Full wwPDB NMR Structure Validation Report (i)

Sep 14, 2020 – 08:15 PM BST

PDB ID	:	6CLZ
Title	:	MT1-MMP HPX domain with Blade 4 Loop Bound to Nanodiscs
Authors	:	Marcink, T.C.; Van Doren, S.R.
Deposited on	:	2018-03-02

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 following versions of software and data (see references (1)) were used in the production of this report:

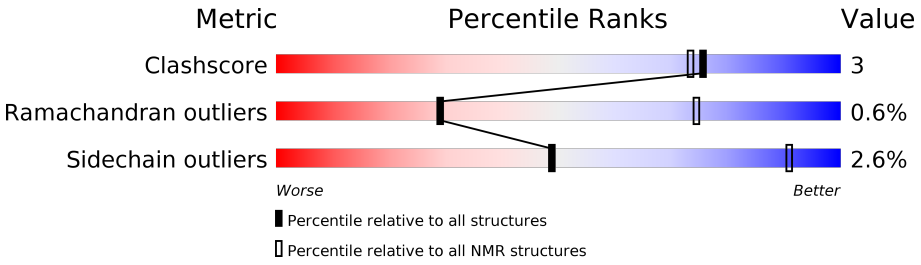
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.14.4.dev1
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.4.dev1

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 3%.

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	196	76% 23% .
2	B	211	85% 14%
2	C	211	85% 14%

2 Ensemble composition and analysis

This entry contains 15 models. Model 9 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:316-A:511, B:55-B:265, C:55-C:265 (618)	0.92	9

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 4 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6
2	7, 8, 9, 10
3	13, 14, 15
4	11, 12

3 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 35924 atoms, of which 20751 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Matrix metalloproteinase-14.

Mol	Chain	Residues	Atoms						Trace
1	A	196	Total	C	H	N	O	S	0
			3202	1067	1565	277	284	9	

- Molecule 2 is a protein called Apolipoprotein A-I.

Mol	Chain	Residues	Atoms						Trace
2	B	211	Total	C	H	N	O	S	0
			3498	1101	1745	308	340	4	
2	C	211	Total	C	H	N	O	S	0
			3498	1101	1745	308	340	4	

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	99	PRO	-	insertion	UNP P02647
B	100	TYR	-	insertion	UNP P02647
B	101	LEU	-	insertion	UNP P02647
B	102	ASP	-	insertion	UNP P02647
B	103	ASP	-	insertion	UNP P02647
B	104	PHE	-	insertion	UNP P02647
B	105	GLN	-	insertion	UNP P02647
B	106	LYS	-	insertion	UNP P02647
B	107	LYS	-	insertion	UNP P02647
B	108	TRP	-	insertion	UNP P02647
B	109	GLN	-	insertion	UNP P02647
B	110	GLU	-	insertion	UNP P02647
B	111	GLU	-	insertion	UNP P02647
B	112	MET	-	insertion	UNP P02647
B	113	GLU	-	insertion	UNP P02647
B	114	LEU	-	insertion	UNP P02647
B	115	TYR	-	insertion	UNP P02647
B	116	ARG	-	insertion	UNP P02647
B	117	GLN	-	insertion	UNP P02647
B	118	LYS	-	insertion	UNP P02647
B	119	VAL	-	insertion	UNP P02647
B	120	GLU	-	insertion	UNP P02647
C	99	PRO	-	insertion	UNP P02647

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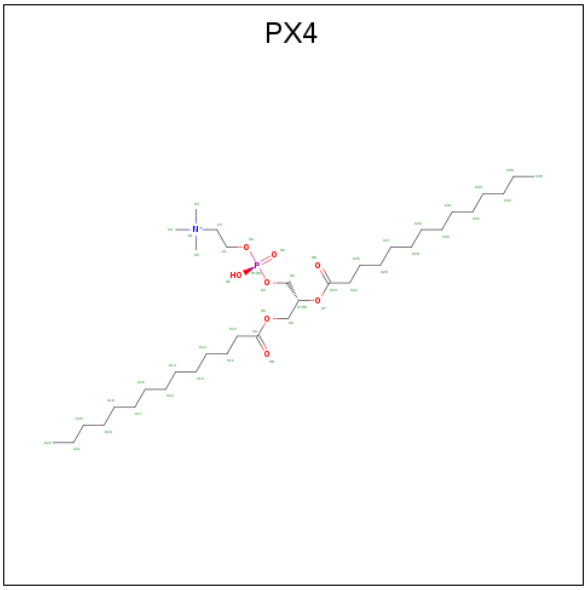
Chain	Residue	Modelled	Actual	Comment	Reference
C	100	TYR	-	insertion	UNP P02647
C	101	LEU	-	insertion	UNP P02647
C	102	ASP	-	insertion	UNP P02647
C	103	ASP	-	insertion	UNP P02647
C	104	PHE	-	insertion	UNP P02647
C	105	GLN	-	insertion	UNP P02647
C	106	LYS	-	insertion	UNP P02647
C	107	LYS	-	insertion	UNP P02647
C	108	TRP	-	insertion	UNP P02647
C	109	GLN	-	insertion	UNP P02647
C	110	GLU	-	insertion	UNP P02647
C	111	GLU	-	insertion	UNP P02647
C	112	MET	-	insertion	UNP P02647
C	113	GLU	-	insertion	UNP P02647
C	114	LEU	-	insertion	UNP P02647
C	115	TYR	-	insertion	UNP P02647
C	116	ARG	-	insertion	UNP P02647
C	117	GLN	-	insertion	UNP P02647
C	118	LYS	-	insertion	UNP P02647
C	119	VAL	-	insertion	UNP P02647
C	120	GLU	-	insertion	UNP P02647

- Molecule 3 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PX4) (formula: $C_{36}H_{73}NO_8P$).



Mol	Chain	Residues	Atoms					
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3	A	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	A	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	A	1	Total	C	H	N	O	P
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Mol	Chain	Residues	Atoms					
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3	A	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	A	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	A	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	A	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	A	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	A	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	A	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	A	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	A	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	A	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	A	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	A	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	A	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	A	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	A	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	A	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	A	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	A	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	A	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	A	1	Total 118	C 36	H 72	N 1	O 8	P 1

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Mol	Chain	Residues	Atoms
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3	A	1	Total C H N O P 118 36 72 1 8 1
3	A	1	Total C H N O P 118 36 72 1 8 1
3	A	1	Total C H N O P 118 36 72 1 8 1
3	A	1	Total C H N O P 118 36 72 1 8 1
3	B	1	Total C H N O P 118 36 72 1 8 1
3	B	1	Total C H N O P 118 36 72 1 8 1
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3	B	1	Total	C	H	N	O	P
			118	36	72	1	8	1
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3	B	1	Total	C	H	N	O	P
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			118	36	72	1	8	1

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Mol	Chain	Residues	Atoms					
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			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
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3	C	1	Total	C	H	N	O	P
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			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
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3	C	1	Total	C	H	N	O	P
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			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1

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Mol	Chain	Residues	Atoms					
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1

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Mol	Chain	Residues	Atoms					
3	C	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	C	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	C	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	C	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	C	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	C	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	C	1	Total 118	C 36	H 72	N 1	O 8	P 1

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	
4	A	1	Total 1	Na 1

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	
5	A	1	Total 1	Cl 1

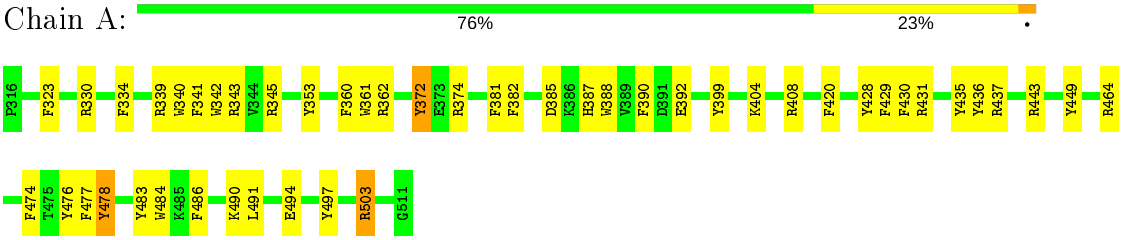
4 Residue-property plots

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.

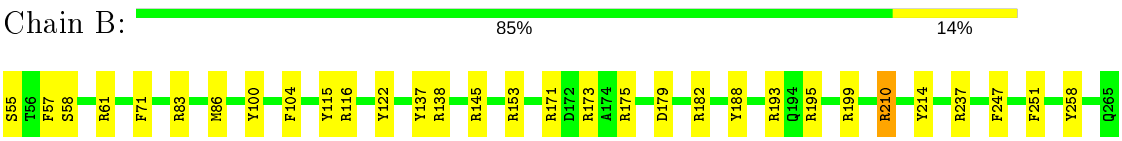
• Molecule 1: Matrix metalloproteinase-14

Chain A:



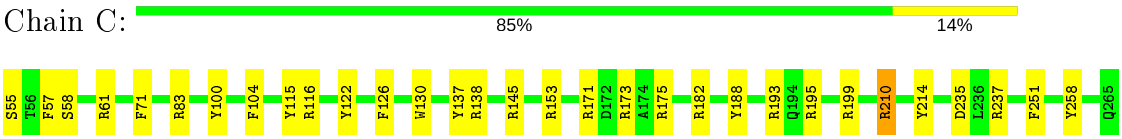
• Molecule 2: Apolipoprotein A-I

Chain B:



• Molecule 2: Apolipoprotein A-I

Chain C:



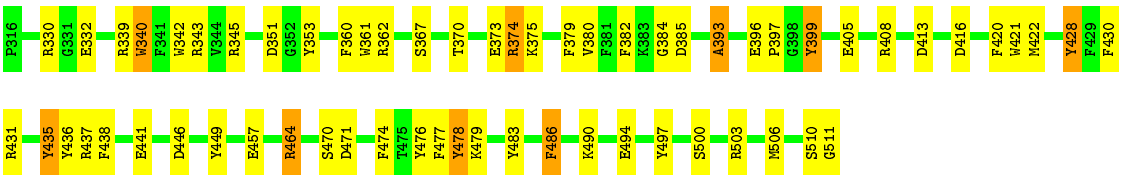
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

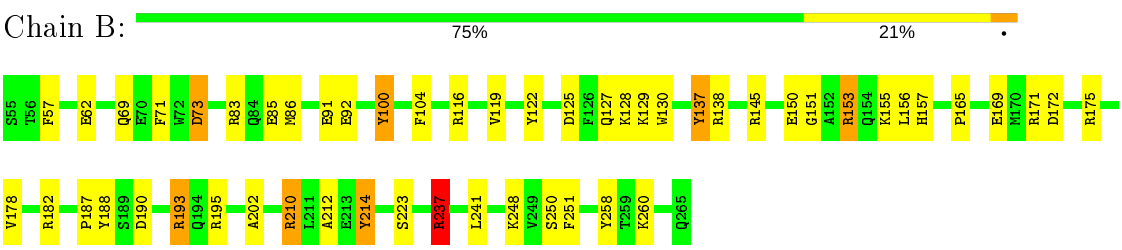
4.2.1 Score per residue for model 1

• Molecule 1: Matrix metalloproteinase-14

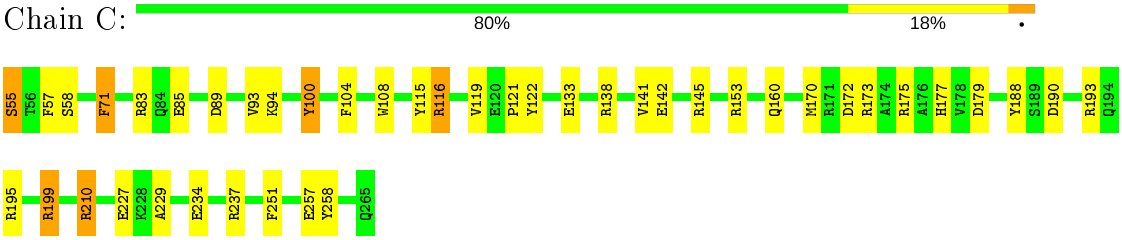
Chain A:



• Molecule 2: Apolipoprotein A-I

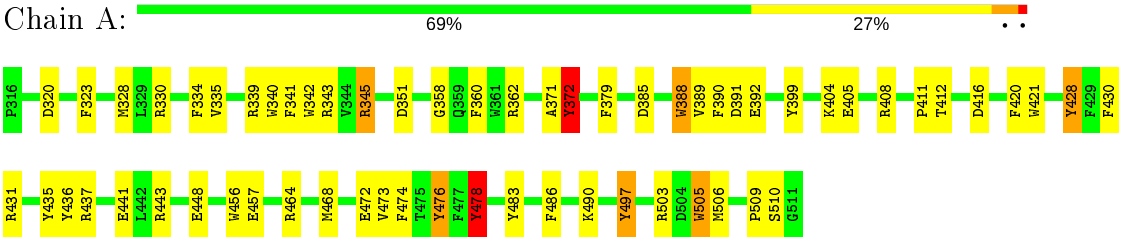


• Molecule 2: Apolipoprotein A-I

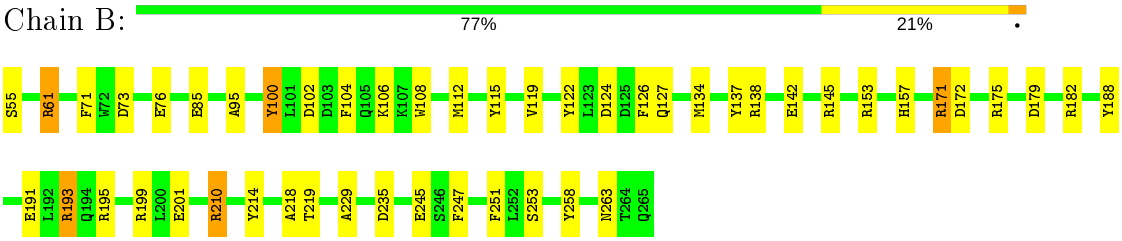


4.2.2 Score per residue for model 2

• Molecule 1: Matrix metalloproteinase-14

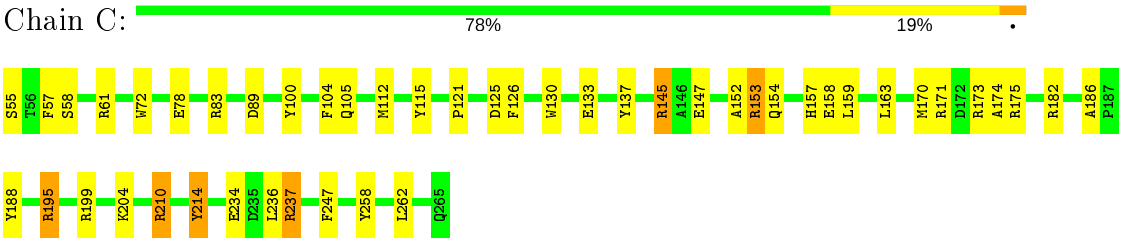


• Molecule 2: Apolipoprotein A-I



• Molecule 2: Apolipoprotein A-I

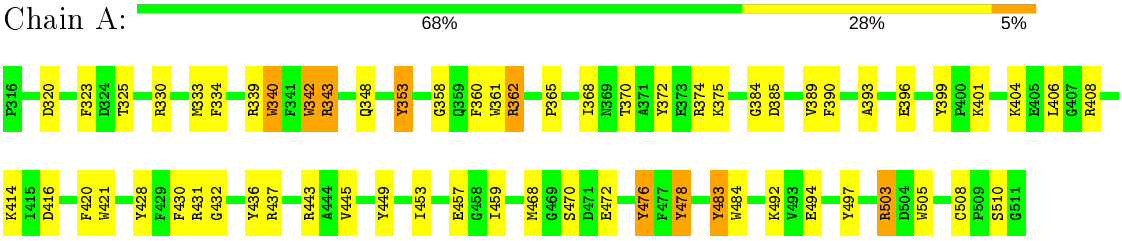
Chain C:



4.2.3 Score per residue for model 3

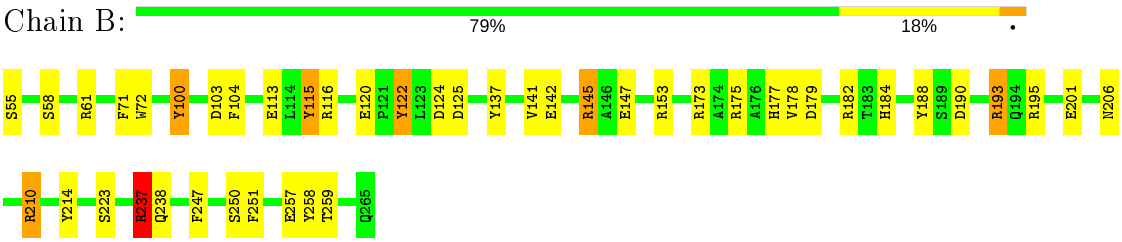
- Molecule 1: Matrix metalloproteinase-14

Chain A:



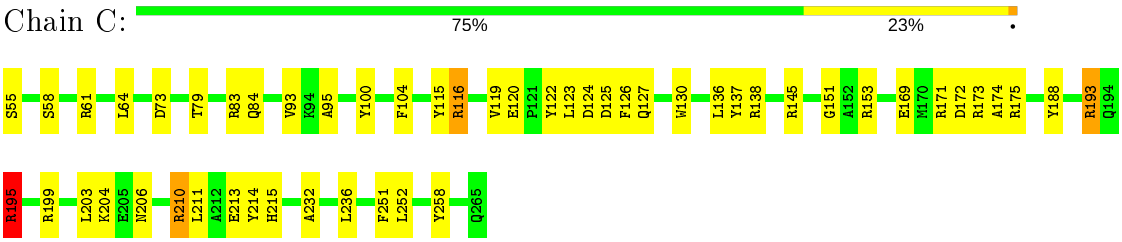
- Molecule 2: Apolipoprotein A-I

Chain B:



