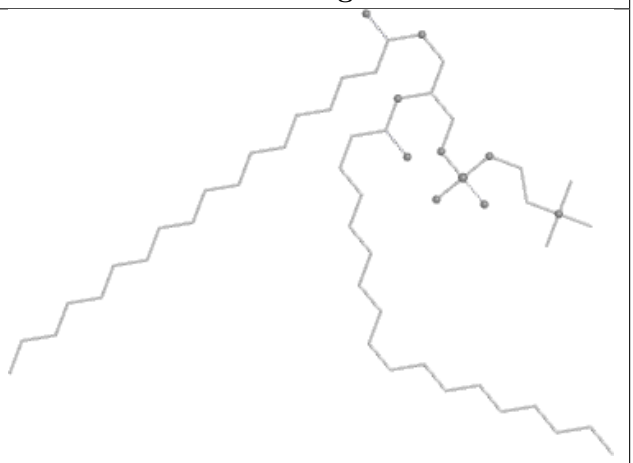
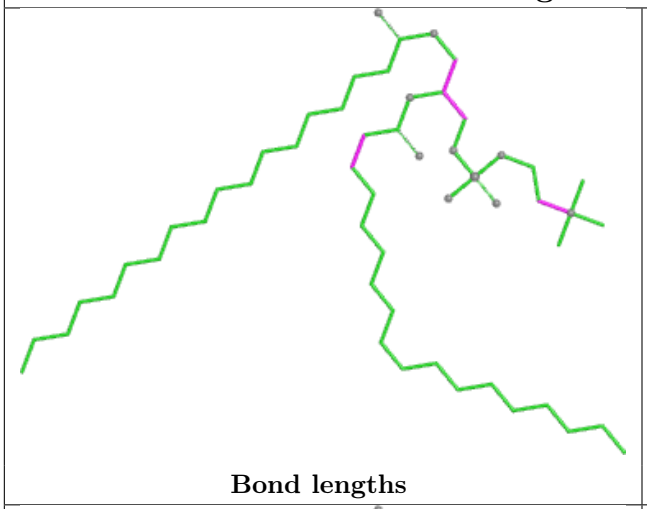
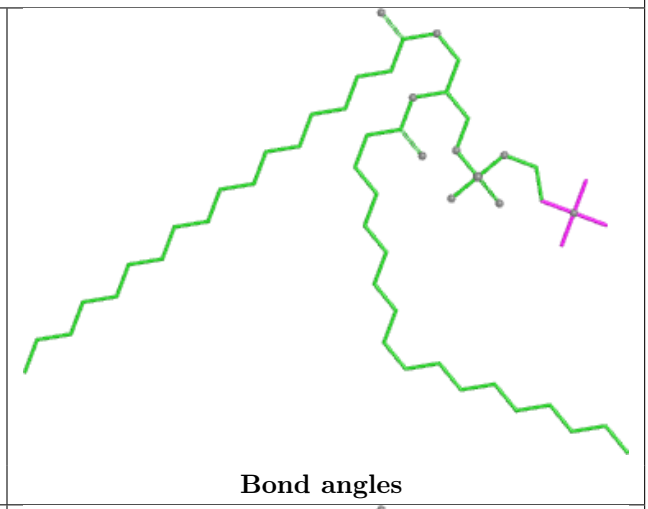


Rings

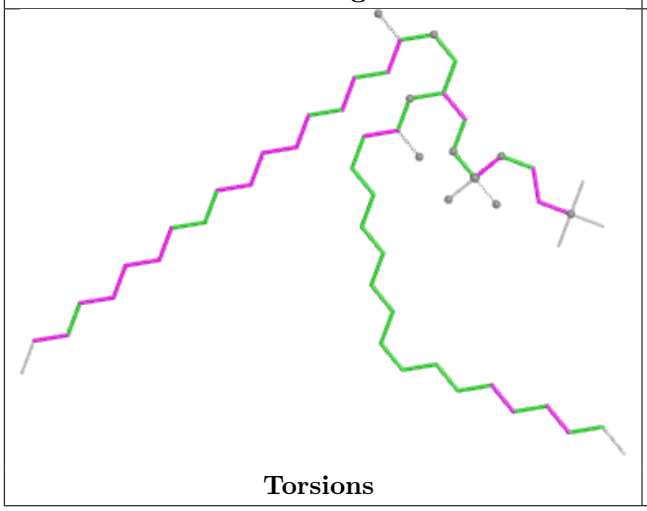
Ligand PCW A 1



Bond lengths



Bond angles



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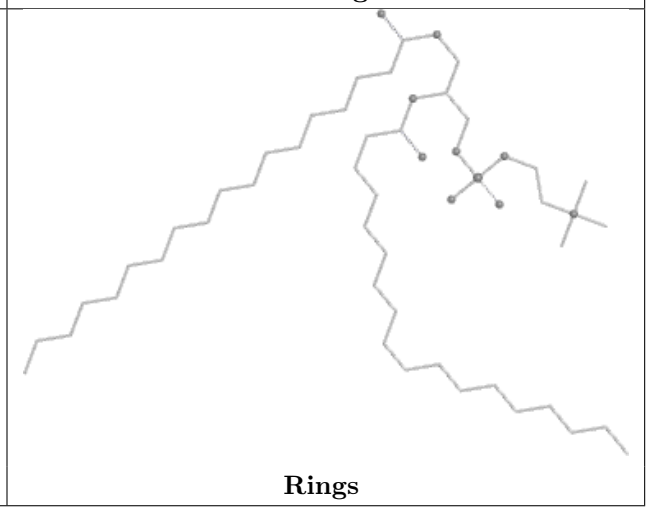
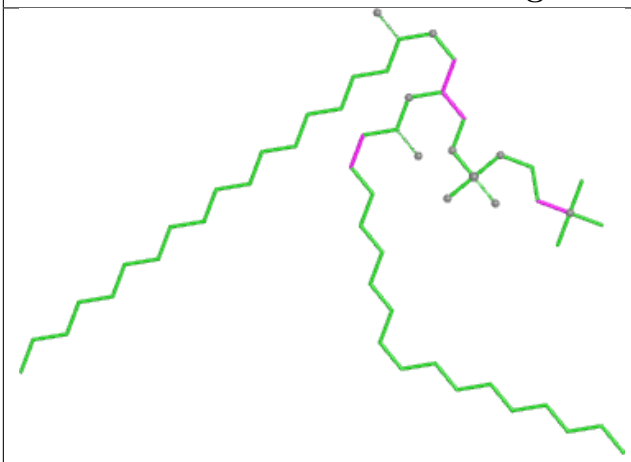


Rings

Ligand PCW A 29



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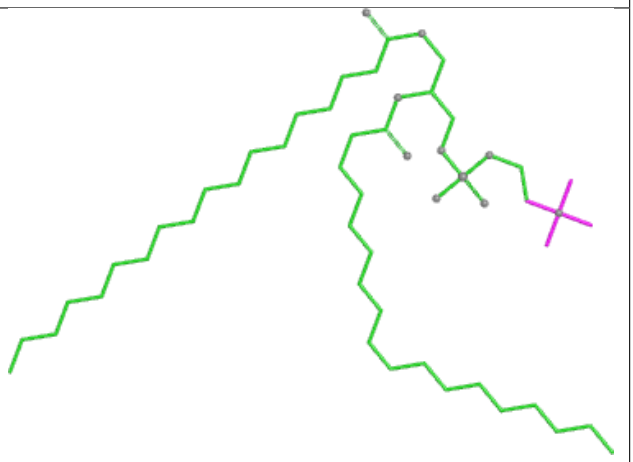
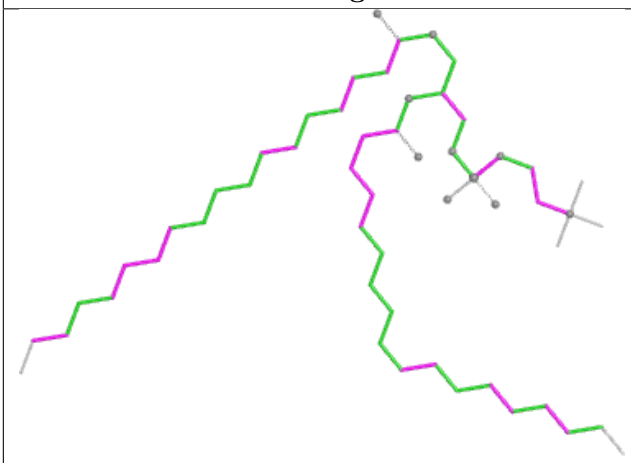
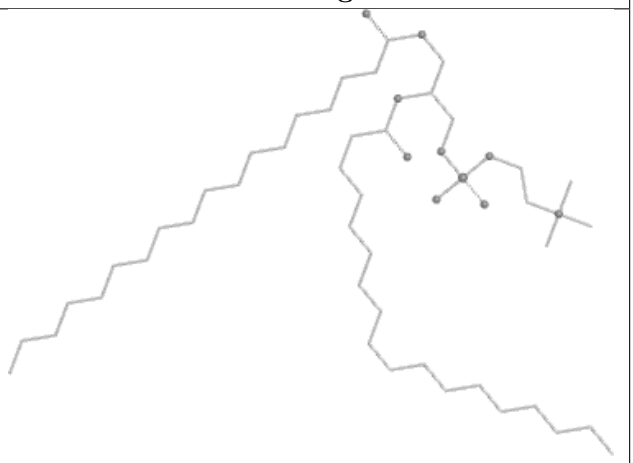


Bond angles

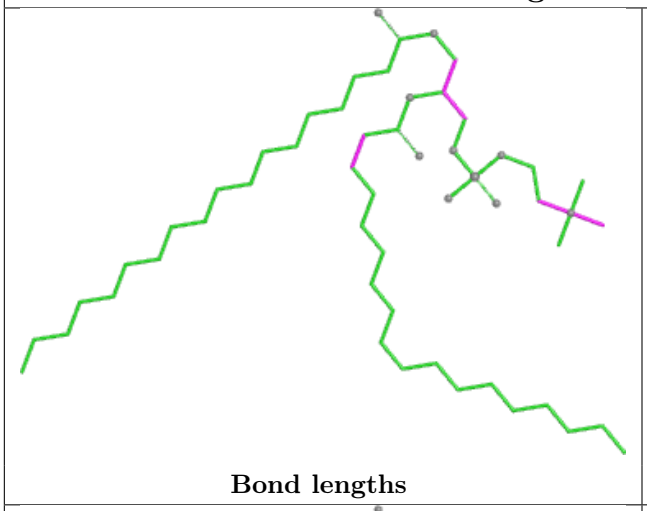


Torsions

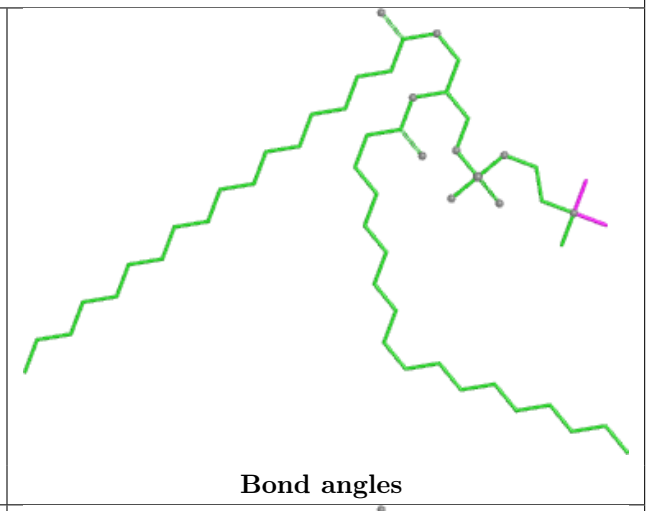


Rings

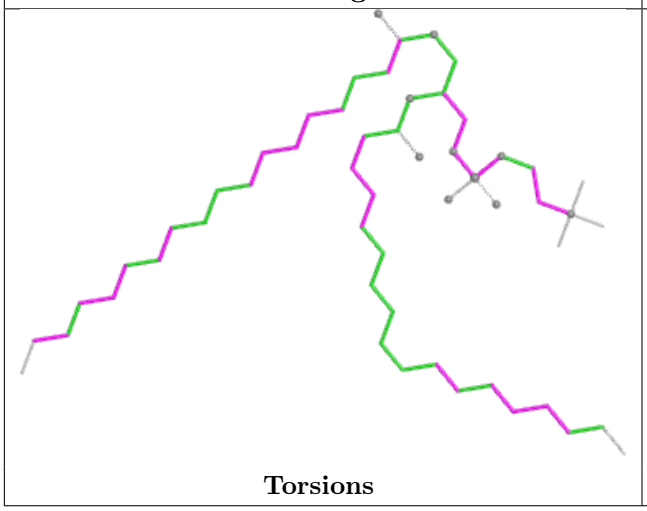
Ligand PCW A 48



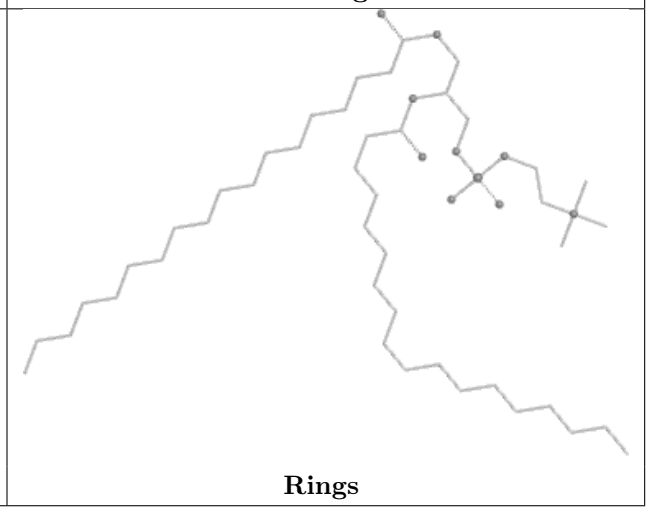
Bond lengths



Bond angles

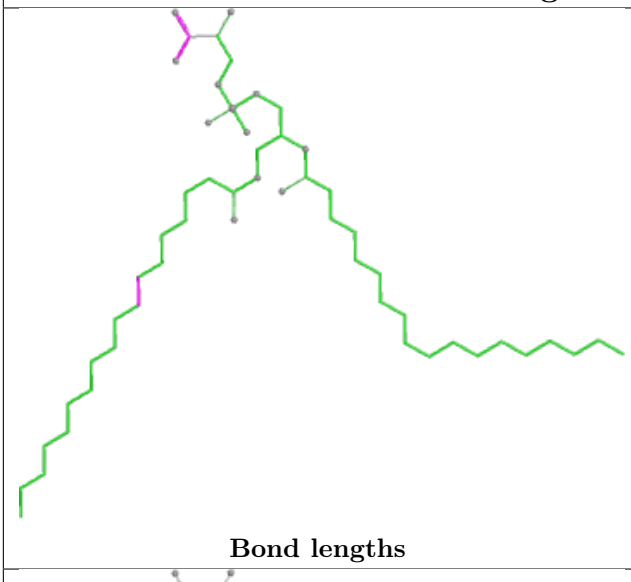


Torsions



Rings

Ligand 17F A 35



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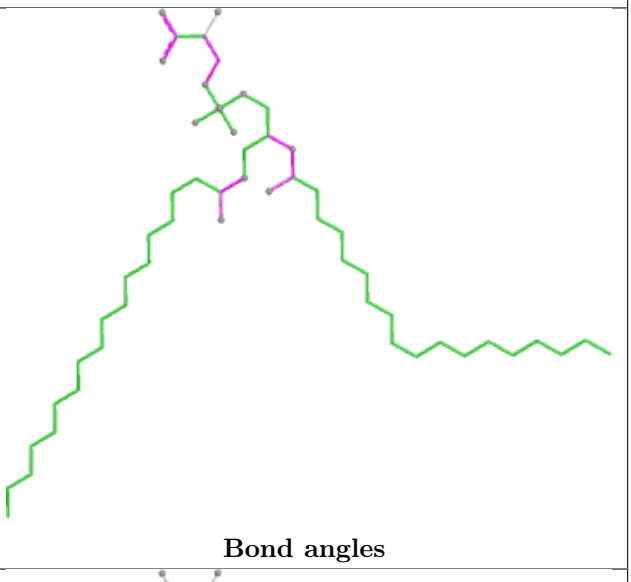
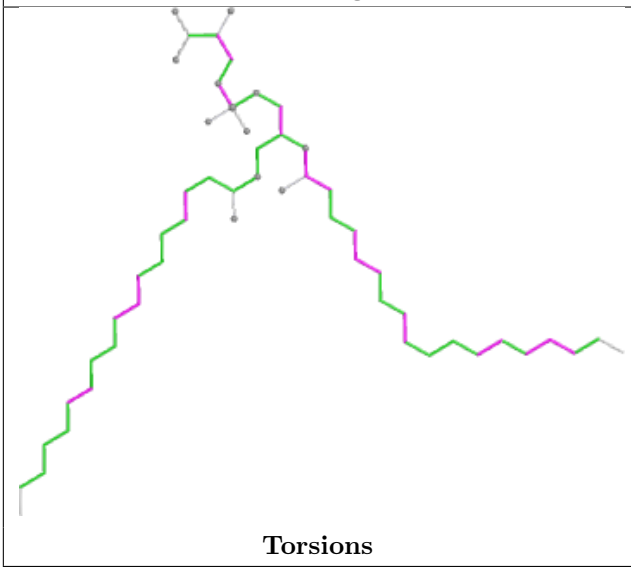
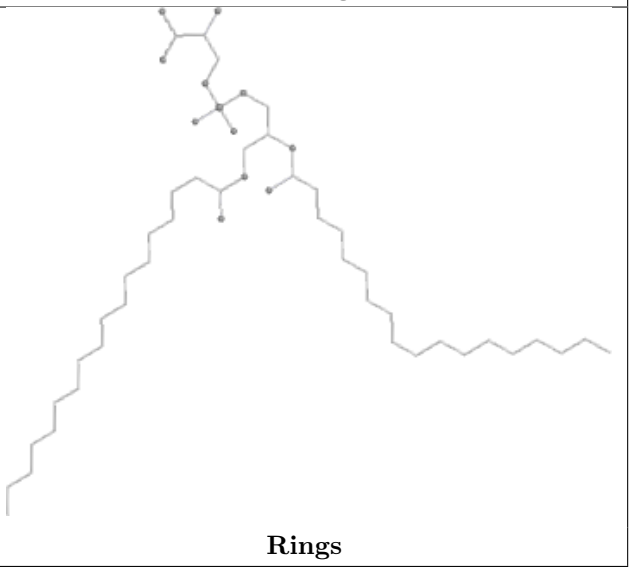


Bond angles

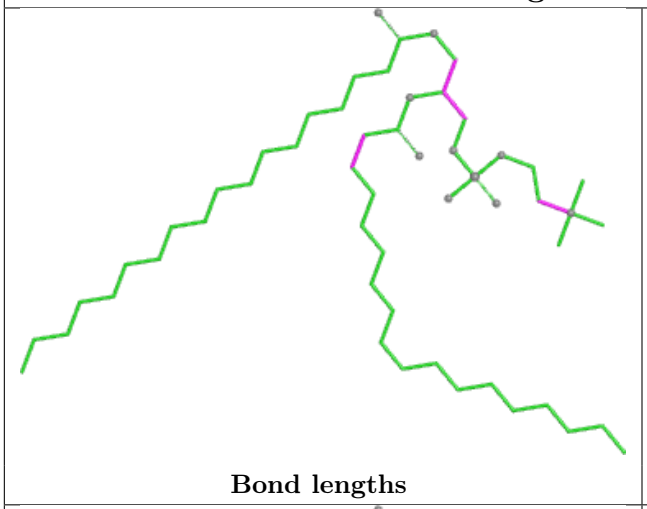


Torsions

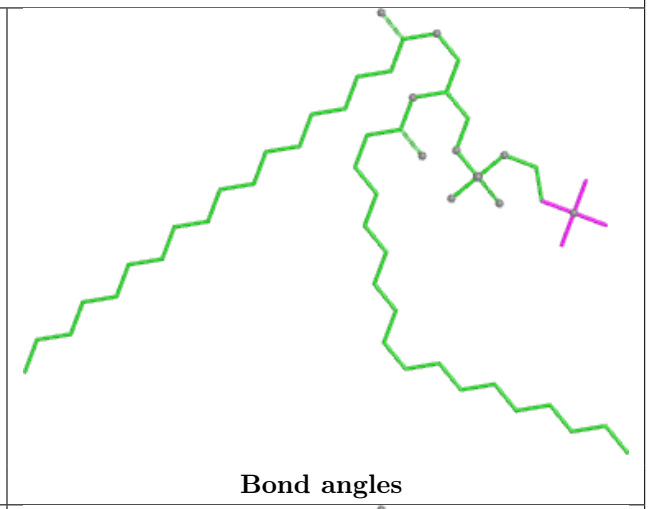


Rings

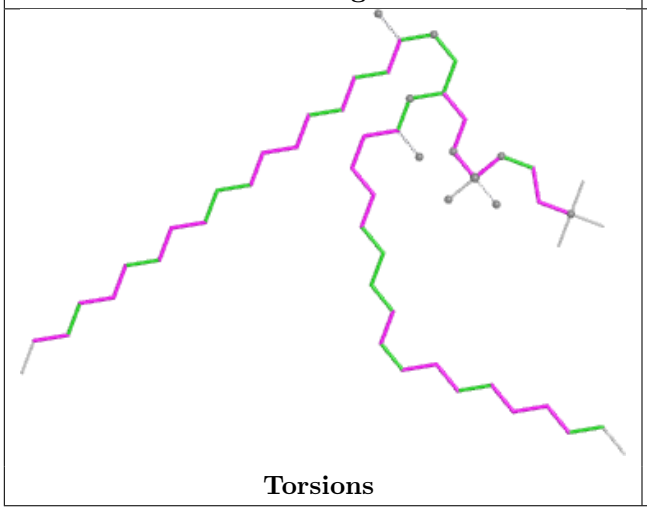
Ligand PCW A 60



Bond lengths



Bond angles



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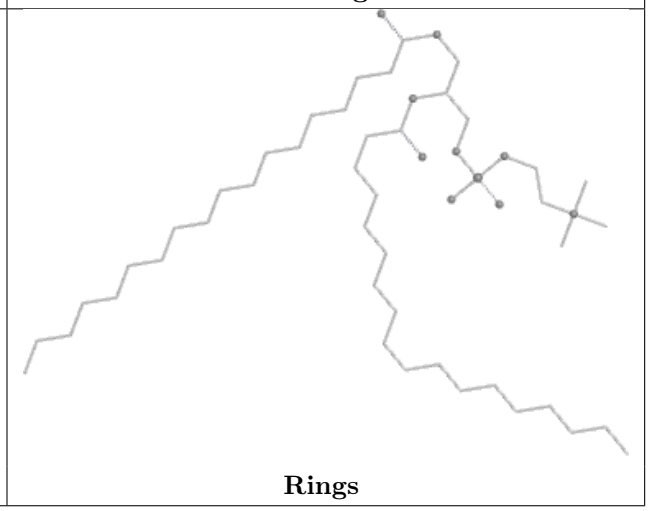
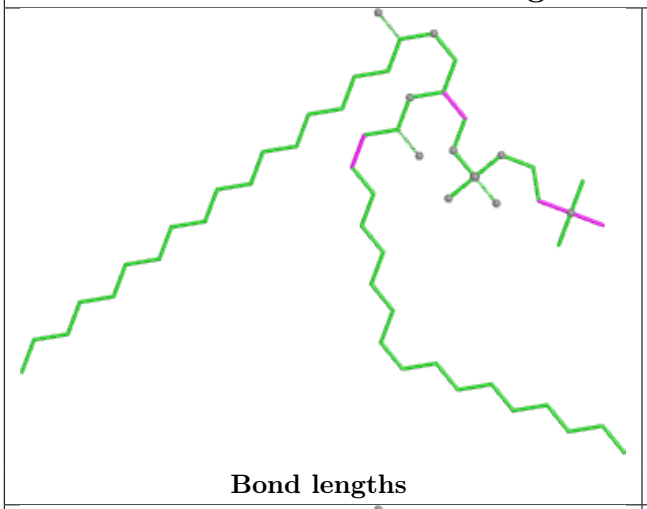
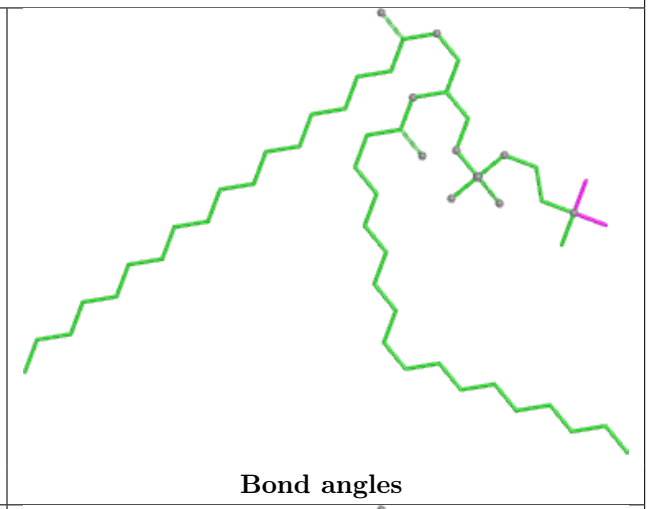


Rings

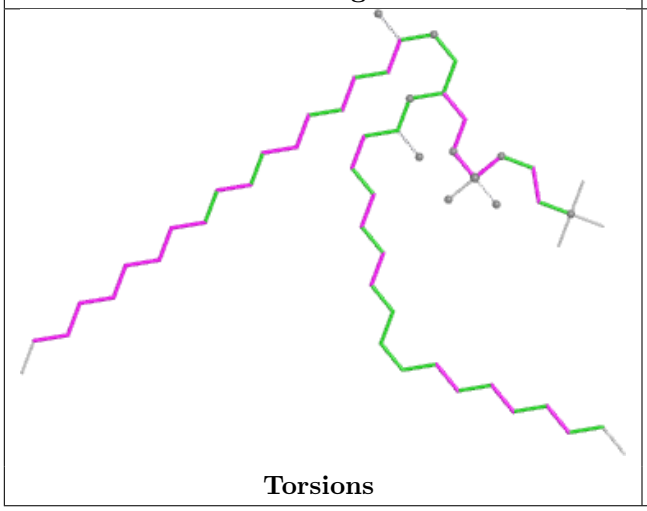
Ligand PCW A 16



Bond lengths



Bond angles



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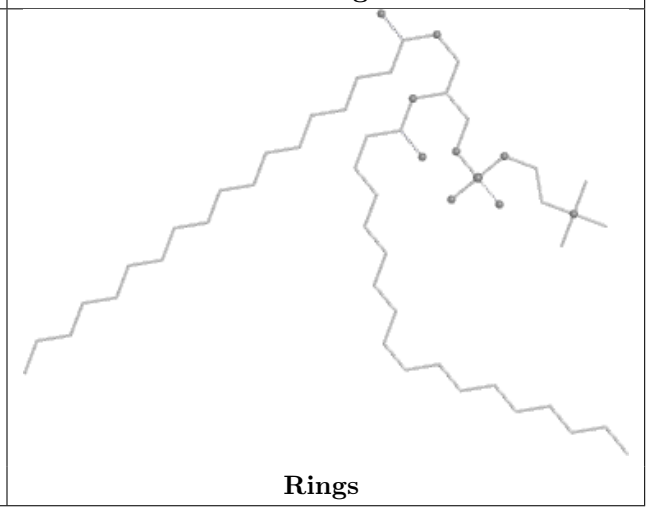
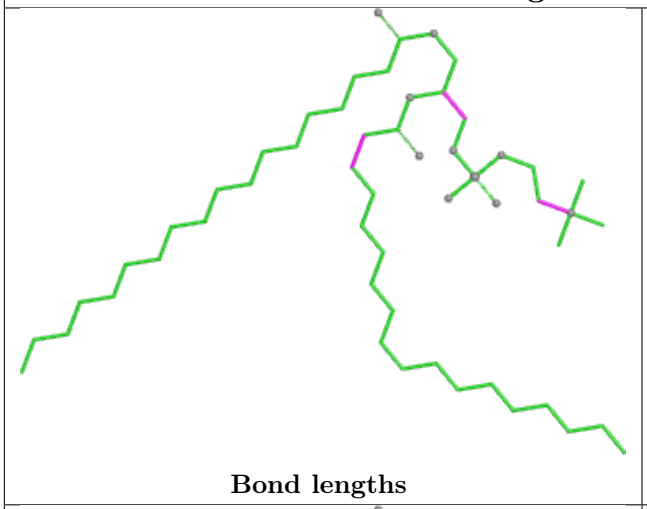
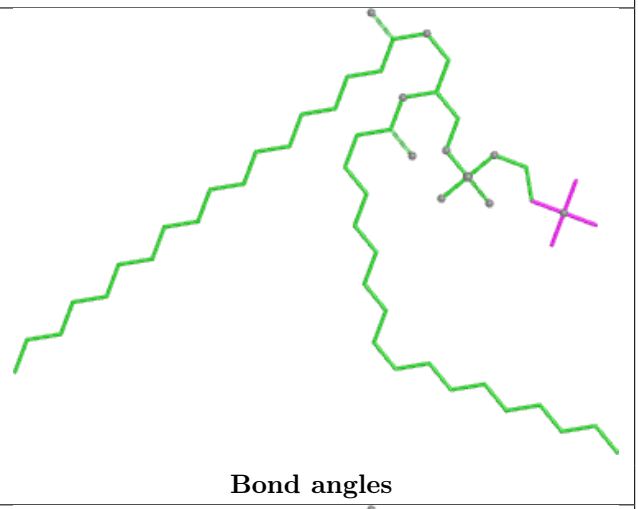