- Molecule 2: Apolipoprotein A-I

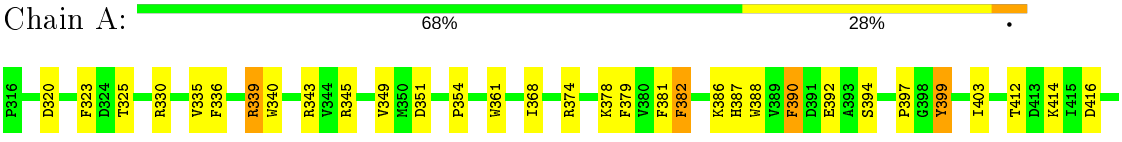
Chain C:



4.2.4 Score per residue for model 4

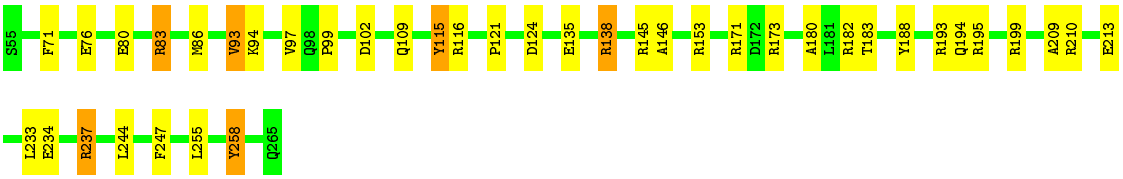
- Molecule 1: Matrix metalloproteinase-14

Chain A:



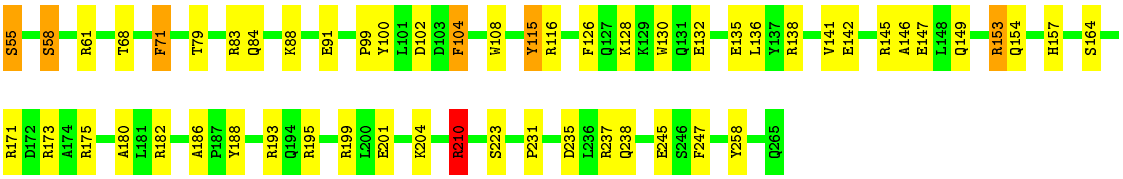
• Molecule 2: Apolipoprotein A-I

Chain B:



• Molecule 2: Apolipoprotein A-I

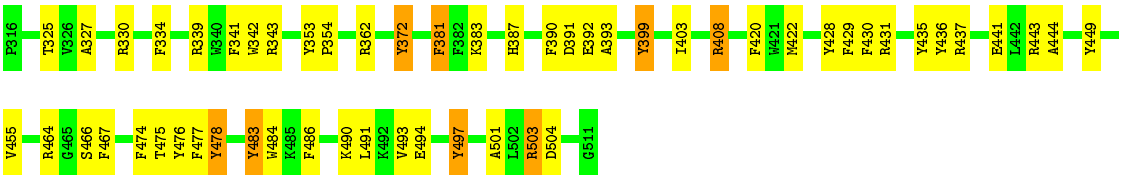
Chain C:



4.2.5 Score per residue for model 5

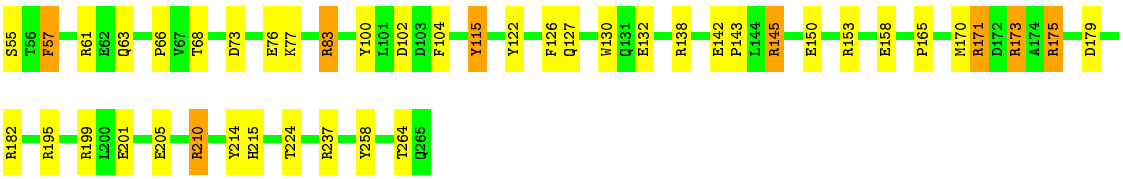
• Molecule 1: Matrix metalloproteinase-14

Chain A:



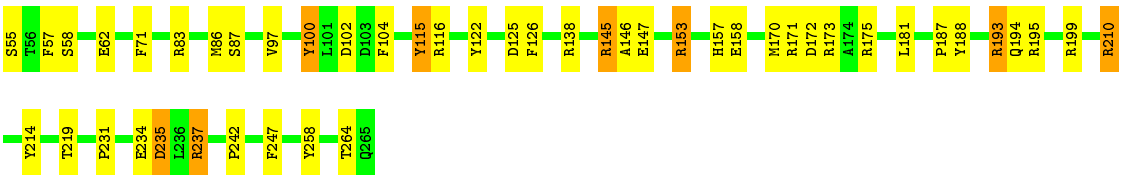
• Molecule 2: Apolipoprotein A-I

Chain B:



• Molecule 2: Apolipoprotein A-I

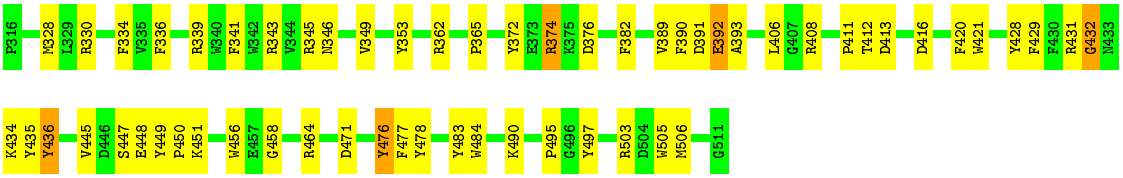
Chain C:



4.2.6 Score per residue for model 6

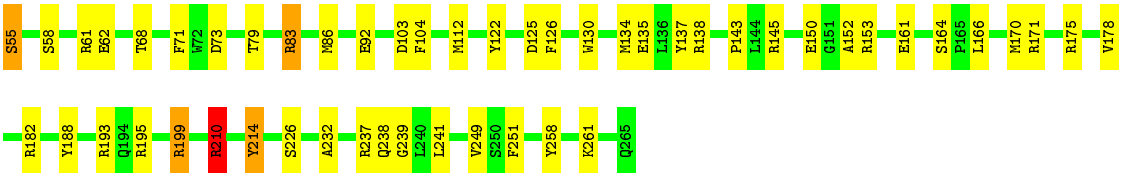
- Molecule 1: Matrix metalloproteinase-14

Chain A:



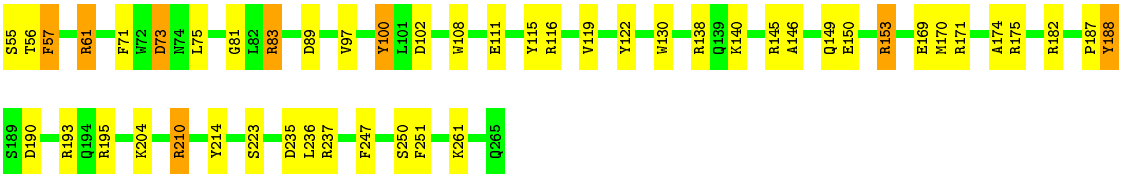
- Molecule 2: Apolipoprotein A-I

Chain B:



- Molecule 2: Apolipoprotein A-I

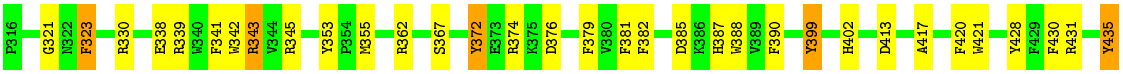
Chain C:



4.2.7 Score per residue for model 7

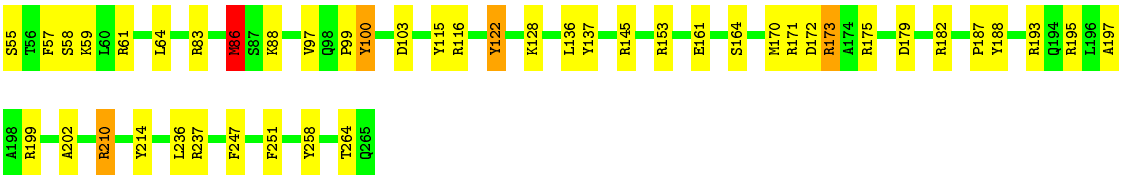
- Molecule 1: Matrix metalloproteinase-14

Chain A:



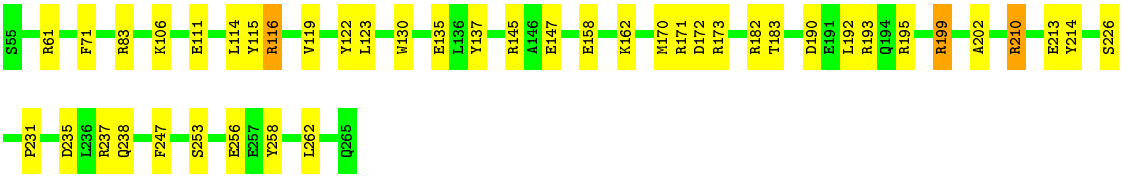
• Molecule 2: Apolipoprotein A-I

Chain B:



• Molecule 2: Apolipoprotein A-I

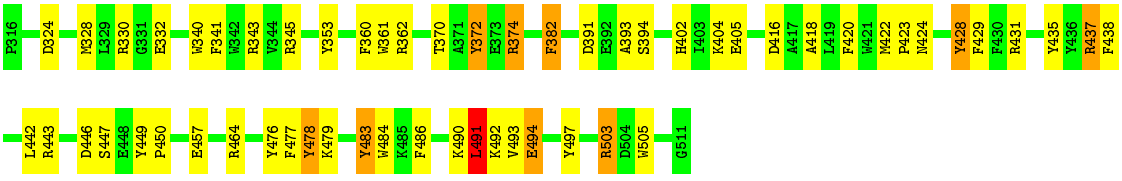
Chain C:



4.2.8 Score per residue for model 8

• Molecule 1: Matrix metalloproteinase-14

Chain A:

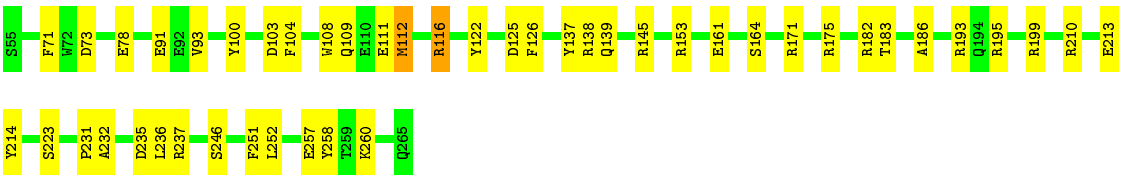


• Molecule 2: Apolipoprotein A-I

Chain B:

• Molecule 2: Apolipoprotein A-I

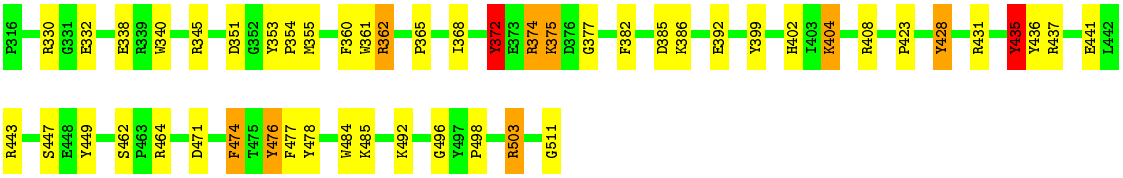
Chain C:



4.2.9 Score per residue for model 9 (medoid)

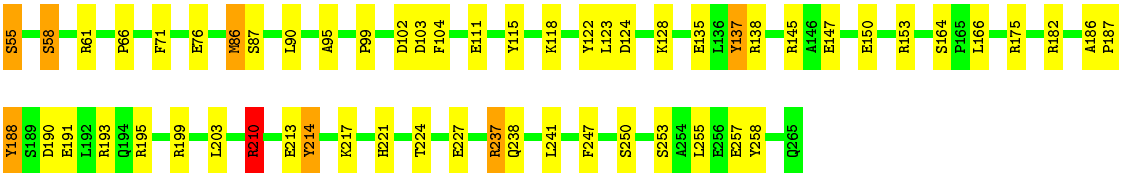
- Molecule 1: Matrix metalloproteinase-14

Chain A:



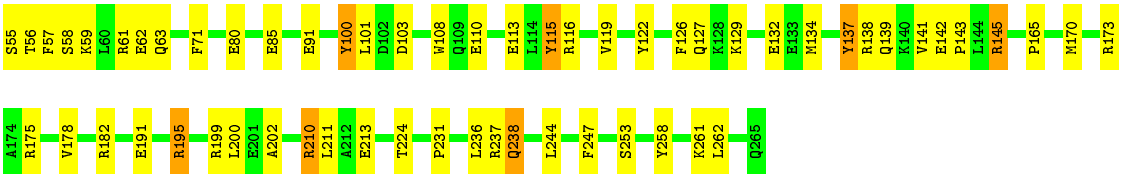
- Molecule 2: Apolipoprotein A-I

Chain B:



- Molecule 2: Apolipoprotein A-I

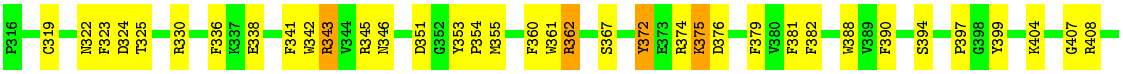
Chain C:

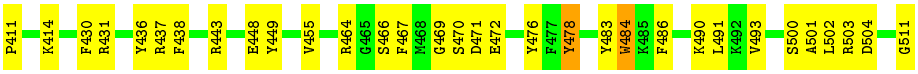


4.2.10 Score per residue for model 10

- Molecule 1: Matrix metalloproteinase-14

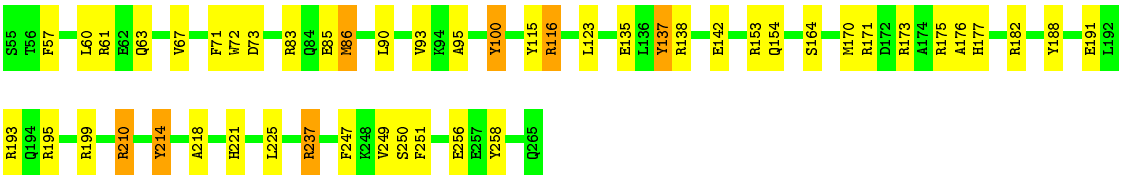
Chain A:





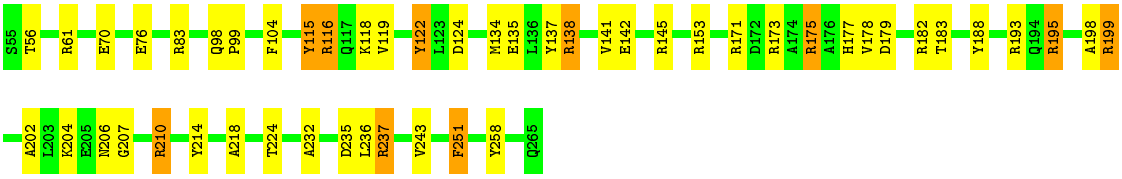
• Molecule 2: Apolipoprotein A-I

Chain B:



• Molecule 2: Apolipoprotein A-I

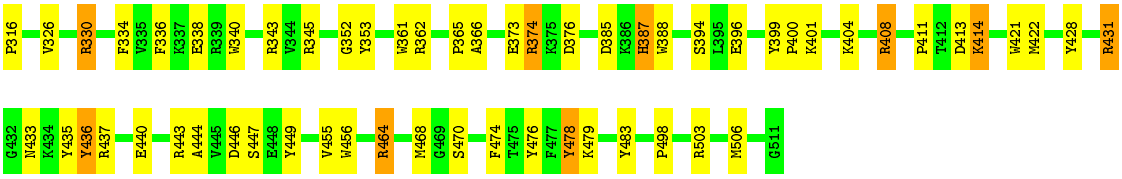
Chain C:



4.2.11 Score per residue for model 11

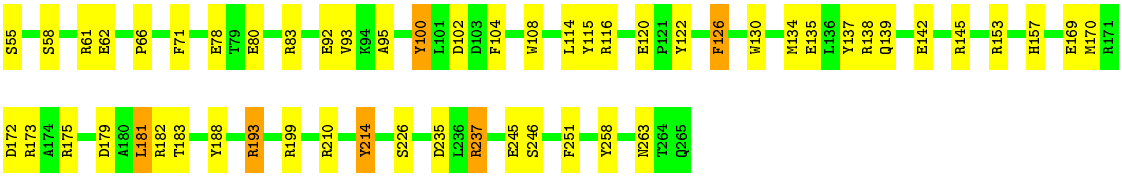
• Molecule 1: Matrix metalloproteinase-14

Chain A:



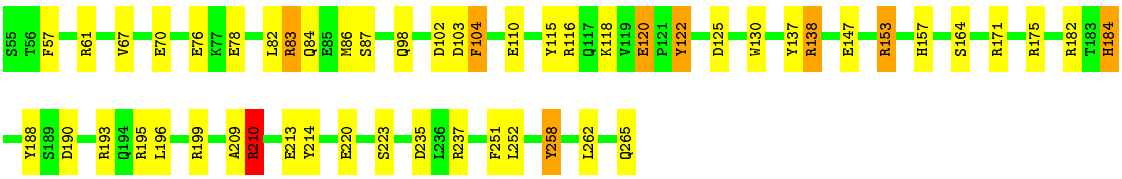
• Molecule 2: Apolipoprotein A-I

Chain B:



• Molecule 2: Apolipoprotein A-I

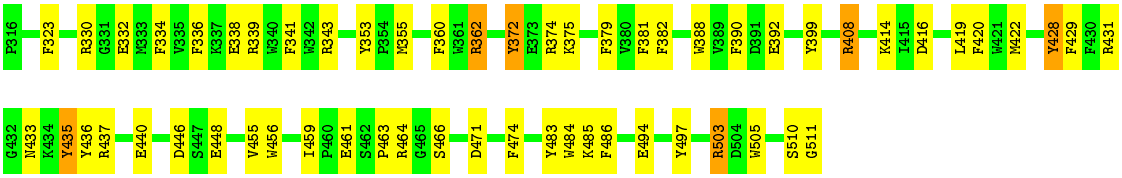
Chain C:



4.2.12 Score per residue for model 12

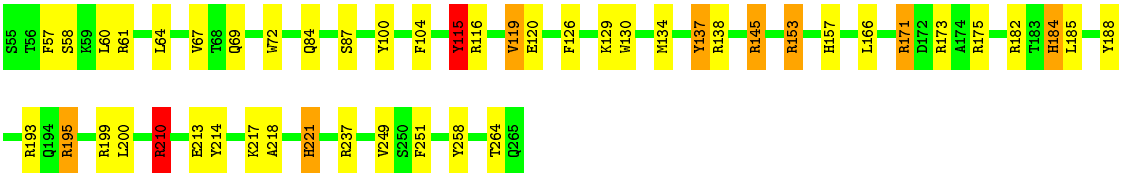
- Molecule 1: Matrix metalloproteinase-14

Chain A:



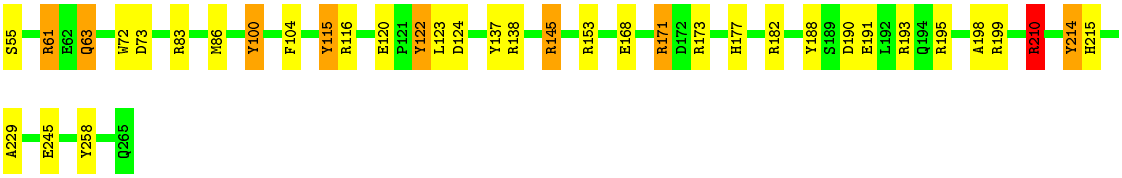
- Molecule 2: Apolipoprotein A-I

Chain B:



- Molecule 2: Apolipoprotein A-I

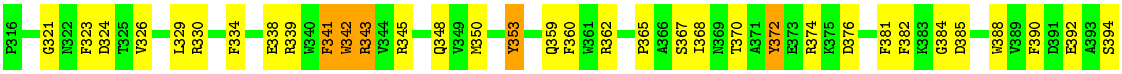
Chain C:



4.2.13 Score per residue for model 13

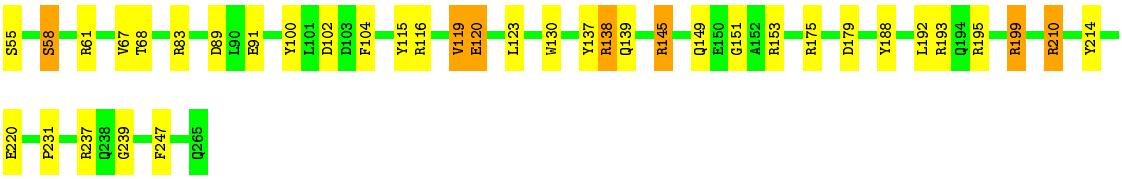
- Molecule 1: Matrix metalloproteinase-14

Chain A:



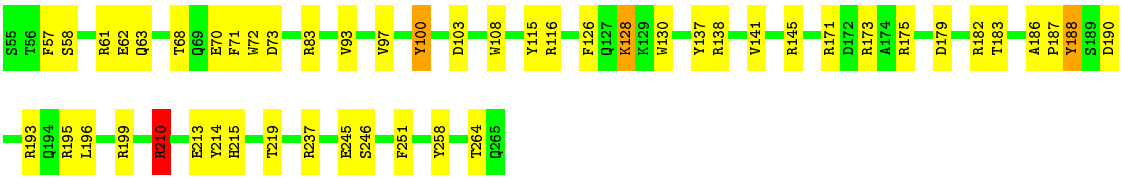
• Molecule 2: Apolipoprotein A-I

Chain B:



• Molecule 2: Apolipoprotein A-I

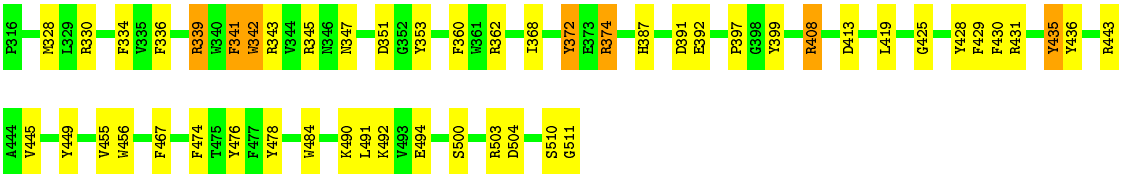
Chain C:



4.2.14 Score per residue for model 14

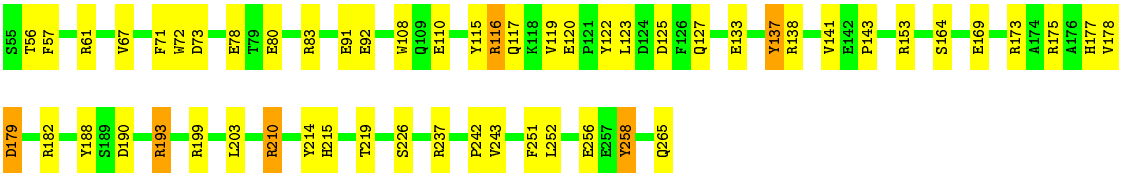
• Molecule 1: Matrix metalloproteinase-14

Chain A:



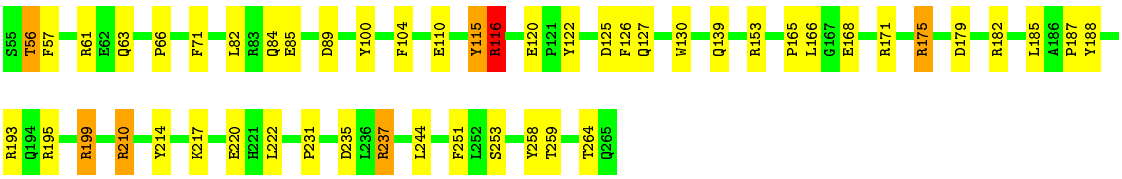
• Molecule 2: Apolipoprotein A-I

Chain B:



• Molecule 2: Apolipoprotein A-I

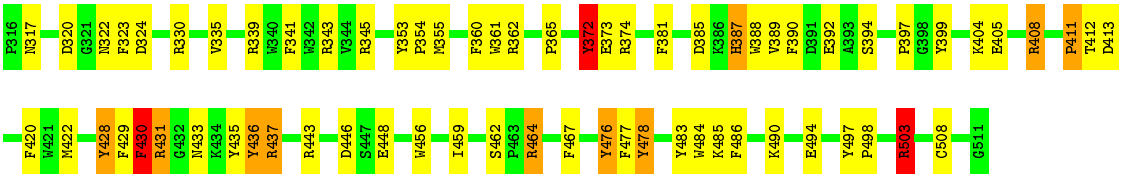
Chain C:



4.2.15 Score per residue for model 15

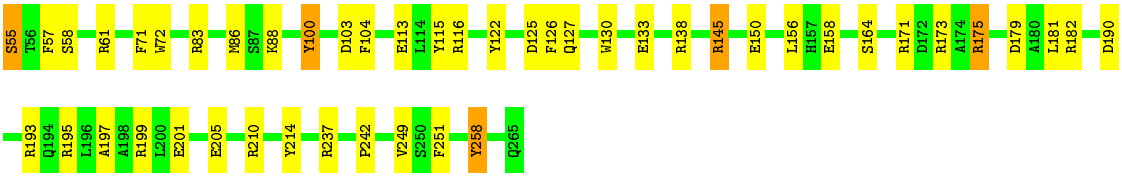
• Molecule 1: Matrix metalloproteinase-14

Chain A:



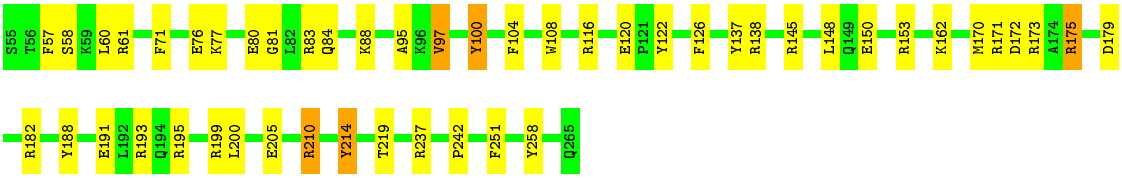
• Molecule 2: Apolipoprotein A-I

Chain B:



• Molecule 2: Apolipoprotein A-I

Chain C:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 500 calculated structures, 15 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
HADDOCK	structure calculation	HADDOCK2.1
NAMD	structure calculation	NAMD2.1 with CUDA GPU processing
NAMD	refinement	NAMD2.1 with CUDA GPU processing

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	324
Number of shifts mapped to atoms	324
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	3%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CL, PX4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.72±0.03	14±4/1696 (0.8± 0.2%)	2.13±0.05	59±5/2286 (2.6± 0.2%)
2	B	1.67±0.03	11±4/1784 (0.6± 0.2%)	2.08±0.08	50±6/2394 (2.1± 0.2%)
2	C	1.67±0.04	11±3/1784 (0.6± 0.2%)	2.08±0.05	50±7/2394 (2.1± 0.3%)
All	All	1.68	534/78960 (0.7%)	2.10	2377/106110 (2.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	8.5±2.2
2	B	0.0±0.0	6.5±1.3
2	C	0.0±0.0	5.7±2.4
All	All	0	310