Rings

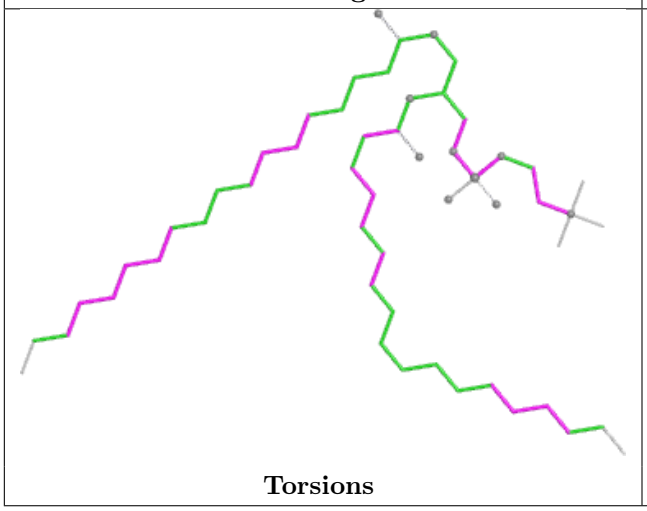
Ligand PCW A 53



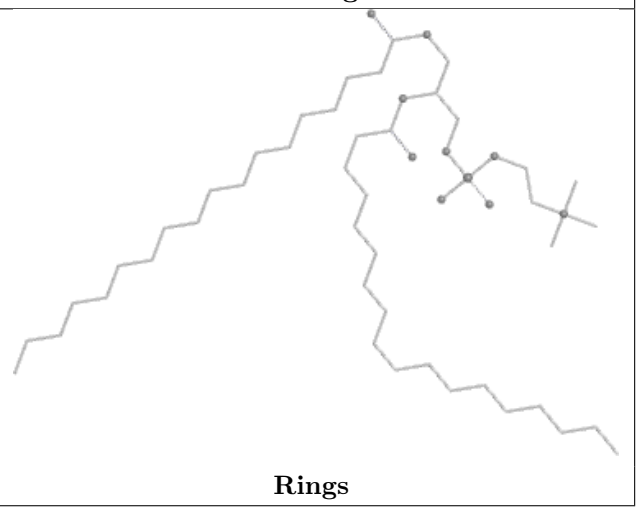
Bond lengths



Bond angles

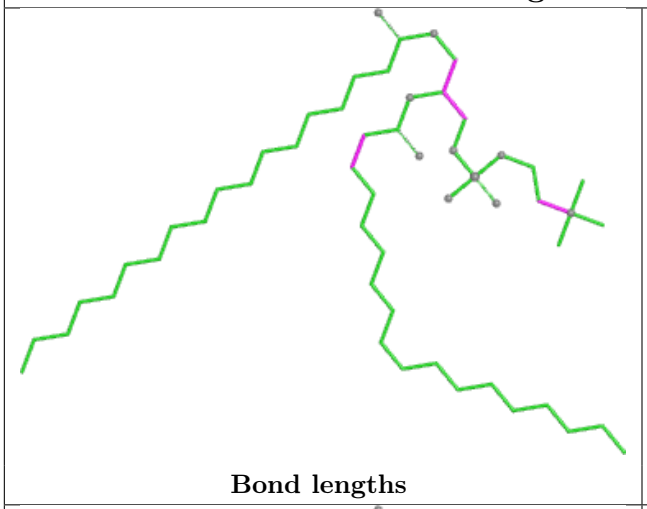


Torsions

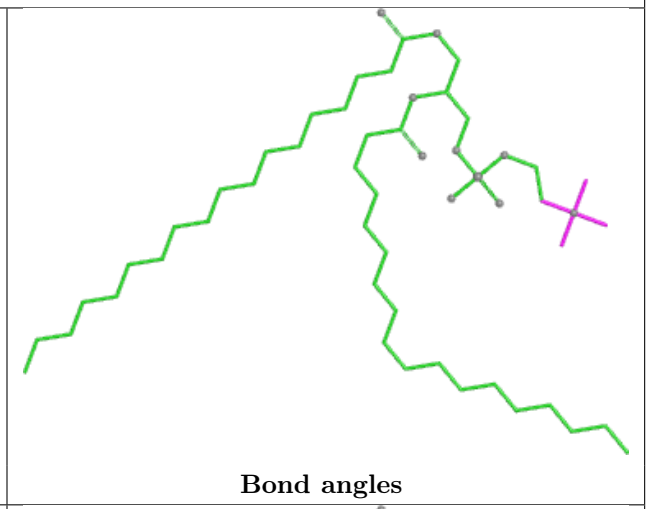


Rings

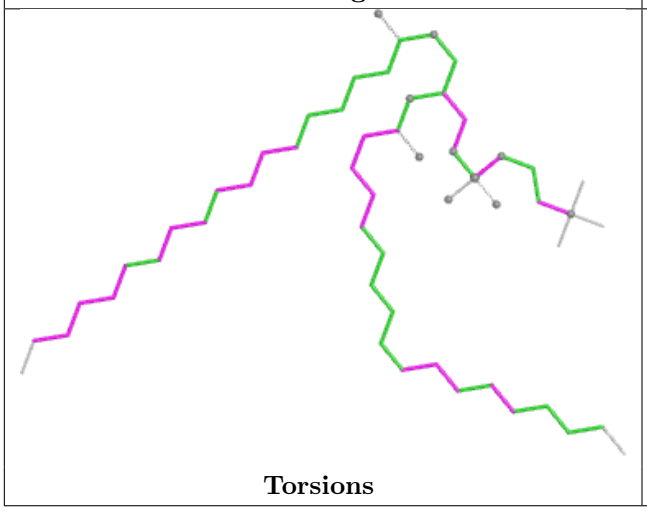
Ligand PCW A 67



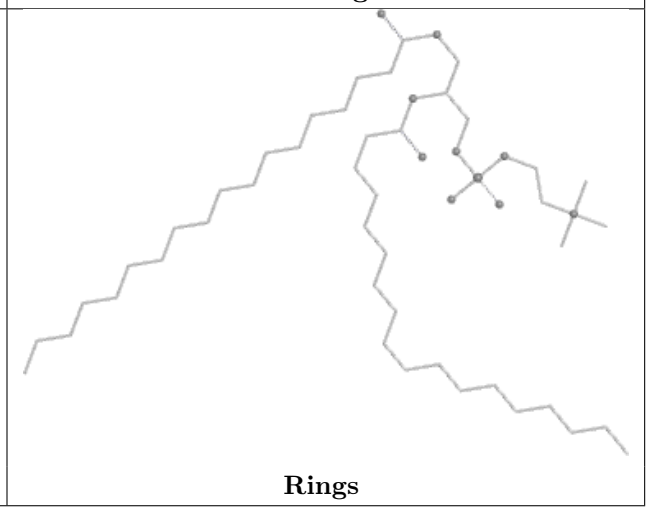
Bond lengths



Bond angles

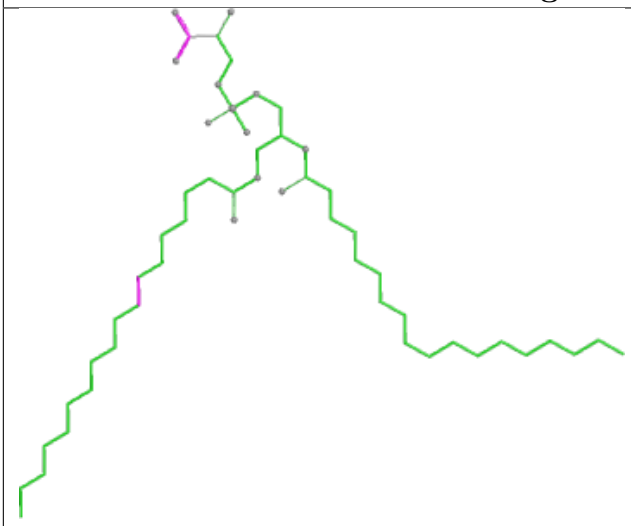


Torsions

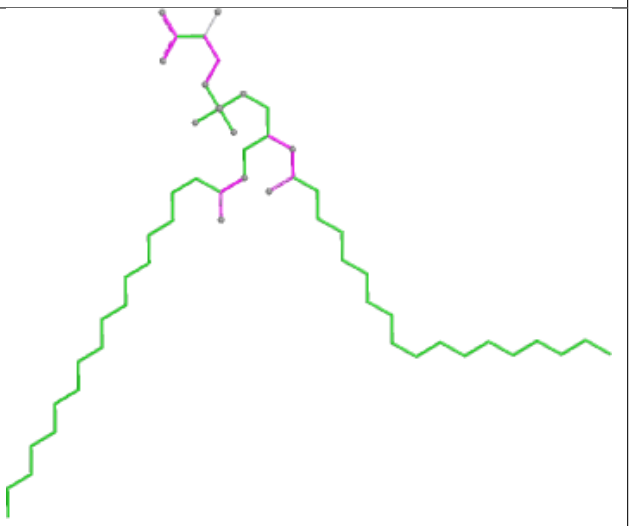


Rings

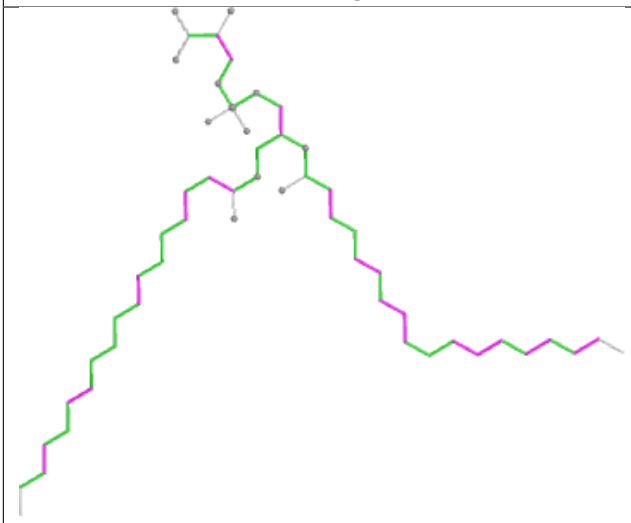
Ligand 17F A 37



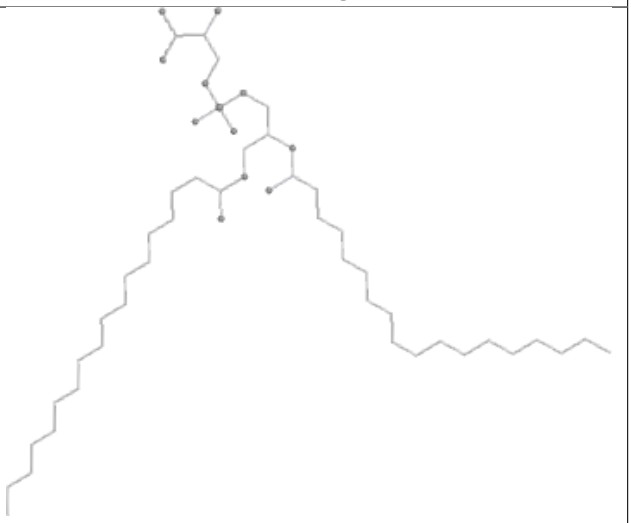
Bond lengths



Bond angles

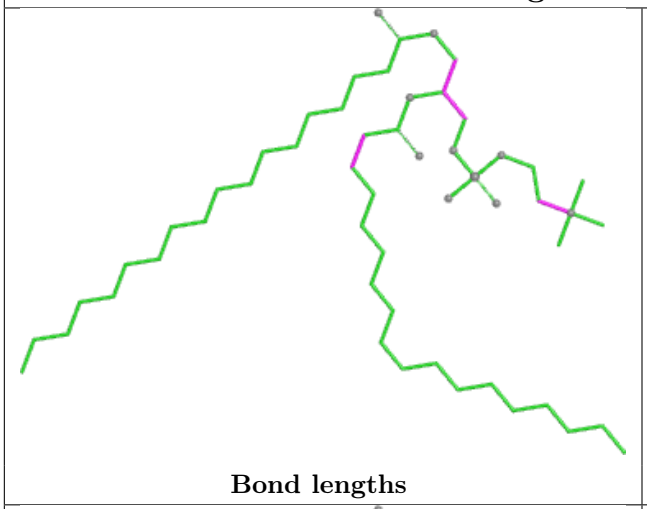


Torsions



Rings

Ligand PCW A 54



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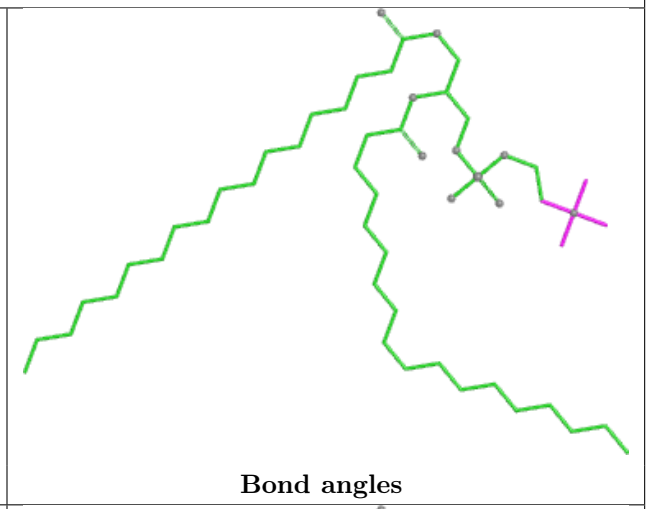
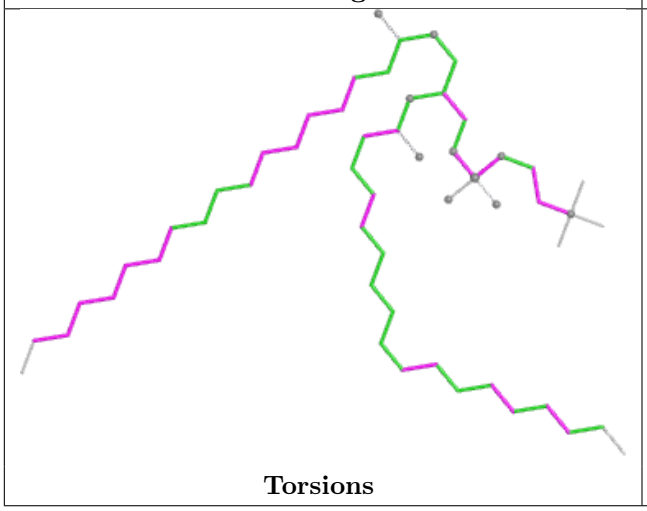
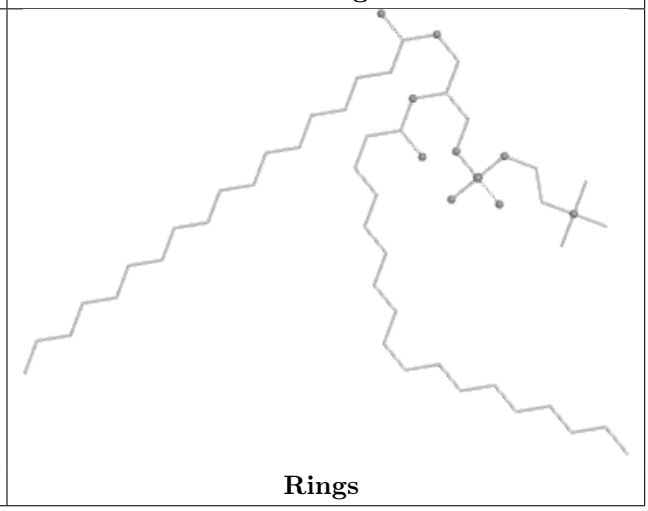


Bond angles

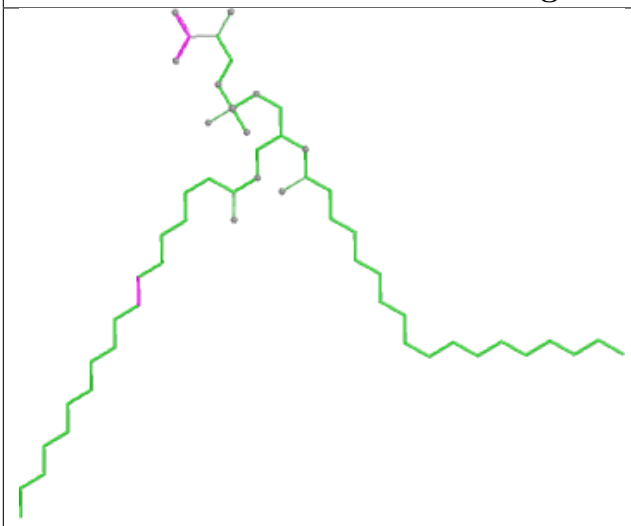


Torsions

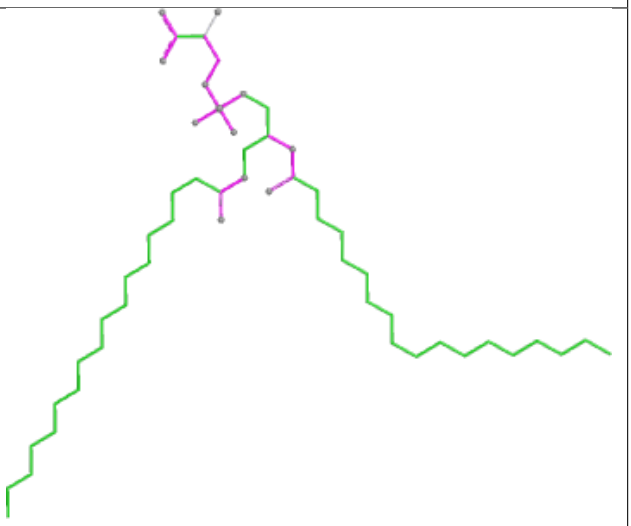


Rings

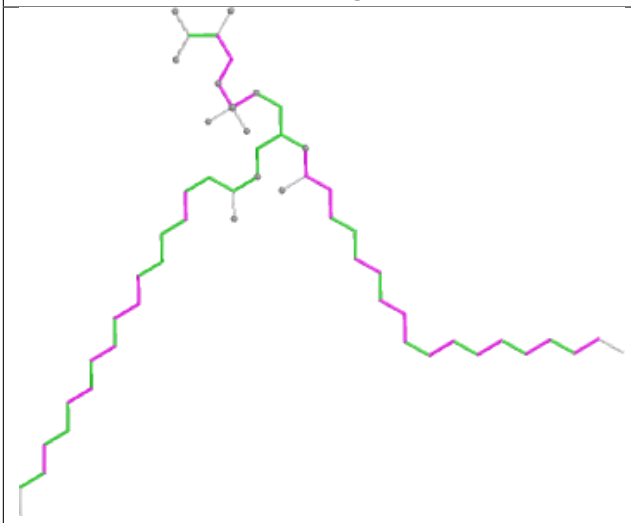
Ligand 17F A 77



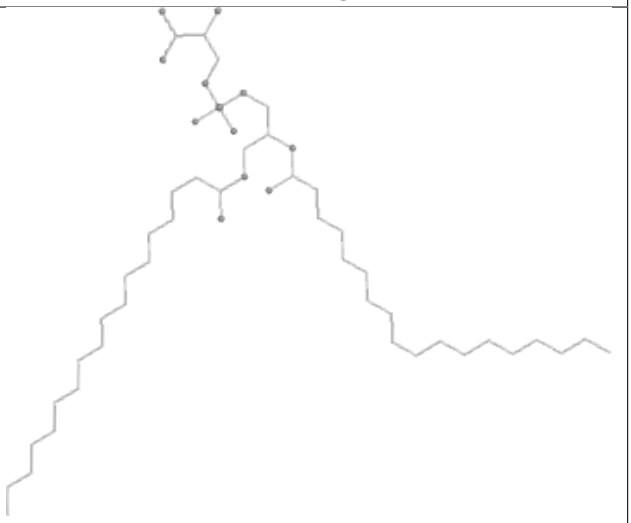
Bond lengths



Bond angles

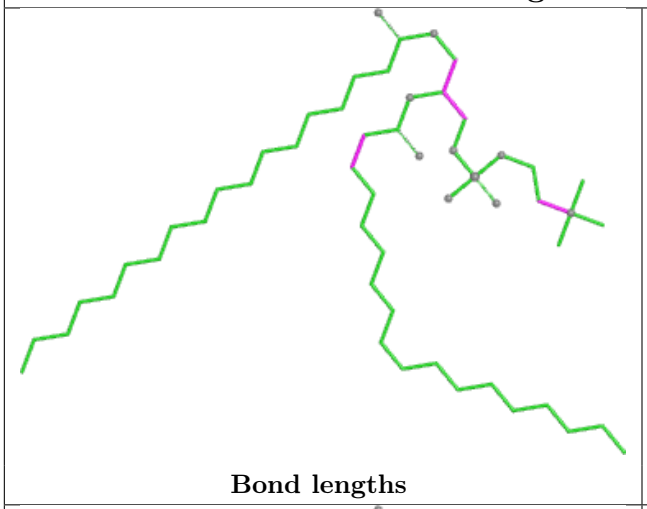


Torsions

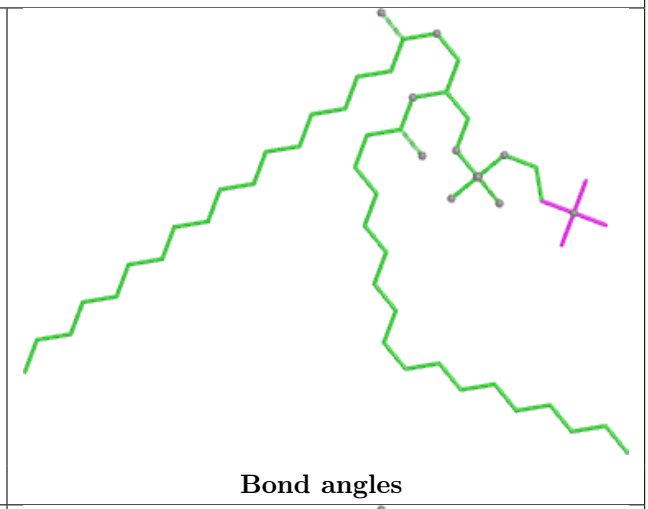


Rings

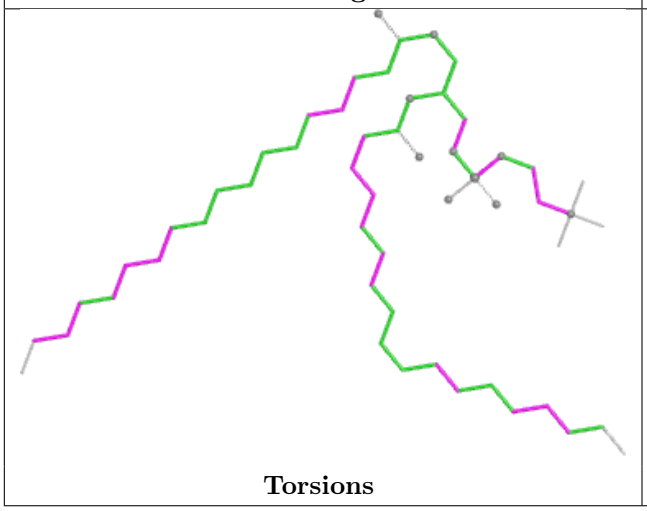
Ligand PCW A 26



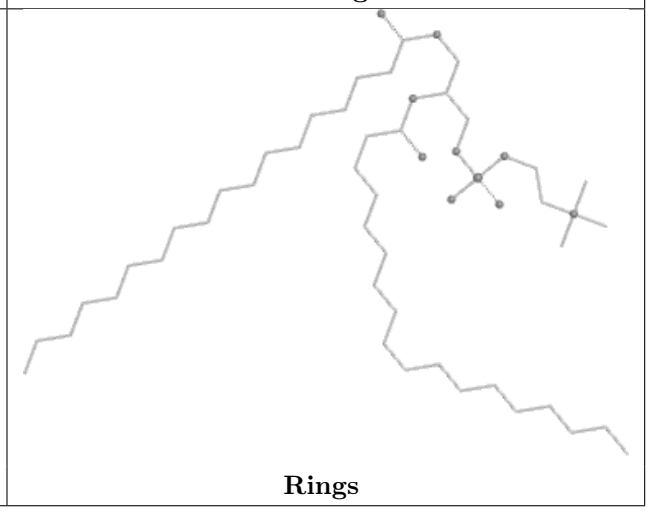
Bond lengths



Bond angles

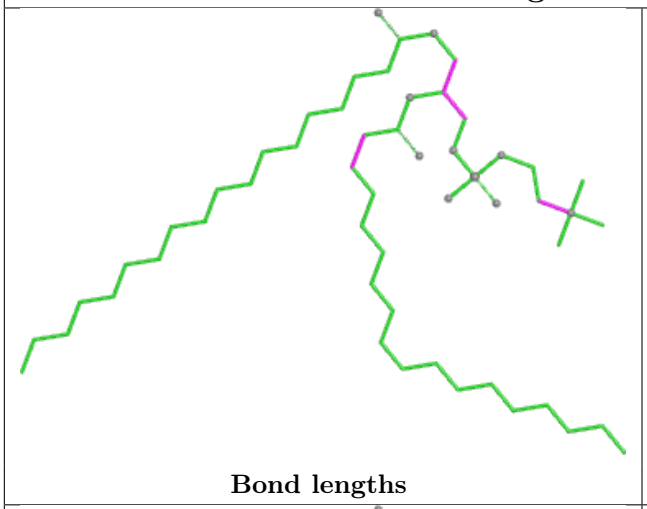


Torsions

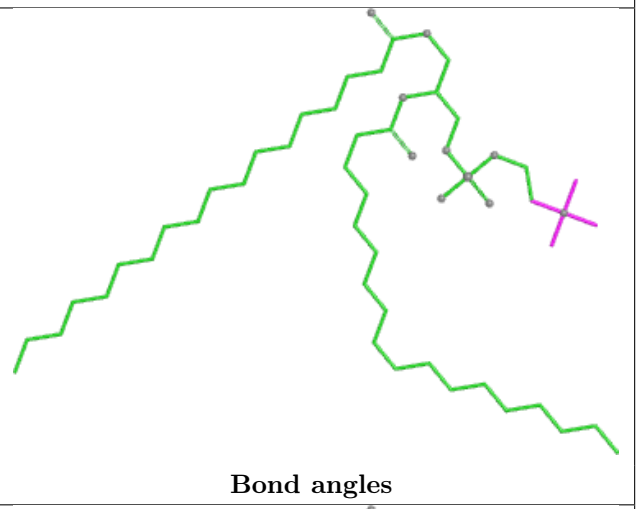


Rings

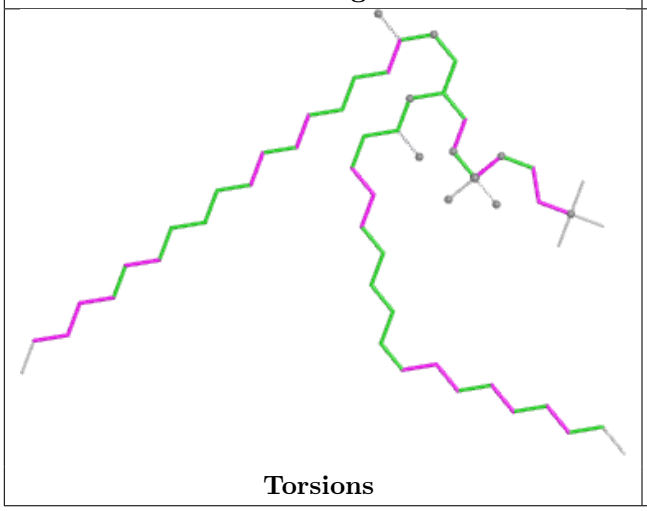
Ligand PCW A 18



Bond lengths



Bond angles



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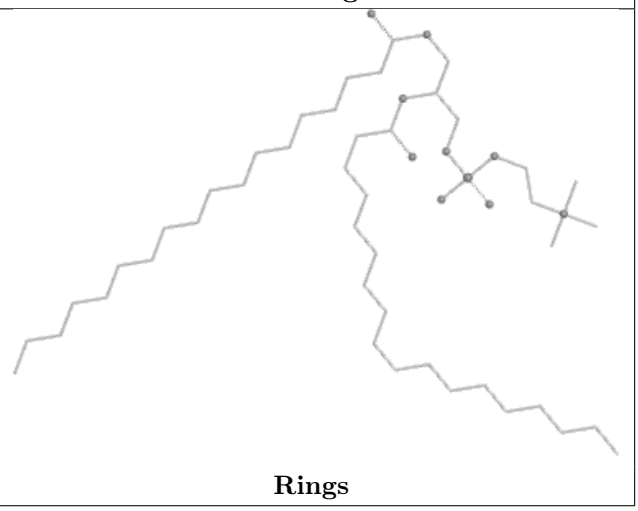
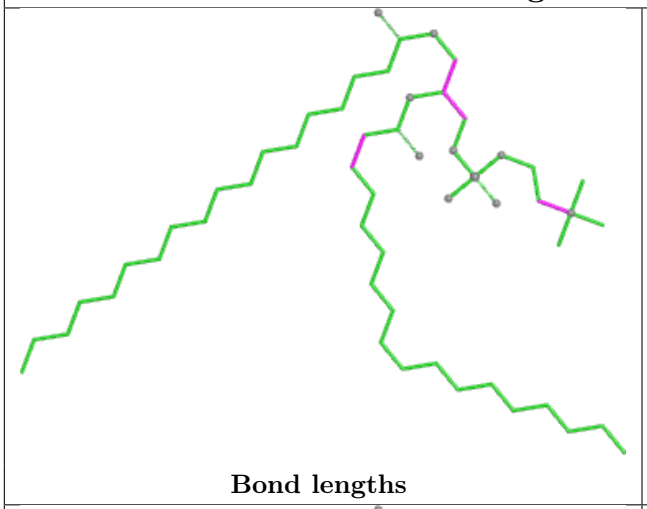
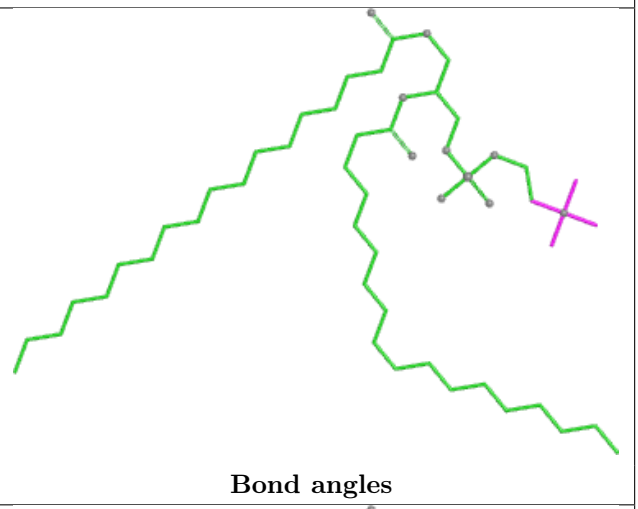


Rings

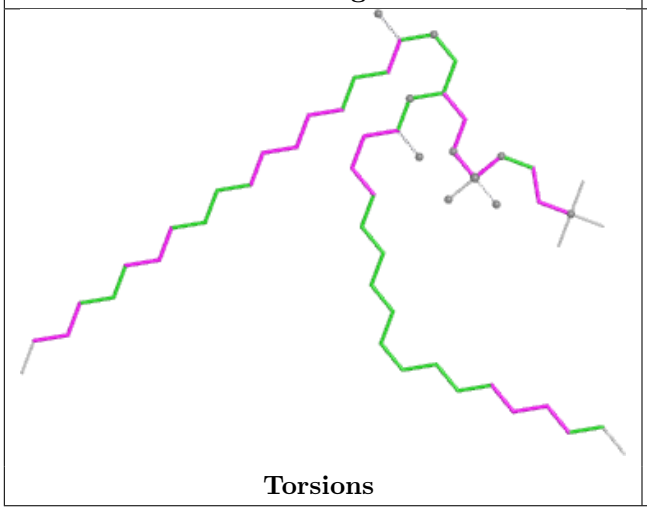
Ligand PCW A 49



Bond lengths



Bond angles



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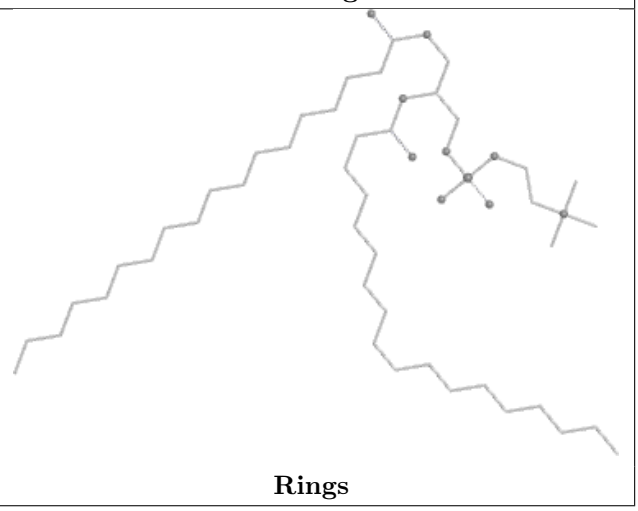
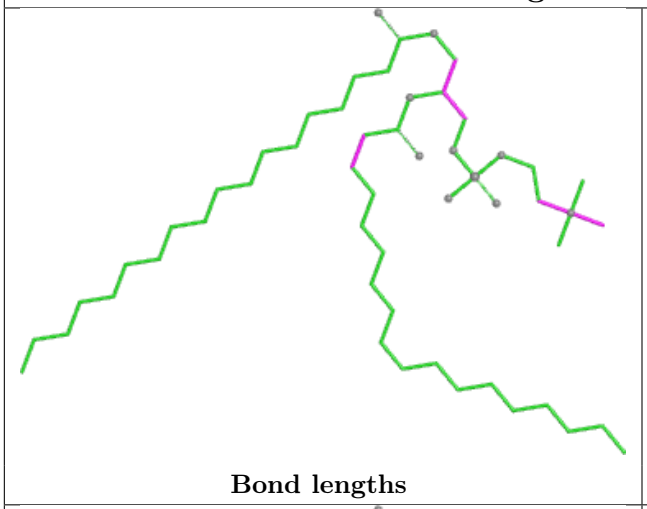
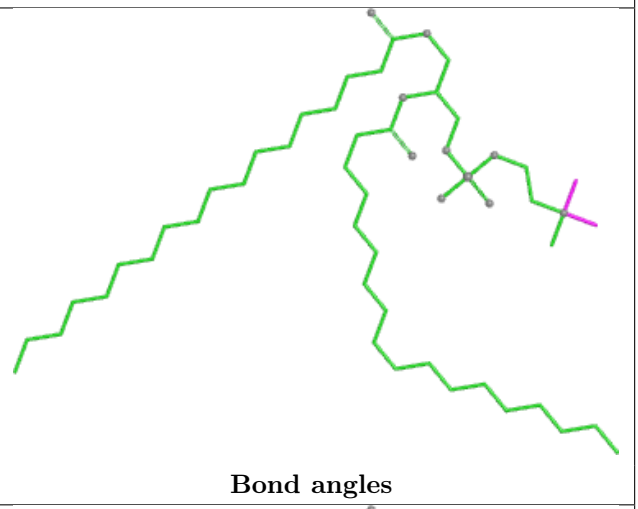


Rings

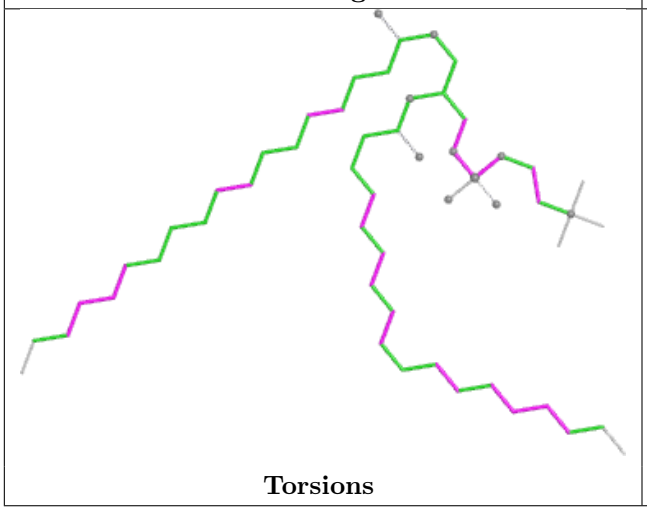
Ligand PCW A 15



Bond lengths



Bond angles



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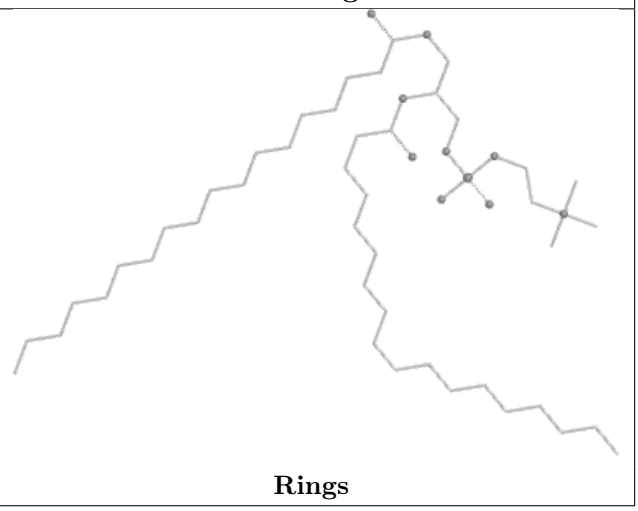
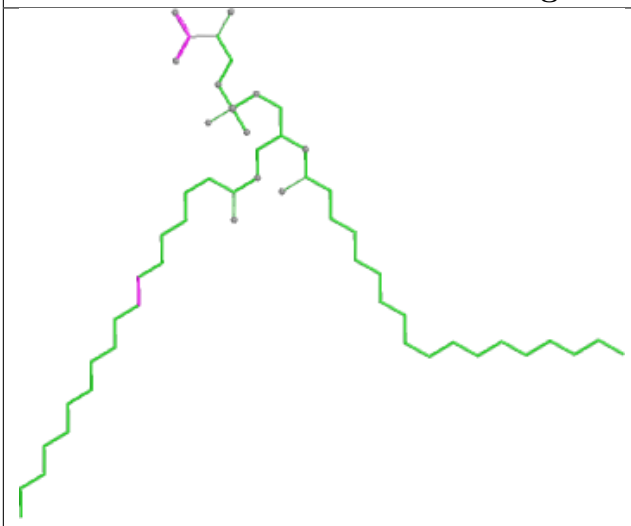
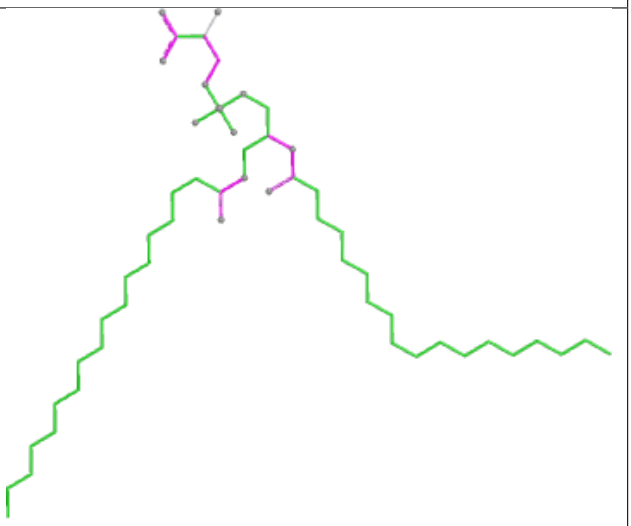