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
2	C	100	TYR	CB-CG	9.02	1.65	1.51	9	1
1	A	428	TYR	CE1-CZ	9.01	1.50	1.38	2	3
1	A	372	TYR	CE1-CZ	8.91	1.50	1.38	6	2
1	A	435	TYR	CG-CD2	8.43	1.50	1.39	13	3
1	A	421	TRP	CD2-CE2	8.36	1.51	1.41	7	1
1	A	353	TYR	CG-CD1	8.20	1.49	1.39	6	1
1	A	470	SER	CA-CB	8.06	1.65	1.52	3	3
2	C	58	SER	CA-CB	8.03	1.65	1.52	13	2
2	B	122	TYR	CG-CD1	8.02	1.49	1.39	5	2
2	B	256	GLU	CD-OE2	7.99	1.34	1.25	14	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	C	223	SER	CA-CB	7.98	1.65	1.52	11	3
2	C	253	SER	CA-CB	7.85	1.64	1.52	9	3
2	B	164	SER	CA-CB	7.82	1.64	1.52	9	2
2	B	169	GLU	CD-OE2	7.78	1.34	1.25	14	1
1	A	421	TRP	NE1-CE2	-7.76	1.27	1.37	1	1
1	A	511	GLY	CA-C	7.71	1.64	1.51	12	3
1	A	342	TRP	NE1-CE2	-7.61	1.27	1.37	3	2
2	B	258	TYR	CE2-CZ	7.58	1.48	1.38	3	2
2	B	137	TYR	CB-CG	-7.56	1.40	1.51	11	1
1	A	436	TYR	CE1-CZ	7.55	1.48	1.38	6	2
2	B	55	SER	CA-CB	7.53	1.64	1.52	15	3
2	C	258	TYR	CG-CD1	7.52	1.49	1.39	1	4
2	B	226	SER	CA-CB	7.52	1.64	1.52	11	2
1	A	353	TYR	CG-CD2	7.46	1.48	1.39	8	1
2	B	85	GLU	CD-OE2	7.42	1.33	1.25	10	2
1	A	458	GLY	N-CA	7.40	1.57	1.46	6	1
2	B	78	GLU	CD-OE2	7.38	1.33	1.25	14	1
2	B	115	TYR	CZ-OH	7.36	1.50	1.37	11	1
2	C	100	TYR	CE2-CZ	7.33	1.48	1.38	14	1
2	B	115	TYR	CD2-CE2	7.27	1.50	1.39	8	1
2	C	165	PRO	N-CD	-7.16	1.37	1.47	9	1
2	C	132	GLU	CB-CG	7.14	1.65	1.52	4	2
2	B	153	ARG	CA-CB	7.09	1.69	1.53	8	1
2	B	57	PHE	CG-CD1	7.08	1.49	1.38	7	1
1	A	361	TRP	CG-CD1	-6.95	1.27	1.36	15	2
1	A	394	SER	CB-OG	6.94	1.51	1.42	13	1
1	A	435	TYR	CD1-CE1	6.92	1.49	1.39	8	1
1	A	503	ARG	CZ-NH2	-6.92	1.24	1.33	11	1
2	B	130	TRP	CD2-CE2	6.91	1.49	1.41	15	1
2	C	135	GLU	CG-CD	-6.90	1.41	1.51	7	1
2	C	214	TYR	CZ-OH	6.89	1.49	1.37	6	2
1	A	467	PHE	CG-CD2	6.83	1.49	1.38	10	1
1	A	367	SER	CA-CB	6.82	1.63	1.52	1	1
2	B	137	TYR	CE1-CZ	6.79	1.47	1.38	13	2
2	B	93	VAL	CB-CG2	6.79	1.67	1.52	4	1
2	C	130	TRP	NE1-CE2	-6.79	1.28	1.37	4	1
2	B	109	GLN	CA-CB	6.75	1.68	1.53	4	1
2	B	115	TYR	CB-CG	-6.75	1.41	1.51	3	1
2	B	92	GLU	CG-CD	6.74	1.62	1.51	6	1
2	B	161	GLU	CB-CG	6.72	1.65	1.52	6	1
2	C	137	TYR	CZ-OH	6.72	1.49	1.37	12	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	449	TYR	CE2-CZ	6.71	1.47	1.38	3	2
2	C	137	TYR	CE1-CZ	6.71	1.47	1.38	2	1
2	B	258	TYR	CE1-CZ	6.70	1.47	1.38	2	2
2	B	214	TYR	CG-CD2	6.68	1.47	1.39	12	1
2	B	111	GLU	CB-CG	6.67	1.64	1.52	9	1
2	B	118	LYS	N-CA	-6.64	1.33	1.46	9	1
2	C	76	GLU	CB-CG	6.64	1.64	1.52	15	1
2	C	57	PHE	CG-CD2	6.63	1.48	1.38	11	1
1	A	372	TYR	CG-CD2	6.63	1.47	1.39	2	1
2	C	122	TYR	CE2-CZ	6.61	1.47	1.38	9	1
1	A	484	TRP	CD2-CE3	6.61	1.50	1.40	10	1
1	A	466	SER	CA-CB	6.58	1.62	1.52	5	2
2	C	81	GLY	CA-C	-6.57	1.41	1.51	15	1
2	C	213	GLU	CD-OE2	6.55	1.32	1.25	3	1
2	B	150	GLU	CB-CG	6.55	1.64	1.52	5	3
2	C	257	GLU	CB-CG	6.54	1.64	1.52	1	1
2	B	247	PHE	CG-CD2	6.51	1.48	1.38	13	1
1	A	436	TYR	CD1-CE1	6.50	1.49	1.39	4	1
2	C	191	GLU	CB-CG	6.50	1.64	1.52	15	2
2	C	122	TYR	CE1-CZ	6.49	1.47	1.38	15	1
2	B	223	SER	CB-OG	-6.48	1.33	1.42	3	1
1	A	484	TRP	CG-CD1	6.44	1.45	1.36	8	1
1	A	366	ALA	CA-CB	6.43	1.66	1.52	11	1
2	B	122	TYR	CG-CD2	6.43	1.47	1.39	11	1
2	B	250	SER	CA-CB	6.43	1.62	1.52	3	3
2	C	182	ARG	CZ-NH1	-6.43	1.24	1.33	12	1
1	A	394	SER	CA-CB	6.42	1.62	1.52	8	4
2	B	120	GLU	CD-OE2	6.42	1.32	1.25	12	1
2	B	122	TYR	CZ-OH	6.42	1.48	1.37	1	2
2	C	191	GLU	CG-CD	-6.42	1.42	1.51	15	1
2	B	169	GLU	CB-CG	6.42	1.64	1.52	1	1
2	C	140	LYS	CA-CB	6.41	1.68	1.53	6	1
2	B	135	GLU	CB-CG	6.40	1.64	1.52	4	2
1	A	340	TRP	NE1-CE2	-6.40	1.29	1.37	3	1
2	C	62	GLU	CB-CG	6.39	1.64	1.52	9	2
2	C	108	TRP	CG-CD1	6.39	1.45	1.36	15	1
2	C	55	SER	CA-CB	6.39	1.62	1.52	6	4
1	A	476	TYR	CZ-OH	6.38	1.48	1.37	7	2
2	C	236	LEU	CA-CB	6.35	1.68	1.53	8	1
1	A	435	TYR	CB-CG	6.34	1.61	1.51	2	2
2	B	92	GLU	CD-OE1	6.34	1.32	1.25	14	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	C	207	GLY	C-N	6.32	1.44	1.33	10	1
2	C	187	PRO	N-CD	6.32	1.56	1.47	6	3
1	A	478	TYR	CE1-CZ	6.31	1.46	1.38	15	1
2	B	250	SER	CB-OG	6.30	1.50	1.42	1	1
1	A	445	VAL	CA-CB	-6.28	1.41	1.54	3	1
1	A	345	ARG	CD-NE	6.24	1.57	1.46	7	2
2	B	214	TYR	CB-CG	6.24	1.61	1.51	14	1
2	C	70	GLU	CD-OE1	6.23	1.32	1.25	11	1
2	B	247	PHE	CD2-CE2	6.22	1.51	1.39	8	1
1	A	486	PHE	CE2-CZ	6.20	1.49	1.37	1	1
1	A	361	TRP	CD1-NE1	-6.19	1.27	1.38	3	1
1	A	373	GLU	CD-OE2	6.19	1.32	1.25	11	1
2	B	132	GLU	CG-CD	6.18	1.61	1.51	5	1
1	A	420	PHE	CG-CD1	6.18	1.48	1.38	4	3
1	A	440	GLU	CG-CD	-6.18	1.42	1.51	7	1
1	A	447	SER	CA-CB	6.18	1.62	1.52	11	2
2	B	227	GLU	CD-OE2	6.18	1.32	1.25	9	1
1	A	500	SER	CA-CB	6.18	1.62	1.52	14	3
2	C	258	TYR	CE1-CZ	6.17	1.46	1.38	5	3
2	B	87	SER	CA-CB	6.14	1.62	1.52	12	1
2	C	111	GLU	CB-CG	6.14	1.63	1.52	7	1
1	A	477	PHE	CG-CD1	6.14	1.48	1.38	13	1
2	C	66	PRO	CA-CB	-6.14	1.41	1.53	14	1
1	A	387	HIS	CB-CG	6.12	1.61	1.50	5	2
2	C	252	LEU	CA-CB	6.11	1.67	1.53	8	1
2	C	245	GLU	CB-CG	6.11	1.63	1.52	13	1
2	B	253	SER	CA-CB	6.10	1.62	1.52	2	1
2	C	100	TYR	CG-CD2	6.10	1.47	1.39	13	1
1	A	483	TYR	CB-CG	6.10	1.60	1.51	10	1
2	B	177	HIS	CB-CG	6.08	1.60	1.50	14	1
2	B	99	PRO	N-CD	-6.08	1.39	1.47	7	1
1	A	336	PHE	CE2-CZ	6.08	1.48	1.37	10	1
2	B	188	TYR	CG-CD2	6.07	1.47	1.39	2	1
2	B	164	SER	CB-OG	6.06	1.50	1.42	15	1
1	A	462	SER	CA-CB	6.06	1.62	1.52	13	1
2	C	55	SER	N-CA	6.05	1.58	1.46	3	2
2	C	161	GLU	CG-CD	-6.05	1.42	1.51	8	1
1	A	358	GLY	N-CA	-6.05	1.36	1.46	3	1
1	A	423	PRO	N-CD	-6.05	1.39	1.47	8	2
2	B	130	TRP	CG-CD1	6.04	1.45	1.36	5	1
1	A	486	PHE	CG-CD1	6.04	1.47	1.38	13	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	C	115	TYR	CE1-CZ	6.03	1.46	1.38	11	1
2	C	85	GLU	CB-CG	6.03	1.63	1.52	14	1
1	A	384	GLY	CA-C	6.01	1.61	1.51	3	2
2	B	193	ARG	CZ-NH2	-6.00	1.25	1.33	8	2
2	C	115	TYR	CB-CG	5.99	1.60	1.51	14	2
1	A	330	ARG	CD-NE	5.98	1.56	1.46	8	1
2	C	171	ARG	CD-NE	5.97	1.56	1.46	7	1
2	B	151	GLY	CA-C	-5.97	1.42	1.51	1	1
1	A	396	GLU	CB-CG	5.96	1.63	1.52	11	2
2	C	137	TYR	CG-CD1	5.96	1.46	1.39	9	1
2	B	171	ARG	CD-NE	5.95	1.56	1.46	4	1
1	A	421	TRP	CG-CD1	5.95	1.45	1.36	6	1
2	B	205	GLU	CD-OE2	5.95	1.32	1.25	15	1
2	B	260	LYS	N-CA	-5.94	1.34	1.46	1	1
1	A	353	TYR	CE1-CZ	5.93	1.46	1.38	3	1
2	B	100	TYR	CG-CD1	5.92	1.46	1.39	1	1
1	A	390	PHE	CG-CD2	5.92	1.47	1.38	3	1
2	B	133	GLU	CD-OE1	-5.91	1.19	1.25	14	1
2	C	210	ARG	CD-NE	5.91	1.56	1.46	11	1
2	C	133	GLU	CB-CG	5.90	1.63	1.52	1	1
1	A	449	TYR	CZ-OH	5.89	1.47	1.37	6	1
1	A	388	TRP	CD2-CE2	5.88	1.48	1.41	4	1
2	C	258	TYR	CE2-CZ	5.88	1.46	1.38	10	1
1	A	476	TYR	CG-CD2	5.88	1.46	1.39	5	1
2	C	149	GLN	CG-CD	5.88	1.64	1.51	6	1
1	A	485	LYS	CA-CB	5.88	1.66	1.53	15	1
2	B	150	GLU	CD-OE1	5.88	1.32	1.25	15	1
1	A	428	TYR	CE2-CZ	5.87	1.46	1.38	14	2
1	A	505	TRP	NE1-CE2	-5.87	1.29	1.37	8	1
2	B	110	GLU	CD-OE2	5.86	1.32	1.25	8	1
2	C	258	TYR	CB-CG	5.86	1.60	1.51	7	1
2	B	80	GLU	CG-CD	5.85	1.60	1.51	4	1
1	A	399	TYR	CE1-CZ	5.84	1.46	1.38	12	2
2	B	221	HIS	CB-CG	5.84	1.60	1.50	10	1
2	B	237	ARG	CD-NE	5.84	1.56	1.46	11	2
1	A	441	GLU	CD-OE2	5.83	1.32	1.25	5	2
1	A	338	GLU	CD-OE2	5.83	1.32	1.25	9	3
2	B	100	TYR	CB-CG	-5.83	1.42	1.51	7	1
2	B	115	TYR	CG-CD2	5.83	1.46	1.39	13	2
2	C	214	TYR	CB-CG	5.83	1.60	1.51	13	1
1	A	476	TYR	CE2-CZ	5.83	1.46	1.38	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	187	PRO	N-CD	-5.82	1.39	1.47	1	1
1	A	484	TRP	CD2-CE2	5.81	1.48	1.41	15	1
2	C	138	ARG	CD-NE	5.80	1.56	1.46	1	1
2	B	137	TYR	CG-CD2	5.80	1.46	1.39	2	1
2	B	62	GLU	CD-OE1	5.79	1.32	1.25	1	1
1	A	327	ALA	CA-C	-5.79	1.37	1.52	5	1
2	B	161	GLU	CG-CD	5.79	1.60	1.51	8	1
2	C	98	GLN	CA-CB	5.79	1.66	1.53	11	1
1	A	478	TYR	CE2-CZ	5.78	1.46	1.38	2	1
2	C	187	PRO	CA-C	-5.78	1.41	1.52	5	1
2	B	92	GLU	CD-OE2	5.78	1.32	1.25	8	2
1	A	505	TRP	CZ2-CH2	5.77	1.48	1.37	4	1
2	C	125	ASP	CA-CB	5.76	1.66	1.53	11	1
2	B	193	ARG	CD-NE	5.76	1.56	1.46	11	2
2	B	237	ARG	CA-CB	5.75	1.66	1.53	1	1
2	B	71	PHE	CG-CD1	-5.74	1.30	1.38	11	1
2	C	158	GLU	CD-OE1	5.74	1.31	1.25	7	1
1	A	372	TYR	CD1-CE1	5.72	1.48	1.39	9	2
2	C	158	GLU	CG-CD	-5.71	1.43	1.51	2	1
1	A	429	PHE	CG-CD2	5.71	1.47	1.38	5	1
1	A	476	TYR	C-N	5.71	1.47	1.34	6	1
2	C	122	TYR	CZ-OH	5.71	1.47	1.37	8	1
2	B	258	TYR	CD2-CE2	5.69	1.47	1.39	7	1
1	A	343	ARG	CZ-NH1	-5.69	1.25	1.33	15	1
2	C	214	TYR	CG-CD1	5.68	1.46	1.39	8	1
2	B	80	GLU	CB-CG	5.68	1.62	1.52	11	2
1	A	483	TYR	CE1-CZ	5.67	1.46	1.38	4	1
2	C	174	ALA	CA-CB	5.66	1.64	1.52	3	1
1	A	447	SER	CB-OG	5.66	1.49	1.42	8	1
2	C	142	GLU	CB-CG	5.65	1.62	1.52	10	2
2	B	78	GLU	CB-CG	5.65	1.62	1.52	11	1
2	C	115	TYR	CE2-CZ	5.64	1.45	1.38	3	1
1	A	456	TRP	CZ2-CH2	5.64	1.48	1.37	14	1
2	B	91	GLU	CD-OE2	5.64	1.31	1.25	13	1
1	A	464	ARG	CZ-NH1	-5.63	1.25	1.33	6	1
1	A	336	PHE	CE1-CZ	5.62	1.48	1.37	4	1
2	B	147	GLU	CA-CB	5.62	1.66	1.53	9	1
2	C	91	GLU	CB-CG	5.62	1.62	1.52	4	2
1	A	474	PHE	CG-CD2	5.61	1.47	1.38	9	1
1	A	381	PHE	CG-CD1	5.60	1.47	1.38	5	2
1	A	365	PRO	N-CD	-5.59	1.40	1.47	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	C	70	GLU	CG-CD	-5.59	1.43	1.51	13	1
1	A	498	PRO	CA-C	-5.59	1.41	1.52	11	1
1	A	435	TYR	CG-CD1	5.59	1.46	1.39	5	1
2	B	135	GLU	CD-OE1	5.58	1.31	1.25	9	1