Rings

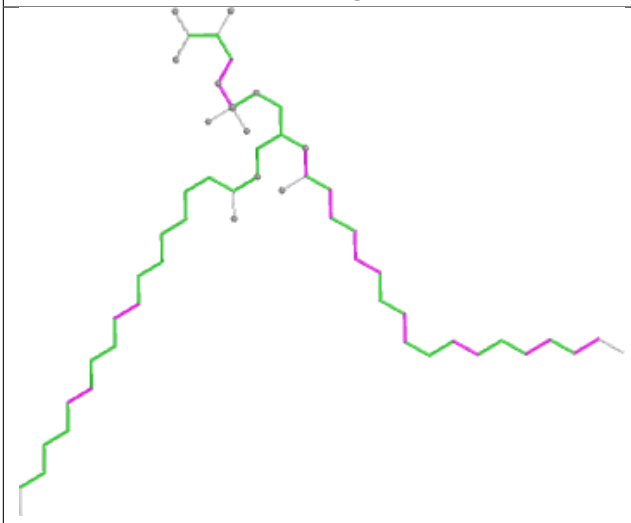
Ligand 17F A 39



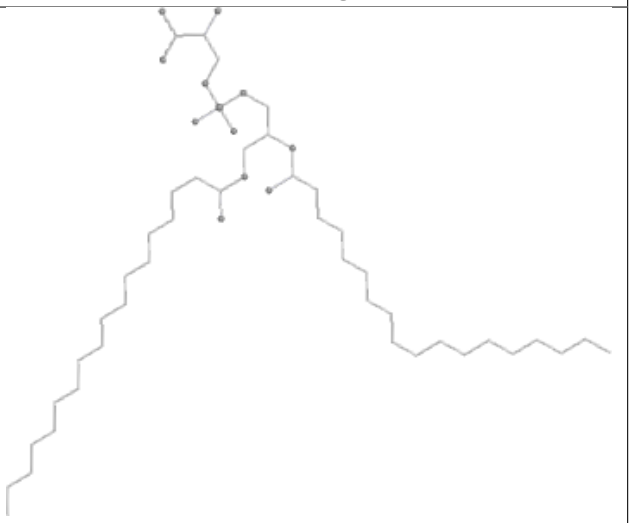
Bond lengths



Bond angles

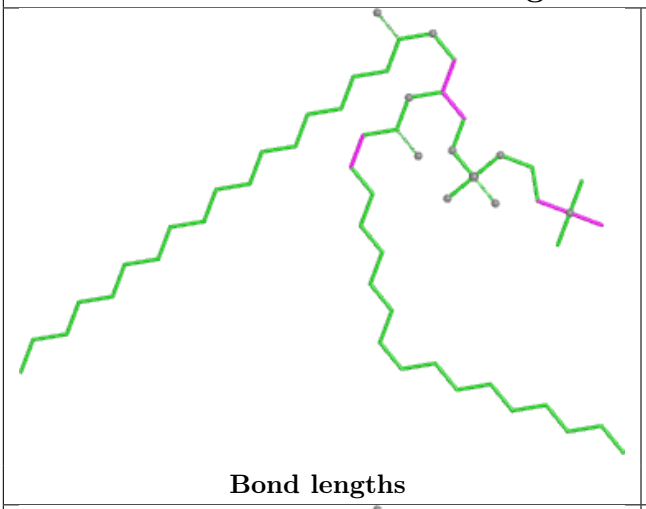


Torsions

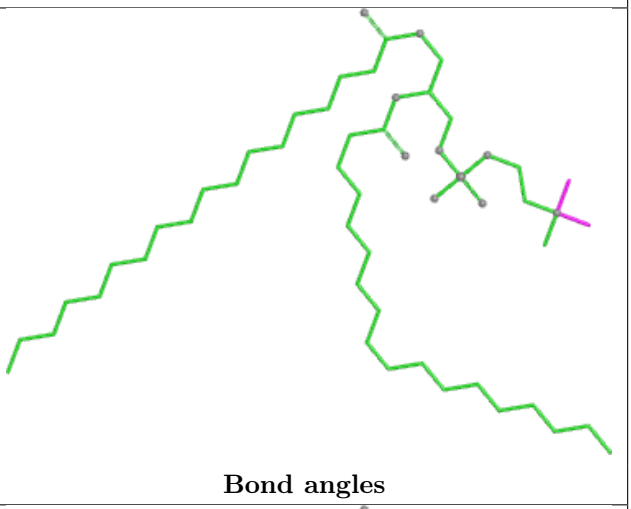


Rings

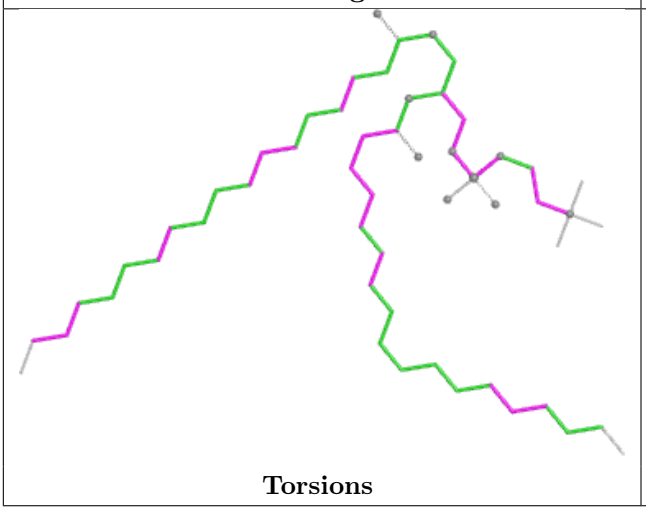
Ligand PCW A 65



Bond lengths



Bond angles



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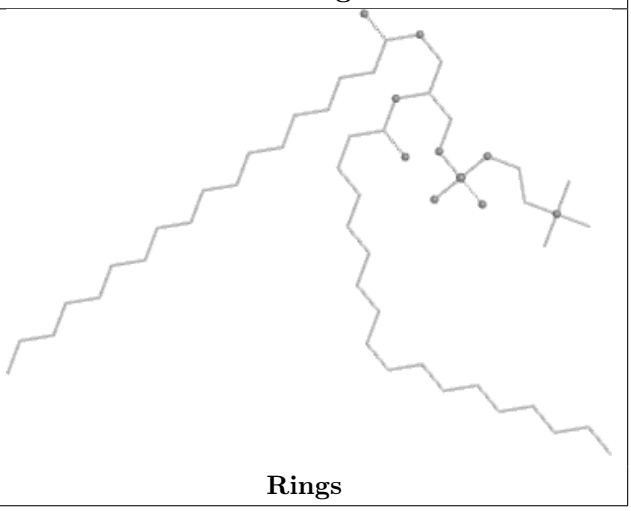
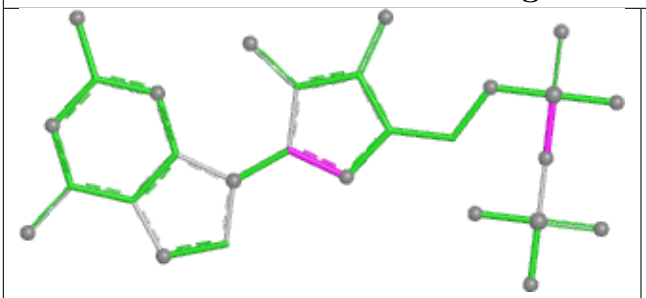
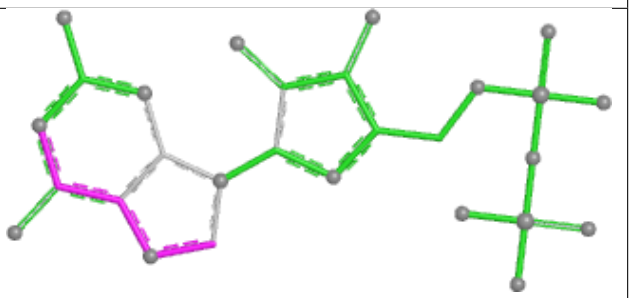


Rings

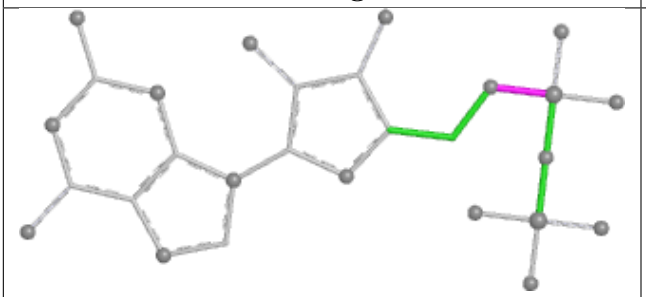
Ligand GDP B 201



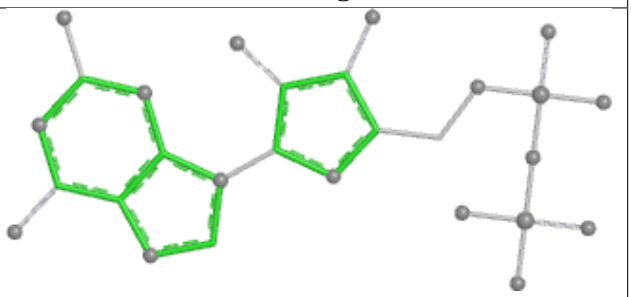
Bond lengths



Bond angles

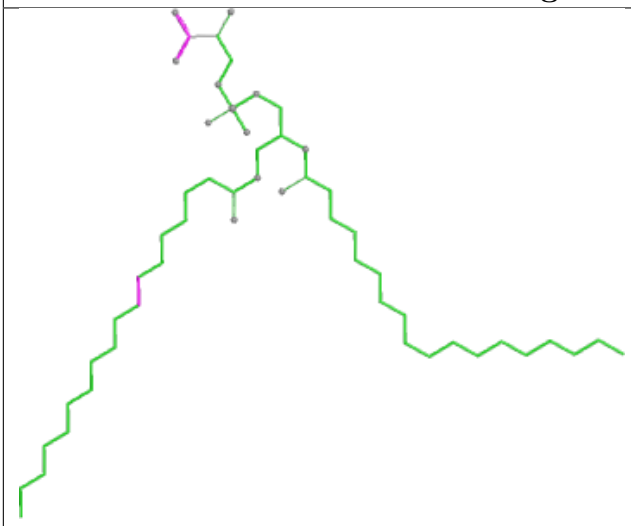


Torsions

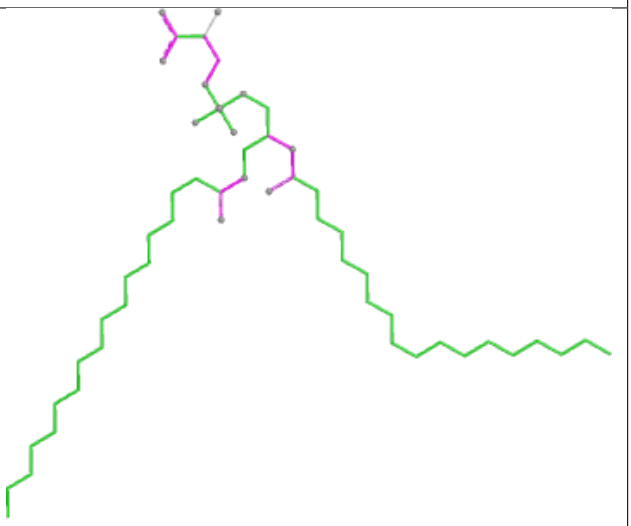


Rings

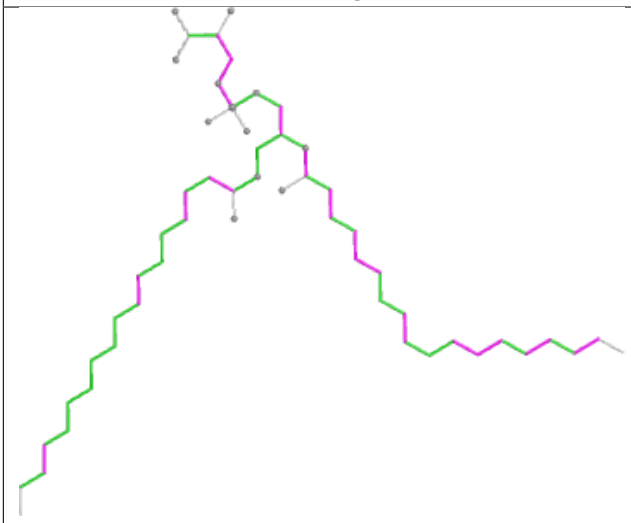
Ligand 17F A 79



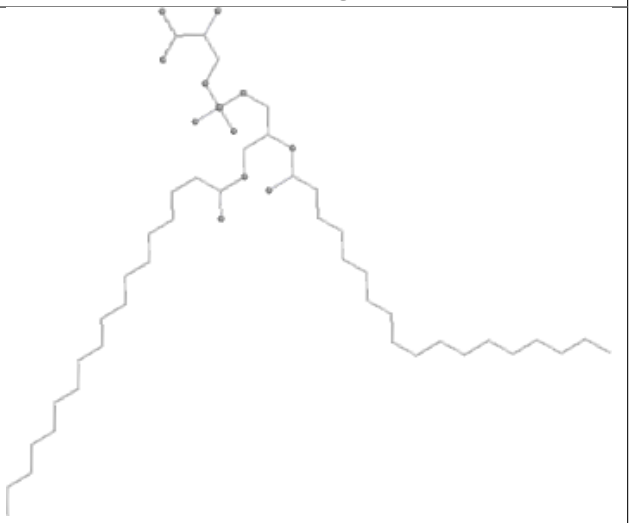
Bond lengths



Bond angles

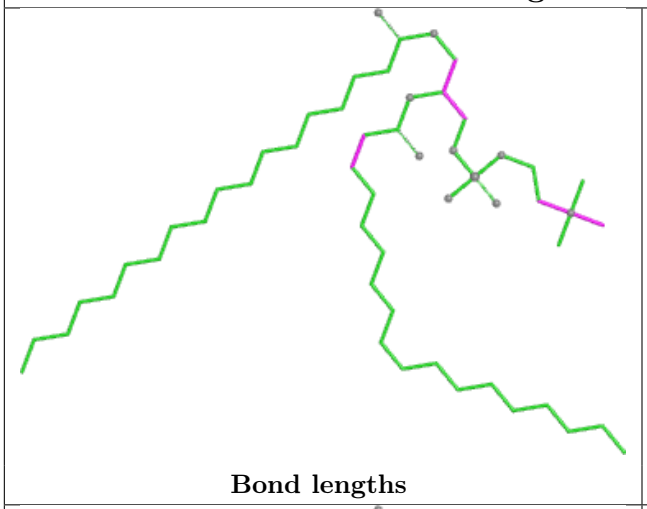


Torsions

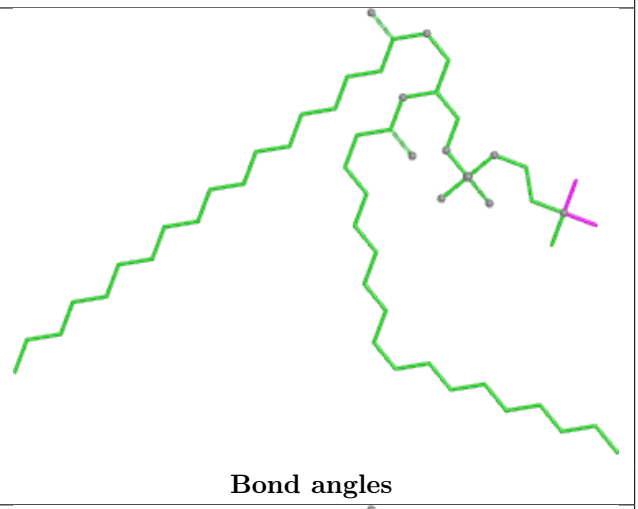


Rings

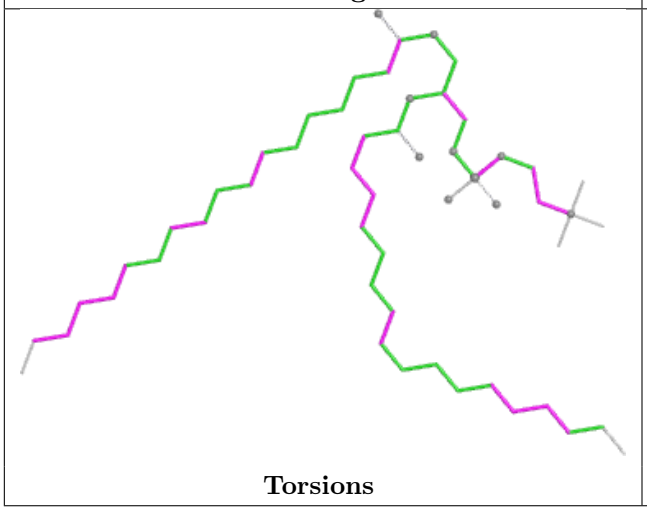
Ligand PCW A 30



Bond lengths



Bond angles



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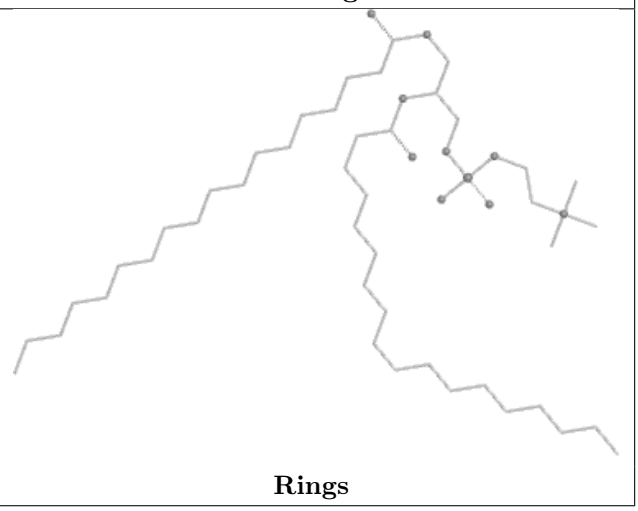
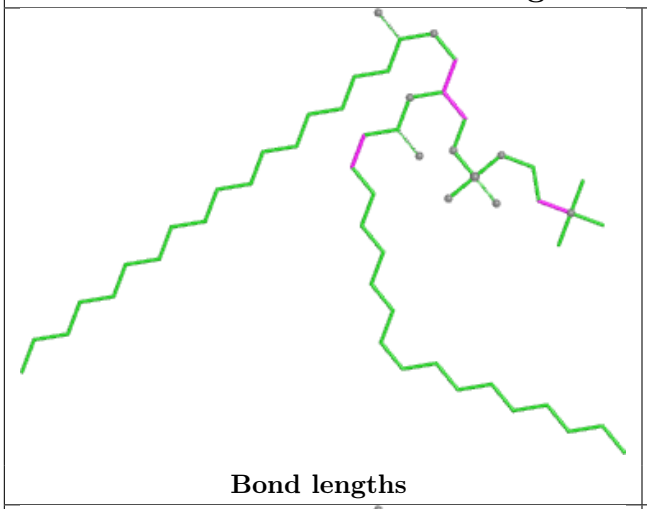
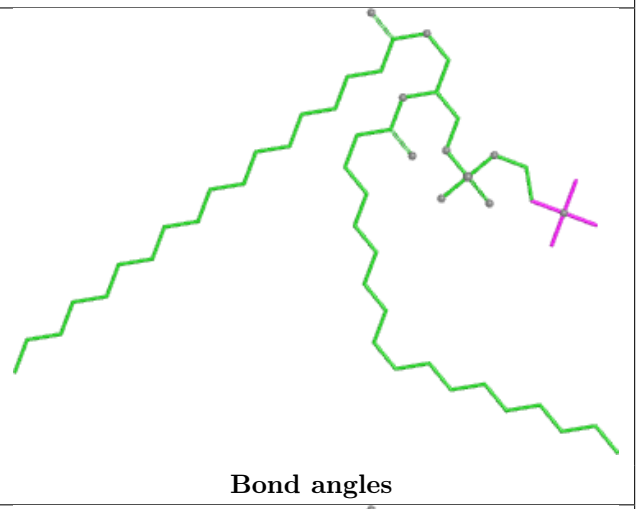


Rings

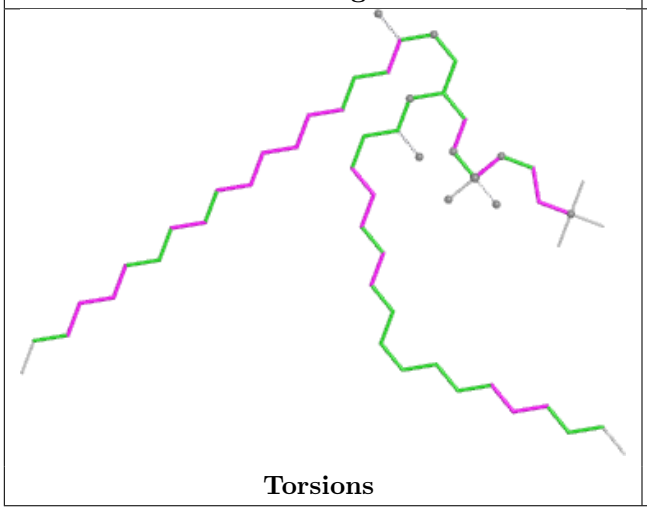
Ligand PCW A 14



Bond lengths



Bond angles



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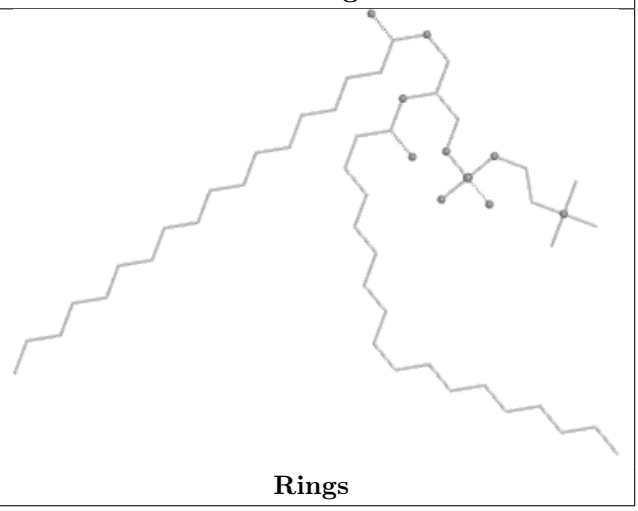
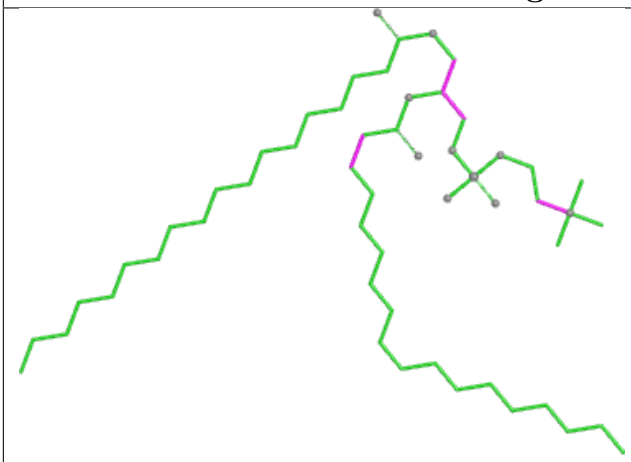
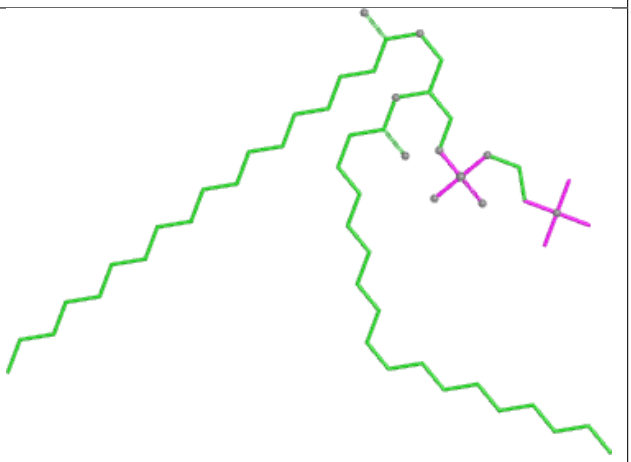


Rings

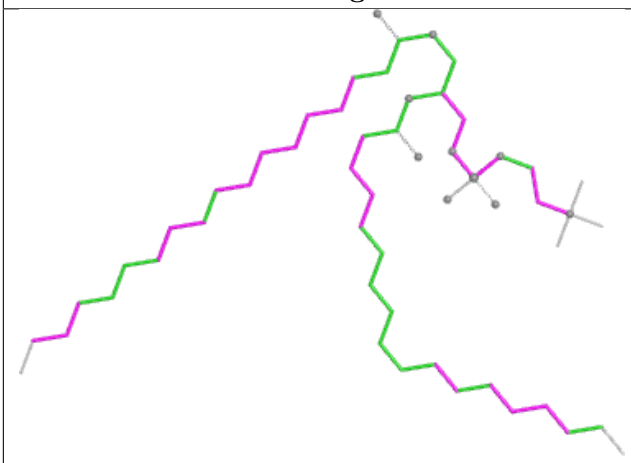
Ligand PCW A 63



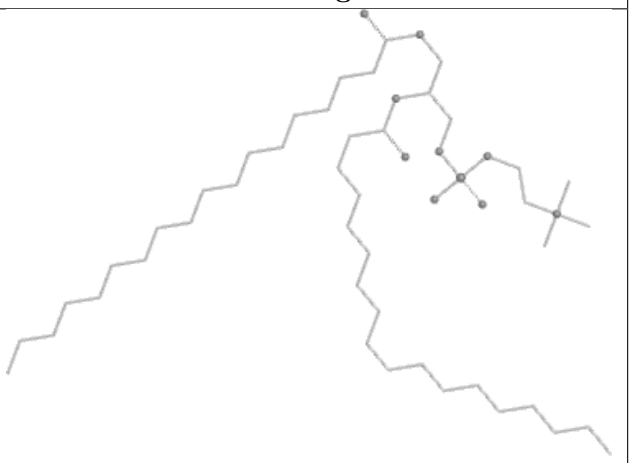
Bond lengths



Bond angles

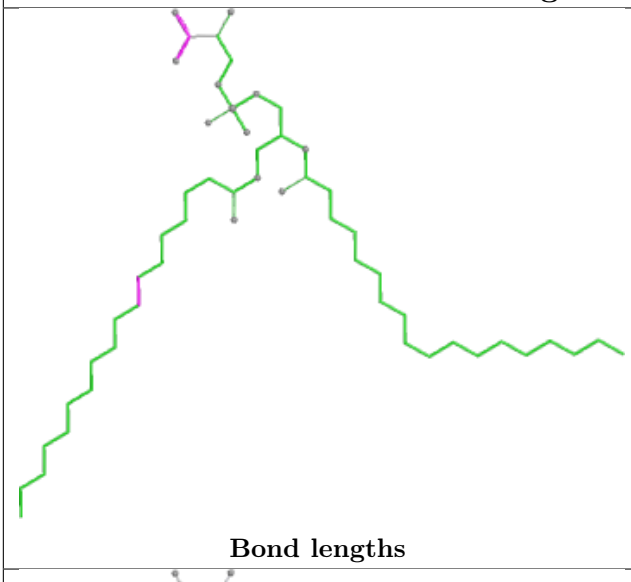


Torsions

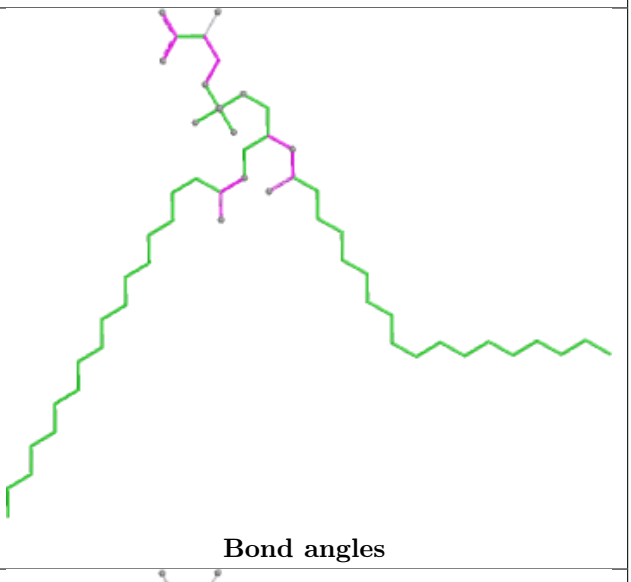


Rings

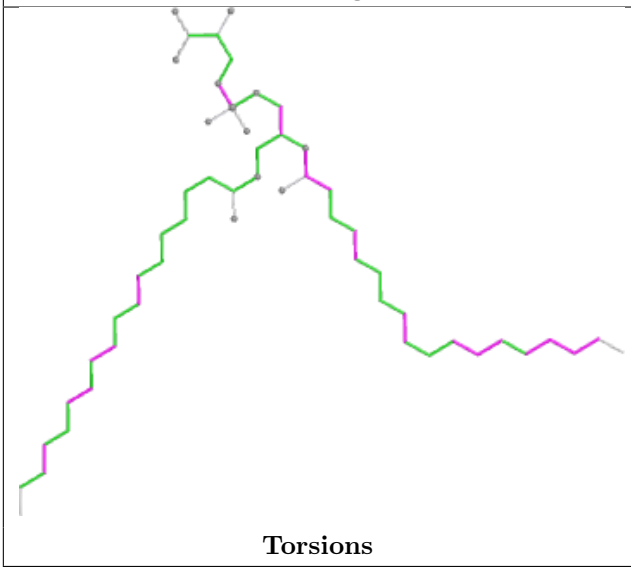
Ligand 17F A 36



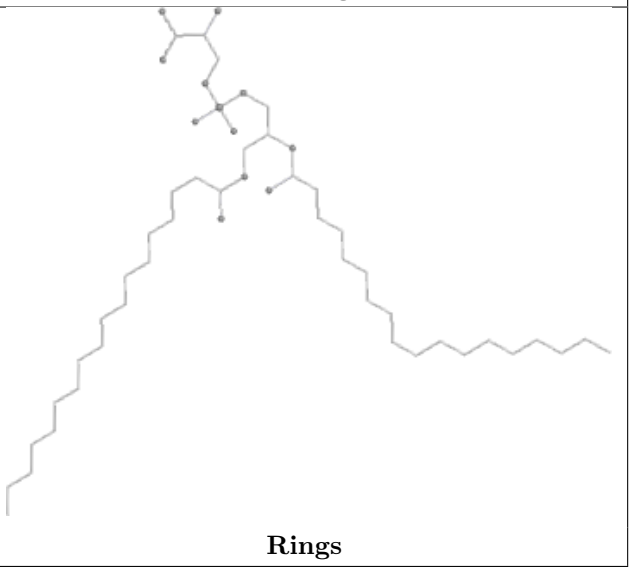
Bond lengths



Bond angles

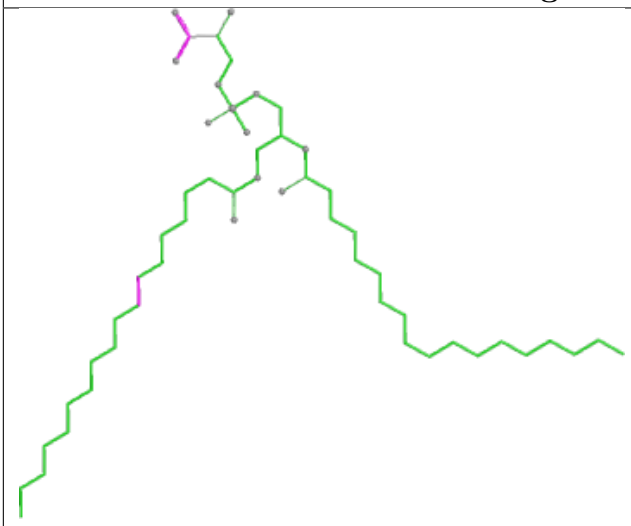


Torsions

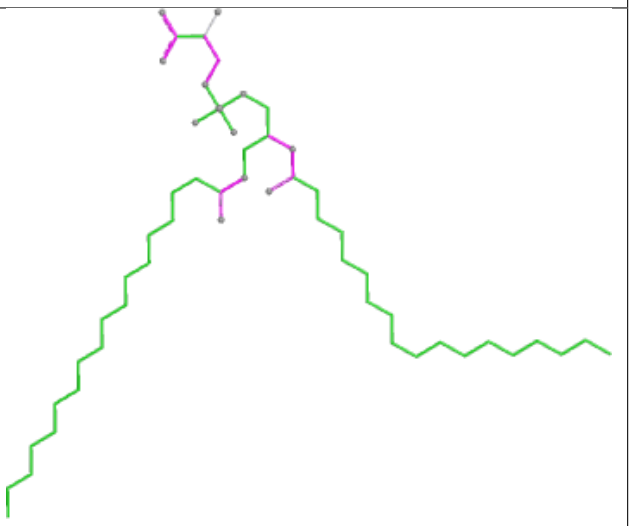


Rings

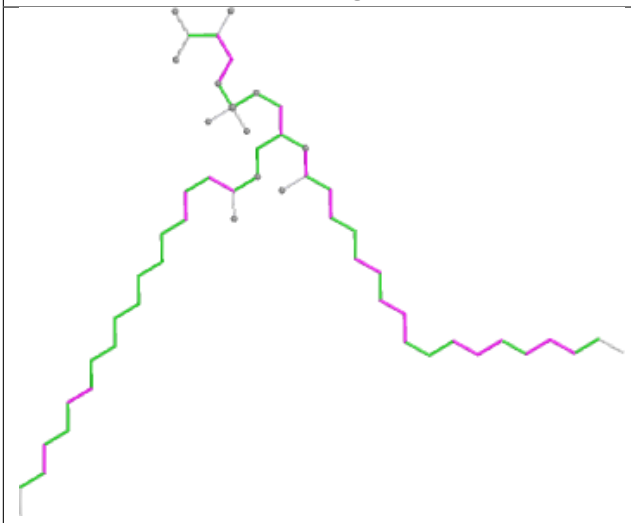
Ligand 17F A 34



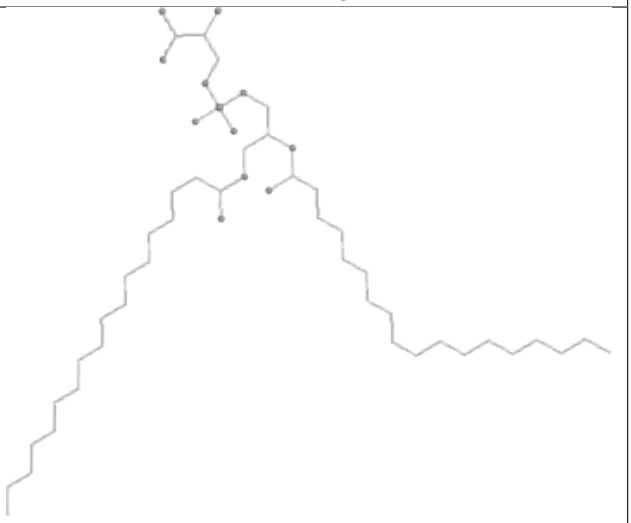
Bond lengths



Bond angles

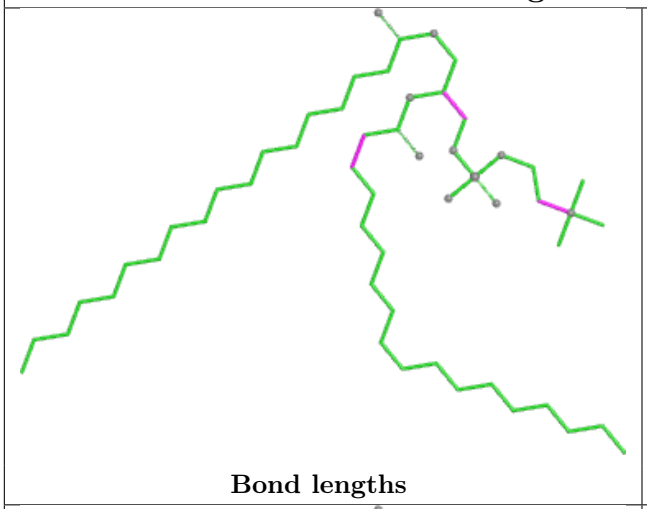


Torsions



Rings

Ligand PCW A 62



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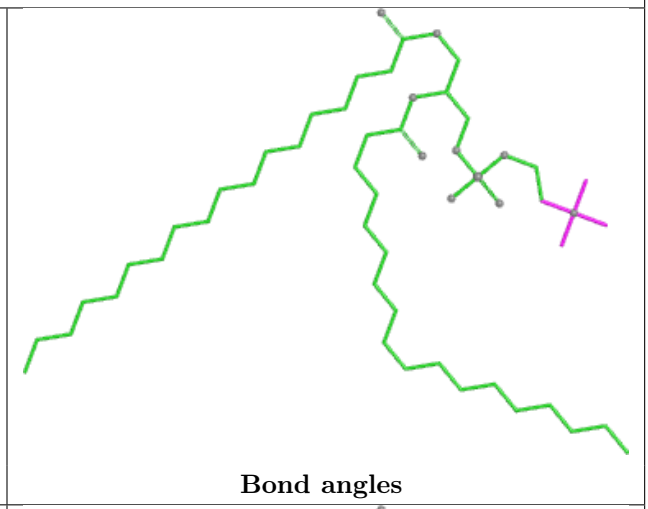
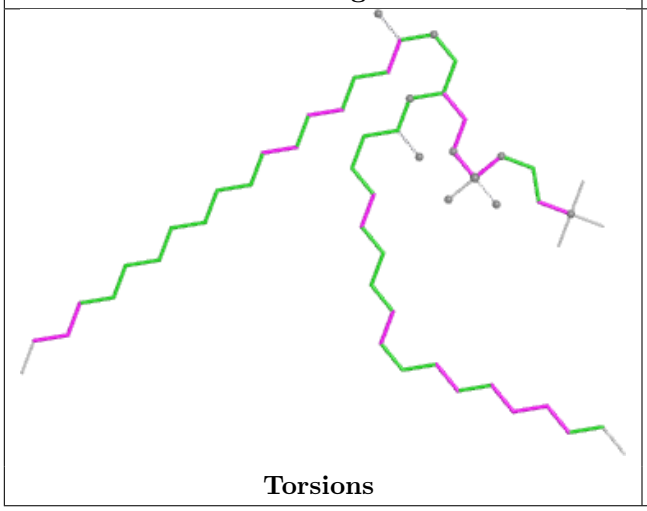