1	A	496	GLY	N-CA	5.58	1.54	1.46	9	1
2	B	145	ARG	CZ-NH1	-5.58	1.25	1.33	8	1
2	C	180	ALA	CA-CB	5.57	1.64	1.52	4	1
1	A	405	GLU	CB-CG	5.57	1.62	1.52	8	1
1	A	472	GLU	CB-CG	5.56	1.62	1.52	2	1
2	B	265	GLN	C-OXT	5.56	1.33	1.23	14	1
2	B	104	PHE	CG-CD2	5.56	1.47	1.38	3	1
1	A	358	GLY	CA-C	-5.55	1.43	1.51	2	1
2	B	120	GLU	CB-CG	5.55	1.62	1.52	3	1
2	B	189	SER	CA-CB	5.55	1.61	1.52	8	1
1	A	511	GLY	N-CA	-5.54	1.37	1.46	7	1
2	C	130	TRP	CA-CB	5.54	1.66	1.53	6	1
2	B	122	TYR	CB-CG	5.54	1.59	1.51	14	1
1	A	388	TRP	CB-CG	5.54	1.60	1.50	11	1
2	B	130	TRP	CG-CD2	5.53	1.53	1.43	1	1
1	A	382	PHE	CA-CB	5.53	1.66	1.53	12	1
2	B	258	TYR	CG-CD2	5.53	1.46	1.39	1	2
2	C	120	GLU	CB-CG	5.53	1.62	1.52	15	1
2	B	76	GLU	CB-CG	5.52	1.62	1.52	4	1
1	A	379	PHE	CG-CD2	5.52	1.47	1.38	1	1
2	B	91	GLU	CD-OE1	5.52	1.31	1.25	1	1
2	C	199	ARG	CZ-NH2	-5.51	1.25	1.33	14	1
1	A	474	PHE	CB-CG	-5.51	1.42	1.51	5	1
2	B	139	GLN	CA-CB	5.50	1.66	1.53	13	1
1	A	339	ARG	CD-NE	5.49	1.55	1.46	7	2
2	C	133	GLU	CD-OE2	5.49	1.31	1.25	2	1
2	B	178	VAL	CB-CG1	5.48	1.64	1.52	3	1
2	C	188	TYR	CG-CD2	5.48	1.46	1.39	6	1
1	A	340	TRP	CD1-NE1	-5.47	1.28	1.38	2	1
1	A	323	PHE	CG-CD2	5.47	1.47	1.38	12	1
1	A	352	GLY	CA-C	-5.46	1.43	1.51	11	1
1	A	483	TYR	CD2-CE2	5.46	1.47	1.39	5	1
2	C	142	GLU	CG-CD	5.46	1.60	1.51	1	1
1	A	494	GLU	CB-CG	5.46	1.62	1.52	7	1
2	C	130	TRP	CZ2-CH2	5.46	1.47	1.37	3	1
2	C	80	GLU	CB-CG	5.45	1.62	1.52	9	1
2	C	126	PHE	CA-CB	5.45	1.66	1.53	14	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	405	GLU	CD-OE1	5.45	1.31	1.25	2	1
2	C	108	TRP	NE1-CE2	-5.44	1.30	1.37	4	1
2	C	81	GLY	N-CA	-5.44	1.37	1.46	6	1
2	B	120	GLU	CD-OE1	5.44	1.31	1.25	13	1
2	B	113	GLU	CB-CG	5.42	1.62	1.52	3	1
1	A	428	TYR	CG-CD2	5.42	1.46	1.39	11	1
1	A	373	GLU	CB-CG	5.42	1.62	1.52	1	1
1	A	464	ARG	CZ-NH2	-5.42	1.26	1.33	7	1
2	C	100	TYR	CZ-OH	5.42	1.47	1.37	6	1
2	C	238	GLN	C-N	5.41	1.42	1.33	4	1
2	B	184	HIS	CB-CG	5.41	1.59	1.50	3	1
2	B	153	ARG	CD-NE	5.41	1.55	1.46	10	2
2	B	77	LYS	CA-CB	5.41	1.65	1.53	5	1
2	C	122	TYR	CG-CD2	5.40	1.46	1.39	6	2
2	B	100	TYR	CA-CB	5.40	1.65	1.53	7	1
2	B	188	TYR	CD1-CE1	5.40	1.47	1.39	9	1
1	A	497	TYR	CG-CD1	5.39	1.46	1.39	6	2
1	A	397	PRO	CA-CB	5.39	1.64	1.53	10	1
2	C	130	TRP	CD2-CE3	5.39	1.48	1.40	14	1
1	A	407	GLY	N-CA	5.39	1.54	1.46	10	1
2	C	108	TRP	CD2-CE2	5.39	1.47	1.41	13	1
1	A	438	PHE	CE1-CZ	5.39	1.47	1.37	7	1
2	C	145	ARG	CB-CG	5.38	1.67	1.52	5	1
2	B	71	PHE	CA-CB	5.38	1.65	1.53	2	1
2	B	62	GLU	CG-CD	5.38	1.60	1.51	6	1
1	A	457	GLU	CD-OE2	5.38	1.31	1.25	8	1
1	A	472	GLU	CD-OE1	-5.38	1.19	1.25	7	1
2	C	72	TRP	CD2-CE2	-5.37	1.34	1.41	12	1
2	C	236	LEU	CA-C	5.36	1.66	1.52	2	1
2	B	213	GLU	CD-OE2	5.36	1.31	1.25	9	1
1	A	437	ARG	CD-NE	5.36	1.55	1.46	10	1
1	A	438	PHE	CG-CD1	5.36	1.46	1.38	1	1
1	A	437	ARG	CZ-NH1	-5.36	1.26	1.33	1	1
1	A	476	TYR	CE1-CZ	-5.36	1.31	1.38	8	1
2	C	220	GLU	CB-CG	5.36	1.62	1.52	11	1
2	C	227	GLU	CD-OE1	5.35	1.31	1.25	1	1
1	A	449	TYR	CG-CD2	5.34	1.46	1.39	7	1
2	C	145	ARG	CD-NE	5.34	1.55	1.46	5	1
2	C	223	SER	CB-OG	5.34	1.49	1.42	4	1
2	C	247	PHE	CG-CD2	5.34	1.46	1.38	4	1
2	C	150	GLU	CD-OE2	5.34	1.31	1.25	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	201	GLU	CG-CD	5.33	1.59	1.51	3	1
1	A	360	PHE	CG-CD1	5.33	1.46	1.38	10	1
1	A	404	LYS	CA-C	5.33	1.66	1.52	9	1
2	B	72	TRP	NE1-CE2	-5.33	1.30	1.37	10	1
2	C	108	TRP	CD2-CE3	5.32	1.48	1.40	9	1
2	B	134	MET	N-CA	-5.32	1.35	1.46	6	1
2	B	127	GLN	CG-CD	5.32	1.63	1.51	2	1
2	B	137	TYR	CE2-CZ	5.32	1.45	1.38	9	1
2	B	197	ALA	N-CA	5.32	1.56	1.46	15	1
2	C	99	PRO	N-CD	-5.31	1.40	1.47	10	2
2	C	164	SER	N-CA	-5.31	1.35	1.46	11	1
2	B	85	GLU	CD-OE1	-5.31	1.19	1.25	1	1
2	C	83	ARG	CZ-NH2	-5.29	1.26	1.33	3	1
1	A	406	LEU	C-N	5.29	1.42	1.33	3	2
1	A	399	TYR	CG-CD2	5.28	1.46	1.39	10	1
1	A	386	LYS	CA-CB	5.28	1.65	1.53	4	1
2	C	100	TYR	CE1-CZ	5.28	1.45	1.38	12	1
2	B	213	GLU	CB-CG	5.27	1.62	1.52	4	1
1	A	388	TRP	CD2-CE3	5.27	1.48	1.40	10	1
1	A	340	TRP	CD2-CE2	5.27	1.47	1.41	4	1
2	C	161	GLU	CB-CG	5.26	1.62	1.52	8	1
2	B	135	GLU	CG-CD	5.26	1.59	1.51	10	1
2	B	247	PHE	CE2-CZ	5.26	1.47	1.37	3	1
1	A	345	ARG	CZ-NH1	-5.26	1.26	1.33	7	1
1	A	408	ARG	CD-NE	5.26	1.55	1.46	10	1
1	A	340	TRP	CG-CD1	5.26	1.44	1.36	8	1
2	C	135	GLU	CA-CB	-5.26	1.42	1.53	4	1
2	C	91	GLU	CG-CD	-5.26	1.44	1.51	8	1
2	B	137	TYR	CZ-OH	5.26	1.46	1.37	9	1
2	B	129	LYS	N-CA	-5.25	1.35	1.46	1	1
1	A	377	GLY	CA-C	-5.25	1.43	1.51	9	1
1	A	500	SER	CB-OG	5.25	1.49	1.42	14	2
1	A	483	TYR	CD1-CE1	5.25	1.47	1.39	13	1
2	C	171	ARG	CZ-NH2	-5.24	1.26	1.33	6	1
2	B	151	GLY	N-CA	5.24	1.53	1.46	13	1
1	A	510	SER	CA-CB	5.24	1.60	1.52	13	1
2	B	61	ARG	CD-NE	5.24	1.55	1.46	9	1
1	A	323	PHE	CA-CB	5.23	1.65	1.53	3	1
2	B	258	TYR	CZ-OH	5.23	1.46	1.37	11	1
1	A	360	PHE	CG-CD2	5.23	1.46	1.38	1	1
2	C	138	ARG	NE-CZ	5.23	1.39	1.33	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	C	182	ARG	CZ-NH2	-5.23	1.26	1.33	6	1
1	A	388	TRP	CE2-CZ2	5.23	1.48	1.39	10	1
2	B	157	HIS	CA-CB	5.23	1.65	1.53	12	1
2	B	258	TYR	CB-CG	-5.23	1.43	1.51	15	2
2	B	165	PRO	N-CD	-5.22	1.40	1.47	8	1
2	B	145	ARG	CG-CD	5.22	1.65	1.51	9	1
2	C	213	GLU	CB-CG	5.22	1.62	1.52	13	1
2	C	191	GLU	CD-OE2	5.22	1.31	1.25	15	1
2	C	169	GLU	CA-CB	-5.22	1.42	1.53	3	1
2	C	188	TYR	CA-CB	5.22	1.65	1.53	12	1
2	C	76	GLU	CD-OE1	5.21	1.31	1.25	11	1
2	B	69	GLN	N-CA	-5.21	1.35	1.46	12	1
2	B	145	ARG	CD-NE	5.21	1.55	1.46	13	1
1	A	372	TYR	CE2-CZ	5.20	1.45	1.38	5	1
1	A	431	ARG	N-CA	-5.20	1.35	1.46	5	1
2	B	122	TYR	CA-CB	5.20	1.65	1.53	3	1
1	A	436	TYR	CB-CG	5.20	1.59	1.51	9	1
2	C	193	ARG	CD-NE	5.20	1.55	1.46	12	1
1	A	372	TYR	N-CA	5.19	1.56	1.46	8	1
1	A	349	VAL	CB-CG2	5.19	1.63	1.52	4	1
2	C	121	PRO	N-CA	5.19	1.56	1.47	2	1
2	C	145	ARG	CZ-NH1	-5.19	1.26	1.33	9	1
1	A	432	GLY	CA-C	5.18	1.60	1.51	6	1
1	A	334	PHE	CG-CD1	5.18	1.46	1.38	11	1
2	B	130	TRP	NE1-CE2	5.18	1.44	1.37	6	1
2	B	201	GLU	CD-OE1	5.17	1.31	1.25	2	1
1	A	360	PHE	CE1-CZ	5.17	1.47	1.37	3	1
1	A	435	TYR	CE1-CZ	5.17	1.45	1.38	13	1
1	A	338	GLU	CD-OE1	-5.17	1.20	1.25	11	1
1	A	428	TYR	CG-CD1	5.17	1.45	1.39	12	1
2	B	173	ARG	CZ-NH1	-5.17	1.26	1.33	11	1
2	B	238	GLN	C-N	5.16	1.42	1.33	9	1
2	C	237	ARG	CZ-NH2	-5.16	1.26	1.33	15	1
1	A	431	ARG	CD-NE	5.15	1.55	1.46	5	1
1	A	425	GLY	CA-C	-5.15	1.43	1.51	14	1
1	A	372	TYR	CG-CD1	5.15	1.45	1.39	13	2
1	A	342	TRP	CD2-CE2	-5.15	1.35	1.41	13	1
1	A	505	TRP	CE2-CZ2	-5.15	1.31	1.39	6	1
2	C	150	GLU	C-N	5.14	1.42	1.33	15	1
2	C	119	VAL	CB-CG1	5.14	1.63	1.52	1	1
2	C	145	ARG	CZ-NH2	-5.14	1.26	1.33	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	246	SER	CB-OG	5.13	1.49	1.42	11	1
2	C	147	GLU	CB-CG	5.13	1.61	1.52	11	1
2	B	70	GLU	CB-CG	5.13	1.61	1.52	8	1
2	C	137	TYR	CE2-CZ	5.13	1.45	1.38	9	1
2	C	87	SER	CA-CB	-5.13	1.45	1.52	11	2
2	B	245	GLU	CD-OE1	5.13	1.31	1.25	2	1
2	B	171	ARG	CZ-NH2	-5.13	1.26	1.33	5	1
2	C	168	GLU	CD-OE1	5.13	1.31	1.25	14	1
2	B	153	ARG	CZ-NH2	-5.12	1.26	1.33	2	1
2	C	110	GLU	CA-CB	5.12	1.65	1.53	9	1
2	C	234	GLU	CD-OE1	5.12	1.31	1.25	2	1
1	A	436	TYR	CG-CD2	5.12	1.45	1.39	10	1
2	B	231	PRO	N-CA	5.12	1.55	1.47	13	1
2	C	154	GLN	CG-CD	5.11	1.62	1.51	2	1
2	B	220	GLU	CB-CG	5.11	1.61	1.52	13	1
1	A	443	ARG	CD-NE	5.10	1.55	1.46	3	1
1	A	343	ARG	CD-NE	5.10	1.55	1.46	5	1
1	A	332	GLU	CD-OE2	5.10	1.31	1.25	12	1
2	B	150	GLU	CD-OE2	5.09	1.31	1.25	1	1
2	B	57	PHE	CB-CG	5.09	1.60	1.51	12	1
2	B	161	GLU	CD-OE1	-5.09	1.20	1.25	7	1
2	C	120	GLU	CD-OE1	5.09	1.31	1.25	12	1
2	C	127	GLN	N-CA	-5.09	1.36	1.46	14	1
2	C	193	ARG	CZ-NH2	-5.09	1.26	1.33	14	1
1	A	494	GLU	CG-CD	5.08	1.59	1.51	5	1
2	B	258	TYR	CG-CD1	5.08	1.45	1.39	14	1
2	B	58	SER	CA-CB	5.08	1.60	1.52	13	1
2	C	237	ARG	CD-NE	5.08	1.55	1.46	14	1
1	A	450	PRO	N-CD	5.08	1.54	1.47	4	1
2	B	87	SER	CB-OG	5.08	1.48	1.42	9	1
2	C	246	SER	CB-OG	-5.08	1.35	1.42	8	1
1	A	332	GLU	CA-CB	5.07	1.65	1.53	1	1
2	B	103	ASP	CA-CB	5.07	1.65	1.53	3	1
1	A	505	TRP	CD2-CE2	5.07	1.47	1.41	3	1
1	A	430	PHE	CG-CD2	5.07	1.46	1.38	14	1
2	C	100	TYR	CD2-CE2	5.07	1.47	1.39	15	1
1	A	498	PRO	N-CD	-5.07	1.40	1.47	15	1
1	A	420	PHE	CG-CD2	5.06	1.46	1.38	2	1
1	A	497	TYR	CG-CD2	5.06	1.45	1.39	2	1
2	C	104	PHE	CG-CD1	5.06	1.46	1.38	8	1
2	C	137	TYR	CG-CD2	5.06	1.45	1.39	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	C	76	GLU	CD-OE2	5.06	1.31	1.25	10	1
1	A	405	GLU	CD-OE2	5.06	1.31	1.25	15	1
2	B	191	GLU	CB-CG	5.06	1.61	1.52	2	1
1	A	486	PHE	CG-CD2	5.05	1.46	1.38	8	1
1	A	430	PHE	CE1-CZ	5.05	1.47	1.37	10	1
1	A	354	PRO	N-CD	-5.04	1.40	1.47	15	1
1	A	390	PHE	CE1-CZ	5.04	1.47	1.37	2	1
2	C	151	GLY	N-CA	-5.04	1.38	1.46	3	1
2	B	76	GLU	CD-OE2	-5.03	1.20	1.25	4	1
2	C	111	GLU	CG-CD	-5.03	1.44	1.51	8	1
2	C	196	LEU	CB-CG	5.03	1.67	1.52	11	1
2	B	182	ARG	CD-NE	5.02	1.54	1.46	9	1
1	A	319	CYS	CB-SG	5.02	1.90	1.82	10	1
2	B	127	GLN	CA-CB	5.02	1.65	1.53	14	1
2	C	261	LYS	CA-CB	5.02	1.65	1.53	9	1
2	C	213	GLU	CA-CB	5.01	1.65	1.53	8	1
2	B	55	SER	N-CA	5.01	1.56	1.46	5	1
1	A	397	PRO	CA-C	-5.01	1.42	1.52	1	1
1	A	353	TYR	CD2-CE2	5.01	1.46	1.39	7	1
2	C	214	TYR	CA-CB	5.00	1.65	1.53	7	1
2	B	239	GLY	N-CA	5.00	1.53	1.46	6	1

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
2	B	193	ARG	NE-CZ-NH2	24.46	132.53	120.30	8	11
2	C	61	ARG	NE-CZ-NH2	23.11	131.86	120.30	11	9
2	C	116	ARG	NE-CZ-NH2	22.39	131.49	120.30	10	9
2	B	199	ARG	NE-CZ-NH2	22.28	131.44	120.30	14	9
2	C	153	ARG	NE-CZ-NH2	22.11	131.35	120.30	12	11
2	B	116	ARG	NE-CZ-NH2	21.07	130.84	120.30	12	9
2	C	83	ARG	NE-CZ-NH2	20.85	130.72	120.30	12	9
2	B	175	ARG	NE-CZ-NH2	20.80	130.70	120.30	13	12
2	B	173	ARG	NE-CZ-NH1	-20.58	110.01	120.30	5	8
2	C	61	ARG	NE-CZ-NH1	-20.44	110.08	120.30	11	5
2	B	195	ARG	NE-CZ-NH2	20.40	130.50	120.30	3	12
2	C	175	ARG	NE-CZ-NH2	19.86	130.23	120.30	2	10
2	B	214	TYR	CB-CG-CD1	19.51	132.71	121.00	11	6
1	A	464	ARG	NE-CZ-NH2	19.51	130.06	120.30	1	10
2	C	195	ARG	NE-CZ-NH2	19.48	130.04	120.30	4	11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	343	ARG	NE-CZ-NH2	19.29	129.94	120.30	4	11
2	C	171	ARG	NE-CZ-NH1	-19.20	110.70	120.30	14	10
2	C	237	ARG	NE-CZ-NH2	19.04	129.82	120.30	14	10
2	C	138	ARG	NE-CZ-NH2	18.87	129.74	120.30	9	7
2	B	237	ARG	NE-CZ-NH2	18.66	129.63	120.30	8	8
2	C	171	ARG	NE-CZ-NH2	18.62	129.61	120.30	15	13
1	A	437	ARG	NE-CZ-NH1	18.42	129.51	120.30	2	8
2	B	61	ARG	NE-CZ-NH2	18.40	129.50	120.30	7	5
2	C	145	ARG	NE-CZ-NH2	18.23	129.42	120.30	1	12
2	C	210	ARG	NE-CZ-NH2	18.14	129.37	120.30	9	12
2	B	83	ARG	NE-CZ-NH2	17.47	129.03	120.30	13	10
2	B	173	ARG	NE-CZ-NH2	17.35	128.98	120.30	14	7
1	A	343	ARG	NE-CZ-NH1	-17.34	111.63	120.30	4	9
2	B	153	ARG	NE-CZ-NH2	17.03	128.81	120.30	14	12
2	C	199	ARG	NE-CZ-NH2	16.92	128.76	120.30	14	9
1	A	345	ARG	NE-CZ-NH1	-16.75	111.93	120.30	15	10
2	B	61	ARG	NE-CZ-NH1	16.73	128.67	120.30	11	8
1	A	362	ARG	NE-CZ-NH1	16.70	128.65	120.30	5	10
2	B	195	ARG	NE-CZ-NH1	-16.61	111.99	120.30	7	9
2	C	122	TYR	CB-CG-CD2	16.60	130.96	121.00	8	7
2	C	193	ARG	NE-CZ-NH2	16.53	128.57	120.30	4	10
1	A	339	ARG	NE-CZ-NH1	16.45	128.53	120.30	3	8
1	A	464	ARG	NE-CZ-NH1	-16.31	112.14	120.30	1	7
1	A	408	ARG	NE-CZ-NH2	16.19	128.39	120.30	13	11
2	B	182	ARG	NE-CZ-NH2	16.18	128.39	120.30	12	12
2	B	175	ARG	NE-CZ-NH1	-16.13	112.23	120.30	11	10
1	A	408	ARG	NE-CZ-NH1	-16.06	112.27	120.30	15	8
2	B	251	PHE	CB-CG-CD1	15.93	131.95	120.80	11	4
2	C	182	ARG	NE-CZ-NH1	-15.91	112.34	120.30	7	8
2	B	258	TYR	CB-CG-CD2	-15.85	111.49	121.00	11	4
2	C	182	ARG	NE-CZ-NH2	15.56	128.08	120.30	8	7
2	B	145	ARG	NE-CZ-NH1	-15.56	112.52	120.30	12	8
2	C	153	ARG	NE-CZ-NH1	-15.39	112.60	120.30	5	8
2	B	199	ARG	NE-CZ-NH1	-15.37	112.61	120.30	14	9
1	A	345	ARG	NE-CZ-NH2	15.34	127.97	120.30	6	5
2	B	145	ARG	NE-CZ-NH2	15.17	127.88	120.30	7	8
2	B	210	ARG	NE-CZ-NH2	15.08	127.84	120.30	5	7
1	A	431	ARG	NE-CZ-NH2	14.80	127.70	120.30	14	11
1	A	503	ARG	NE-CZ-NH1	-14.79	112.91	120.30	11	10
1	A	399	TYR	CB-CG-CD2	-14.76	112.15	121.00	5	5
2	C	214	TYR	CB-CG-CD1	-14.72	112.17	121.00	13	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	330	ARG	NE-CZ-NH1	14.70	127.65	120.30	5	7
2	C	210	ARG	NE-CZ-NH1	-14.58	113.01	120.30	10	10
1	A	443	ARG	NE-CZ-NH1	-14.51	113.05	120.30	9	5
2	C	122	TYR	CB-CG-CD1	-14.34	112.39	121.00	8	5
2	B	193	ARG	NE-CZ-NH1	-14.11	113.25	120.30	1	9
1	A	372	TYR	CB-CG-CD1	14.07	129.44	121.00	3	5
2	C	173	ARG	NE-CZ-NH2	14.04	127.32	120.30	3	10
2	B	214	TYR	CB-CG-CD2	-13.88	112.67	121.00	11	8
2	B	237	ARG	NE-CZ-NH1	-13.67	113.47	120.30	6	12
2	C	138	ARG	NE-CZ-NH1	-13.57	113.52	120.30	1	6
1	A	467	PHE	CB-CG-CD2	-13.54	111.33	120.80	7	2
2	B	153	ARG	NE-CZ-NH1	-13.48	113.56	120.30	11	9
2	B	89	ASP	CB-CG-OD2	-13.45	106.19	118.30	13	1
1	A	478	TYR	CB-CG-CD2	-13.39	112.97	121.00	9	7
1	A	477	PHE	CB-CG-CD1	13.35	130.14	120.80	8	5
2	C	145	ARG	NE-CZ-NH1	-13.21	113.70	120.30	2	7
1	A	431	ARG	NE-CZ-NH1	-13.19	113.70	120.30	5	7
2	C	195	ARG	NE-CZ-NH1	-13.09	113.76	120.30	9	7
2	C	199	ARG	NE-CZ-NH1	-13.00	113.80	120.30	1	8
1	A	477	PHE	CB-CG-CD2	-12.86	111.80	120.80	8	4
1	A	474	PHE	CB-CG-CD1	-12.85	111.81	120.80	14	5
2	B	247	PHE	CB-CG-CD1	-12.85	111.81	120.80	9	4
1	A	330	ARG	NE-CZ-NH2	12.77	126.69	120.30	9	11
1	A	374	ARG	NE-CZ-NH2	12.73	126.67	120.30	9	7
2	B	171	ARG	NE-CZ-NH2	12.70	126.65	120.30	12	9
2	B	171	ARG	NE-CZ-NH1	-12.60	114.00	120.30	8	5
2	C	116	ARG	NE-CZ-NH1	12.57	126.58	120.30	13	7
2	C	126	PHE	CB-CG-CD1	-12.44	112.09	120.80	4	1
2	B	188	TYR	CB-CG-CD2	-12.42	113.55	121.00	1	4
1	A	435	TYR	CB-CG-CD2	-12.35	113.59	121.00	13	6
1	A	437	ARG	NE-CZ-NH2	-12.19	114.21	120.30	12	6
2	C	175	ARG	NE-CZ-NH1	-12.11	114.25	120.30	5	8
2	B	83	ARG	NE-CZ-NH1	-12.10	114.25	120.30	10	5
1	A	353	TYR	CB-CG-CD2	-12.09	113.74	121.00	3	2
2	C	104	PHE	CB-CG-CD2	-11.99	112.40	120.80	3	6
1	A	429	PHE	CB-CG-CD1	-11.98	112.41	120.80	15	3
1	A	483	TYR	CB-CG-CD1	11.98	128.19	121.00	15	5
1	A	360	PHE	CB-CG-CD2	11.91	129.14	120.80	14	5
2	B	138	ARG	NE-CZ-NH1	-11.89	114.35	120.30	8	6
2	C	247	PHE	CB-CG-CD1	11.88	129.11	120.80	7	4
2	C	251	PHE	CB-CG-CD2	-11.79	112.55	120.80	3	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	443	ARG	NE-CZ-NH2	11.77	126.19	120.30	14	10
2	B	179	ASP	CB-CG-OD2	11.72	128.85	118.30	7	7
2	B	137	TYR	CB-CG-CD2	11.67	128.00	121.00	7	7
1	A	385	ASP	CB-CG-OD2	-11.61	107.85	118.30	1	5
1	A	381	PHE	CB-CG-CD2	-11.59	112.69	120.80	15	5
1	A	362	ARG	NE-CZ-NH2	-11.55	114.53	120.30	10	6
2	B	122	TYR	CB-CG-CD1	-11.54	114.07	121.00	3	4
1	A	379	PHE	CB-CG-CD2	11.46	128.82	120.80	2	3
1	A	385	ASP	CB-CG-OD1	11.33	128.50	118.30	2	5
1	A	446	ASP	CB-CG-OD2	-11.31	108.12	118.30	4	3
2	B	182	ARG	NE-CZ-NH1	-11.30	114.65	120.30	3	7
1	A	374	ARG	NE-CZ-NH1	-11.29	114.66	120.30	3	6
2	B	247	PHE	CB-CG-CD2	11.27	128.69	120.80	9	7
1	A	372	TYR	CB-CG-CD2	-11.14	114.32	121.00	3	4
2	B	210	ARG	NE-CZ-NH1	-11.10	114.75	120.30	1	11
2	C	103	ASP	CB-CG-OD2	10.94	128.15	118.30	8	2
2	B	100	TYR	CG-CD1-CE1	-10.92	112.56	121.30	10	2
1	A	339	ARG	NE-CZ-NH2	-10.89	114.85	120.30	1	6
2	B	115	TYR	CB-CG-CD1	10.88	127.53	121.00	2	6
2	B	115	TYR	CB-CG-CD2	-10.87	114.48	121.00	14	6
2	B	100	TYR	CB-CG-CD1	-10.85	114.49	121.00	10	5
2	B	61	ARG	NH1-CZ-NH2	-10.85	107.46	119.40	7	5
1	A	436	TYR	CB-CG-CD1	-10.84	114.50	121.00	11	7
1	A	476	TYR	CB-CG-CD2	10.83	127.50	121.00	14	6
1	A	471	ASP	CB-CG-OD2	10.78	128.00	118.30	12	6
2	C	137	TYR	CB-CG-CD2	-10.74	114.56	121.00	15	5
2	C	115	TYR	CB-CG-CD2	-10.73	114.56	121.00	12	6
1	A	497	TYR	CB-CG-CD2	-10.68	114.59	121.00	6	5
2	B	188	TYR	CG-CD2-CE2	-10.58	112.83	121.30	3	5
2	C	116	ARG	NH1-CZ-NH2	-10.51	107.83	119.40	10	3
1	A	478	TYR	CB-CG-CD1	10.51	127.31	121.00	3	4
2	C	214	TYR	CB-CG-CD2	10.49	127.30	121.00	13	6
2	C	235	ASP	CB-CG-OD2	-10.49	108.86	118.30	5	5
2	C	100	TYR	CB-CG-CD2	10.46	127.27	121.00	1	8
1	A	341	PHE	CB-CG-CD2	-10.37	113.54	120.80	2	3
2	C	173	ARG	NE-CZ-NH1	-10.36	115.12	120.30	5	7
2	C	137	TYR	CB-CG-CD1	-10.35	114.79	121.00	10	5
1	A	435	TYR	CB-CG-CD1	10.32	127.19	121.00	13	7
1	A	449	TYR	CB-CG-CD2	10.27	127.16	121.00	13	4
2	B	57	PHE	CB-CG-CD2	-10.26	113.62	120.80	5	5
2	C	237	ARG	NE-CZ-NH1	-10.20	115.20	120.30	14	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	235	ASP	CB-CG-OD1	-10.08	109.23	118.30	11	6
1	A	345	ARG	NH1-CZ-NH2	-10.05	108.34	119.40	6	3
2	C	125	ASP	CB-CG-OD1	9.99	127.29	118.30	3	3
1	A	486	PHE	CB-CG-CD1	-9.99	113.81	120.80	10	3
1	A	497	TYR	CG-CD2-CE2	-9.99	113.31	121.30	6	2
1	A	428	TYR	CB-CG-CD2	-9.95	115.03	121.00	8	5
1	A	399	TYR	CB-CG-CD1	-9.94	115.03	121.00	11	4
2	C	100	TYR	CB-CG-CD1	-9.94	115.03	121.00	14	5
2	C	251	PHE	CB-CG-CD1	-9.91	113.86	120.80	15	5
1	A	381	PHE	CB-CG-CD1	9.91	127.74	120.80	15	2
1	A	476	TYR	CB-CG-CD1	-9.87	115.08	121.00	14	6
2	B	124	ASP	CB-CG-OD1	-9.82	109.46	118.30	2	3
2	C	193	ARG	NH1-CZ-NH2	-9.79	108.62	119.40	4	2
2	C	83	ARG	NH1-CZ-NH2	-9.78	108.65	119.40	12	4
1	A	430	PHE	CB-CG-CD2	9.78	127.64	120.80	13	5
2	C	193	ARG	NE-CZ-NH1	-9.77	115.42	120.30	1	7
1	A	390	PHE	CB-CG-CD1	9.74	127.62	120.80	5	4
1	A	430	PHE	CB-CG-CD1	-9.73	113.99	120.80	5	5
1	A	379	PHE	CB-CG-CD1	-9.69	114.02	120.80	2	2
2	C	83	ARG	NE-CZ-NH1	-9.61	115.50	120.30	1	2
1	A	341	PHE	CB-CG-CD1	9.60	127.52	120.80	2	6
2	B	258	TYR	CB-CG-CD1	-9.58	115.25	121.00	12	4
1	A	446	ASP	CB-CG-OD1	9.51	126.86	118.30	4	3
2	B	134	MET	CG-SD-CE	9.47	115.35	100.20	12	3
1	A	436	TYR	CB-CG-CD2	9.40	126.64	121.00	3	5
2	B	100	TYR	CB-CG-CD2	9.34	126.61	121.00	8	5
1	A	391	ASP	CB-CG-OD1	-9.34	109.89	118.30	14	3
2	B	172	ASP	CB-CG-OD2	9.30	126.67	118.30	11	3
2	C	73	ASP	CB-CG-OD1	9.29	126.66	118.30	6	4
2	C	258	TYR	CG-CD2-CE2	-9.26	113.90	121.30	4	1
1	A	503	ARG	NE-CZ-NH2	9.22	124.91	120.30	5	9
2	C	89	ASP	CB-CG-OD2	9.21	126.59	118.30	2	3
2	B	116	ARG	NE-CZ-NH1	-9.14	115.73	120.30	3	3
2	C	237	ARG	NH1-CZ-NH2	-9.13	109.35	119.40	8	4
2	B	122	TYR	CB-CG-CD2	9.12	126.47	121.00	3	4
2	B	199	ARG	NH1-CZ-NH2	-9.11	109.38	119.40	10	2
2	C	104	PHE	CB-CG-CD1	9.11	127.18	120.80	8	5
1	A	478	TYR	CG-CD1-CE1	-9.11	114.01	121.30	11	5
1	A	353	TYR	CB-CG-CD1	-9.08	115.55	121.00	7	3
2	B	188	TYR	CZ-CE2-CD2	9.02	127.92	119.80	3	1
1	A	390	PHE	CB-CG-CD2	-8.95	114.54	120.80	10	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	138	ARG	NE-CZ-NH2	8.91	124.75	120.30	12	10
2	C	126	PHE	CB-CG-CD2	-8.86	114.59	120.80	9	4
1	A	476	TYR	CD1-CE1-CZ	8.87	127.78	119.80	10	1
2	C	258	TYR	CB-CG-CD2	8.79	126.27	121.00	13	7
2	B	126	PHE	CB-CG-CD1	8.68	126.88	120.80	5	2
2	C	170	MET	CG-SD-CE	-8.68	86.31	100.20	5	6
2	C	172	ASP	CB-CG-OD2	8.66	126.09	118.30	1	4
1	A	355	MET	CG-SD-CE	-8.61	86.42	100.20	9	5
1	A	334	PHE	CB-CG-CD1	-8.59	114.79	120.80	13	4
2	C	247	PHE	CB-CG-CD2	-8.57	114.80	120.80	7	3
1	A	422	MET	CG-SD-CE	-8.55	86.52	100.20	1	2
2	C	73	ASP	CB-CG-OD2	-8.54	110.61	118.30	3	1
2	B	172	ASP	CB-CG-OD1	-8.52	110.64	118.30	11	2
2	B	179	ASP	CB-CG-OD1	-8.52	110.64	118.30	13	2
2	C	258	TYR	CB-CG-CD1	-8.49	115.91	121.00	4	7
1	A	484	TRP	CD1-NE1-CE2	8.48	116.63	109.00	8	3
1	A	413	ASP	CB-CG-OD2	8.45	125.90	118.30	7	4
2	B	108	TRP	CB-CG-CD2	8.40	137.52	126.60	14	3
2	C	173	ARG	NH1-CZ-NH2	8.40	128.64	119.40	10	2
1	A	476	TYR	CG-CD2-CE2	-8.39	114.58	121.30	13	1
1	A	389	VAL	CG1-CB-CG2	-8.36	97.52	110.90	6	2
2	B	137	TYR	CB-CG-CD1	-8.35	115.99	121.00	12	7
1	A	428	TYR	CB-CG-CD1	-8.33	116.00	121.00	12	5
2	B	130	TRP	CB-CG-CD2	8.29	137.38	126.60	15	4
2	C	103	ASP	CB-CG-OD1	-8.29	110.83	118.30	11	2
2	B	102	ASP	CB-CG-OD2	-8.26	110.87	118.30	11	5
1	A	360	PHE	CB-CG-CD1	8.24	126.57	120.80	15	6
1	A	320	ASP	CB-CG-OD1	8.23	125.70	118.30	3	3
1	A	484	TRP	CB-CG-CD1	-8.23	116.30	127.00	10	5
2	B	173	ARG	NH1-CZ-NH2	-8.22	110.36	119.40	15	3
1	A	382	PHE	CB-CG-CD1	8.15	126.51	120.80	8	5
2	B	130	TRP	CB-CG-CD1	-8.13	116.42	127.00	15	4
1	A	351	ASP	CB-CG-OD1	8.12	125.61	118.30	4	4
1	A	467	PHE	CB-CG-CD1	8.12	126.48	120.80	5	2
1	A	431	ARG	NH1-CZ-NH2	-8.11	110.48	119.40	12	3
2	C	130	TRP	CE3-CZ3-CH2	-8.11	112.28	121.20	11	2
1	A	420	PHE	CB-CG-CD2	8.11	126.48	120.80	15	6
1	A	421	TRP	CB-CG-CD2	8.11	137.14	126.60	2	1
1	A	320	ASP	CB-CG-OD2	-8.07	111.03	118.30	2	2
2	B	181	LEU	CB-CG-CD2	8.05	124.68	111.00	11	1
2	B	104	PHE	CB-CG-CD2	-8.04	115.17	120.80	6	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	455	VAL	CA-CB-CG2	8.01	122.91	110.90	12	2
2	B	126	PHE	CB-CG-CD2	-8.00	115.20	120.80	5	3
2	B	124	ASP	CB-CG-OD2	7.94	125.45	118.30	9	2
1	A	416	ASP	CB-CG-OD2	-7.94	111.16	118.30	6	4
2	C	122	TYR	CG-CD1-CE1	-7.94	114.95	121.30	10	2
2	C	130	TRP	CB-CG-CD2	7.93	136.92	126.60	4	3
1	A	388	TRP	CD1-NE1-CE2	7.93	116.14	109.00	13	1
2	C	188	TYR	CB-CG-CD2	7.92	125.75	121.00	12	4
1	A	393	ALA	N-CA-CB	-7.91	99.03	110.10	5	1