Bond angles



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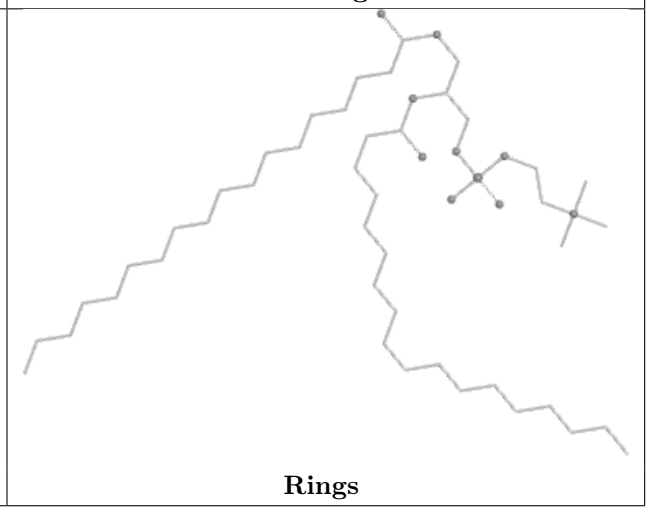
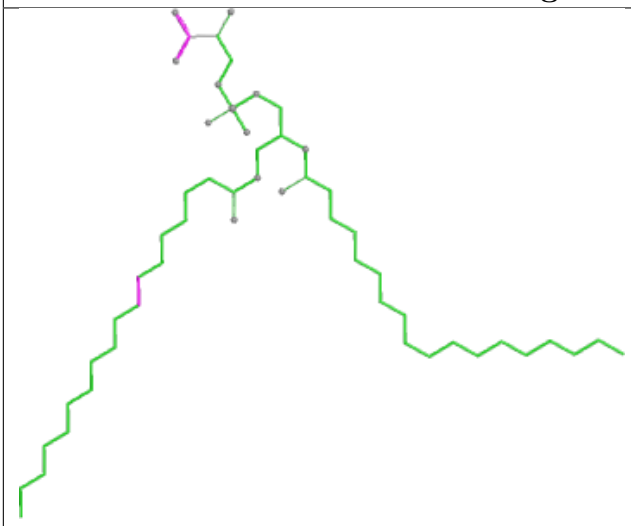


Rings

Ligand 17F A 76



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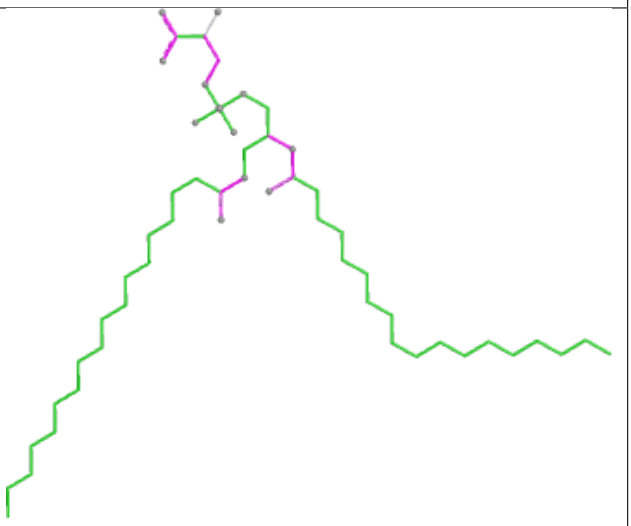
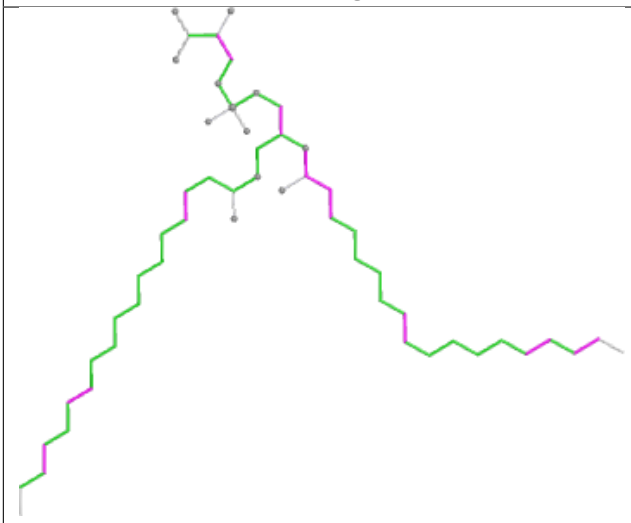


Bond angles



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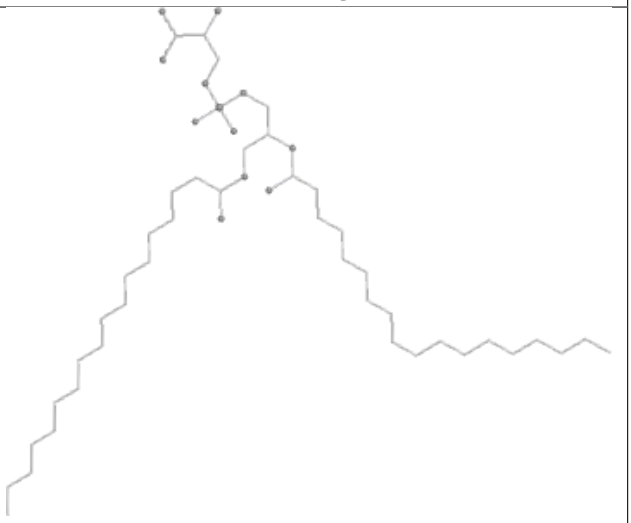
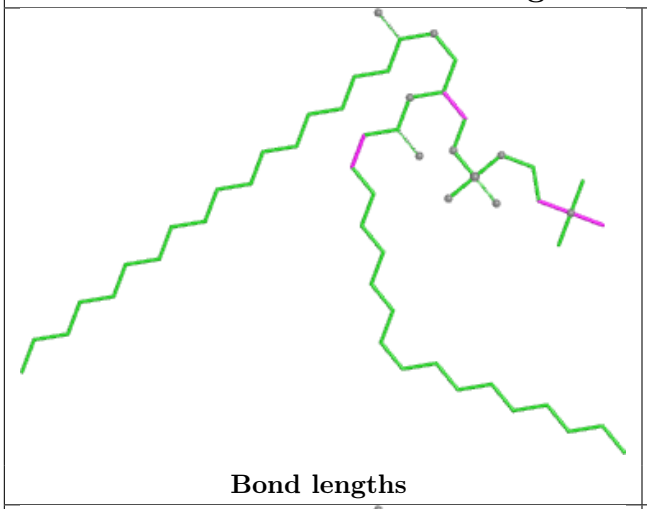


Rings

Ligand PCW A 50



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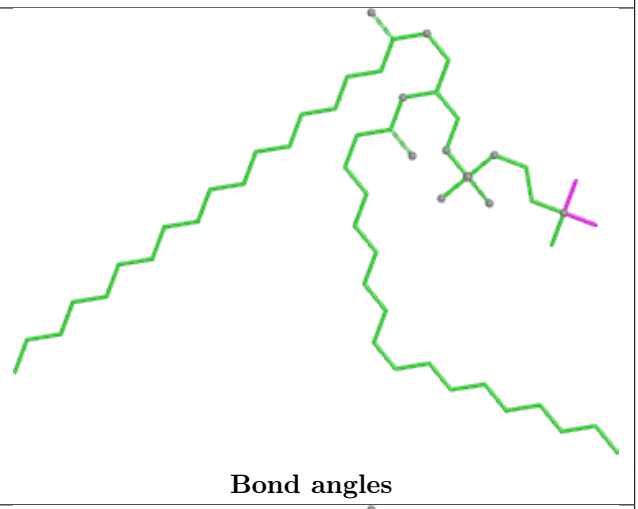
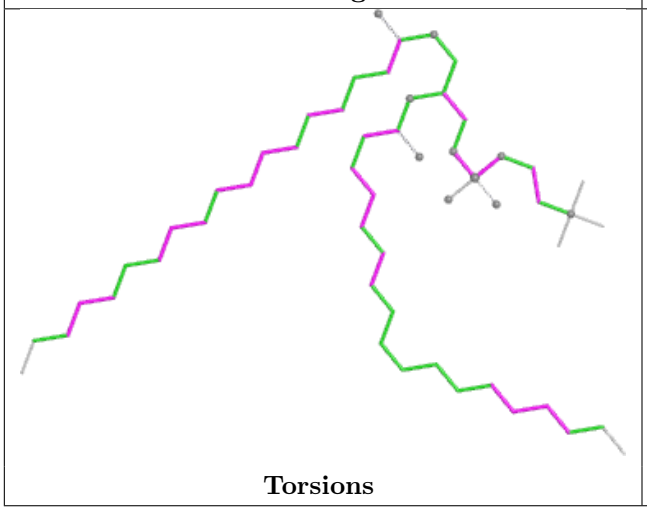


Bond angles



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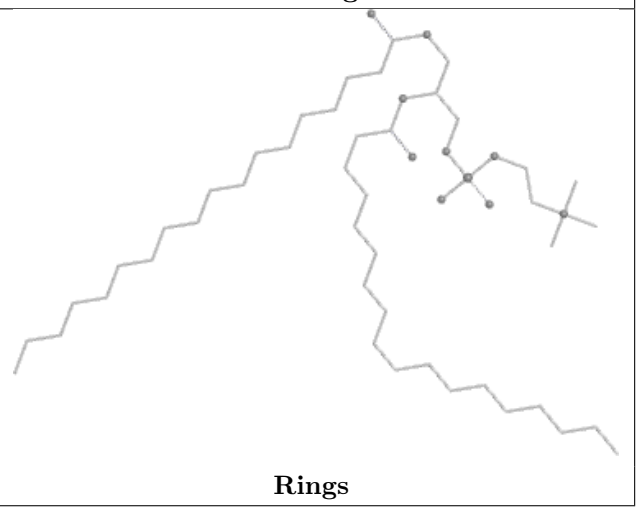
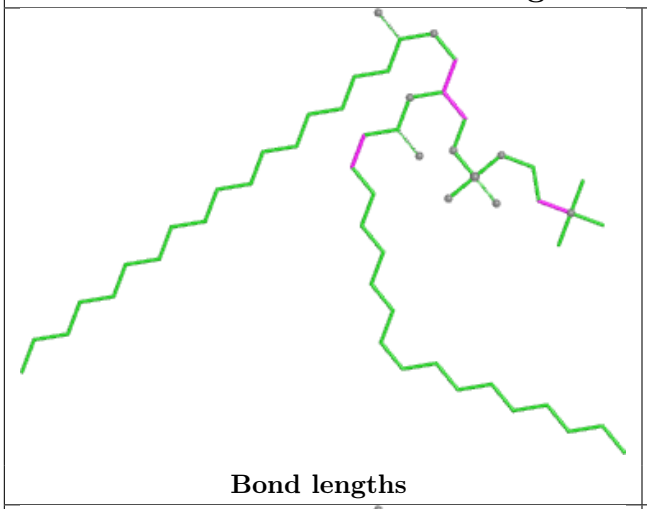


Rings

Ligand PCW A 24



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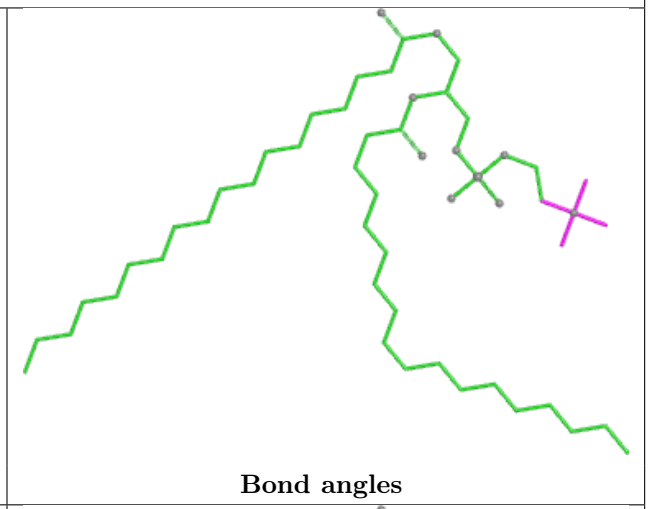
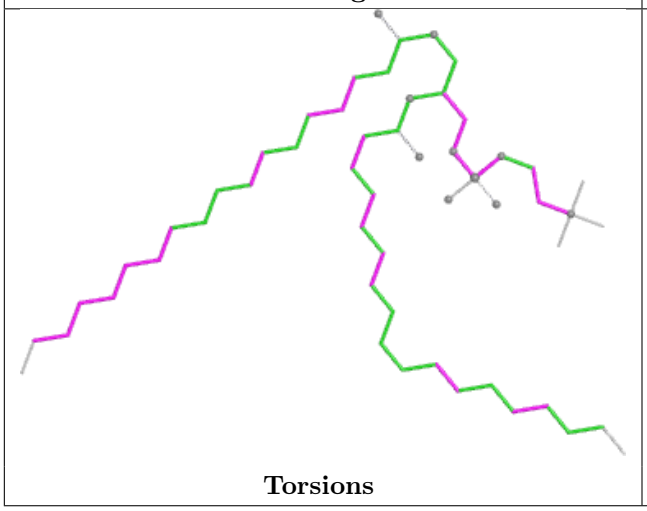


Bond angles



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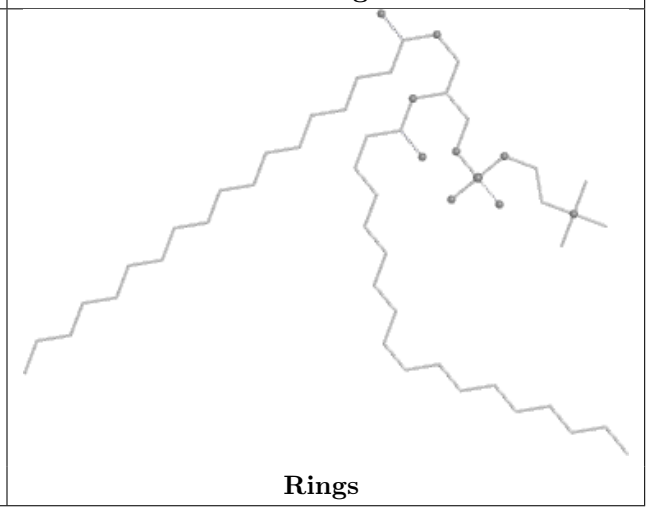
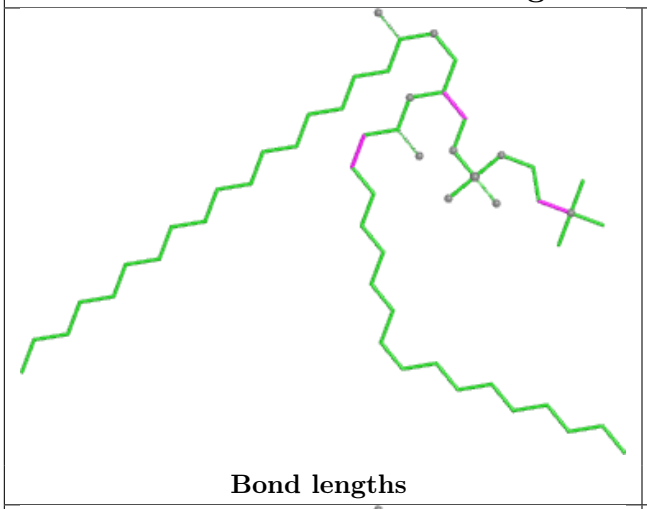


Rings

Ligand PCW A 69



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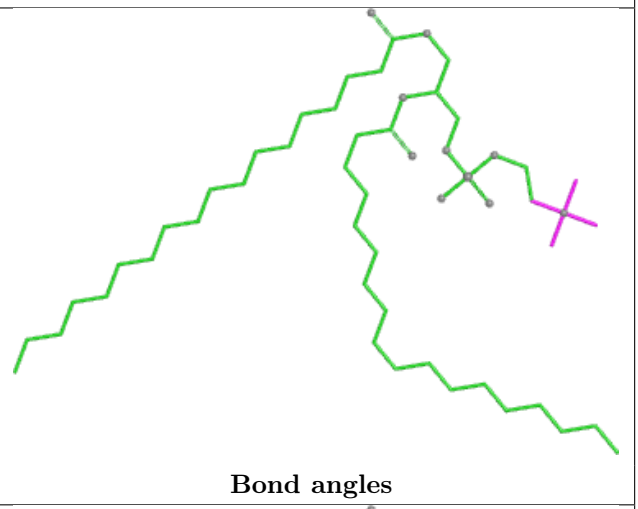
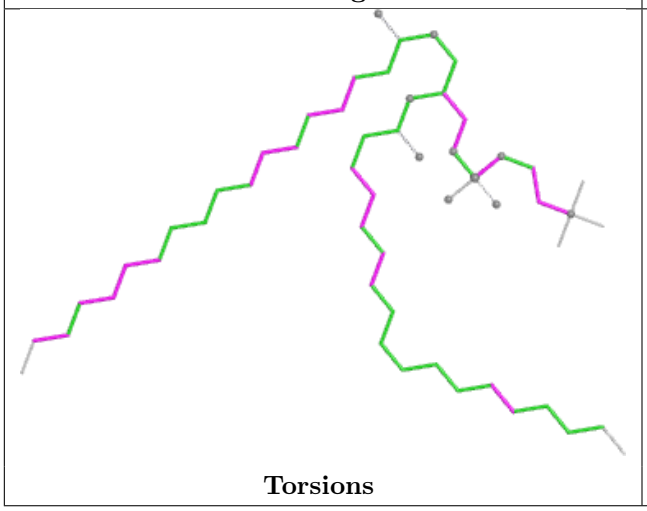


Bond angles



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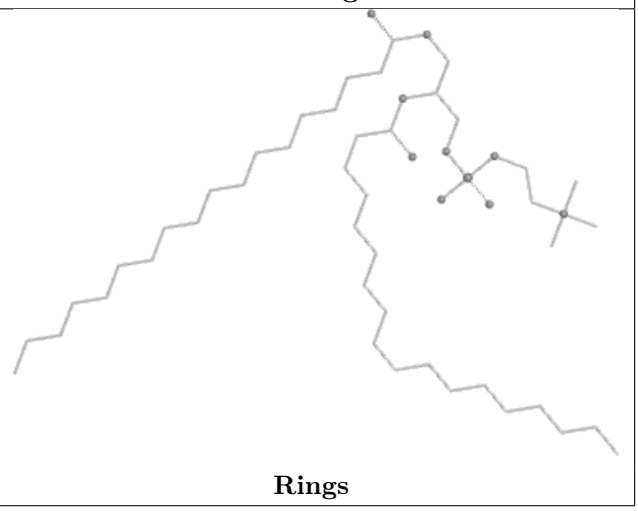
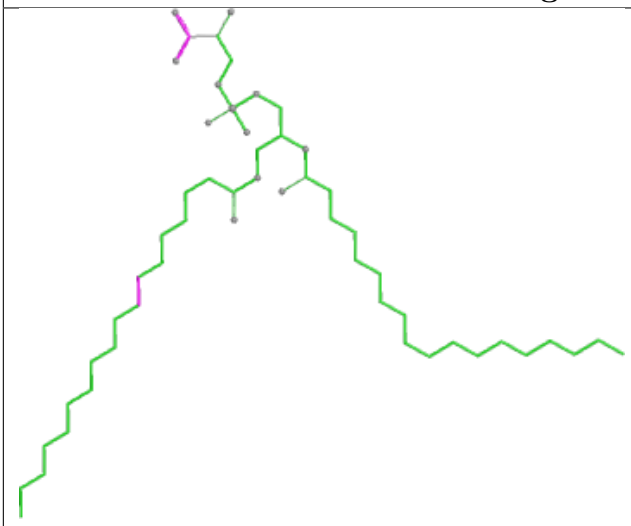


Rings

Ligand 17F A 78



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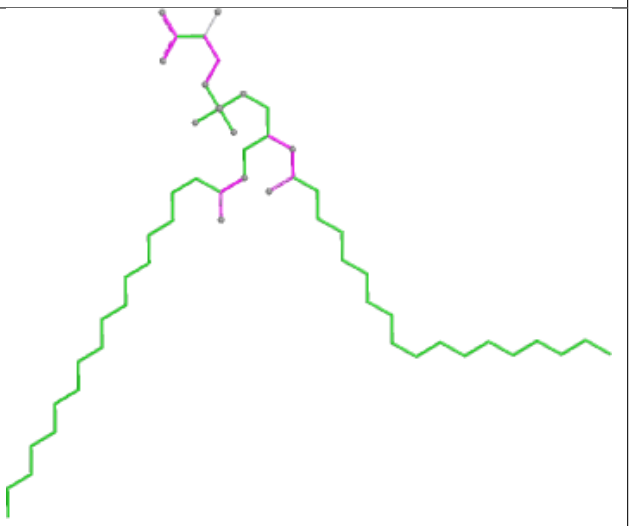
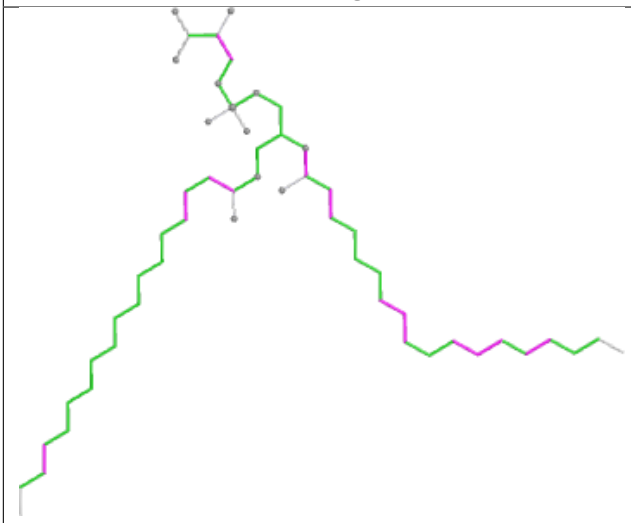


Bond angles



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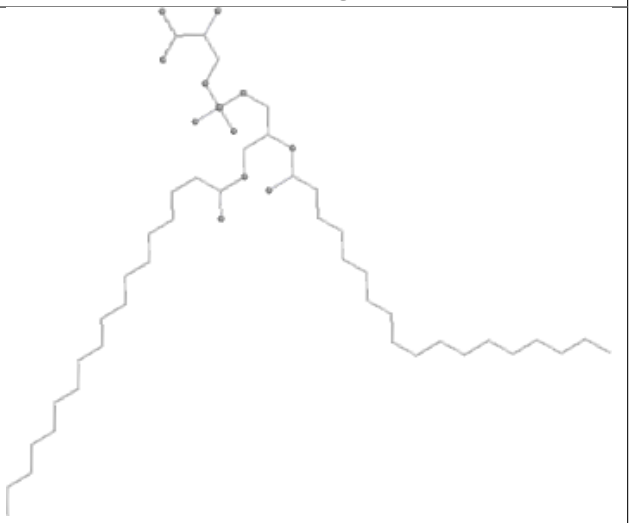
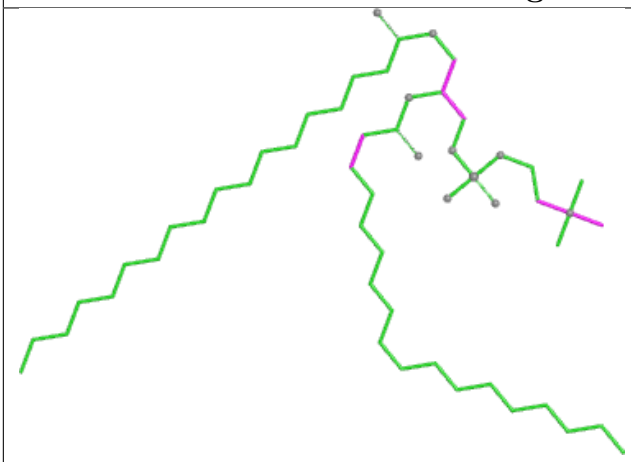


Rings

Ligand PCW A 19



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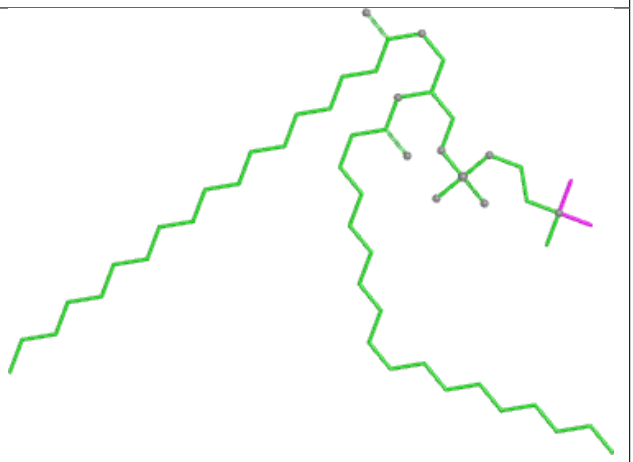
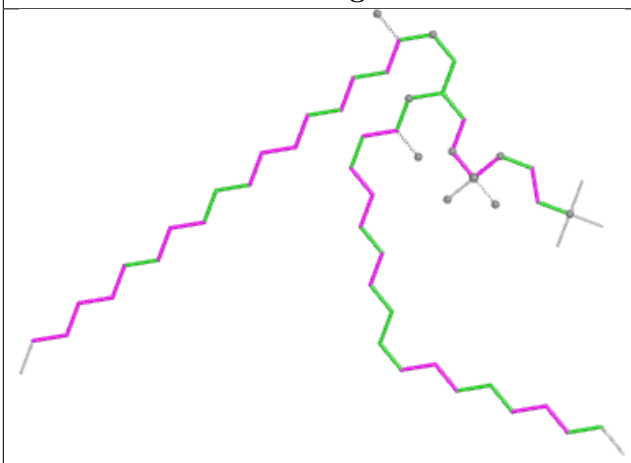
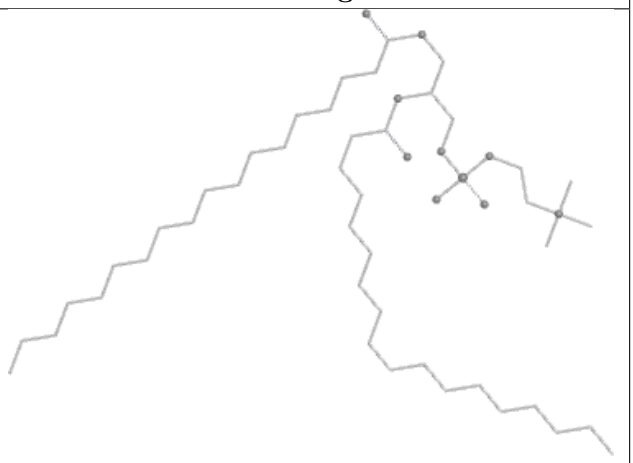


Bond angles

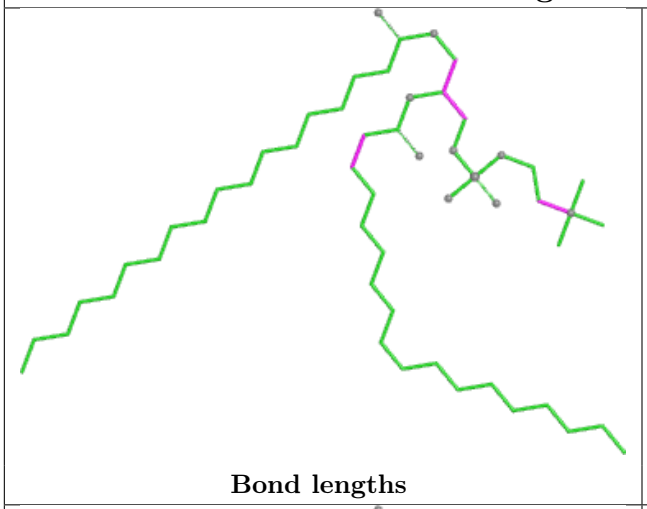


Torsions



Rings

Ligand PCW A 6



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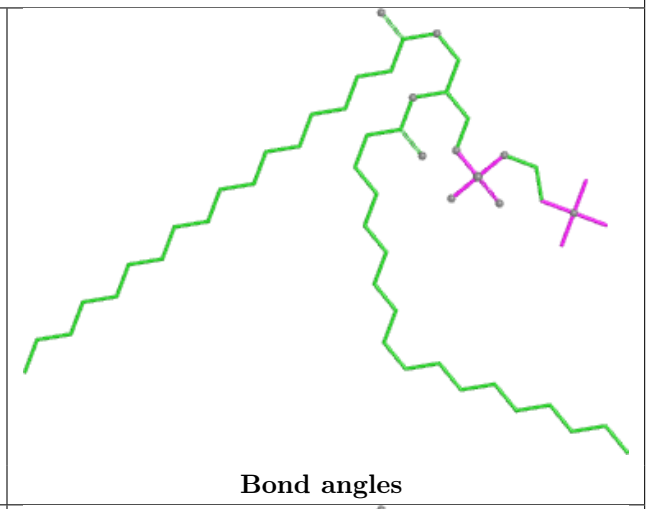
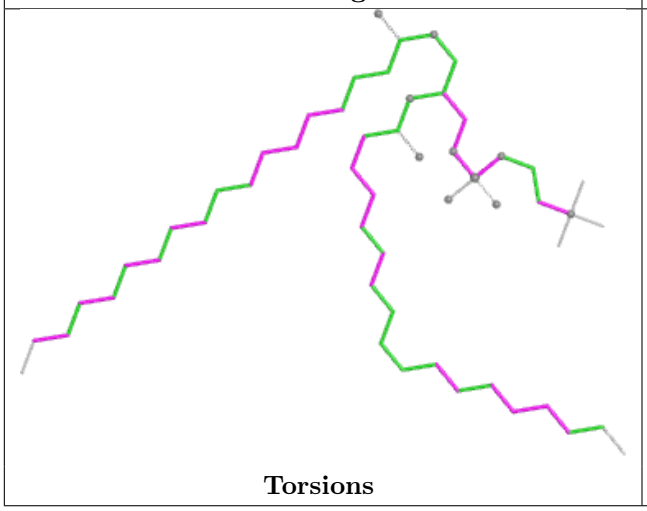
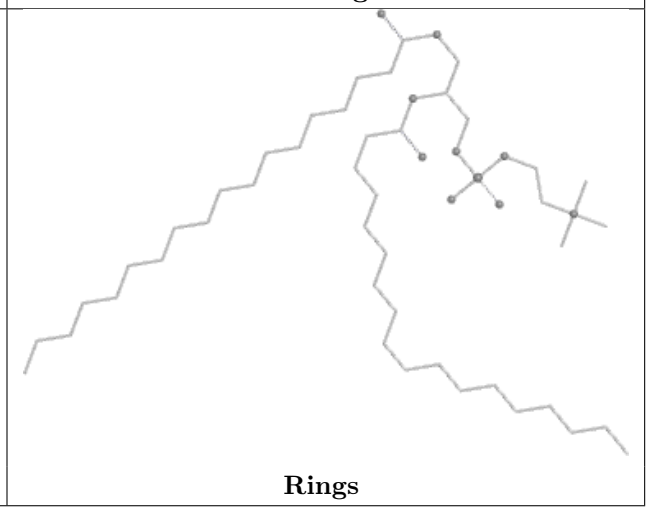


Bond angles

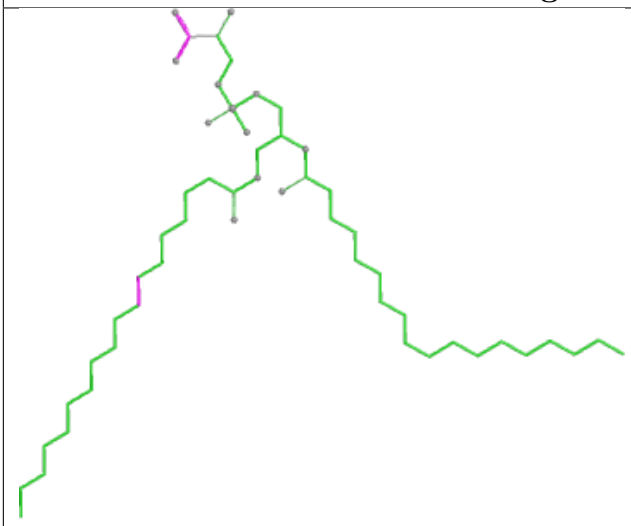


Torsions

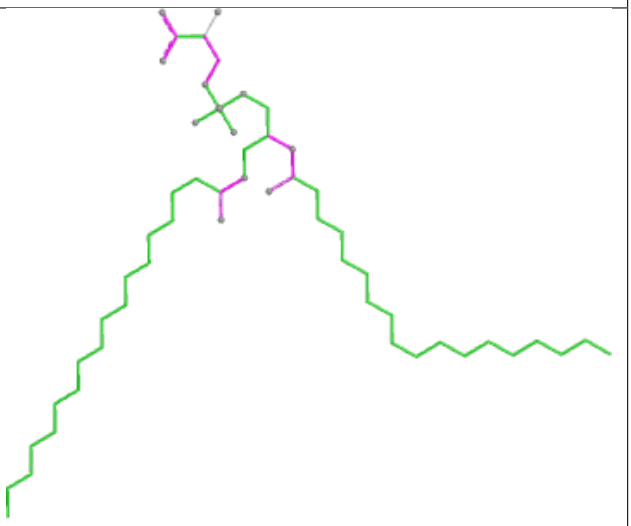


Rings

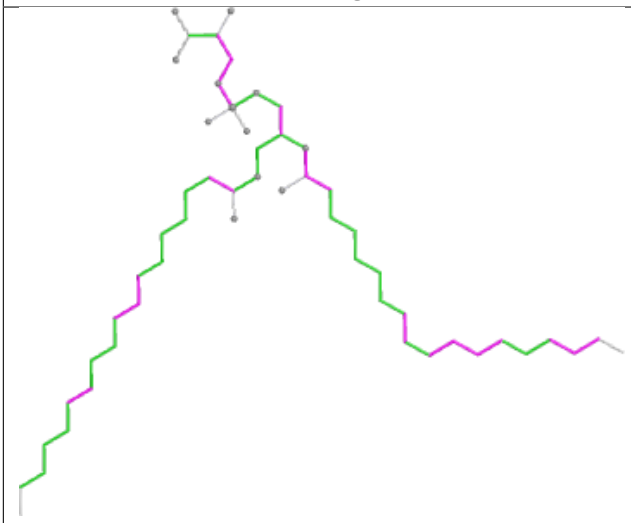
Ligand 17F A 75



Bond lengths



Bond angles



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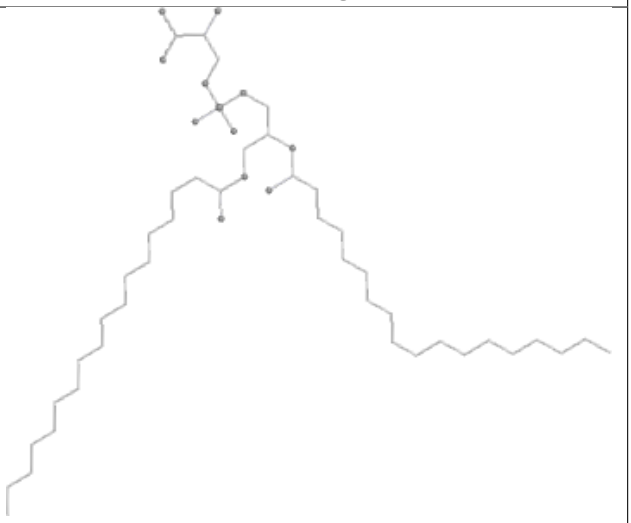
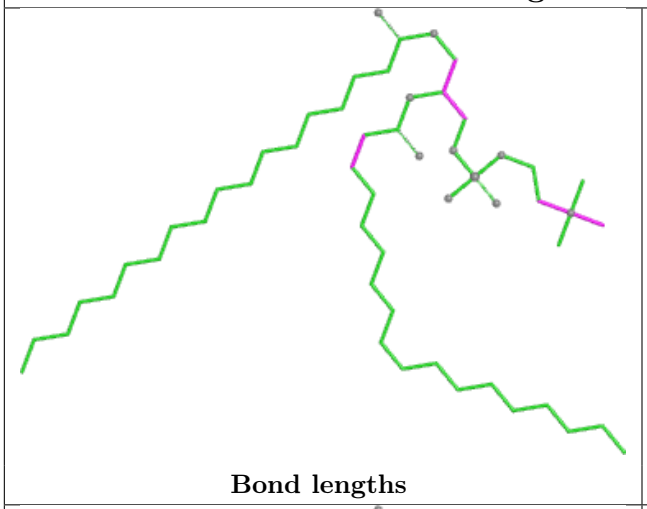


Rings

Ligand PCW A 47



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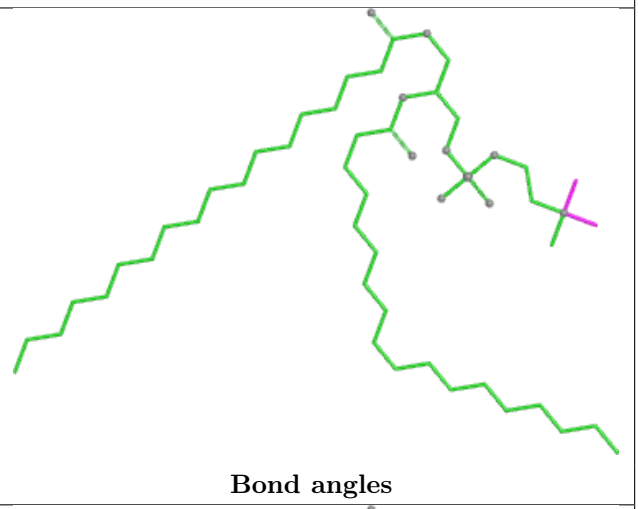
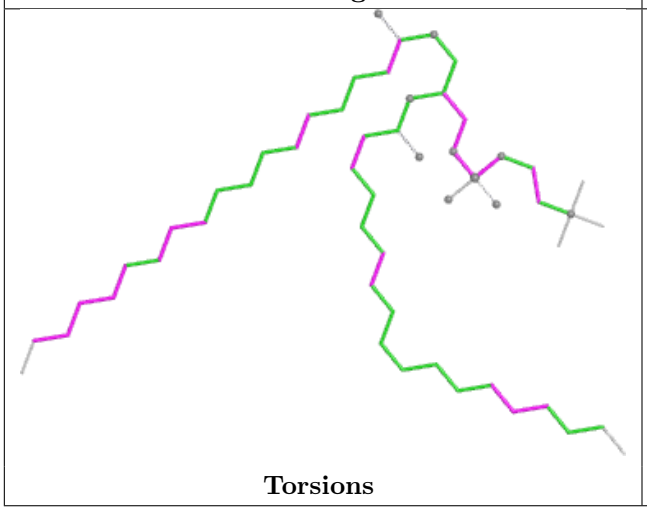
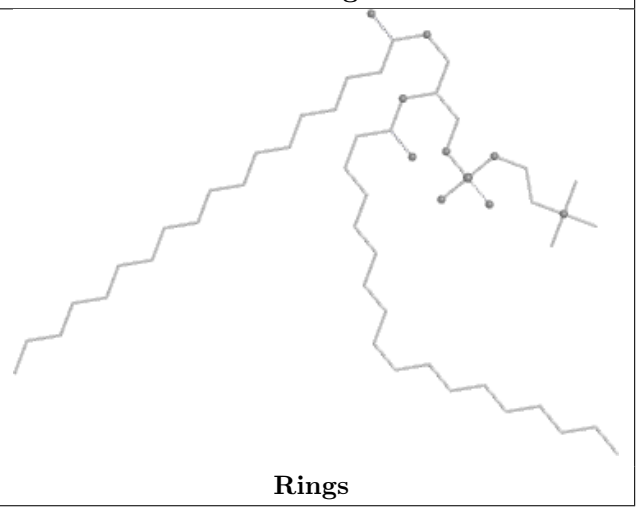


Bond angles

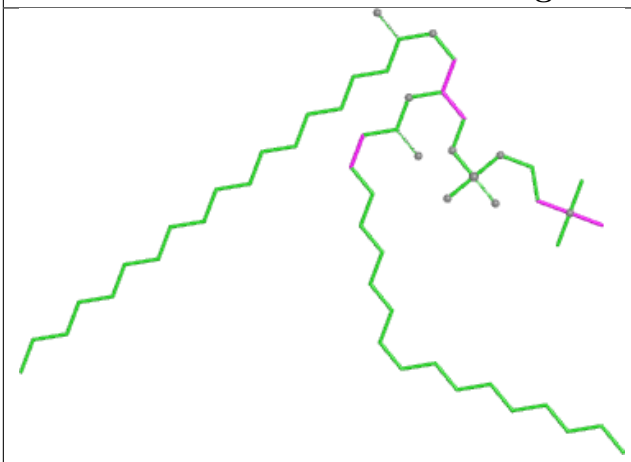


Torsions

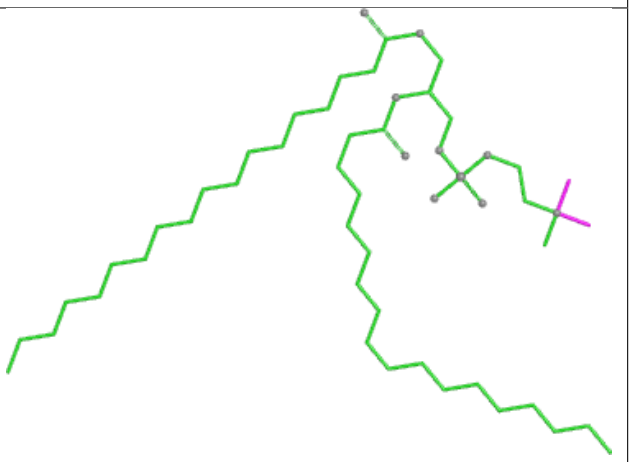


Rings

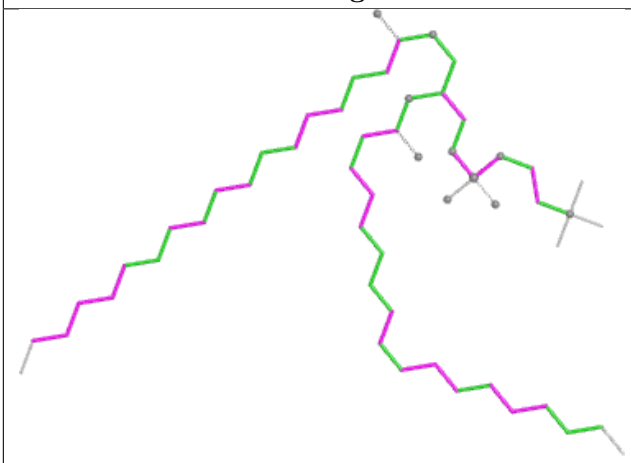
Ligand PCW A 8



Bond lengths



Bond angles



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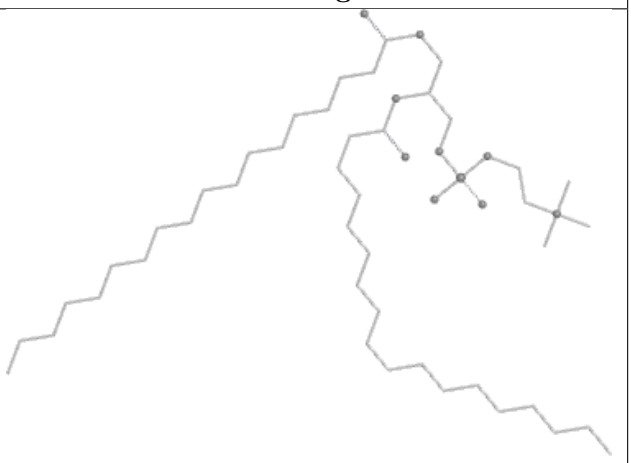
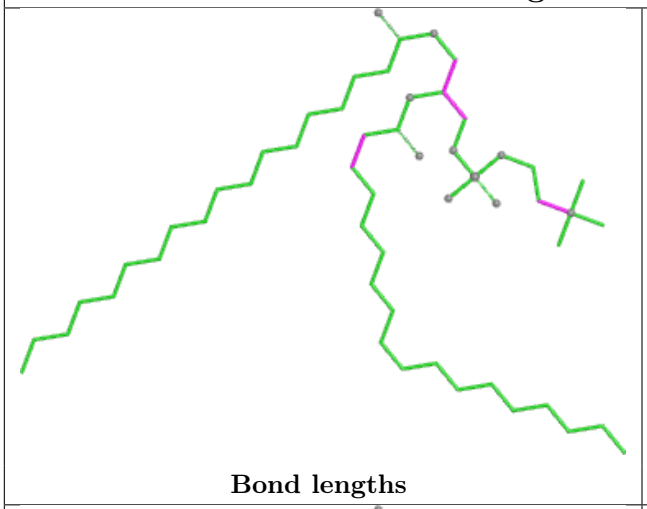
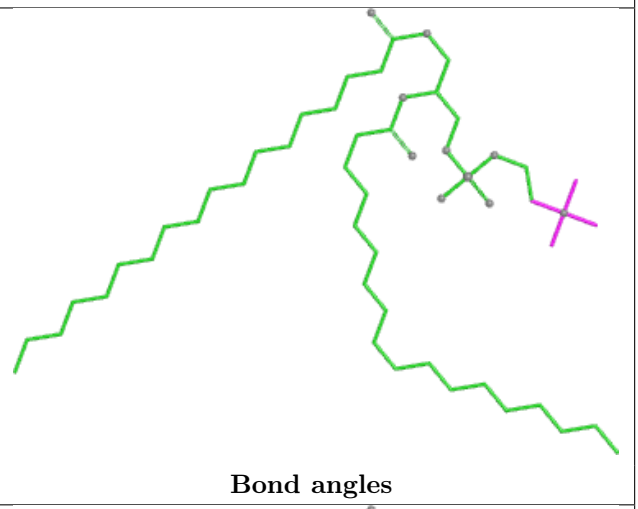


Rings

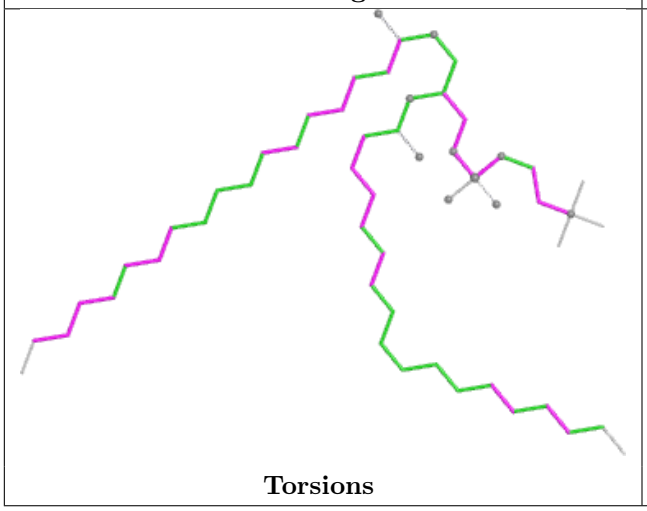
Ligand PCW A 61



Bond lengths



Bond angles



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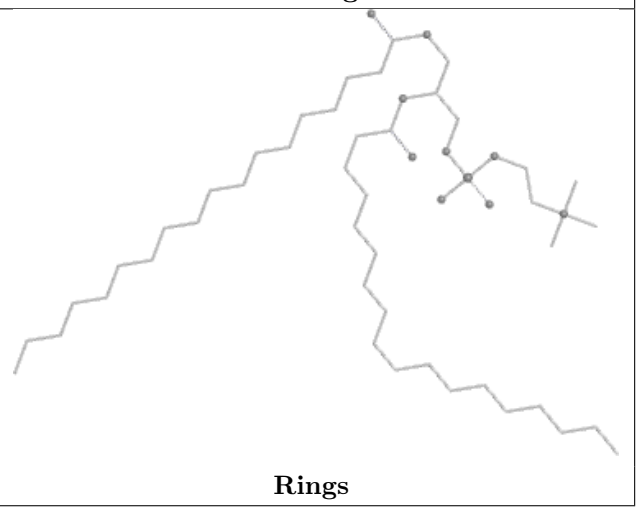
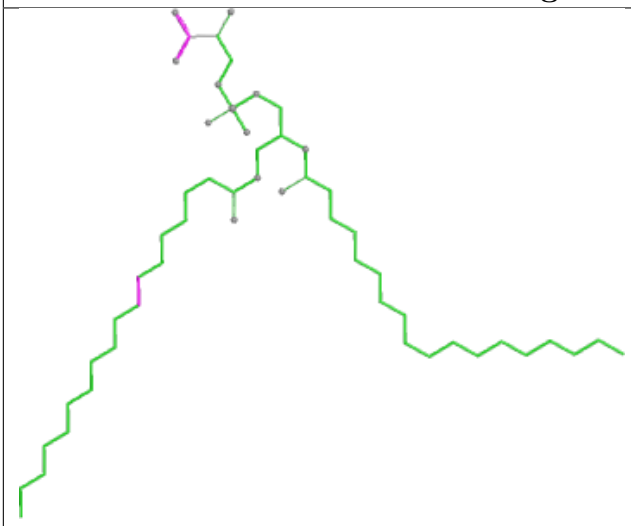
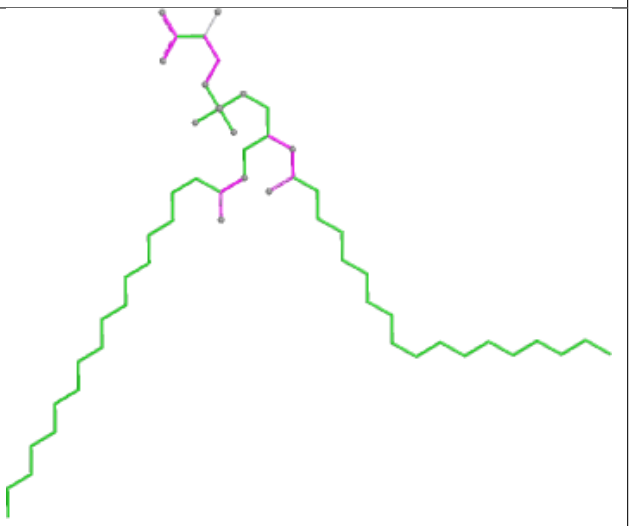


Rings

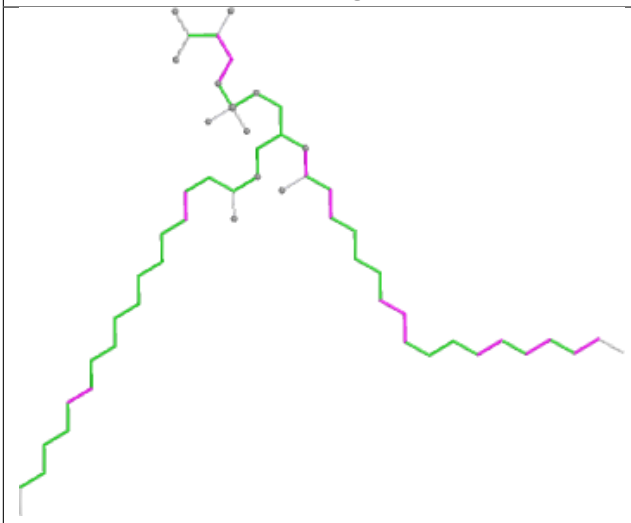
Ligand 17F A 73



Bond lengths



Bond angles



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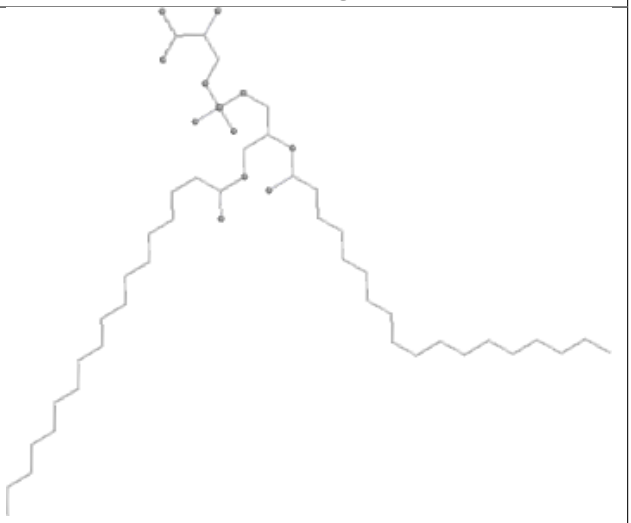
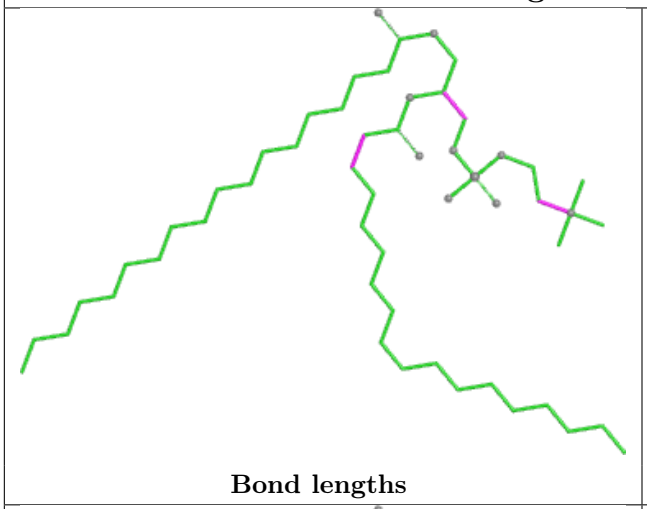
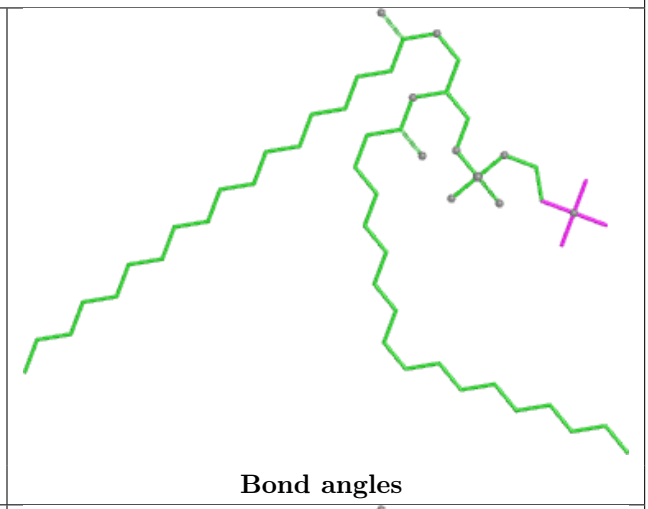


Rings

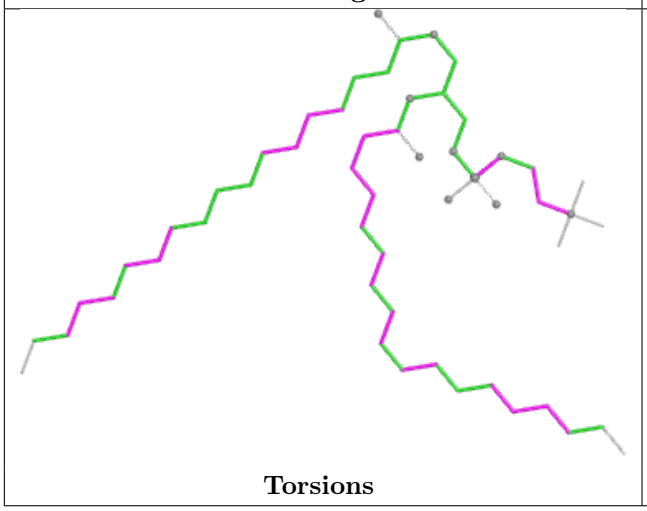
Ligand PCW A 51



Bond lengths



Bond angles



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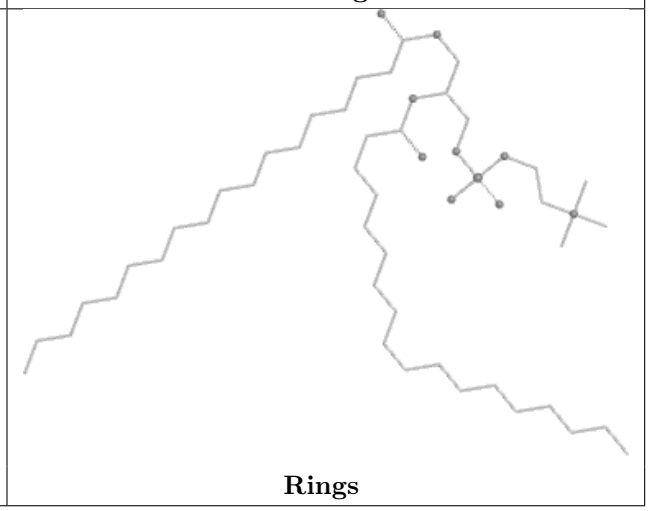
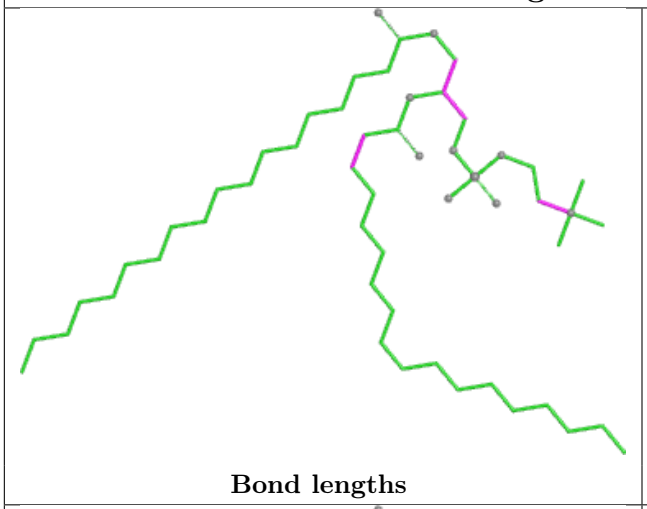
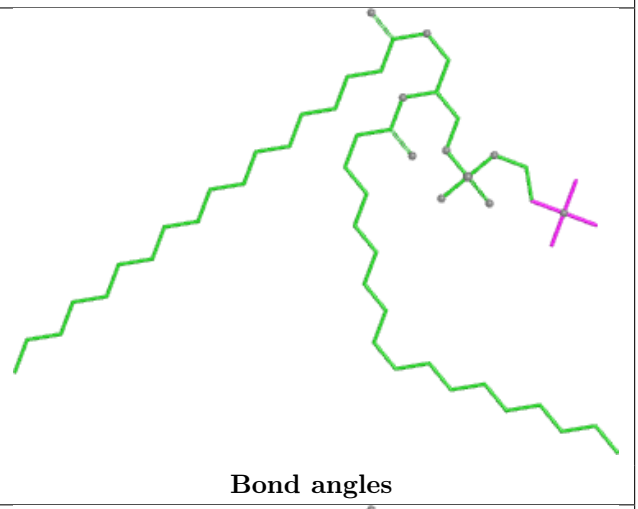


Rings

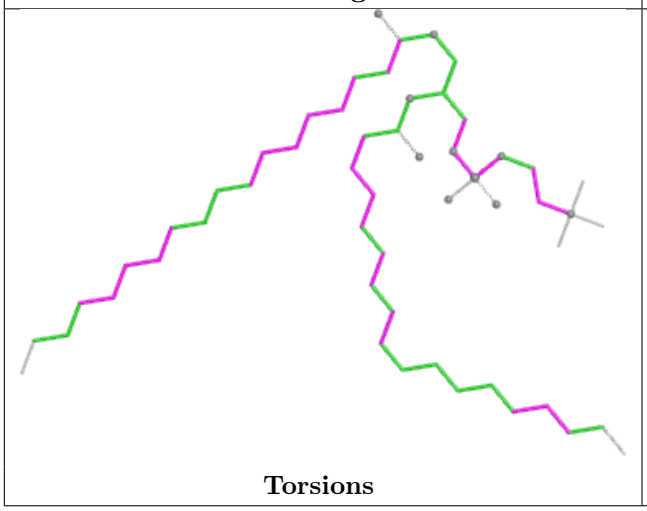
Ligand PCW A 46



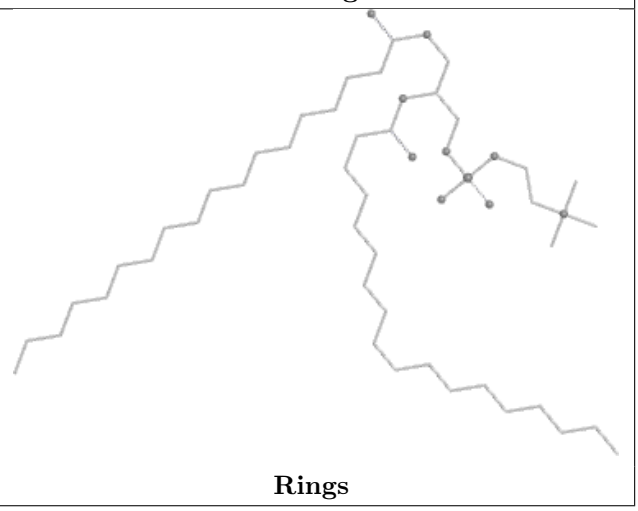
Bond lengths



Bond angles

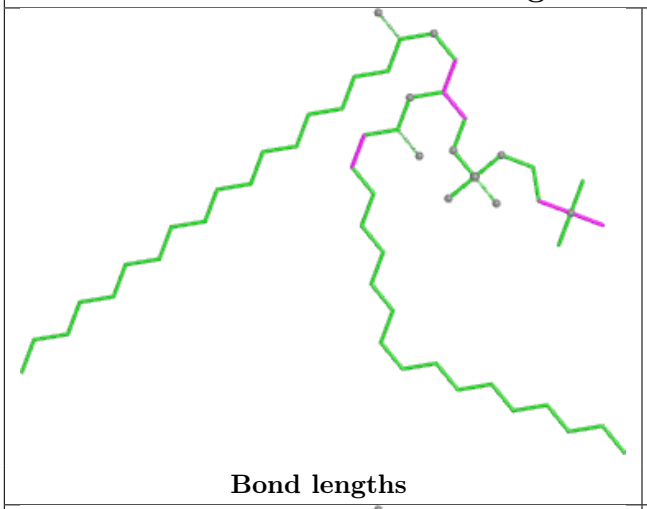


Torsions

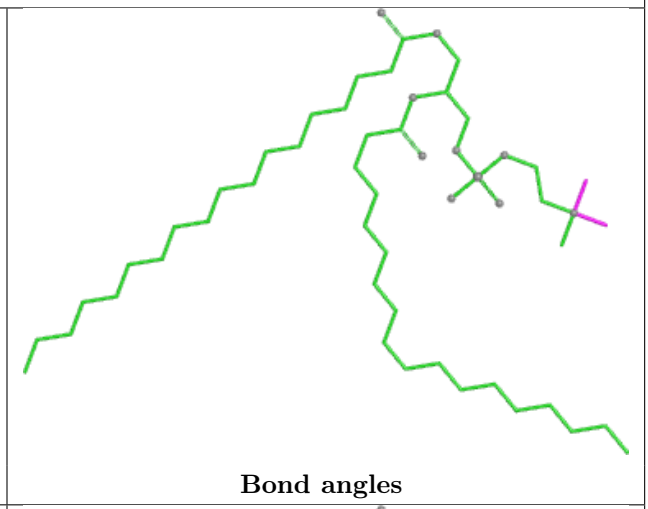


Rings

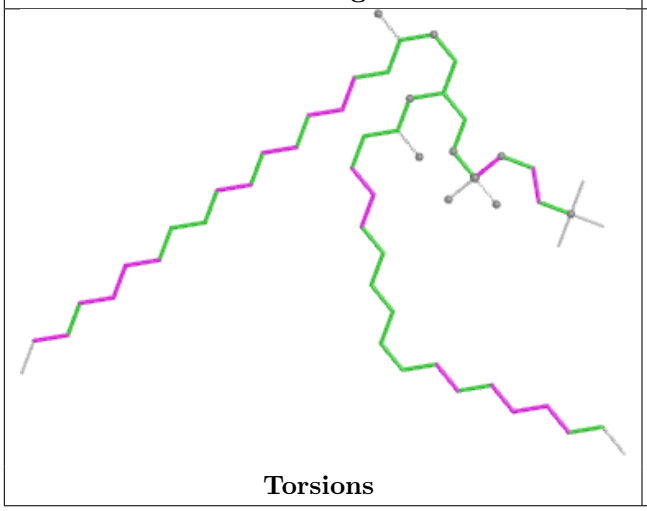
Ligand PCW A 11



Bond lengths



Bond angles



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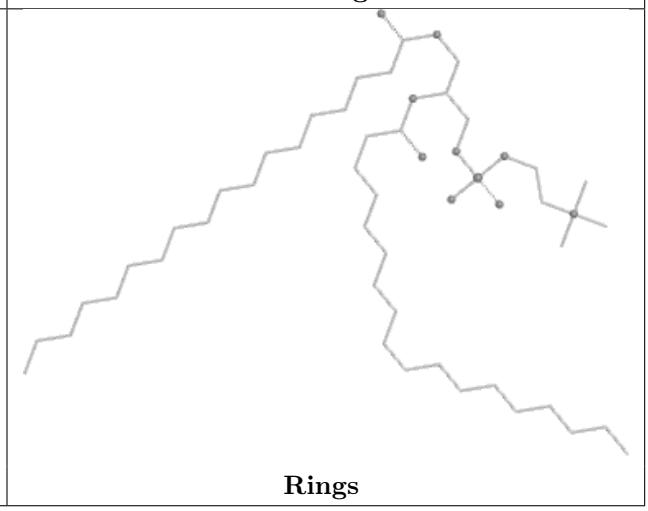
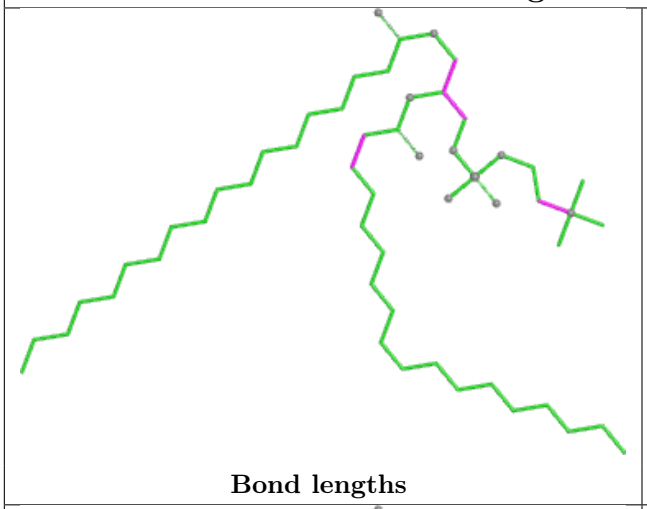
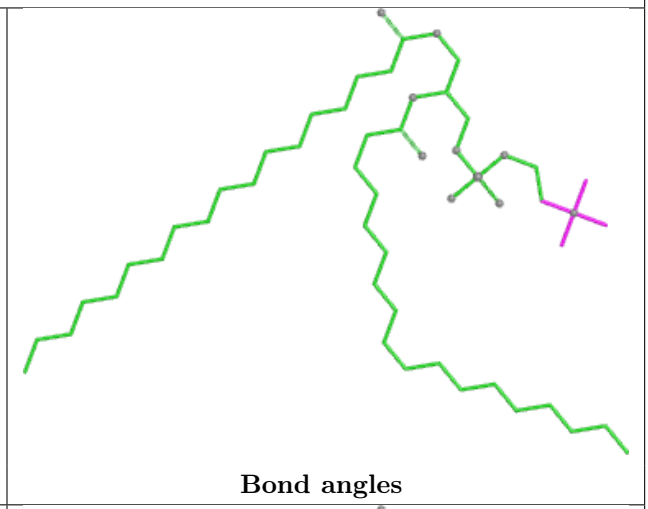


Rings

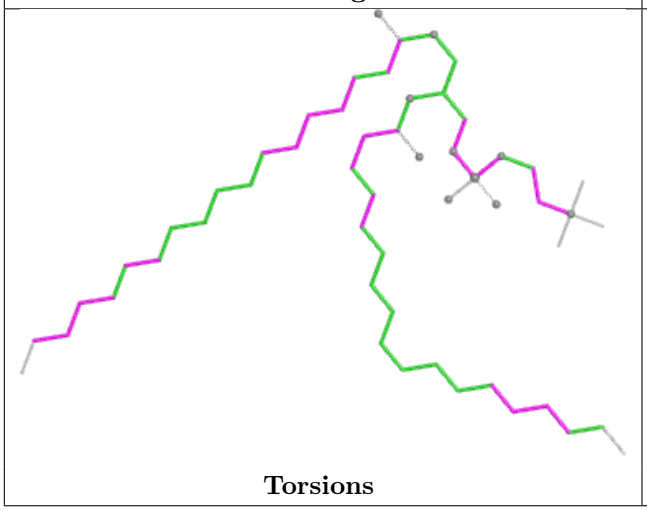
Ligand PCW A 71



Bond lengths



Bond angles



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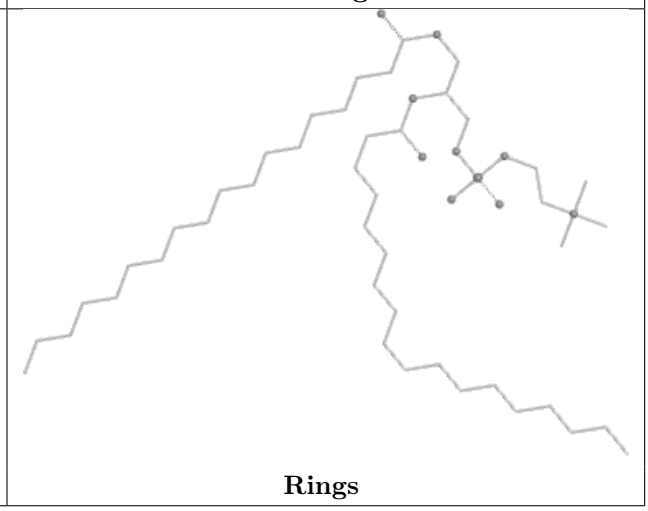
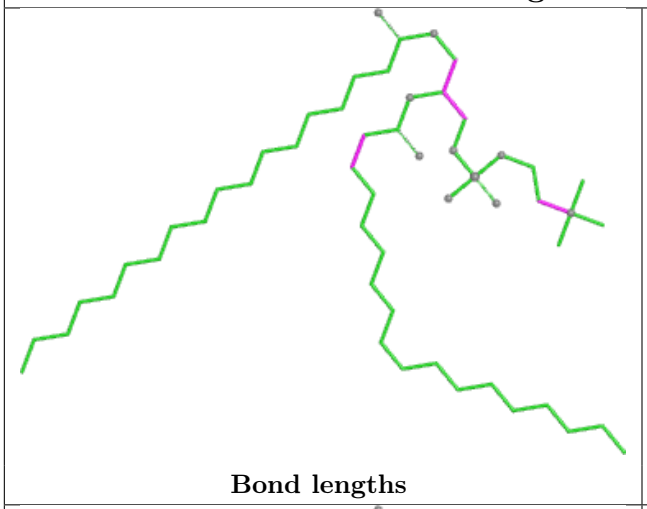
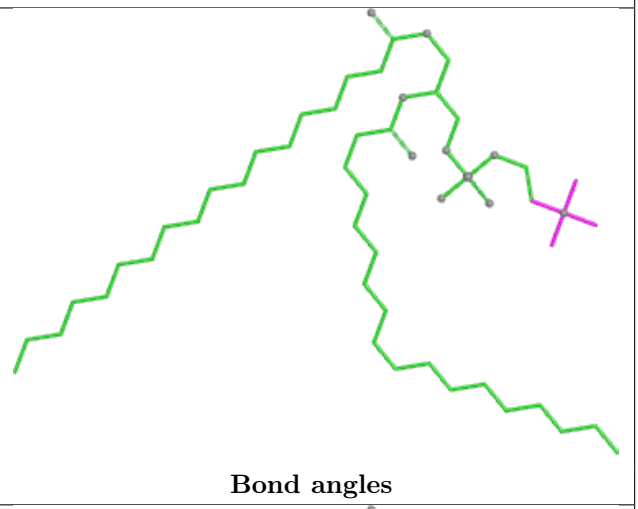