1	A	484	TRP	CB-CG-CD2	7.85	136.81	126.60	10	5
2	B	226	SER	N-CA-CB	7.85	122.27	110.50	6	1
2	C	79	THR	CA-CB-CG2	-7.84	101.42	112.40	3	2
2	B	83	ARG	NH1-CZ-NH2	-7.83	110.78	119.40	11	2
1	A	438	PHE	CB-CG-CD1	-7.83	115.32	120.80	10	3
2	B	193	ARG	NH1-CZ-NH2	7.82	128.01	119.40	14	4
2	C	188	TYR	CB-CG-CD1	-7.81	116.31	121.00	5	7
1	A	449	TYR	CB-CG-CD1	7.81	125.68	121.00	9	4
2	B	183	THR	CA-CB-CG2	-7.79	101.49	112.40	4	1
1	A	504	ASP	CB-CG-OD2	7.76	125.29	118.30	5	1
2	B	71	PHE	CB-CG-CD1	-7.76	115.37	120.80	3	5
2	B	104	PHE	CB-CG-CD1	7.76	126.23	120.80	11	3
2	B	102	ASP	CB-CG-OD1	7.75	125.27	118.30	13	4
2	B	188	TYR	CG-CD1-CE1	-7.74	115.11	121.30	12	4
1	A	388	TRP	CE2-CD2-CG	-7.72	101.12	107.30	12	1
2	B	181	LEU	CB-CG-CD1	7.72	124.12	111.00	15	1
2	C	124	ASP	CB-CG-OD2	7.70	125.23	118.30	3	2
2	C	130	TRP	CG-CD2-CE3	-7.67	127.00	133.90	13	2
1	A	336	PHE	CB-CG-CD1	7.66	126.16	120.80	6	2
1	A	483	TYR	CB-CG-CD2	-7.62	116.43	121.00	13	4
1	A	414	LYS	CA-CB-CG	7.61	130.13	113.40	11	1
1	A	323	PHE	CB-CG-CD2	-7.60	115.48	120.80	15	4
2	C	82	LEU	CB-CG-CD1	7.59	123.90	111.00	11	1
2	C	100	TYR	CG-CD1-CE1	-7.57	115.24	121.30	6	2
1	A	336	PHE	CB-CG-CD2	-7.53	115.53	120.80	6	2
1	A	347	ASN	N-CA-CB	7.52	124.14	110.60	14	1
2	B	86	MET	CG-SD-CE	-7.50	88.20	100.20	9	3
2	C	61	ARG	NH1-CZ-NH2	-7.48	111.17	119.40	9	2
2	C	57	PHE	CB-CG-CD2	-7.48	115.56	120.80	1	5
2	C	115	TYR	CG-CD1-CE1	-7.46	115.33	121.30	1	2
2	C	175	ARG	NH1-CZ-NH2	-7.45	111.20	119.40	6	3
1	A	437	ARG	NH1-CZ-NH2	-7.42	111.24	119.40	9	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	471	ASP	CB-CG-OD1	-7.42	111.63	118.30	12	3
1	A	450	PRO	N-CA-C	7.41	131.36	112.10	6	2
2	B	251	PHE	CB-CG-CD2	-7.40	115.62	120.80	11	6
2	C	108	TRP	CG-CD2-CE3	-7.40	127.24	133.90	15	1
2	C	115	TYR	CB-CG-CD1	-7.37	116.58	121.00	6	4
2	B	73	ASP	CB-CG-OD2	-7.36	111.68	118.30	6	2
2	C	122	TYR	CG-CD2-CE2	7.35	127.18	121.30	11	1
2	B	188	TYR	CB-CG-CD1	7.33	125.40	121.00	10	6
1	A	506	MET	CG-SD-CE	-7.31	88.51	100.20	2	6
2	C	234	GLU	O-C-N	-7.30	111.01	122.70	5	1
1	A	421	TRP	CB-CG-CD1	-7.30	117.52	127.00	2	1
1	A	354	PRO	N-CD-CG	7.28	114.12	103.20	5	1
1	A	374	ARG	NH1-CZ-NH2	-7.26	111.42	119.40	9	2
1	A	440	GLU	OE1-CD-OE2	-7.25	114.60	123.30	12	2
1	A	361	TRP	CB-CG-CD1	7.24	136.41	127.00	10	1
2	C	72	TRP	CB-CG-CD2	7.22	135.99	126.60	2	2
1	A	408	ARG	NH1-CZ-NH2	-7.22	111.46	119.40	9	4
2	B	115	TYR	CG-CD1-CE1	-7.21	115.53	121.30	5	1
2	C	130	TRP	CD1-CG-CD2	-7.19	100.55	106.30	4	1
2	C	179	ASP	CB-CG-OD2	7.18	124.77	118.30	1	2
2	C	70	GLU	OE1-CD-OE2	-7.17	114.70	123.30	11	3
1	A	342	TRP	CZ3-CH2-CZ2	-7.16	113.01	121.60	13	1
1	A	328	MET	CG-SD-CE	-7.15	88.76	100.20	2	4
2	C	145	ARG	NH1-CZ-NH2	-7.14	111.55	119.40	10	3
2	B	258	TYR	CD1-CE1-CZ	-7.13	113.38	119.80	10	3
2	C	86	MET	CG-SD-CE	-7.09	88.85	100.20	12	2
2	B	57	PHE	CB-CG-CD1	-7.08	115.84	120.80	14	3
1	A	420	PHE	CB-CG-CD1	7.08	125.75	120.80	5	5
2	C	258	TYR	CD1-CG-CD2	7.07	125.68	117.90	4	1
1	A	433	ASN	CB-CA-C	7.07	124.54	110.40	11	1
2	B	108	TRP	CB-CG-CD1	-7.01	117.89	127.00	2	2
1	A	478	TYR	CD1-CG-CD2	7.00	125.60	117.90	9	2
1	A	429	PHE	CB-CG-CD2	-6.98	115.91	120.80	12	5
2	B	125	ASP	CB-CG-OD2	6.98	124.58	118.30	6	3
2	B	120	GLU	OE1-CD-OE2	-6.97	114.94	123.30	11	1
1	A	339	ARG	NH1-CZ-NH2	-6.96	111.75	119.40	3	1
1	A	428	TYR	CZ-CE2-CD2	6.96	126.06	119.80	12	3
2	B	175	ARG	NH1-CZ-NH2	6.94	127.04	119.40	2	4
2	C	130	TRP	CB-CG-CD1	-6.94	117.98	127.00	2	1
1	A	503	ARG	NH1-CZ-NH2	-6.93	111.77	119.40	15	3
2	B	258	TYR	CG-CD1-CE1	6.93	126.85	121.30	6	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	71	PHE	CB-CG-CD2	-6.92	115.95	120.80	6	4
1	A	391	ASP	CB-CG-OD2	6.91	124.52	118.30	14	4
2	B	76	GLU	OE1-CD-OE2	6.90	131.59	123.30	5	2
1	A	474	PHE	CB-CG-CD2	6.89	125.62	120.80	7	3
2	B	116	ARG	NH1-CZ-NH2	-6.89	111.83	119.40	12	2
2	C	188	TYR	CG-CD1-CE1	-6.88	115.79	121.30	13	2
2	C	115	TYR	CZ-CE2-CD2	6.88	125.99	119.80	13	3
2	B	192	LEU	CB-CG-CD1	6.87	122.68	111.00	13	1
2	B	71	PHE	CB-CG-CD2	-6.86	116.00	120.80	14	3
1	A	361	TRP	NE1-CE2-CD2	6.86	114.16	107.30	11	1
2	B	103	ASP	CB-CG-OD1	-6.85	112.13	118.30	3	3
1	A	505	TRP	CB-CG-CD2	-6.84	117.70	126.60	2	1
2	C	188	TYR	CG-CD2-CE2	-6.84	115.83	121.30	13	2
1	A	435	TYR	CG-CD2-CE2	-6.84	115.83	121.30	6	2
1	A	392	GLU	OE1-CD-OE2	-6.83	115.10	123.30	6	1
1	A	456	TRP	CB-CG-CD1	6.83	135.88	127.00	11	1
2	B	190	ASP	CB-CG-OD2	-6.83	112.15	118.30	8	2
2	B	190	ASP	CB-CG-OD1	6.82	124.44	118.30	1	4
1	A	342	TRP	CB-CG-CD1	-6.82	118.14	127.00	2	1
2	B	64	LEU	CB-CG-CD2	-6.82	99.42	111.00	12	2
1	A	475	THR	O-C-N	-6.81	111.80	122.70	5	1
1	A	416	ASP	CB-CG-OD1	6.81	124.43	118.30	3	5
1	A	353	TYR	CG-CD1-CE1	-6.81	115.85	121.30	3	2
2	B	237	ARG	N-CA-CB	6.80	122.83	110.60	9	5
1	A	334	PHE	CB-CG-CD2	-6.79	116.05	120.80	12	3
1	A	510	SER	CB-CA-C	6.77	122.95	110.10	12	1
2	B	122	TYR	CD1-CG-CD2	6.74	125.32	117.90	2	1
2	B	166	LEU	CB-CG-CD2	6.74	122.46	111.00	12	1
2	C	179	ASP	CB-CG-OD1	6.74	124.37	118.30	15	3
2	B	66	PRO	N-CA-CB	6.73	111.37	103.30	9	1
2	C	186	ALA	CA-C-N	6.72	135.91	117.10	4	1
2	B	97	VAL	CA-CB-CG2	-6.71	100.84	110.90	7	1
2	B	182	ARG	CD-NE-CZ	6.70	132.99	123.60	4	1
2	B	176	ALA	N-CA-CB	-6.70	100.72	110.10	10	1
2	C	252	LEU	CB-CG-CD1	6.70	122.39	111.00	11	1
1	A	324	ASP	CB-CG-OD1	6.70	124.33	118.30	8	3
2	B	153	ARG	NH1-CZ-NH2	-6.69	112.05	119.40	14	2
2	B	71	PHE	CB-CA-C	6.68	123.77	110.40	2	1
1	A	376	ASP	CB-CG-OD1	6.68	124.31	118.30	13	2
1	A	382	PHE	N-CA-CB	6.67	122.61	110.60	1	3
1	A	372	TYR	CA-CB-CG	6.66	126.06	113.40	5	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	99	PRO	N-CA-CB	6.66	111.29	103.30	9	1
1	A	388	TRP	CB-CG-CD2	-6.65	117.96	126.60	12	4
2	B	250	SER	N-CA-CB	6.64	120.46	110.50	9	1
2	C	191	GLU	OE1-CD-OE2	-6.63	115.34	123.30	15	2
2	B	218	ALA	N-CA-CB	-6.63	100.81	110.10	10	3
2	B	244	LEU	CB-CG-CD2	6.62	122.26	111.00	4	1
1	A	456	TRP	CB-CG-CD2	-6.62	118.00	126.60	11	2
2	C	237	ARG	CD-NE-CZ	6.61	132.85	123.60	9	2
2	C	125	ASP	N-CA-CB	-6.61	98.71	110.60	5	1
1	A	505	TRP	CB-CG-CD1	6.59	135.56	127.00	2	1
1	A	382	PHE	CB-CG-CD2	-6.59	116.19	120.80	9	3
2	C	153	ARG	NH1-CZ-NH2	-6.58	112.17	119.40	3	2
2	B	93	VAL	CA-CB-CG1	-6.57	101.05	110.90	10	1
1	A	486	PHE	CB-CG-CD2	6.56	125.39	120.80	10	4
2	B	169	GLU	OE1-CD-OE2	-6.56	115.43	123.30	11	1
2	C	85	GLU	OE1-CD-OE2	-6.55	115.44	123.30	9	2
2	B	170	MET	O-C-N	-6.55	112.22	122.70	10	1
2	C	128	LYS	O-C-N	-6.55	112.22	122.70	4	1
2	B	92	GLU	OE1-CD-OE2	-6.55	115.44	123.30	14	2
1	A	370	THR	CA-CB-CG2	6.55	121.57	112.40	8	2
1	A	333	MET	CA-CB-CG	6.54	124.43	113.30	3	1
2	C	100	TYR	CG-CD2-CE2	-6.54	116.06	121.30	13	2
2	B	93	VAL	CA-CB-CG2	-6.54	101.09	110.90	11	1
2	C	198	ALA	N-CA-CB	-6.54	100.94	110.10	10	2
2	B	165	PRO	N-CA-CB	6.53	111.13	103.30	1	2
2	B	191	GLU	O-C-N	-6.52	112.26	122.70	10	2
1	A	417	ALA	CB-CA-C	-6.51	100.33	110.10	7	1
1	A	380	VAL	CA-CB-CG2	-6.51	101.14	110.90	1	1
1	A	382	PHE	CG-CD2-CE2	6.50	127.95	120.80	4	1
2	C	195	ARG	NH1-CZ-NH2	-6.50	112.25	119.40	4	2
2	B	154	GLN	O-C-N	-6.49	112.31	122.70	10	1
1	A	353	TYR	CG-CD2-CE2	-6.49	116.11	121.30	6	2
1	A	443	ARG	NH1-CZ-NH2	-6.48	112.27	119.40	10	2
2	C	178	VAL	CA-CB-CG2	-6.48	101.18	110.90	9	1
1	A	497	TYR	CD1-CG-CD2	6.46	125.01	117.90	8	1
1	A	351	ASP	CB-CG-OD2	-6.45	112.49	118.30	1	4
2	C	72	TRP	CB-CG-CD1	-6.45	118.61	127.00	2	2
2	B	103	ASP	CB-CG-OD2	6.45	124.11	118.30	3	4
2	C	210	ARG	NH1-CZ-NH2	-6.45	112.31	119.40	4	6
1	A	442	LEU	CB-CA-C	-6.45	97.95	110.20	8	1
1	A	497	TYR	CB-CG-CD1	6.44	124.87	121.00	12	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	493	VAL	CA-CB-CG2	6.44	120.56	110.90	5	1
2	B	170	MET	CG-SD-CE	-6.44	89.89	100.20	7	5
1	A	379	PHE	CG-CD1-CE1	6.44	127.88	120.80	7	1
1	A	412	THR	CA-CB-CG2	6.43	121.41	112.40	15	3
2	C	68	THR	CA-CB-CG2	6.41	121.38	112.40	4	1
1	A	343	ARG	NH1-CZ-NH2	-6.41	112.34	119.40	11	2
2	B	89	ASP	CB-CG-OD1	6.41	124.07	118.30	13	1
2	C	110	GLU	OE1-CD-OE2	-6.41	115.61	123.30	11	1
2	C	57	PHE	CB-CG-CD1	-6.41	116.31	120.80	6	3
2	B	253	SER	N-CA-CB	6.41	120.12	110.50	9	1
2	C	130	TRP	CZ3-CH2-CZ2	-6.40	113.92	121.60	4	2
2	C	71	PHE	CB-CG-CD1	6.40	125.28	120.80	13	4
2	C	195	ARG	CD-NE-CZ	6.40	132.56	123.60	5	1
2	B	63	GLN	N-CA-CB	-6.40	99.09	110.60	5	1
2	C	184	HIS	O-C-N	-6.40	112.47	122.70	11	1
2	C	95	ALA	N-CA-CB	-6.39	101.15	110.10	15	1
2	C	93	VAL	CA-CB-CG2	-6.39	101.32	110.90	3	1
2	B	133	GLU	OE1-CD-OE2	-6.39	115.64	123.30	15	1
2	C	94	LYS	O-C-N	-6.38	112.49	122.70	1	1
2	C	172	ASP	CB-CG-OD1	6.38	124.04	118.30	7	2
2	C	148	LEU	N-CA-CB	-6.38	97.64	110.40	15	1
1	A	361	TRP	CB-CG-CD2	-6.38	118.31	126.60	10	2
2	B	128	LYS	N-CA-CB	-6.37	99.13	110.60	7	1
2	B	188	TYR	CD1-CE1-CZ	6.37	125.53	119.80	7	1
1	A	463	PRO	N-CA-CB	6.37	110.94	103.30	4	1
2	C	111	GLU	OE1-CD-OE2	-6.36	115.66	123.30	6	1
2	B	191	GLU	OE1-CD-OE2	-6.35	115.67	123.30	9	1
2	B	235	ASP	CB-CG-OD1	6.35	124.02	118.30	2	2
2	B	72	TRP	CB-CG-CD1	-6.35	118.75	127.00	15	1
2	B	202	ALA	N-CA-CB	-6.35	101.21	110.10	7	2
2	C	188	TYR	CD1-CE1-CZ	6.35	125.51	119.80	13	1
2	B	122	TYR	CG-CD1-CE1	-6.33	116.24	121.30	2	3
1	A	323	PHE	CB-CG-CD1	6.33	125.23	120.80	15	3
1	A	464	ARG	NH1-CZ-NH2	-6.32	112.44	119.40	8	1
1	A	418	ALA	CB-CA-C	-6.32	100.62	110.10	8	1
2	C	202	ALA	N-CA-CB	-6.32	101.26	110.10	7	2
2	B	158	GLU	OE1-CD-OE2	-6.31	115.73	123.30	15	2
1	A	445	VAL	CA-CB-CG1	6.31	120.36	110.90	14	1
2	C	258	TYR	N-CA-CB	-6.31	99.25	110.60	2	1
2	B	178	VAL	CA-CB-CG1	6.30	120.35	110.90	6	1
1	A	435	TYR	CB-CA-C	6.29	122.98	110.40	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	361	TRP	NE1-CE2-CZ2	-6.28	123.49	130.40	1	1
2	B	147	GLU	OE1-CD-OE2	-6.28	115.76	123.30	9	2
2	C	264	THR	CA-CB-CG2	-6.28	103.60	112.40	5	1
1	A	449	TYR	CG-CD2-CE2	-6.28	116.27	121.30	14	3
2	B	183	THR	N-CA-CB	6.28	122.24	110.30	11	1
1	A	372	TYR	CG-CD1-CE1	-6.27	116.28	121.30	7	2
1	A	413	ASP	O-C-N	-6.27	112.66	122.70	11	2
2	C	232	ALA	N-CA-CB	-6.27	101.32	110.10	3	3
2	C	250	SER	N-CA-CB	6.27	119.91	110.50	6	1
2	C	199	ARG	NH1-CZ-NH2	-6.27	112.51	119.40	10	3
1	A	353	TYR	CZ-CE2-CD2	6.25	125.43	119.80	6	3
1	A	362	ARG	NH1-CZ-NH2	-6.25	112.53	119.40	11	1
1	A	428	TYR	CD1-CE1-CZ	6.24	125.42	119.80	11	2
2	B	137	TYR	CZ-CE2-CD2	-6.24	114.18	119.80	7	1
2	B	142	GLU	OE1-CD-OE2	-6.24	115.81	123.30	3	2
1	A	478	TYR	CG-CD2-CE2	-6.23	116.31	121.30	9	2
1	A	477	PHE	CB-CA-C	-6.23	97.95	110.40	15	1
1	A	413	ASP	CB-CG-OD1	-6.22	112.70	118.30	7	3
2	C	100	TYR	CD1-CE1-CZ	-6.21	114.21	119.80	2	1
1	A	464	ARG	CD-NE-CZ	6.21	132.29	123.60	5	1
2	C	183	THR	CA-CB-CG2	-6.21	103.71	112.40	8	2
1	A	332	GLU	OE1-CD-OE2	-6.20	115.86	123.30	8	2
2	B	125	ASP	CB-CA-C	-6.20	98.01	110.40	14	1
2	B	73	ASP	CB-CG-OD1	6.19	123.87	118.30	6	1
1	A	349	VAL	CG1-CB-CG2	6.19	120.80	110.90	6	1
2	C	147	GLU	CG-CD-OE2	6.19	130.67	118.30	11	1
2	B	249	VAL	CG1-CB-CG2	-6.18	101.00	110.90	6	3
2	B	95	ALA	CB-CA-C	6.18	119.37	110.10	2	2
1	A	428	TYR	CG-CD2-CE2	-6.17	116.36	121.30	9	2
1	A	349	VAL	CA-CB-CG1	-6.17	101.64	110.90	6	1
1	A	379	PHE	CD1-CE1-CZ	-6.17	112.69	120.10	7	1
1	A	428	TYR	CD1-CG-CD2	6.16	124.68	117.90	3	1
2	C	190	ASP	CB-CG-OD1	6.15	123.84	118.30	12	2
2	C	102	ASP	CB-CG-OD1	6.15	123.83	118.30	5	1
1	A	374	ARG	CD-NE-CZ	6.15	132.21	123.60	15	2
1	A	436	TYR	CG-CD1-CE1	-6.15	116.38	121.30	7	2
2	C	122	TYR	CD1-CE1-CZ	6.14	125.33	119.80	6	1
2	C	130	TRP	CH2-CZ2-CE2	-6.11	111.29	117.40	2	1
1	A	346	ASN	CA-CB-CG	-6.11	99.96	113.40	10	1
2	C	210	ARG	CA-CB-CG	6.11	126.83	113.40	2	1
2	B	247	PHE	CG-CD1-CE1	6.10	127.51	120.80	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	116	ARG	CD-NE-CZ	6.09	132.12	123.60	13	2
1	A	461	GLU	O-C-N	-6.09	112.96	122.70	12	1
2	B	100	TYR	CD1-CE1-CZ	6.08	125.28	119.80	10	1
2	B	157	HIS	CA-CB-CG	-6.08	103.26	113.60	2	1
1	A	353	TYR	CA-CB-CG	-6.07	101.86	113.40	15	1
2	C	58	SER	N-CA-CB	6.07	119.61	110.50	15	1
1	A	439	ASN	O-C-N	-6.07	112.99	122.70	4	1
1	A	396	GLU	OE1-CD-OE2	-6.07	116.02	123.30	1	1
2	C	64	LEU	O-C-N	-6.06	112.89	123.20	3	1
2	B	197	ALA	N-CA-CB	-6.06	101.62	110.10	7	1
1	A	417	ALA	N-CA-CB	6.06	118.58	110.10	7	1
2	C	188	TYR	O-C-N	-6.05	113.01	122.70	5	1
1	A	459	ILE	CA-C-N	6.04	134.02	117.10	12	2
2	B	164	SER	N-CA-C	6.04	127.31	111.00	10	2
2	C	89	ASP	CB-CG-OD1	-6.04	112.87	118.30	1	2
2	B	264	THR	CA-CB-CG2	-6.04	103.95	112.40	7	1
2	B	237	ARG	NH1-CZ-NH2	-6.04	112.76	119.40	8	3
2	C	134	MET	N-CA-CB	-6.04	99.73	110.60	10	1
1	A	491	LEU	CB-CA-C	6.03	121.66	110.20	14	1
2	B	135	GLU	CB-CA-C	6.03	122.46	110.40	6	1
2	B	185	LEU	N-CA-CB	-6.02	98.36	110.40	12	1
2	B	250	SER	CB-CA-C	6.02	121.54	110.10	1	1
2	C	141	VAL	CA-CB-CG2	-6.02	101.88	110.90	4	3
2	C	120	GLU	CA-C-N	6.02	133.94	117.10	15	2
2	B	95	ALA	N-CA-CB	-6.01	101.68	110.10	9	2
1	A	404	LYS	O-C-N	-6.00	113.10	122.70	15	3
2	B	138	ARG	NH1-CZ-NH2	-6.00	112.80	119.40	10	2
2	C	115	TYR	CD1-CE1-CZ	6.00	125.20	119.80	14	1
2	C	214	TYR	CG-CD1-CE1	-6.00	116.50	121.30	12	4
2	B	55	SER	N-CA-CB	5.98	119.48	110.50	2	1
2	B	91	GLU	OE1-CD-OE2	-5.98	116.12	123.30	13	1
1	A	367	SER	N-CA-CB	5.98	119.47	110.50	1	3
2	C	108	TRP	CG-CD1-NE1	5.98	116.08	110.10	13	2
2	C	141	VAL	CG1-CB-CG2	-5.98	101.34	110.90	13	1
2	C	114	LEU	CB-CG-CD1	-5.97	100.84	111.00	7	1
1	A	462	SER	N-CA-CB	5.97	119.46	110.50	4	2
2	B	62	GLU	OE1-CD-OE2	-5.97	116.14	123.30	11	1
2	B	117	GLN	CA-CB-CG	5.97	126.53	113.40	14	1
2	B	258	TYR	CG-CD2-CE2	-5.97	116.53	121.30	5	2
2	C	178	VAL	CG1-CB-CG2	-5.96	101.36	110.90	10	1
1	A	343	ARG	CD-NE-CZ	5.96	131.95	123.60	2	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	119	VAL	CA-CB-CG1	5.96	119.84	110.90	12	2
2	C	108	TRP	NE1-CE2-CD2	-5.96	101.34	107.30	1	1
2	B	232	ALA	CB-CA-C	-5.95	101.17	110.10	6	1
1	A	467	PHE	CZ-CE2-CD2	5.95	127.24	120.10	14	2
2	C	149	GLN	O-C-N	-5.94	113.20	122.70	4	1
1	A	476	TYR	CG-CD1-CE1	-5.94	116.55	121.30	10	2
2	C	56	THR	OG1-CB-CG2	-5.94	96.34	110.00	14	1
1	A	428	TYR	CG-CD1-CE1	-5.93	116.55	121.30	1	2
2	C	137	TYR	CG-CD2-CE2	-5.93	116.55	121.30	13	1
2	C	175	ARG	CB-CA-C	5.93	122.27	110.40	15	1
1	A	381	PHE	CZ-CE2-CD2	-5.93	112.98	120.10	12	1
2	C	121	PRO	N-CA-CB	5.93	110.42	103.30	1	1
2	C	106	LYS	O-C-N	-5.93	113.21	122.70	7	1
2	B	71	PHE	CG-CD2-CE2	-5.93	114.28	120.80	9	1
1	A	341	PHE	CD1-CE1-CZ	-5.93	112.98	120.10	10	1
2	B	238	GLN	N-CA-CB	5.92	121.27	110.60	6	1
2	C	134	MET	O-C-N	-5.92	113.22	122.70	9	1
2	C	124	ASP	N-CA-CB	-5.91	99.96	110.60	10	1
2	C	100	TYR	O-C-N	-5.91	113.24	122.70	9	1
2	C	146	ALA	N-CA-CB	-5.91	101.83	110.10	4	2
1	A	375	LYS	O-C-N	-5.91	113.25	122.70	3	1
2	C	244	LEU	CB-CG-CD1	5.90	121.03	111.00	9	1
2	C	214	TYR	CZ-CE2-CD2	5.89	125.10	119.80	12	2
2	B	115	TYR	CG-CD2-CE2	-5.88	116.60	121.30	12	2
1	A	446	ASP	O-C-N	-5.87	113.30	122.70	12	2
2	B	141	VAL	CG1-CB-CG2	-5.87	101.50	110.90	3	1
2	B	67	VAL	CB-CA-C	5.87	122.56	111.40	14	1
2	B	71	PHE	CD1-CG-CD2	5.87	125.93	118.30	9	1
2	C	202	ALA	C-N-CA	5.87	136.37	121.70	9	1
1	A	491	LEU	N-CA-CB	5.86	122.12	110.40	10	1
1	A	403	ILE	CB-CA-C	5.86	123.32	111.60	4	1
1	A	361	TRP	CH2-CZ2-CE2	5.86	123.26	117.40	9	1
1	A	452	ASN	CB-CA-C	5.86	122.11	110.40	13	1
1	A	361	TRP	CE2-CD2-CG	-5.85	102.62	107.30	9	2
2	B	171	ARG	NH1-CZ-NH2	-5.85	112.96	119.40	10	4
1	A	387	HIS	CA-CB-CG	5.85	123.55	113.60	5	4
1	A	416	ASP	CB-CA-C	-5.85	98.70	110.40	4	1
2	B	203	LEU	O-C-N	-5.85	113.34	122.70	9	2
2	C	179	ASP	O-C-N	-5.85	113.34	122.70	10	1
1	A	456	TRP	CG-CD2-CE3	-5.84	128.64	133.90	6	1
1	A	510	SER	N-CA-CB	5.84	119.25	110.50	13	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	163	LEU	CB-CG-CD2	5.83	120.91	111.00	2	1
2	C	174	ALA	N-CA-CB	5.83	118.26	110.10	6	1
1	A	455	VAL	CA-CB-CG1	5.83	119.64	110.90	10	2
2	B	234	GLU	OE1-CD-OE2	-5.82	116.32	123.30	4	1
1	A	341	PHE	CB-CA-C	5.82	122.04	110.40	5	1
2	C	186	ALA	N-CA-CB	-5.82	101.96	110.10	8	2
1	A	484	TRP	CG-CD1-NE1	-5.82	104.28	110.10	5	2
2	B	166	LEU	CB-CG-CD1	5.82	120.89	111.00	6	1
2	B	63	GLN	O-C-N	-5.80	113.41	122.70	10	1
2	B	212	ALA	N-CA-CB	-5.80	101.98	110.10	1	1
1	A	438	PHE	CB-CG-CD2	-5.80	116.74	120.80	7	2
2	B	108	TRP	CE3-CZ3-CH2	5.80	127.58	121.20	8	1
2	C	258	TYR	CG-CD1-CE1	-5.80	116.66	121.30	4	4
2	B	123	LEU	CB-CG-CD2	5.80	120.85	111.00	13	1
1	A	326	VAL	CG1-CB-CG2	-5.79	101.63	110.90	13	1
1	A	462	SER	CB-CA-C	5.79	121.11	110.10	9	1
2	C	142	GLU	OE1-CD-OE2	-5.79	116.36	123.30	4	1
2	B	236	LEU	CB-CG-CD2	-5.78	101.17	111.00	7	1
2	C	104	PHE	CG-CD2-CE2	-5.78	114.44	120.80	3	1
1	A	501	ALA	N-CA-CB	5.78	118.19	110.10	5	1
2	B	186	ALA	CA-C-N	5.78	133.28	117.10	9	1
2	C	188	TYR	CZ-CE2-CD2	5.78	125.00	119.80	13	1
1	A	479	LYS	C-N-CA	5.77	134.43	122.30	8	1
2	C	112	MET	CG-SD-CE	5.77	109.44	100.20	2	1
2	C	125	ASP	CB-CG-OD2	5.77	123.50	118.30	14	3
1	A	390	PHE	N-CA-CB	5.77	120.98	110.60	4	1
2	C	259	THR	CA-CB-CG2	-5.77	104.32	112.40	14	1
2	B	68	THR	CA-CB-CG2	-5.76	104.33	112.40	13	2
1	A	326	VAL	O-C-N	-5.75	113.51	122.70	11	1
1	A	387	HIS	N-CA-CB	5.75	120.94	110.60	15	1
1	A	399	TYR	CG-CD1-CE1	-5.75	116.70	121.30	11	3
2	B	100	TYR	CD1-CG-CD2	5.74	124.21	117.90	10	1
2	C	108	TRP	CE2-CD2-CG	5.74	111.89	107.30	1	1
2	C	127	GLN	CG-CD-OE1	5.74	133.07	121.60	3	1
2	B	149	GLN	CA-CB-CG	5.74	126.02	113.40	13	1
2	C	108	TRP	CD2-CE3-CZ3	5.73	126.25	118.80	6	1
2	B	115	TYR	CD1-CE1-CZ	-5.73	114.64	119.80	3	1
2	B	182	ARG	NH1-CZ-NH2	-5.73	113.10	119.40	8	1
2	B	120	GLU	N-CA-C	5.72	126.45	111.00	14	1
1	A	414	LYS	O-C-N	-5.71	113.56	122.70	4	1
2	B	219	THR	CA-CB-CG2	-5.71	104.40	112.40	14	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	97	VAL	CA-CB-CG2	-5.71	102.34	110.90	5	1
1	A	422	MET	CA-C-N	5.71	133.08	117.10	1	1
1	A	399	TYR	CB-CA-C	-5.71	98.99	110.40	12	1
2	B	72	TRP	CH2-CZ2-CE2	5.71	123.11	117.40	12	1
2	B	126	PHE	CD1-CE1-CZ	5.70	126.94	120.10	12	1
2	B	72	TRP	CD2-CE2-CZ2	-5.70	115.46	122.30	12	1
1	A	421	TRP	CE2-CD2-CG	-5.70	102.74	107.30	3	1
1	A	390	PHE	CG-CD2-CE2	5.70	127.07	120.80	5	1
2	C	128	LYS	N-CA-CB	5.70	120.85	110.60	13	1
2	C	71	PHE	CG-CD1-CE1	-5.69	114.54	120.80	4	1
2	B	217	LYS	CB-CA-C	-5.69	99.02	110.40	9	1
2	C	205	GLU	OE1-CD-OE2	-5.69	116.47	123.30	15	1
1	A	376	ASP	N-CA-CB	5.68	120.83	110.60	10	1
1	A	325	THR	N-CA-CB	5.68	121.09	110.30	4	2
1	A	324	ASP	CB-CA-C	-5.68	99.04	110.40	10	1
1	A	486	PHE	O-C-N	-5.68	113.61	122.70	15	1
1	A	317	ASN	CA-CB-CG	-5.67	100.92	113.40	15	1
1	A	335	VAL	CG1-CB-CG2	5.67	119.97	110.90	4	2
2	C	62	GLU	OE1-CD-OE2	-5.67	116.50	123.30	5	1
2	B	164	SER	N-CA-CB	5.67	119.00	110.50	6	2
1	A	484	TRP	CD1-CG-CD2	5.67	110.83	106.30	14	1
2	C	190	ASP	CB-CG-OD2	-5.66	113.20	118.30	6	3
2	B	225	LEU	O-C-N	-5.66	113.64	122.70	10	1
2	B	214	TYR	CG-CD2-CE2	5.66	125.83	121.30	14	1
2	C	71	PHE	CA-CB-CG	5.66	127.48	113.90	14	1
1	A	491	LEU	CB-CG-CD1	-5.66	101.39	111.00	8	2
1	A	376	ASP	CB-CG-OD2	5.66	123.39	118.30	6	2
1	A	321	GLY	C-N-CA	5.65	135.83	121.70	13	1
1	A	477	PHE	N-CA-CB	5.65	120.77	110.60	4	2
2	C	98	GLN	CB-CA-C	5.65	121.70	110.40	10	1
2	B	213	GLU	OE1-CD-OE2	-5.65	116.53	123.30	12	1
2	B	178	VAL	O-C-N	-5.65	113.67	122.70	14	1
1	A	394	SER	N-CA-CB	5.64	118.96	110.50	15	1
2	C	264	THR	N-CA-CB	5.64	121.02	110.30	13	2
1	A	389	VAL	N-CA-CB	5.64	123.90	111.50	3	1
1	A	340	TRP	CD1-NE1-CE2	5.64	114.07	109.00	9	1
2	C	112	MET	CB-CA-C	5.64	121.67	110.40	8	1
1	A	370	THR	N-CA-CB	5.63	121.01	110.30	13	1
2	C	201	GLU	OE1-CD-OE2	-5.63	116.54	123.30	4	1
2	B	214	TYR	CD1-CG-CD2	-5.62	111.71	117.90	1	1
2	C	200	LEU	CB-CA-C	5.62	120.88	110.20	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	403	ILE	O-C-N	-5.62	113.71	122.70	5	1
2	C	82	LEU	CB-CA-C	-5.61	99.54	110.20	14	1
1	A	484	TRP	CZ3-CH2-CZ2	-5.61	114.87	121.60	7	2
2	B	94	LYS	O-C-N	-5.61	113.73	122.70	8	1
2	C	153	ARG	O-C-N	-5.61	113.73	122.70	12	1
1	A	441	GLU	CB-CA-C	-5.60	99.19	110.40	1	1
1	A	505	TRP	N-CA-CB	5.60	120.68	110.60	6	1
2	C	153	ARG	CD-NE-CZ	5.60	131.44	123.60	8	1
2	C	93	VAL	CG1-CB-CG2	-5.59	101.95	110.90	13	2
2	C	138	ARG	N-CA-CB	5.59	120.67	110.60	13	1
2	C	122	TYR	CD1-CG-CD2	-5.59	111.75	117.90	11	1
1	A	447	SER	N-CA-CB	-5.59	102.11	110.50	6	1
2	C	135	GLU	OE1-CD-OE2	-5.58	116.60	123.30	10	1
2	B	264	THR	N-CA-CB	5.58	120.90	110.30	5	1
2	C	111	GLU	CB-CA-C	5.58	121.55	110.40	8	1
2	B	259	THR	O-C-N	-5.58	113.78	122.70	3	1
2	C	97	VAL	CA-CB-CG1	5.58	119.26	110.90	15	2
2	C	190	ASP	O-C-N	-5.57	113.78	122.70	11	1
2	B	112	MET	CA-CB-CG	-5.57	103.83	113.30	6	1
2	B	200	LEU	CB-CG-CD2	-5.57	101.53	111.00	12	1
1	A	497	TYR	CD1-CE1-CZ	-5.57	114.79	119.80	5	3
2	C	78	GLU	OE1-CD-OE2	-5.57	116.62	123.30	8	3
2	B	248	LYS	O-C-N	-5.56	113.81	122.70	1	1
2	C	226	SER	N-CA-CB	-5.56	102.16	110.50	7	1
2	B	86	MET	CA-CB-CG	5.55	122.74	113.30	10	1
2	B	59	LYS	N-CA-CB	-5.55	100.61	110.60	7	1
1	A	497	TYR	CZ-CE2-CD2	5.55	124.79	119.80	6	1
2	B	252	LEU	CB-CG-CD2	5.55	120.43	111.00	14	1
2	B	251	PHE	N-CA-CB	-5.54	100.63	110.60	10	1
2	B	137	TYR	CG-CD1-CE1	-5.54	116.87	121.30	10	1
2	C	175	ARG	CB-CG-CD	5.53	125.99	111.60	6	2
1	A	468	MET	O-C-N	-5.53	113.80	123.20	2	1
2	B	223	SER	CB-CA-C	-5.53	99.60	110.10	1	1
2	C	229	ALA	CB-CA-C	-5.53	101.81	110.10	1	2
1	A	492	LYS	CB-CA-C	-5.52	99.36	110.40	9	1
2	C	119	VAL	O-C-N	-5.52	113.87	122.70	10	1
1	A	340	TRP	CH2-CZ2-CE2	5.51	122.92	117.40	2	1
1	A	322	ASN	CA-CB-CG	-5.51	101.27	113.40	10	1
1	A	486	PHE	CB-CA-C	5.51	121.43	110.40	2	1
1	A	372	TYR	CD1-CE1-CZ	-5.51	114.84	119.80	14	1
2	C	257	GLU	OE1-CD-OE2	-5.51	116.69	123.30	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	110	GLU	O-C-N	-5.51	113.89	122.70	14	1
2	B	201	GLU	O-C-N	-5.51	113.89	122.70	8	1
1	A	479	LYS	O-C-N	-5.50	113.84	123.20	11	1
1	A	422	MET	N-CA-C	5.50	125.86	111.00	1	2
2	B	258	TYR	CD1-CG-CD2	5.50	123.95	117.90	11	1
1	A	495	PRO	CA-C-N	5.50	127.19	116.20	7	1
1	A	501	ALA	O-C-N	-5.49	113.91	122.70	10	1
2	C	102	ASP	O-C-N	-5.49	113.91	122.70	4	2
2	C	214	TYR	CD1-CE1-CZ	5.49	124.74	119.80	12	1
2	B	180	ALA	N-CA-CB	-5.49	102.42	110.10	4	1
2	B	91	GLU	O-C-N	-5.49	113.92	122.70	14	1
2	B	257	GLU	OE1-CD-OE2	-5.49	116.72	123.30	9	2
2	B	241	LEU	CB-CG-CD1	5.49	120.32	111.00	9	1
2	C	119	VAL	CA-CB-CG1	5.48	119.12	110.90	9	1
2	C	193	ARG	N-CA-CB	5.48	120.46	110.60	14	1
2	B	72	TRP	CB-CG-CD2	5.48	133.72	126.60	15	1
1	A	468	MET	CG-SD-CE	-5.47	91.44	100.20	13	2
1	A	424	ASN	O-C-N	-5.47	113.89	123.20	8	1
1	A	422	MET	O-C-N	-5.47	110.71	121.10	1	1
2	C	115	TYR	CG-CD2-CE2	-5.47	116.92	121.30	13	1
2	C	122	TYR	O-C-N	-5.47	113.95	122.70	1	1
2	B	205	GLU	OE1-CD-OE2	-5.47	116.74	123.30	5	1
2	B	245	GLU	OE1-CD-OE2	-5.46	116.74	123.30	11	1
1	A	399	TYR	CA-CB-CG	-5.46	103.02	113.40	15	2
2	C	171	ARG	NH1-CZ-NH2	-5.46	113.40	119.40	15	1
2	C	164	SER	CA-C-N	5.45	132.36	117.10	4	1
2	B	261	LYS	O-C-N	-5.45	113.98	122.70	6	1
2	C	256	GLU	OE1-CD-OE2	-5.45	116.76	123.30	7	1
2	C	152	ALA	O-C-N	-5.45	113.99	122.70	2	1
2	C	186	ALA	CA-C-O	-5.45	108.67	120.10	4	1
2	C	147	GLU	CB-CA-C	5.45	121.29	110.40	7	1
2	C	196	LEU	CB-CA-C	5.44	120.54	110.20	13	1
1	A	342	TRP	CB-CG-CD2	5.44	133.67	126.60	14	1
1	A	353	TYR	CA-C-O	-5.44	108.68	120.10	10	1
1	A	436	TYR	CD1-CE1-CZ	-5.44	114.91	119.80	11	1
2	B	76	GLU	N-CA-CB	5.43