Rings

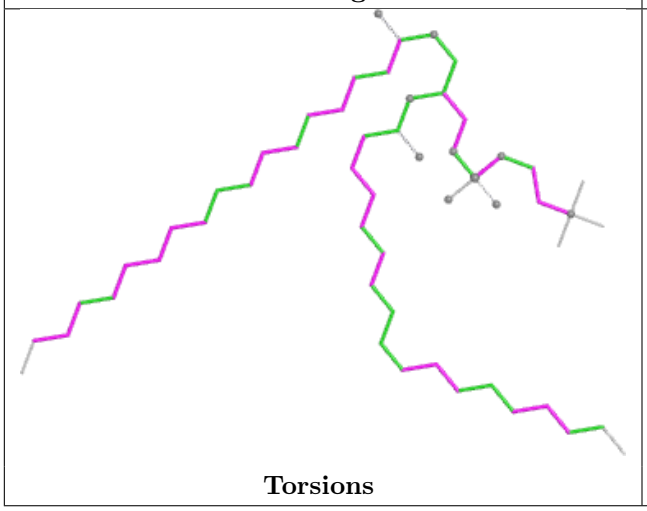
Ligand PCW A 44



Bond lengths



Bond angles



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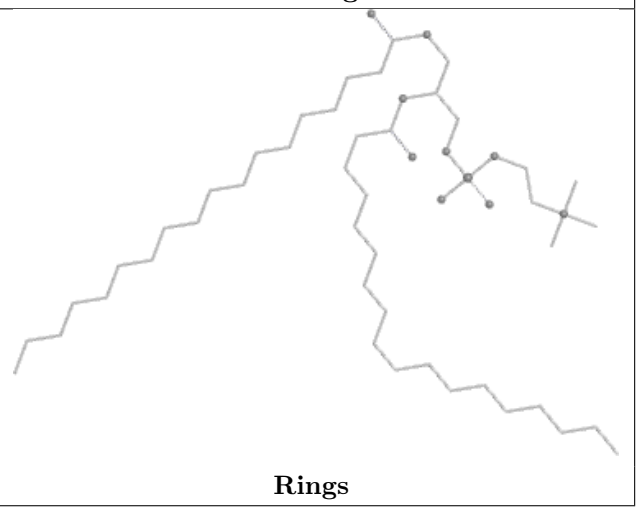
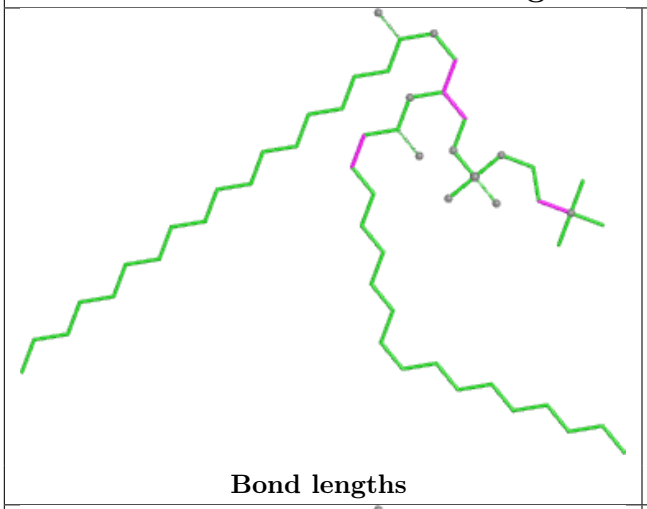
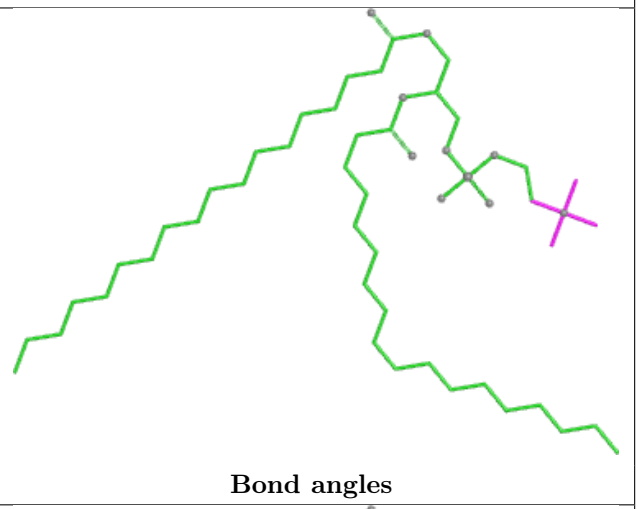


Rings

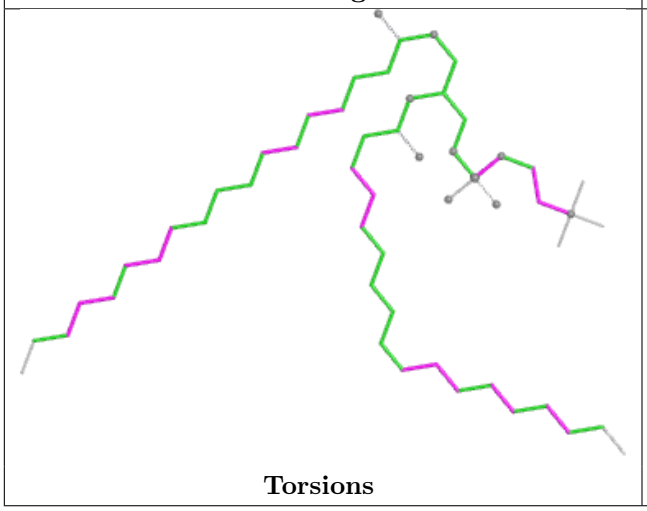
Ligand PCW A 23



Bond lengths



Bond angles



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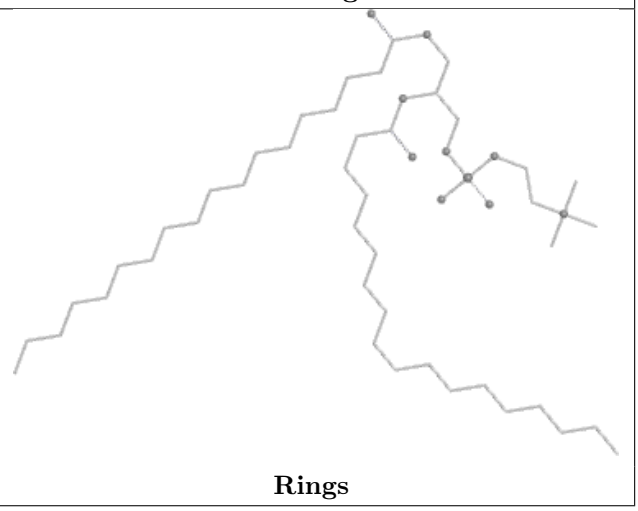
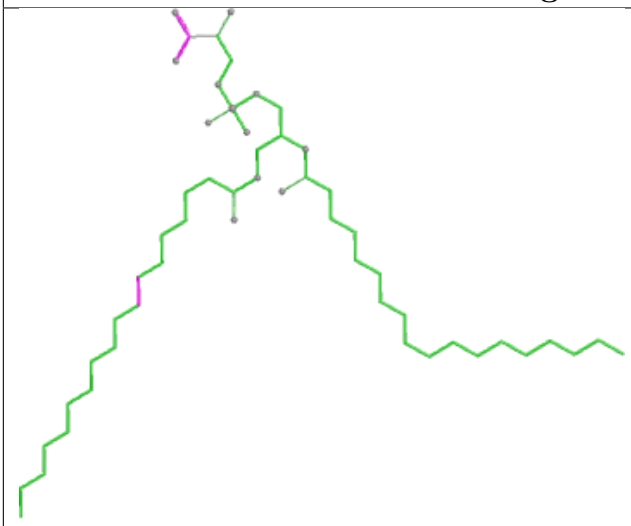


Rings

Ligand 17F A 80



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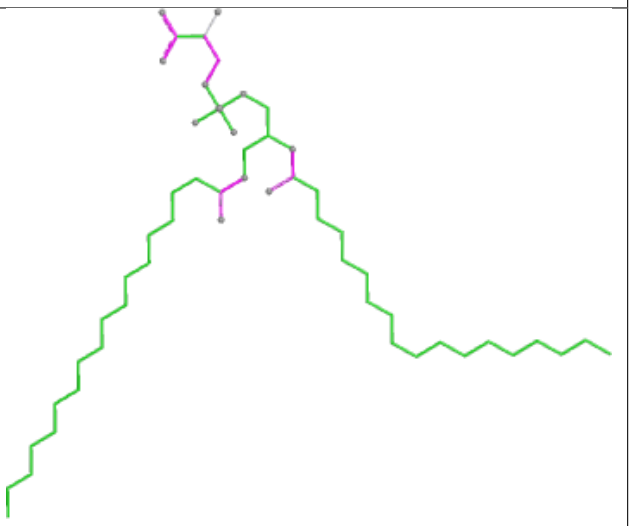
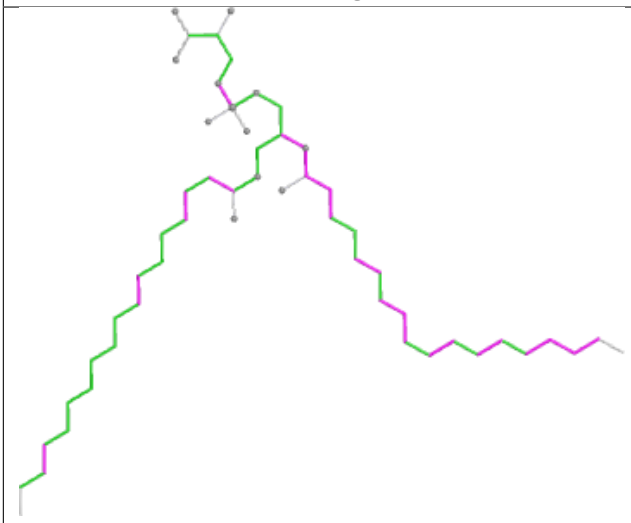


Bond angles



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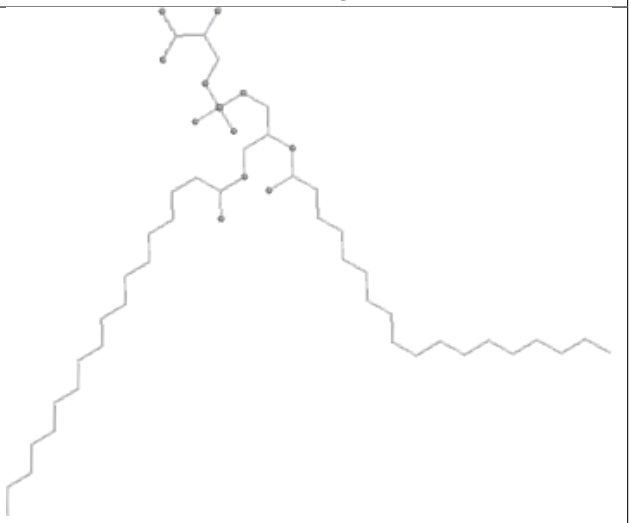
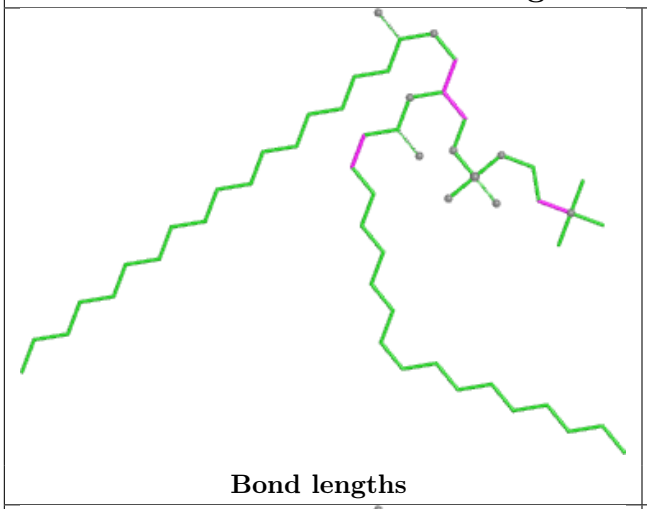


Rings

Ligand PCW A 10



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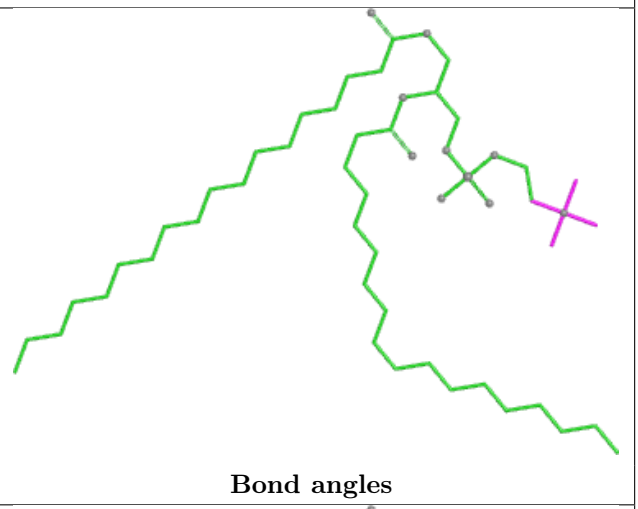
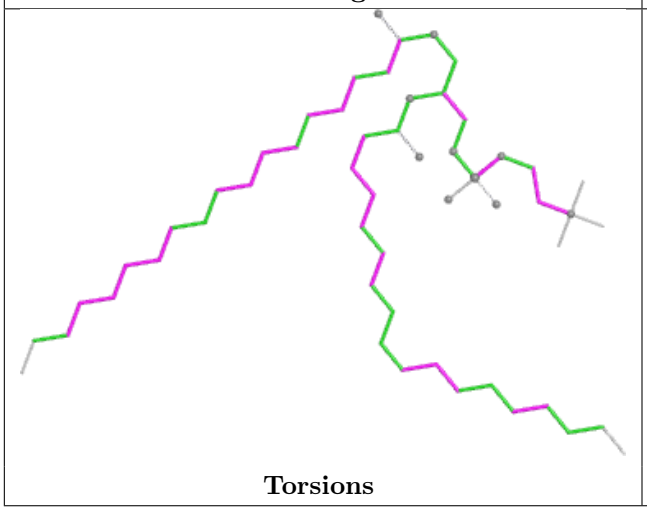


Bond angles



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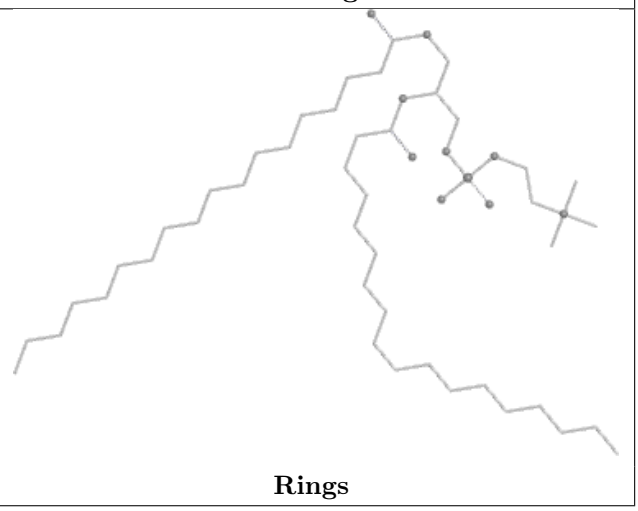
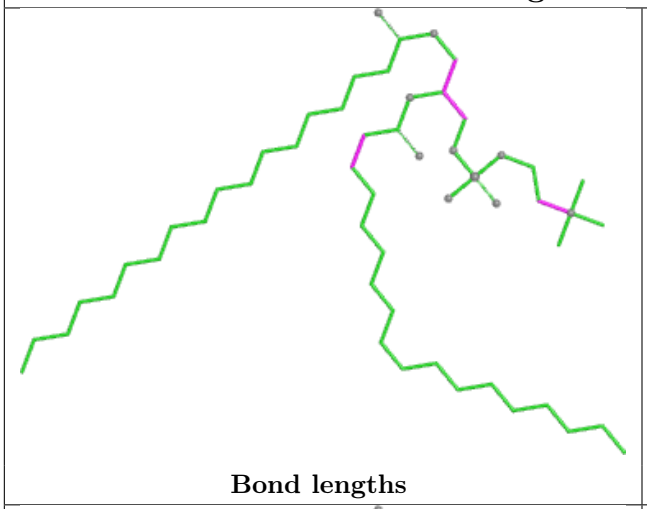


Rings

Ligand PCW A 28



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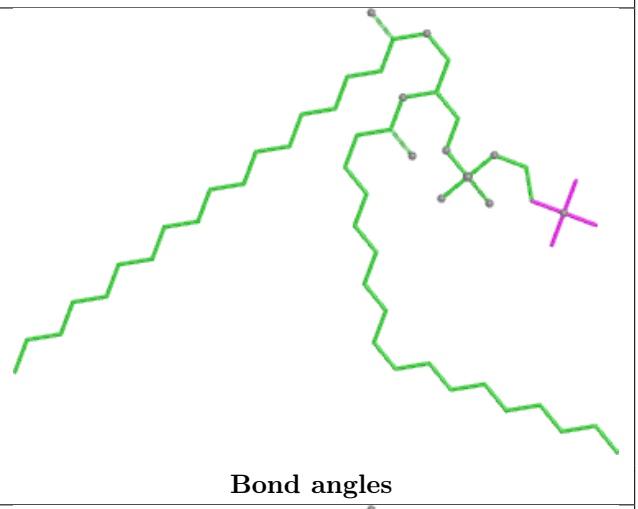
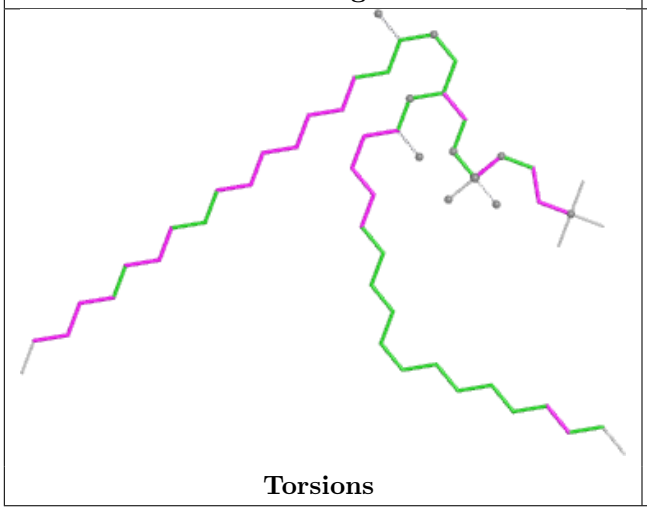


Bond angles



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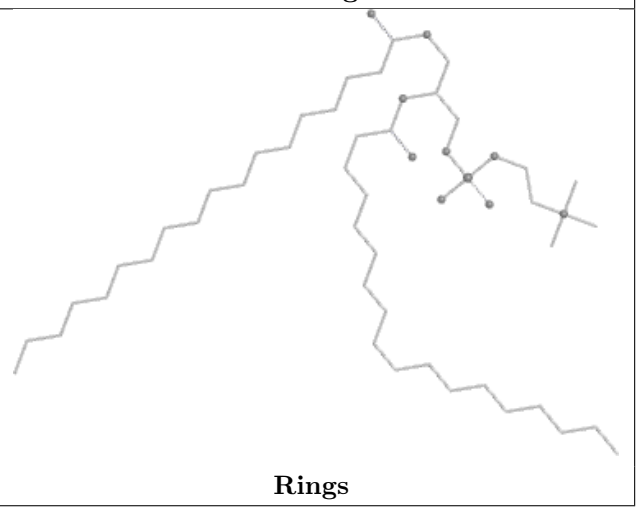
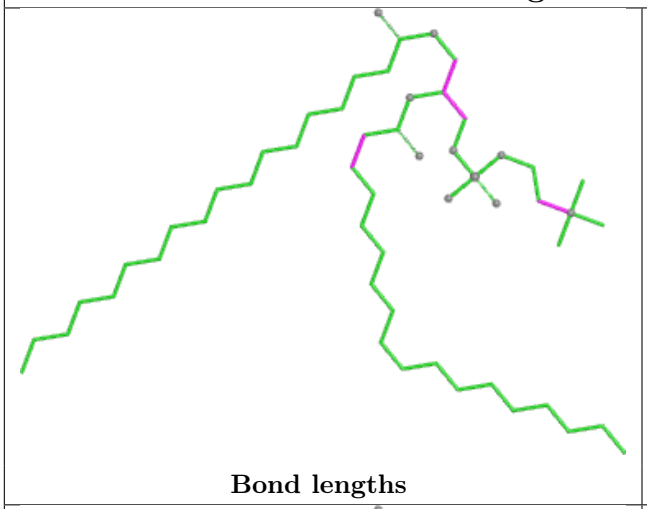
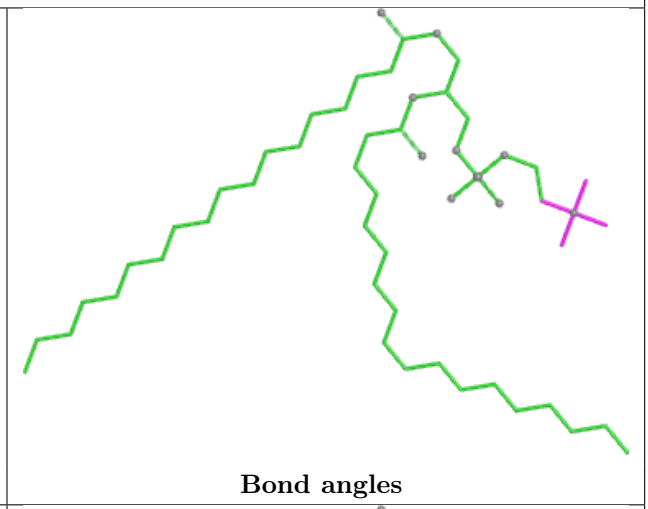


Rings

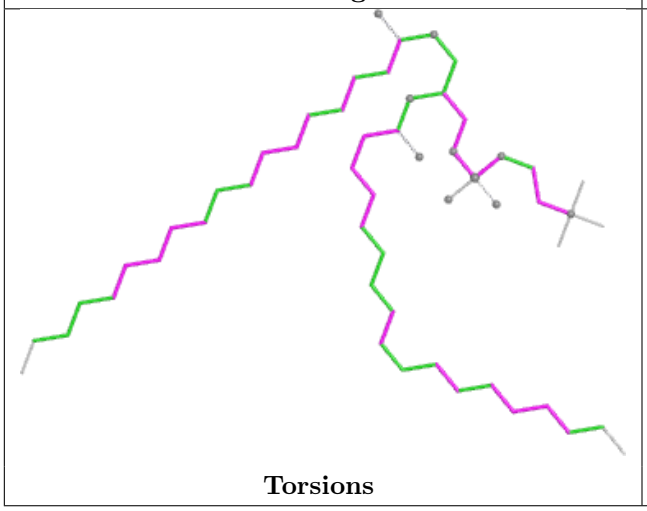
Ligand PCW A 17



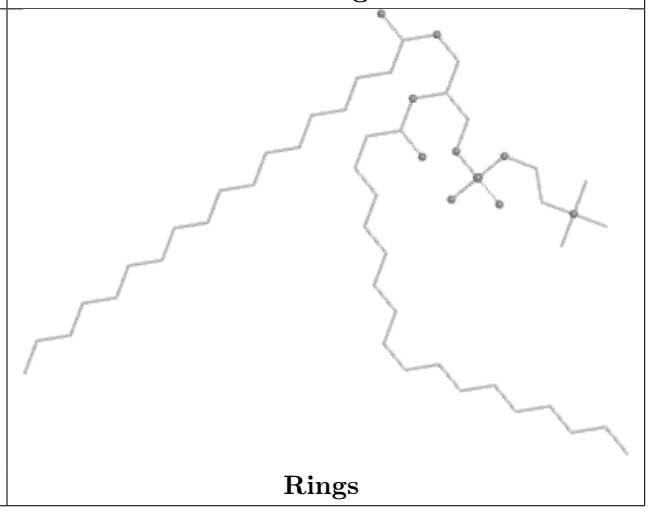
Bond lengths



Bond angles

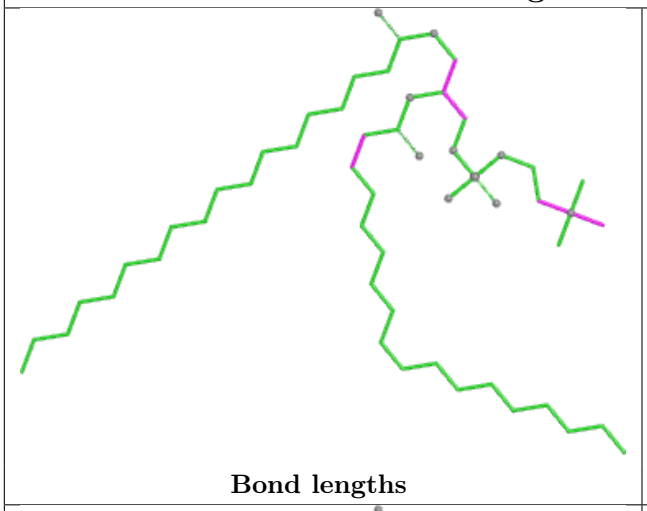


Torsions

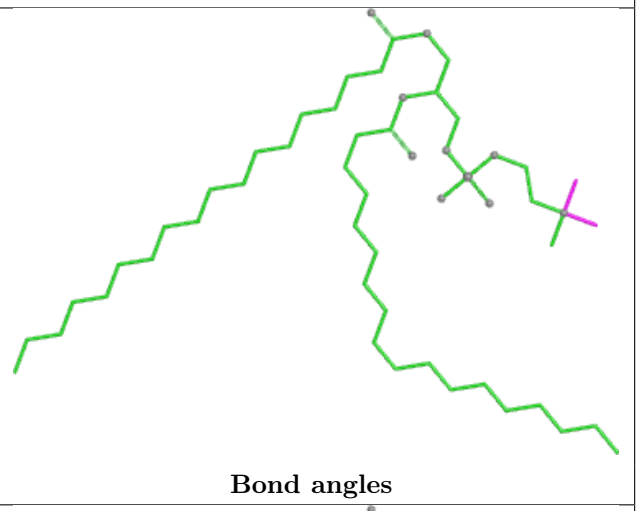


Rings

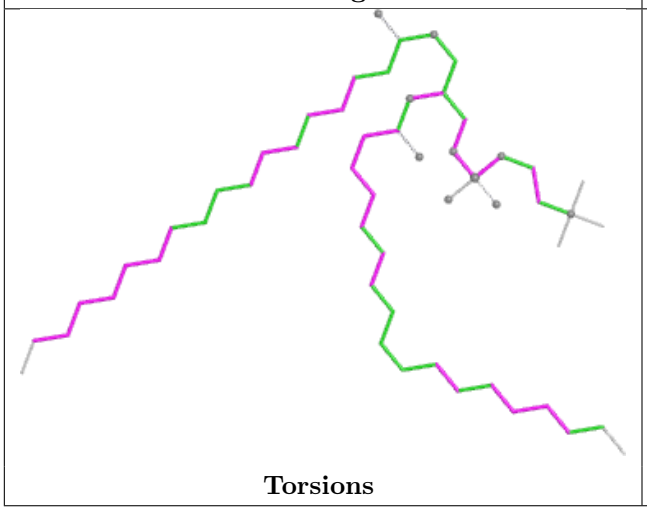
Ligand PCW A 55



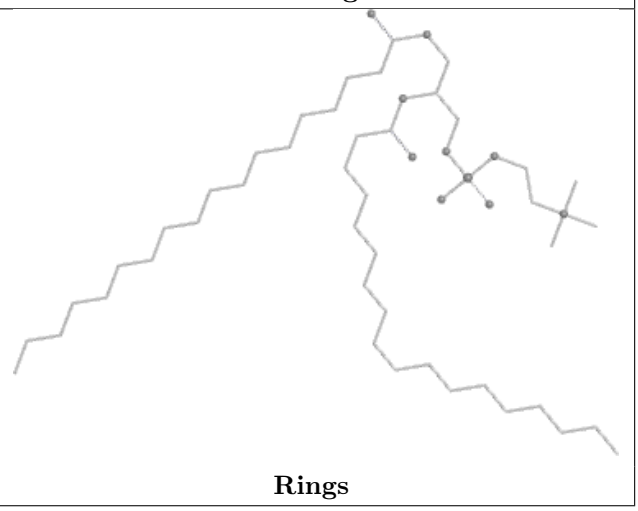
Bond lengths



Bond angles

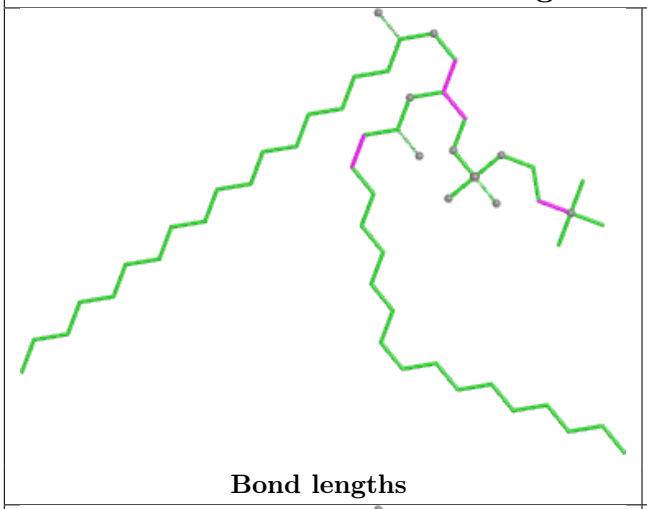


Torsions



Rings

Ligand PCW A 4



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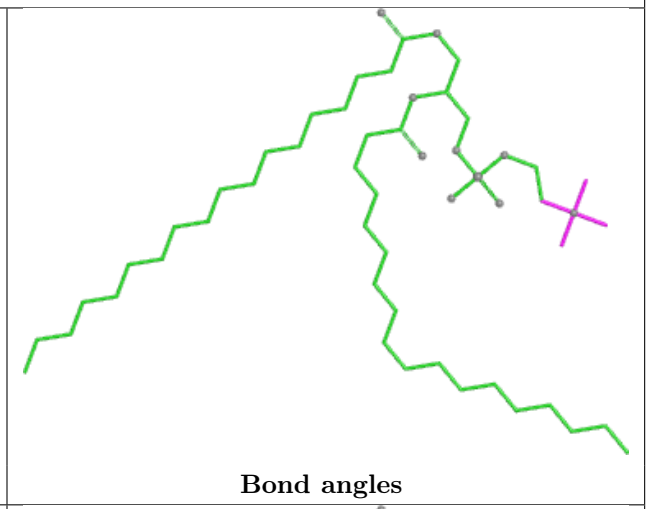
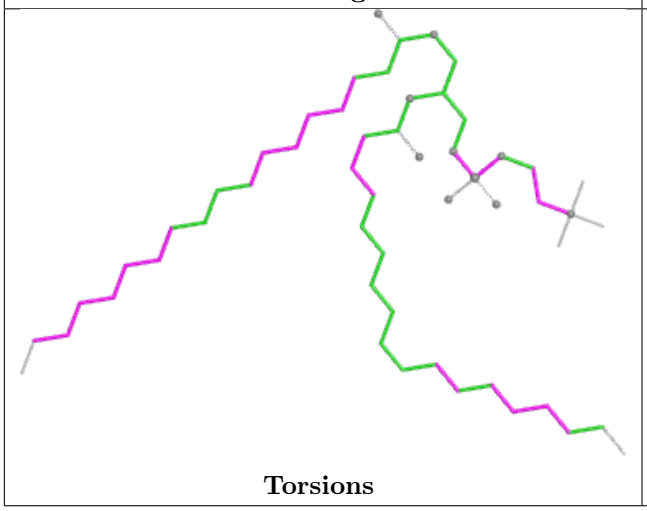
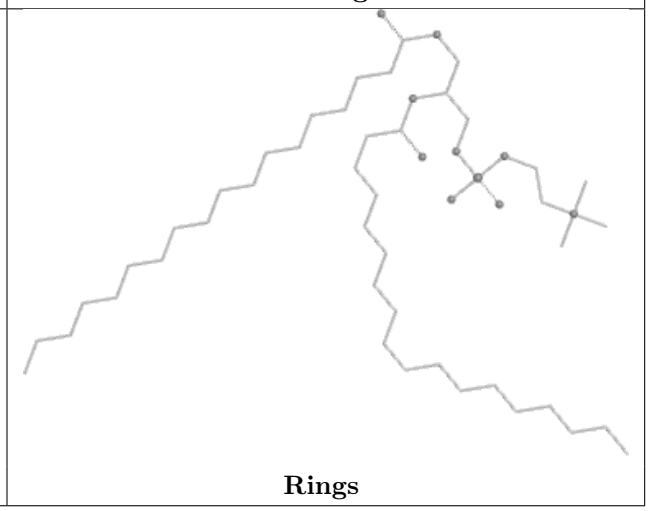


Bond angles

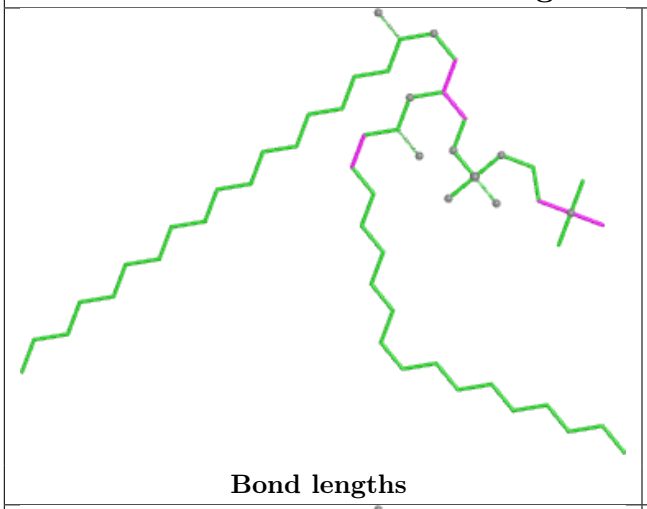


Torsions

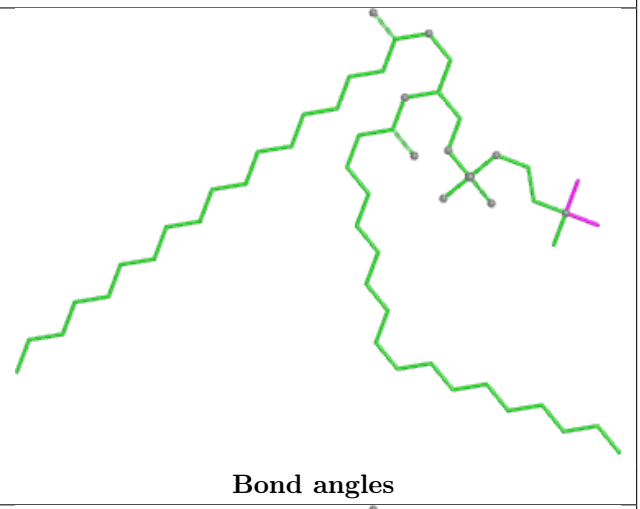


Rings

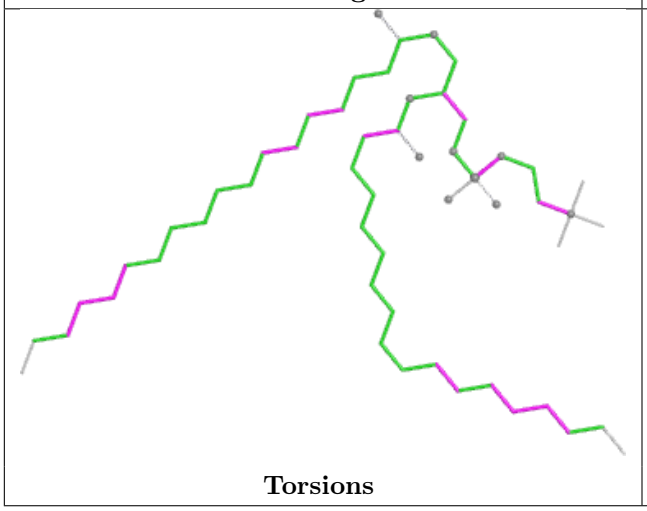
Ligand PCW A 7



Bond lengths



Bond angles



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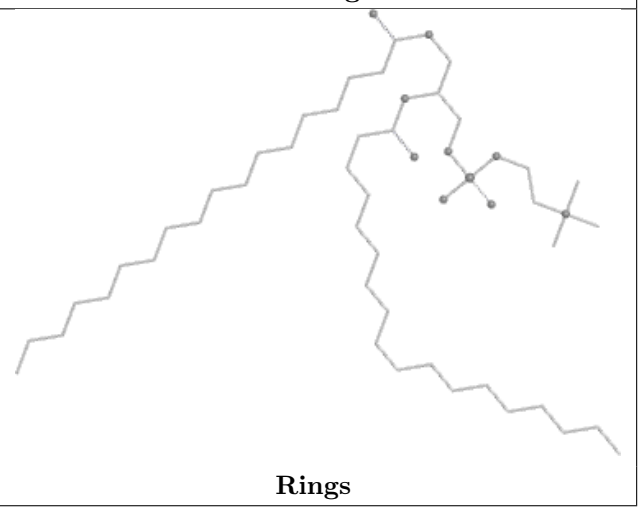
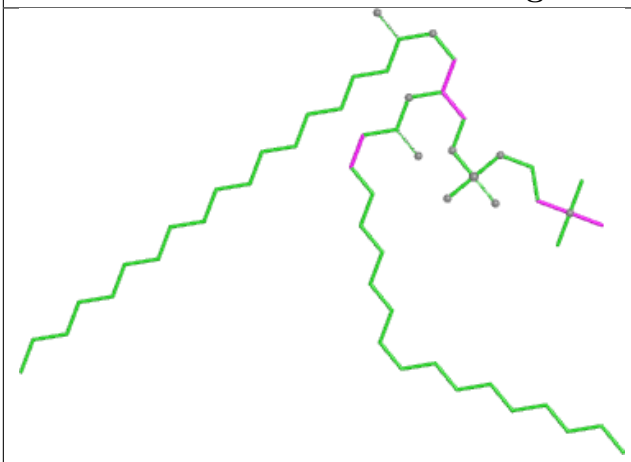
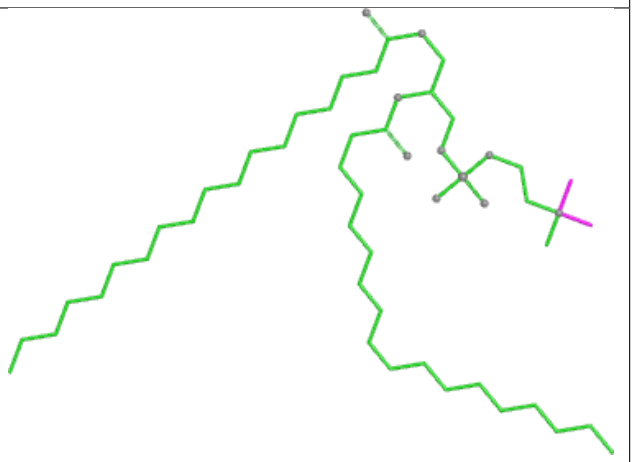


Rings

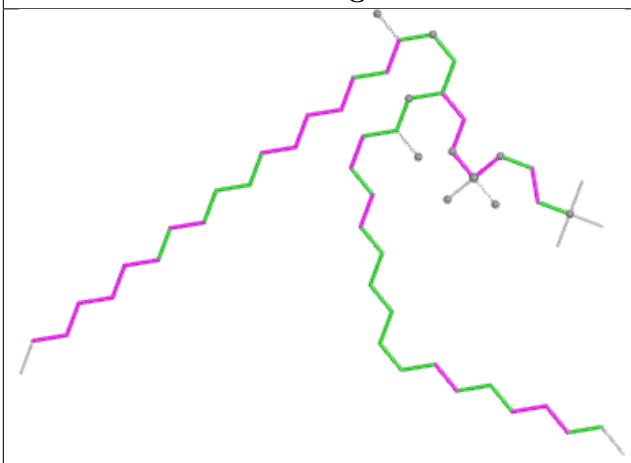
Ligand PCW A 32



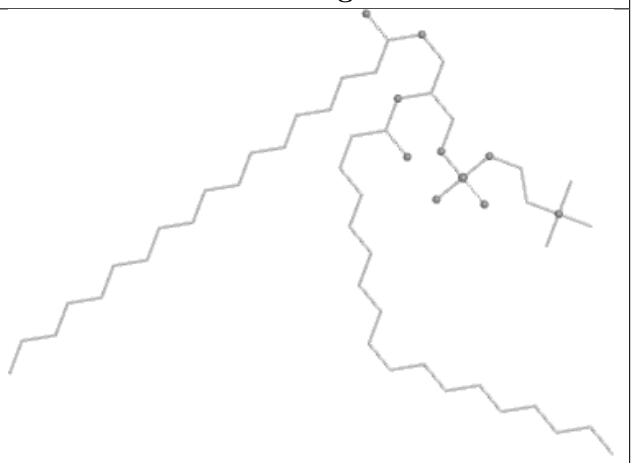
Bond lengths



Bond angles

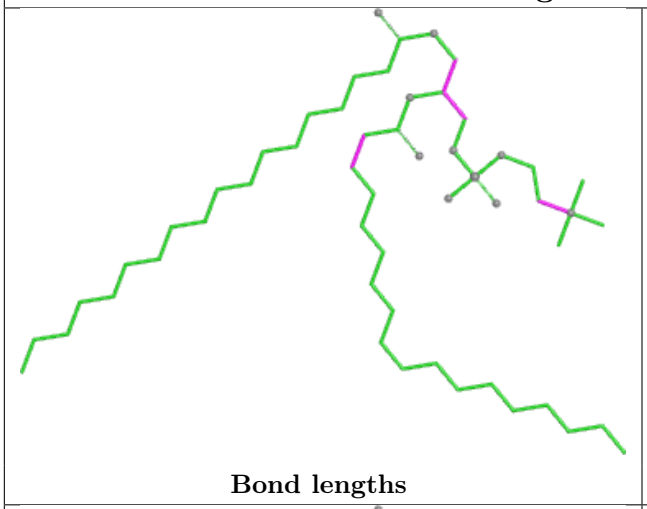


Torsions

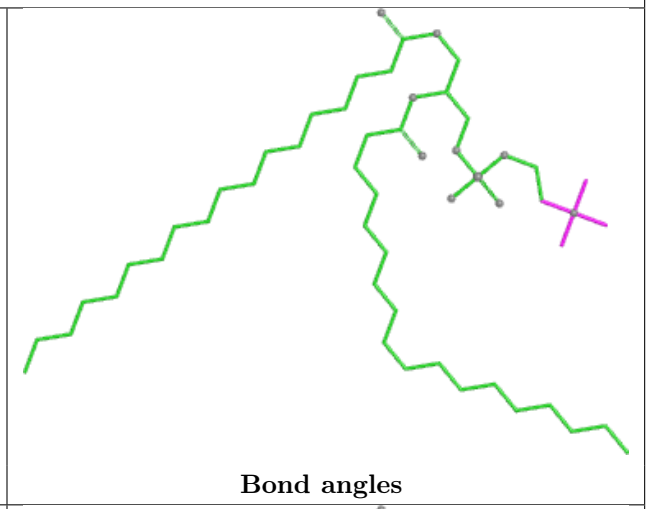


Rings

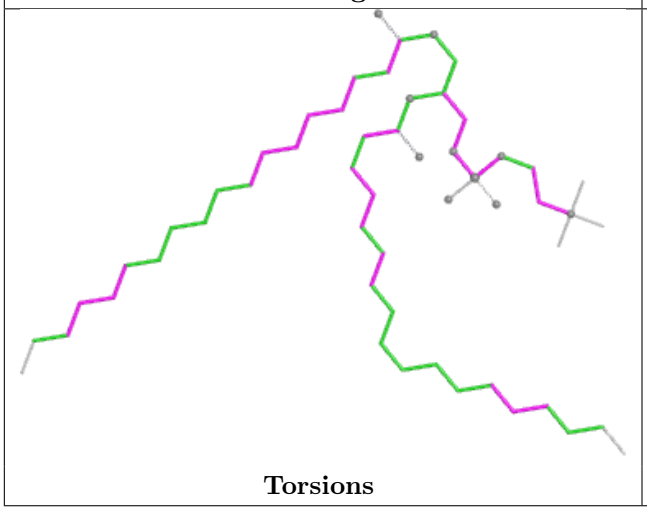
Ligand PCW A 5



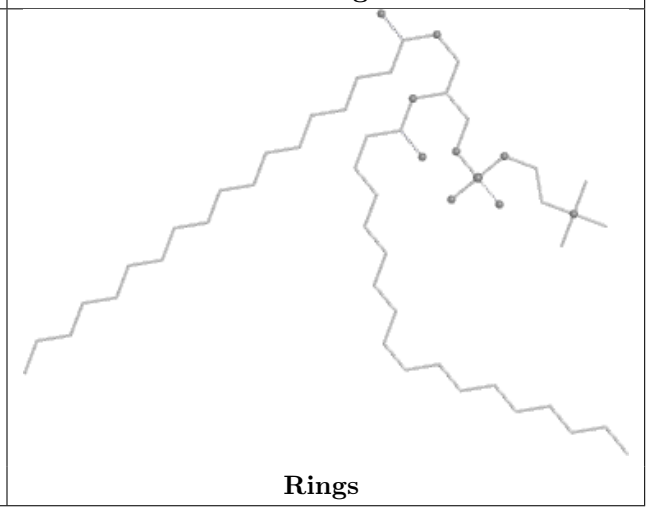
Bond lengths



Bond angles

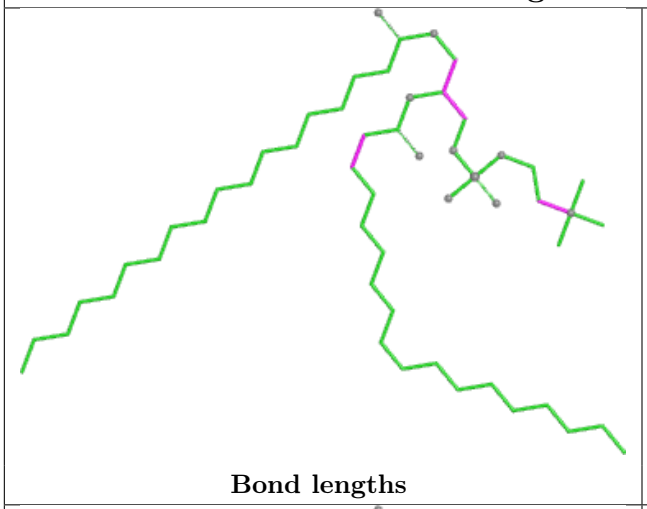


Torsions

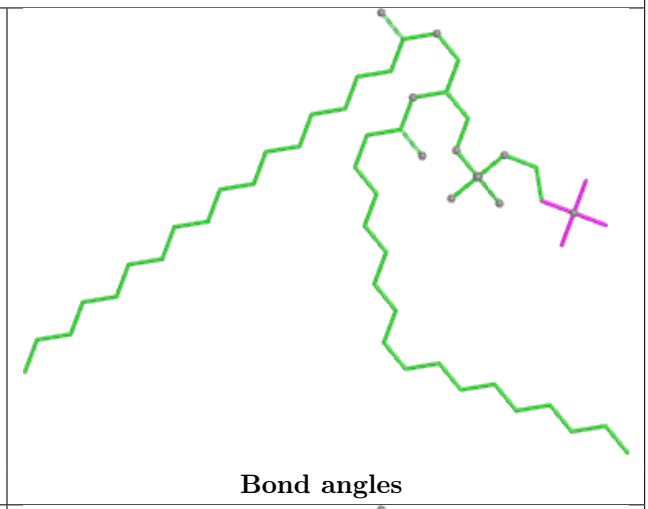


Rings

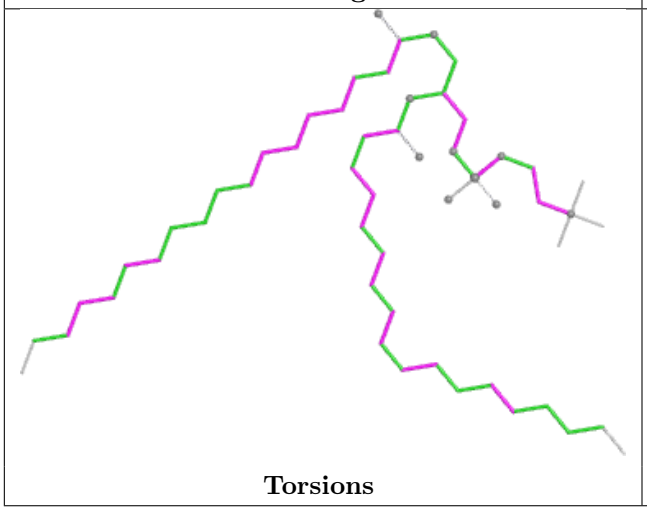
Ligand PCW A 21



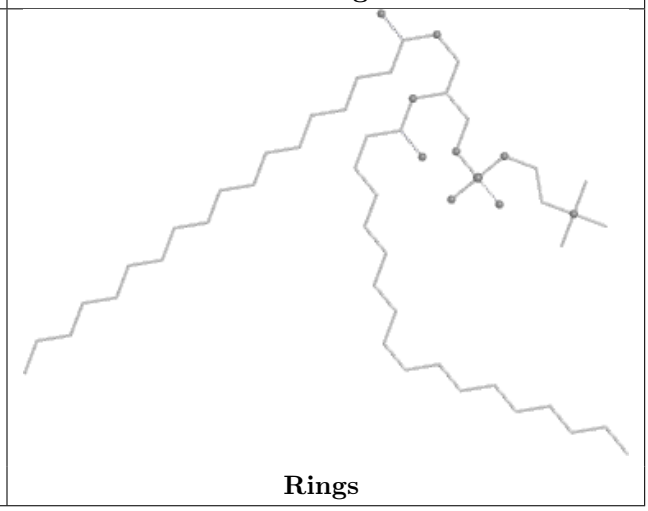
Bond lengths



Bond angles

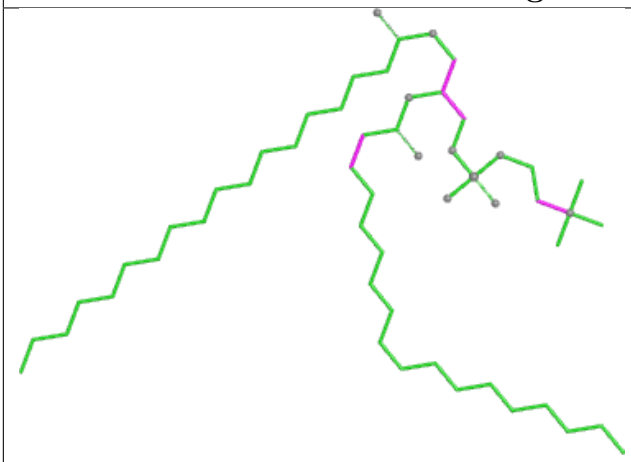


Torsions

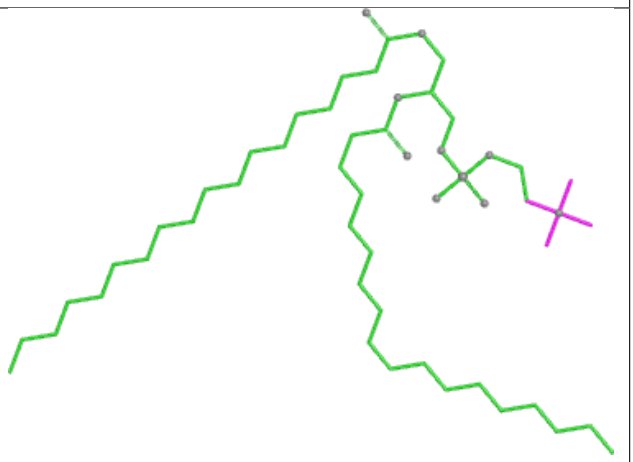


Rings

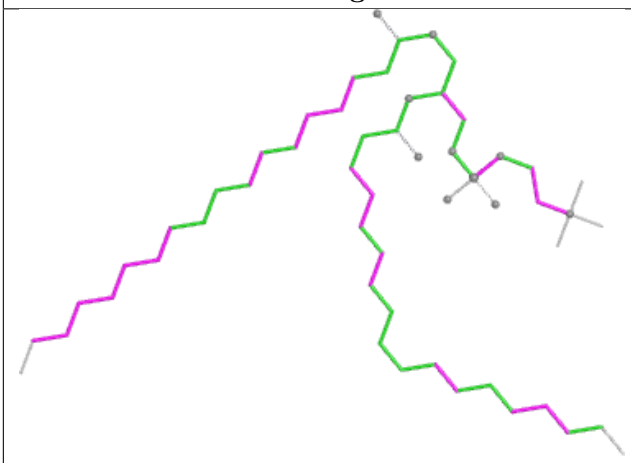
Ligand PCW A 41



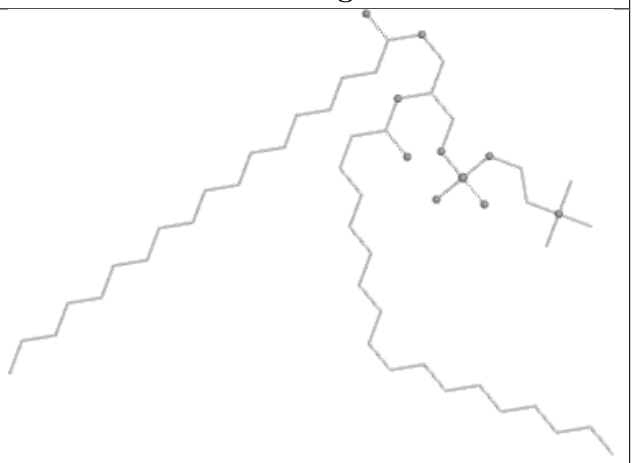
Bond lengths



Bond angles

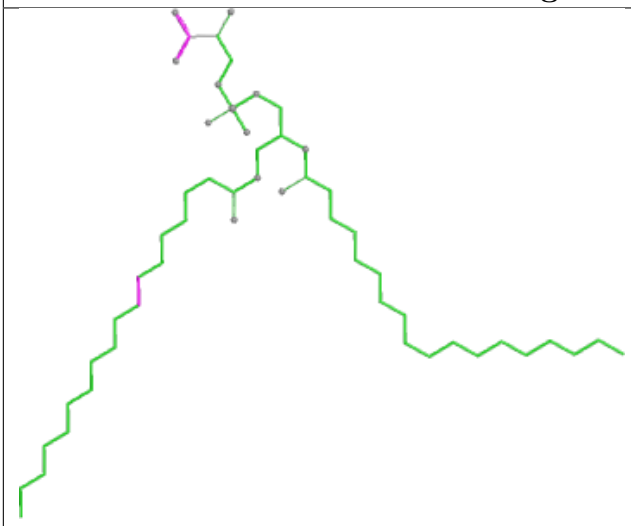


Torsions

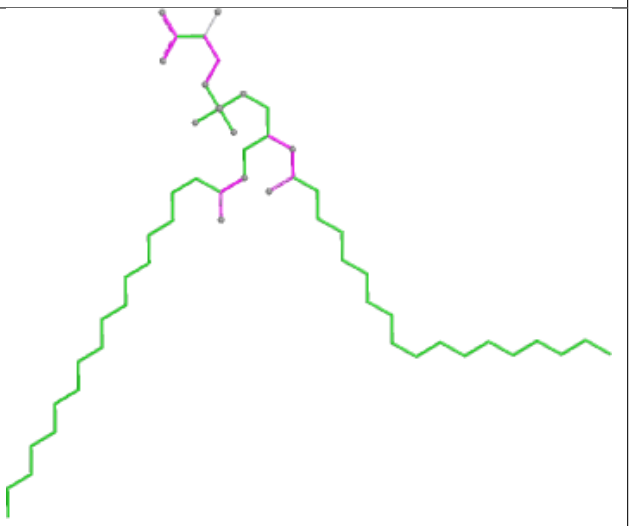


Rings

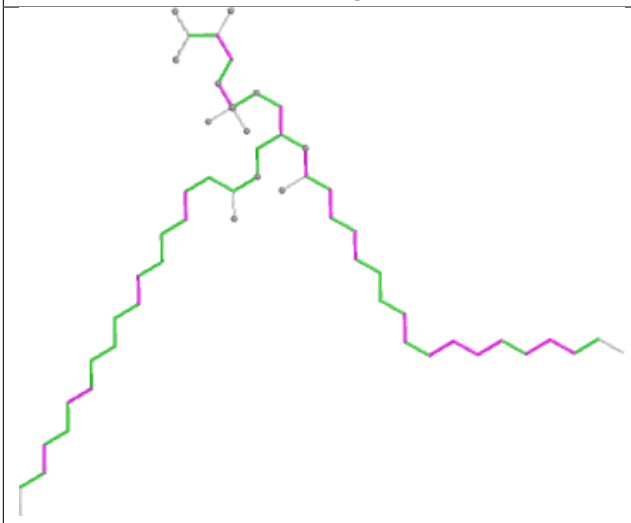
Ligand 17F A 40



Bond lengths



Bond angles



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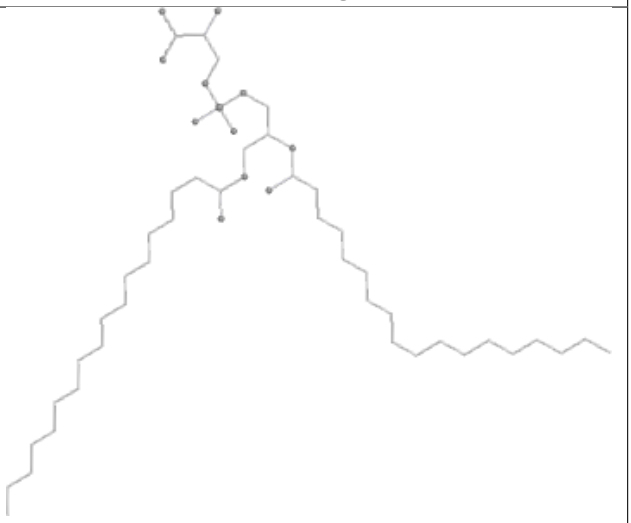
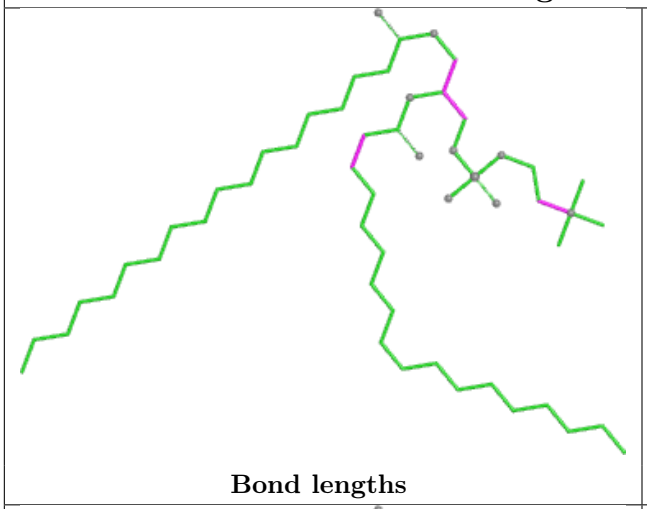
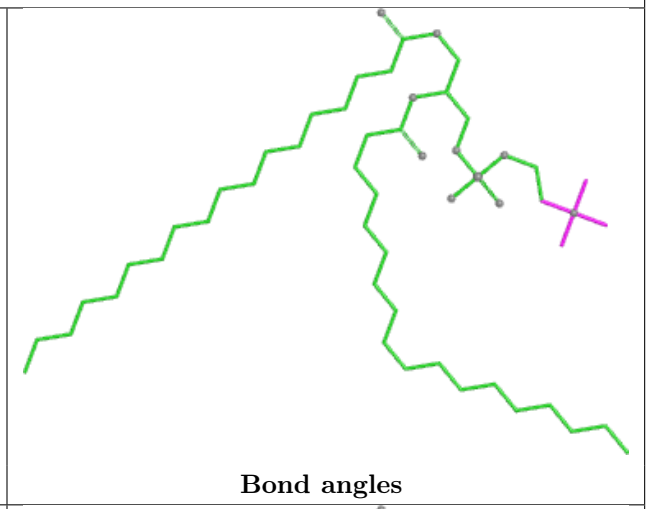


Rings

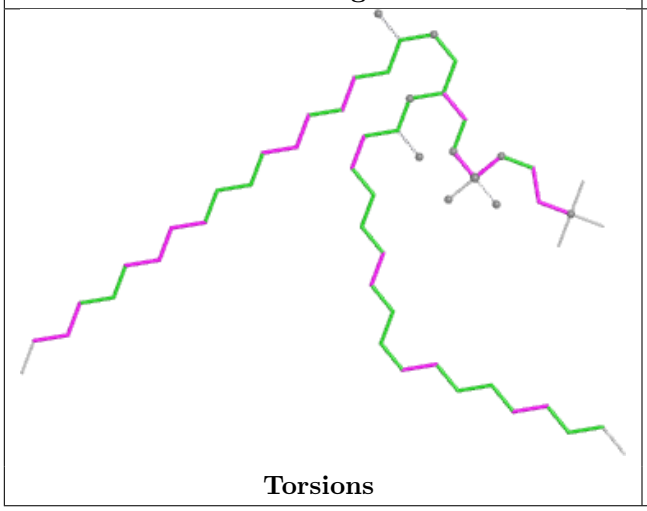
Ligand PCW A 2



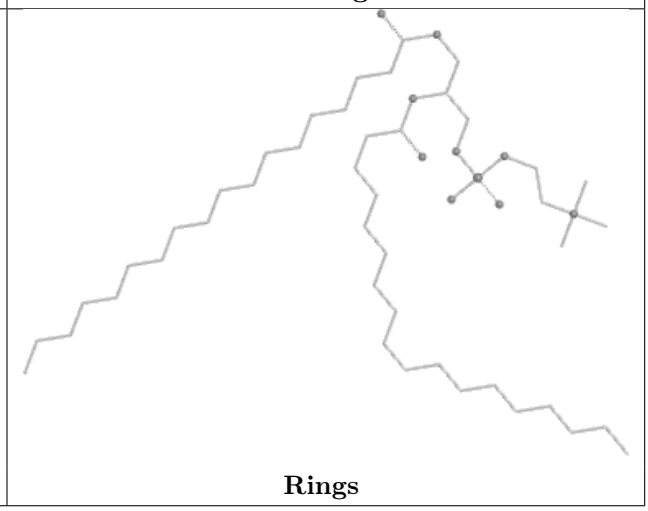
Bond lengths



Bond angles

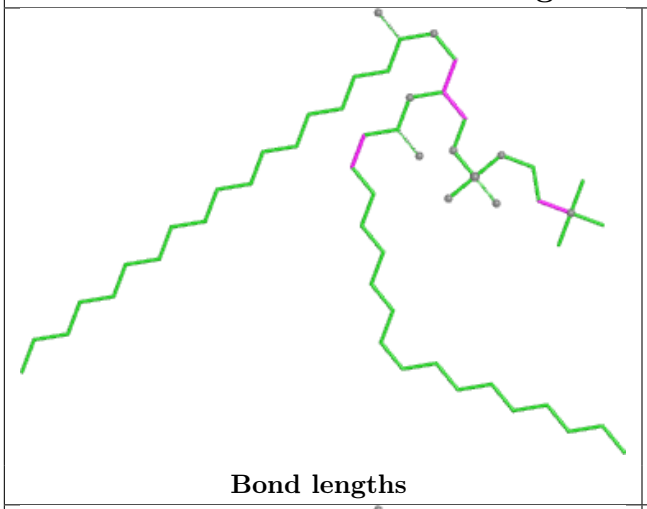


Torsions

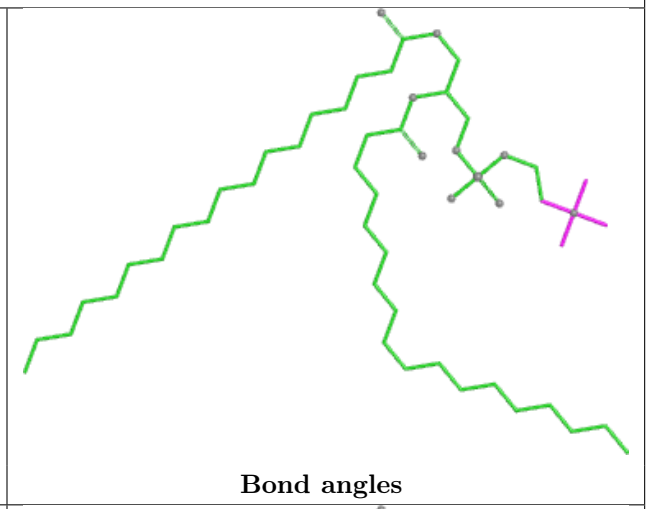


Rings

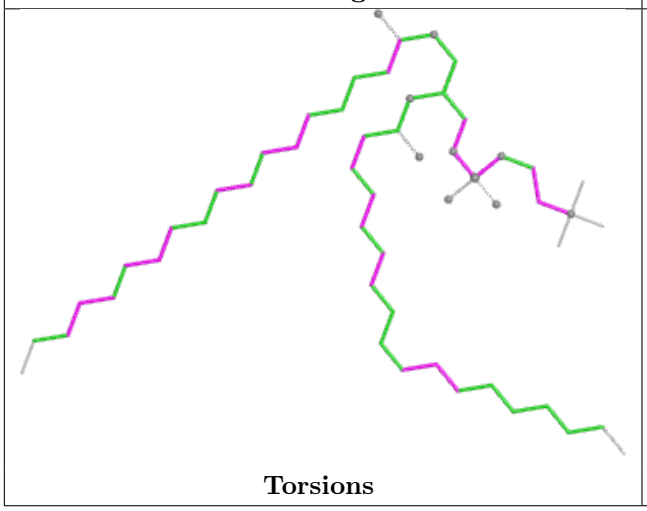
Ligand PCW A 3



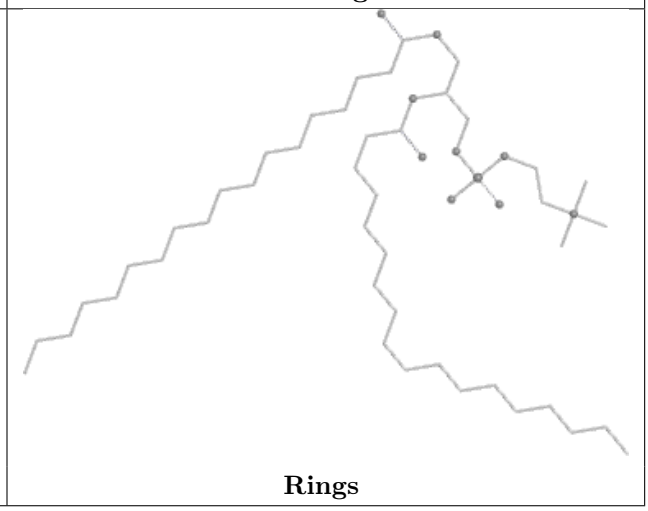
Bond lengths



Bond angles

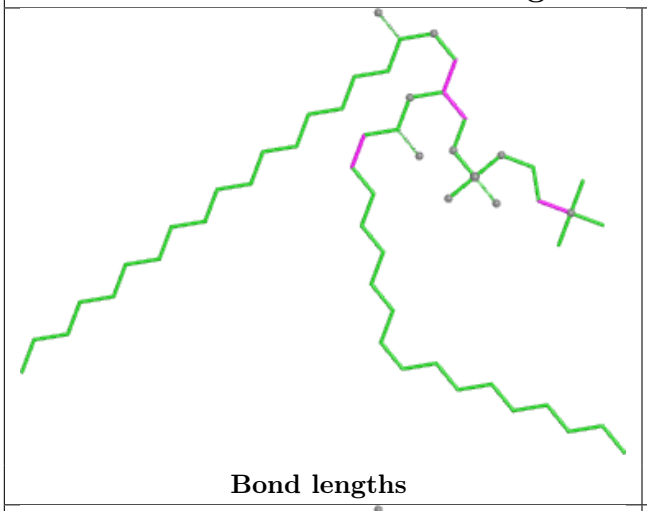


Torsions

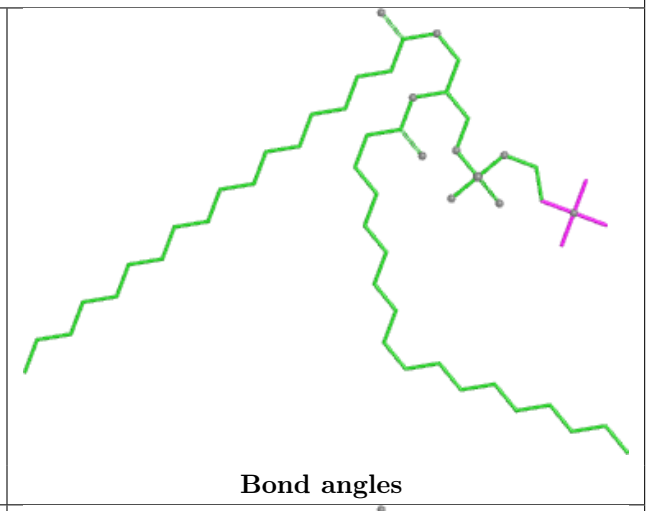


Rings

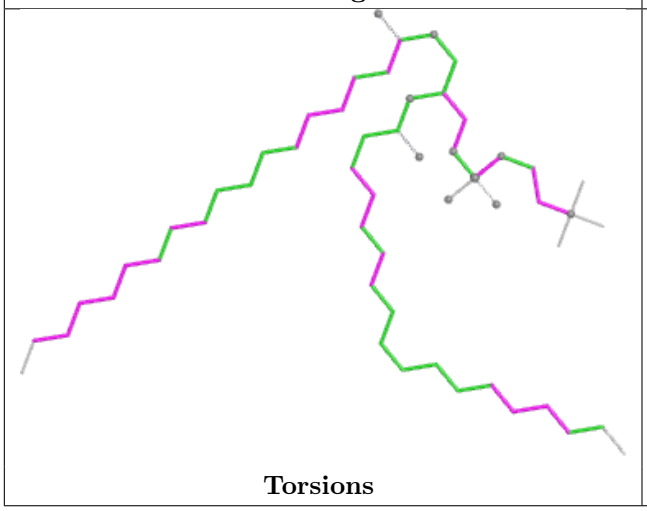
Ligand PCW A 56



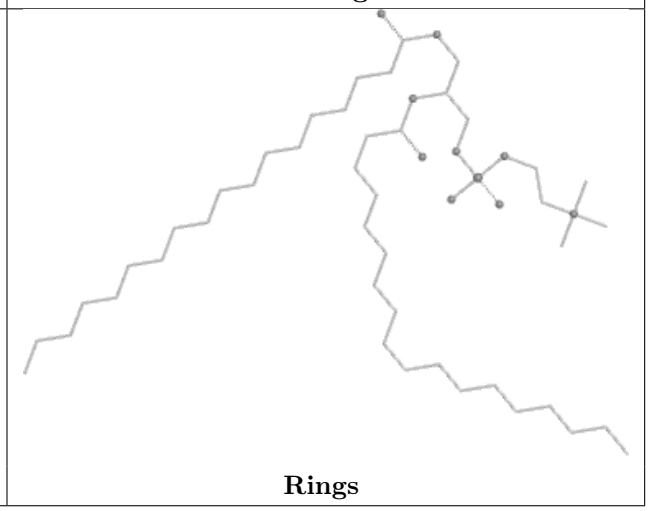
Bond lengths



Bond angles

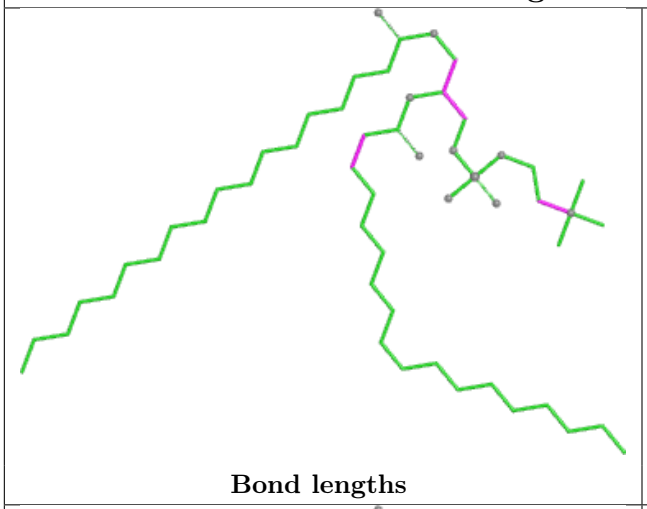


Torsions

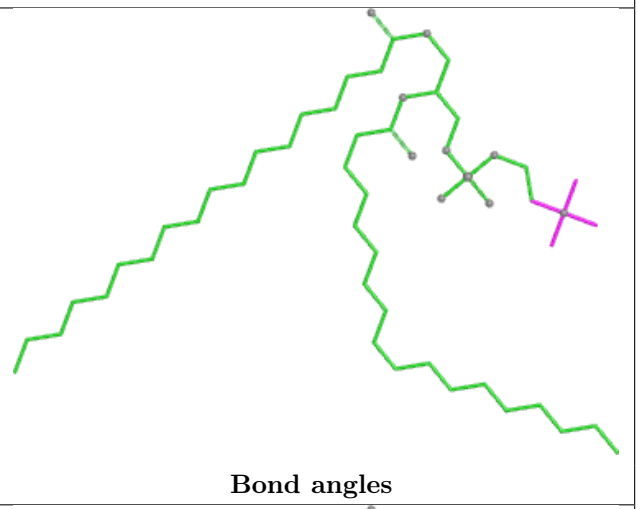


Rings

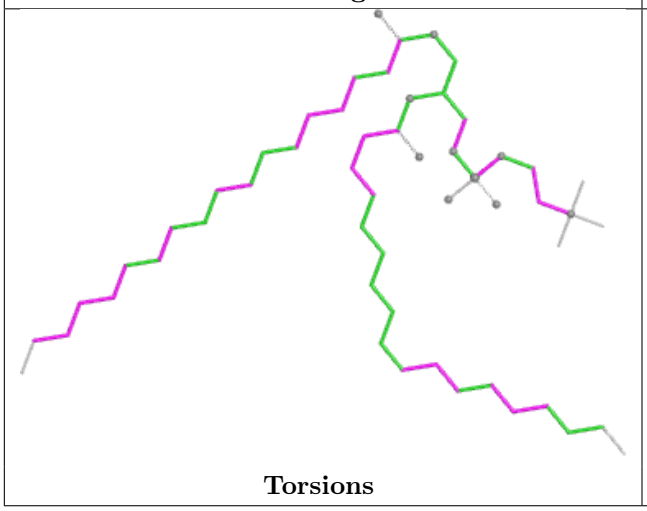
Ligand PCW A 45



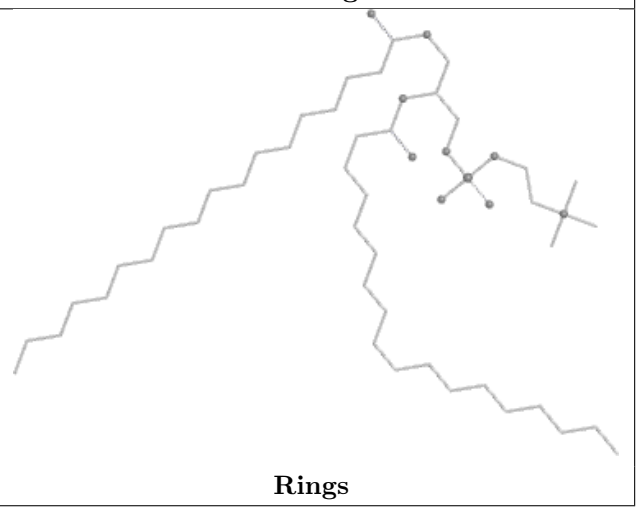
Bond lengths



Bond angles

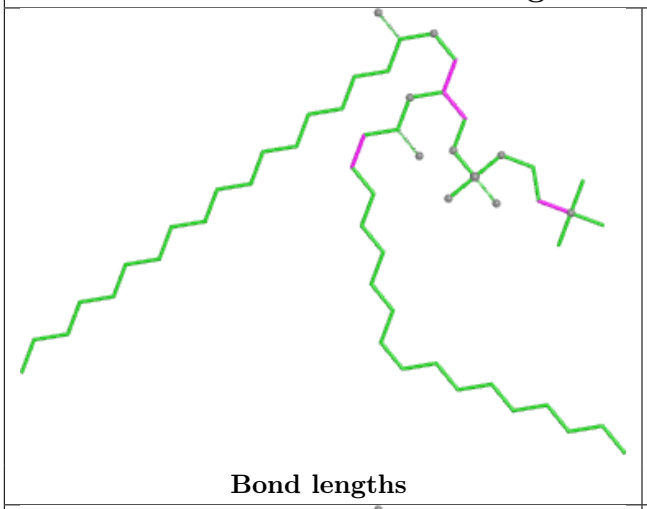


Torsions

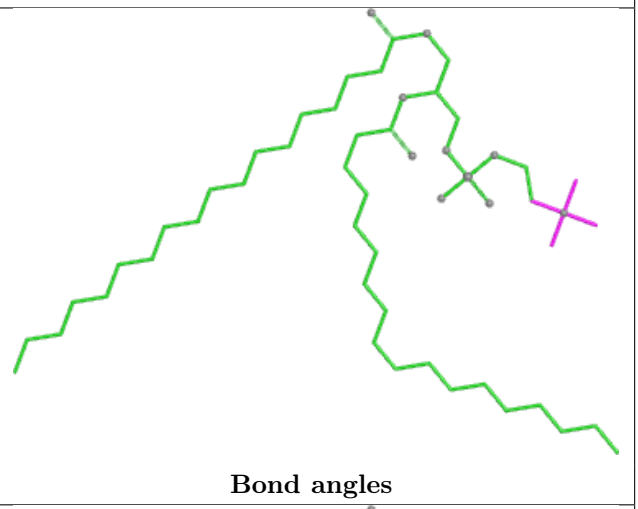


Rings

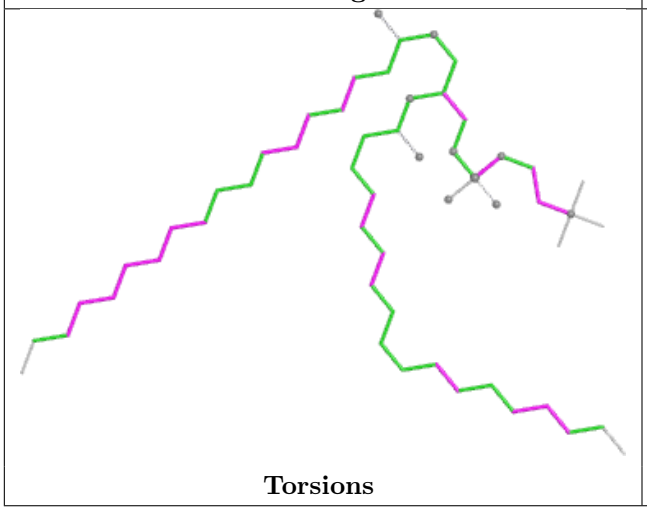
Ligand PCW A 52



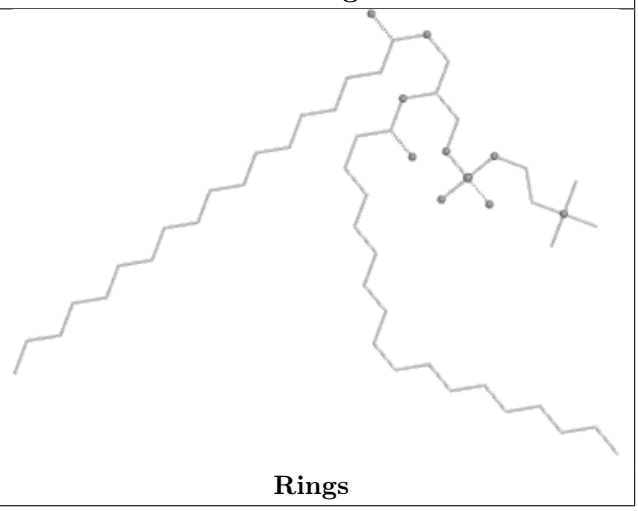
Bond lengths



Bond angles

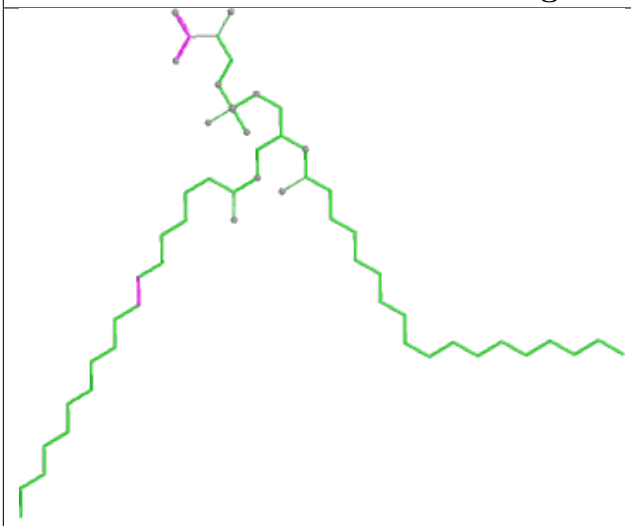


Torsions

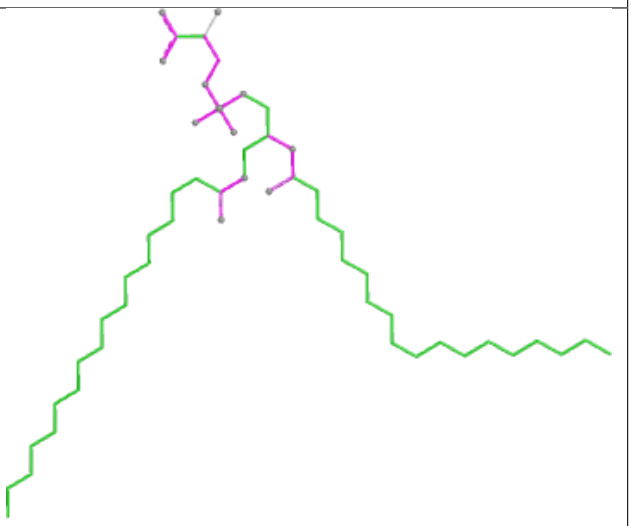


Rings

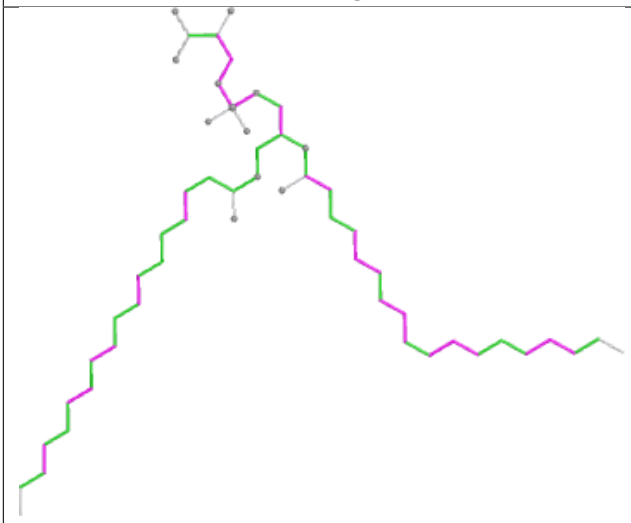
Ligand 17F A 33



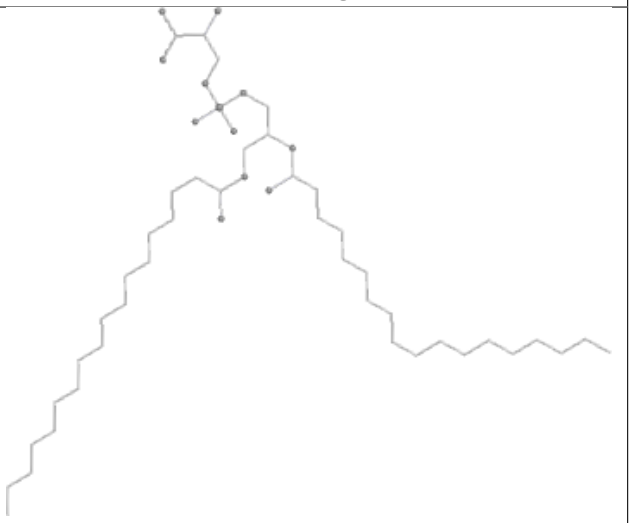
Bond lengths



Bond angles

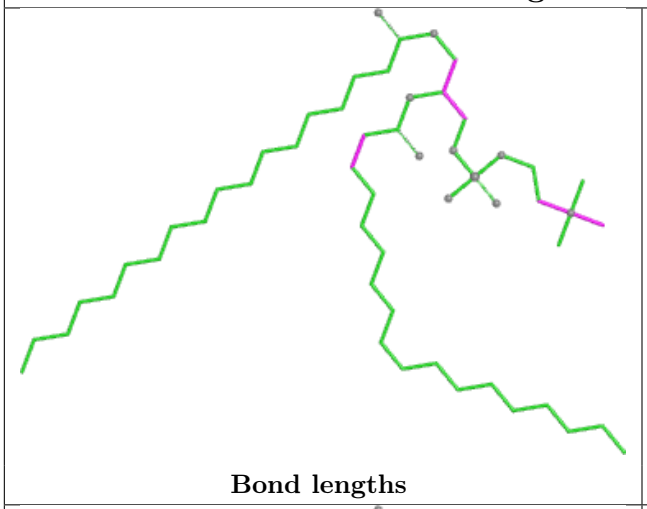


Torsions

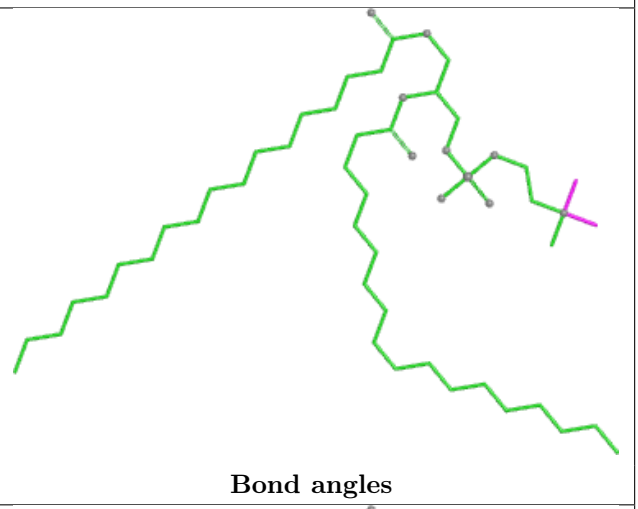


Rings

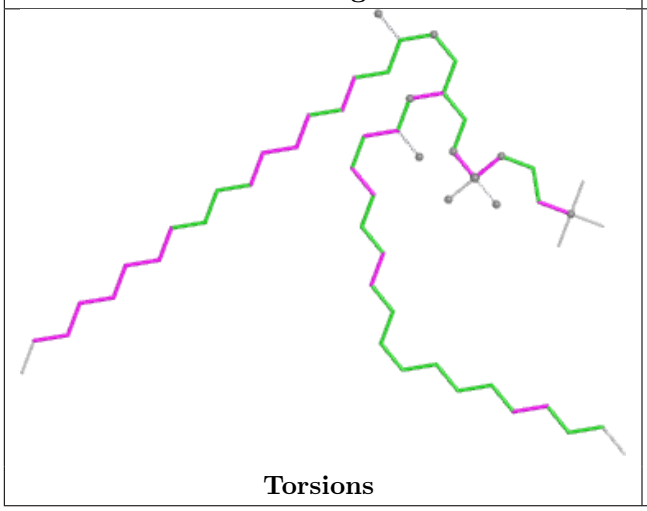
Ligand PCW A 27



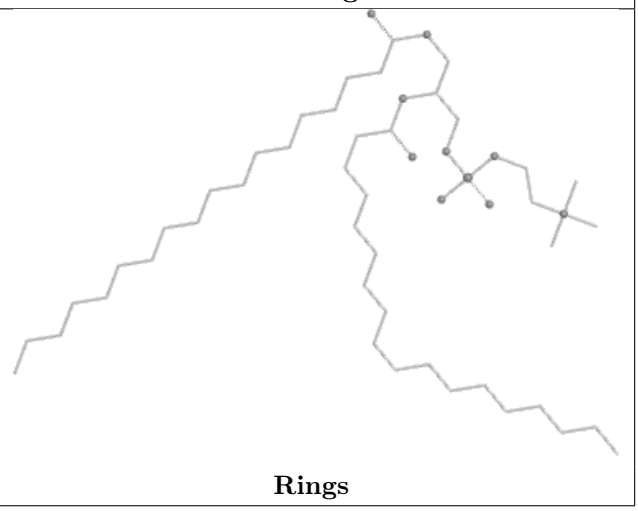
Bond lengths



Bond angles

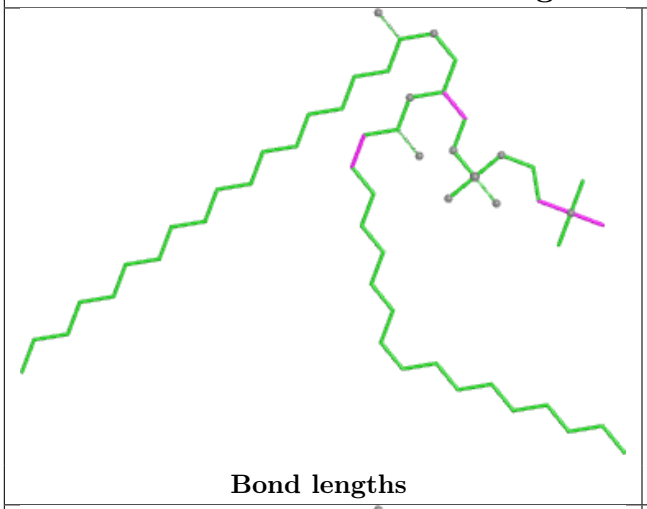


Torsions

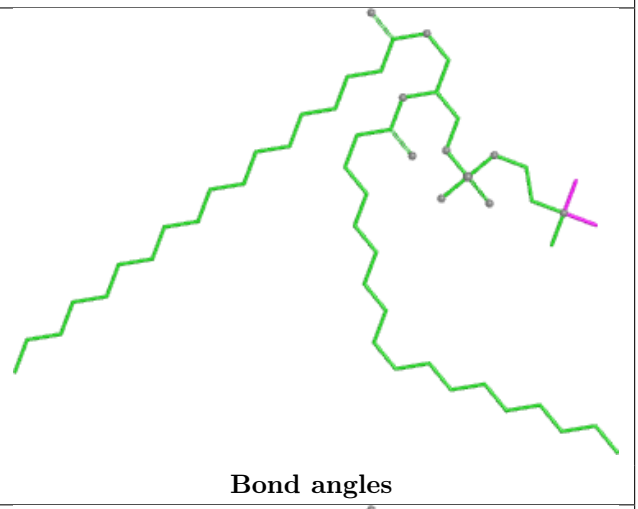


Rings

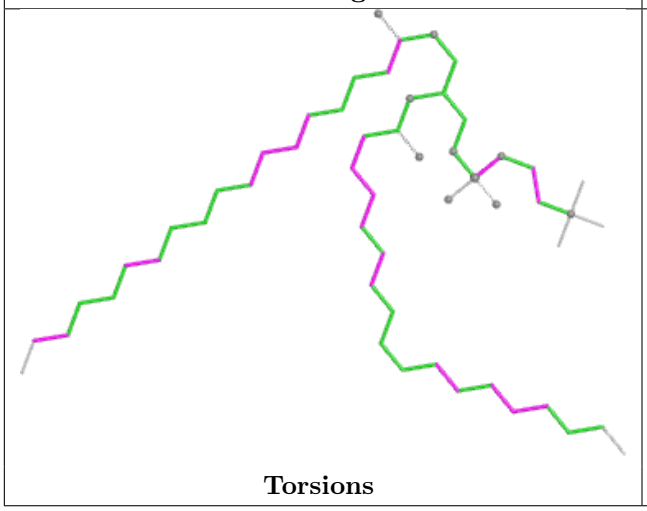
Ligand PCW A 9



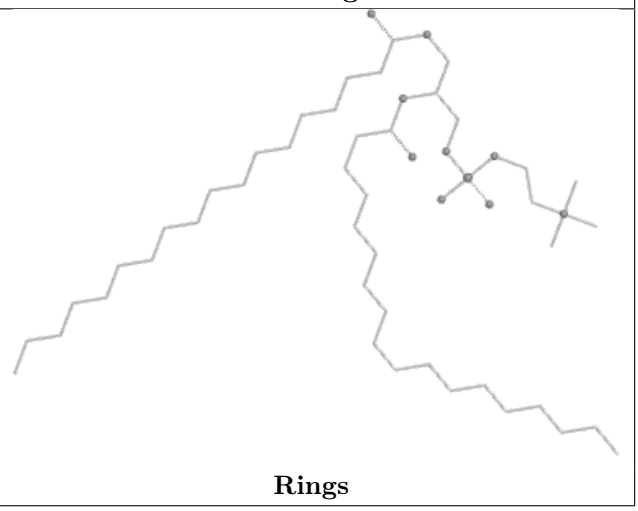
Bond lengths



Bond angles

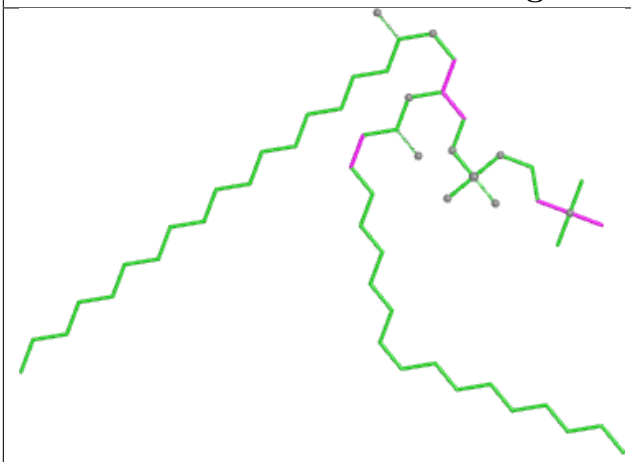


Torsions

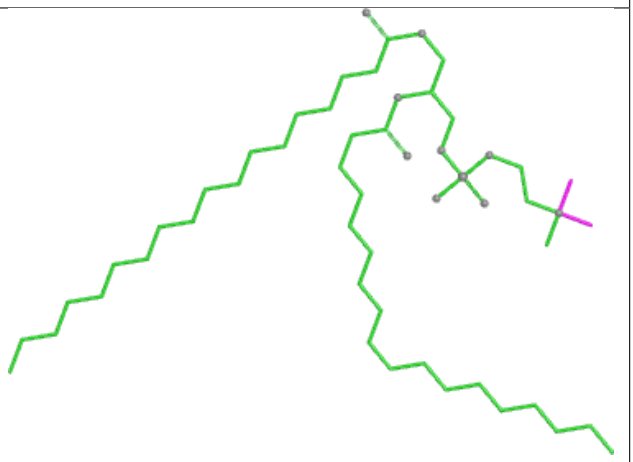


Rings

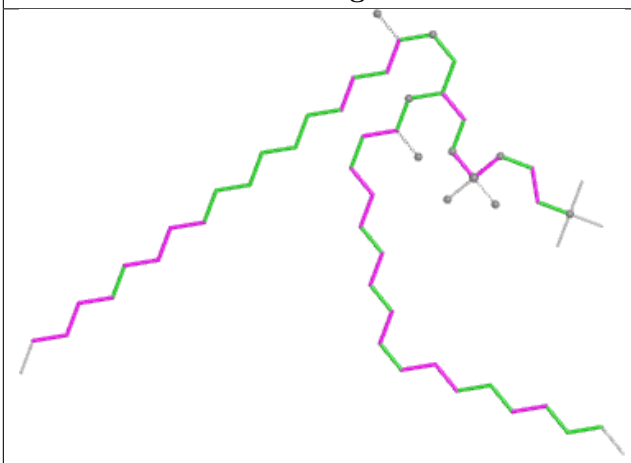
Ligand PCW A 66



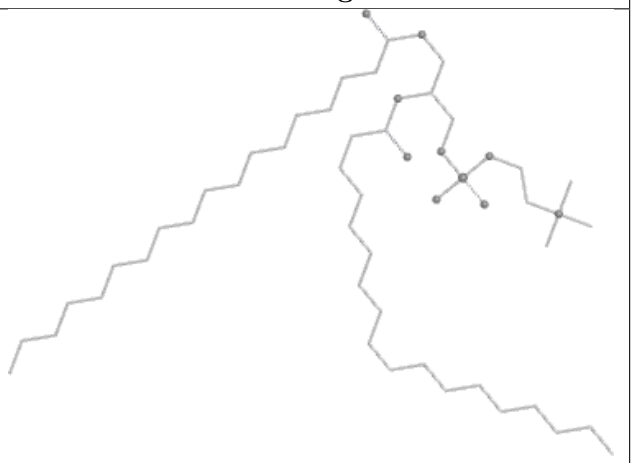
Bond lengths



Bond angles

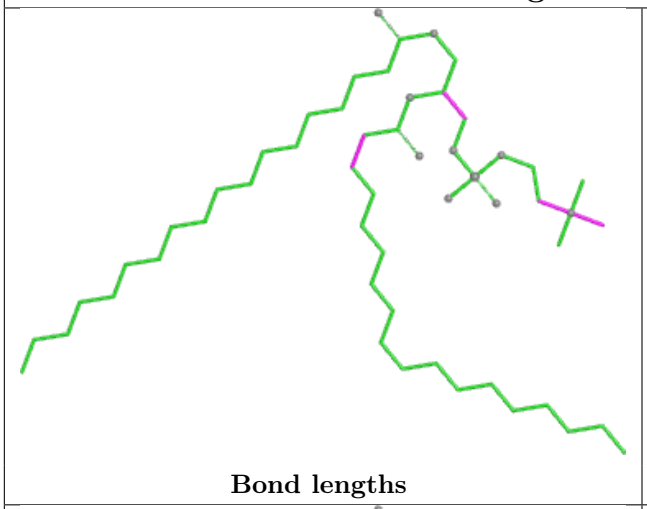


Torsions

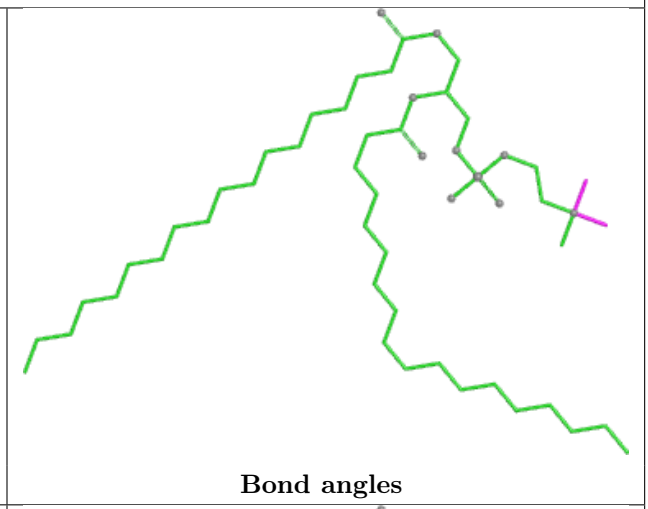


Rings

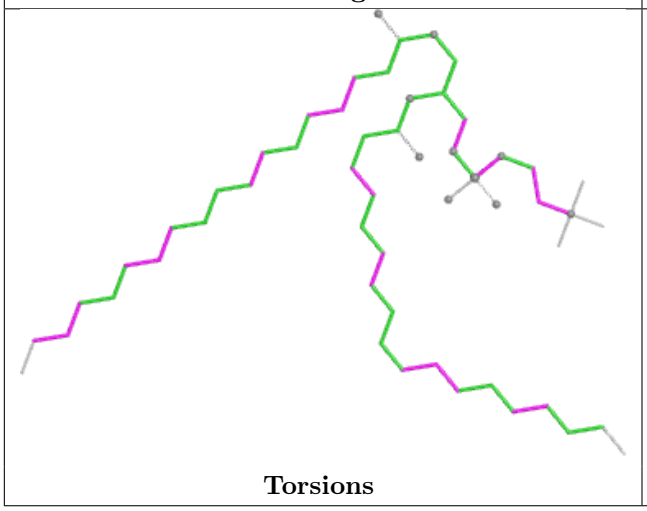
Ligand PCW A 12



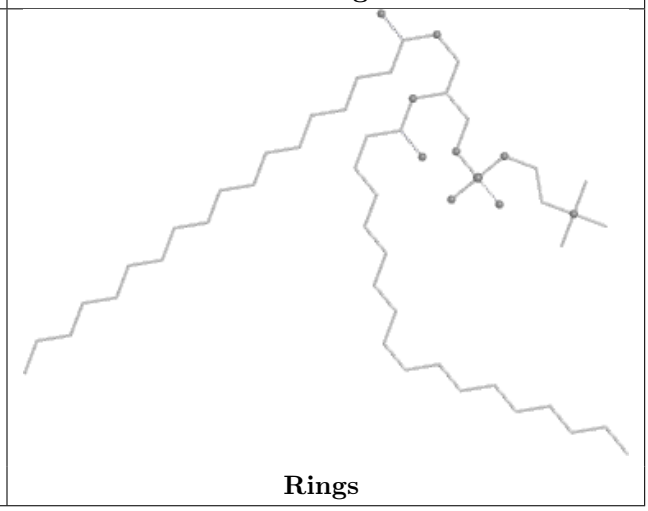
Bond lengths



Bond angles

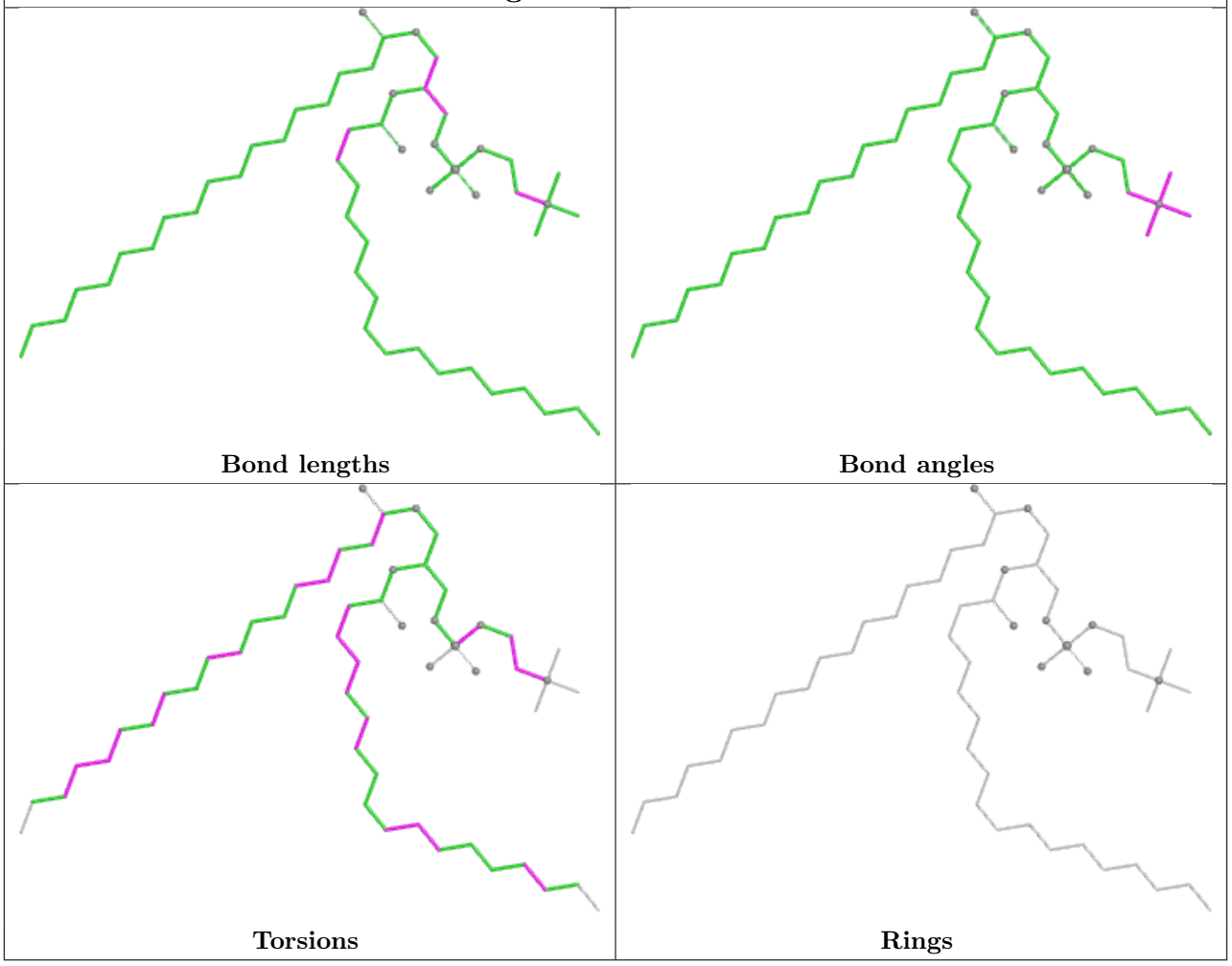


Torsions



Rings

Ligand PCW A 58



6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 1% for the well-defined parts and 1% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	44
Number of shifts mapped to atoms	11
Number of unparsed shifts	0
Number of shifts with mapping errors	33
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 33 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	21	ILE	HD11	0.004	.	1
1	B	21	ILE	HD12	0.004	.	1
1	B	21	ILE	HD13	0.004	.	1
1	B	24	ILE	HD11	0.395	.	1
1	B	24	ILE	HD12	0.395	.	1
1	B	24	ILE	HD13	0.395	.	1
1	B	36	ILE	HD11	0.633	.	1
1	B	36	ILE	HD12	0.633	.	1
1	B	36	ILE	HD13	0.633	.	1
1	B	46	ILE	HD11	0.391	.	1
1	B	46	ILE	HD12	0.391	.	1
1	B	46	ILE	HD13	0.391	.	1
1	B	55	ILE	HD11	0.468	.	1
1	B	55	ILE	HD12	0.468	.	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	55	ILE	HD13	0.468	.	1
1	B	84	ILE	HD11	0.705	.	1
1	B	84	ILE	HD12	0.705	.	1
1	B	84	ILE	HD13	0.705	.	1
1	B	93	ILE	HD11	0.744	.	1
1	B	93	ILE	HD12	0.744	.	1
1	B	93	ILE	HD13	0.744	.	1
1	B	100	ILE	HD11	0.316	.	1
1	B	100	ILE	HD12	0.316	.	1
1	B	100	ILE	HD13	0.316	.	1
1	B	139	ILE	HD11	0.816	.	1
1	B	139	ILE	HD12	0.816	.	1
1	B	139	ILE	HD13	0.816	.	1
1	B	142	ILE	HD11	0.632	.	1
1	B	142	ILE	HD12	0.632	.	1
1	B	142	ILE	HD13	0.632	.	1
1	B	163	ILE	HD11	0.595	.	1
1	B	163	ILE	HD12	0.595	.	1
1	B	163	ILE	HD13	0.595	.	1

7.1.2 Chemical shift referencing

No chemical shift referencing corrections were calculated (not enough data).

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 1%, i.e. 40 atoms were assigned a chemical shift out of a possible 7422. 0 out of 101 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/2643 (0%)	0/1068 (0%)	0/1062 (0%)	0/513 (0%)
Sidechain	40/4332 (1%)	30/2785 (1%)	10/1359 (1%)	0/188 (0%)
Aromatic	0/447 (0%)	0/231 (0%)	0/216 (0%)	0/0 (—%)
Overall	40/7422 (1%)	30/4084 (1%)	10/2637 (0%)	0/701 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 1%, i.e. 44 atoms were assigned a chemical shift out of a possible 8175. 0 out of 108 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/2895 (0%)	0/1170 (0%)	0/1162 (0%)	0/563 (0%)
Sidechain	44/4808 (1%)	33/3087 (1%)	11/1505 (1%)	0/216 (0%)
Aromatic	0/472 (0%)	0/244 (0%)	0/228 (0%)	0/0 (—%)
Overall	44/8175 (1%)	33/4501 (1%)	11/2895 (0%)	0/779 (0%)

7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain B: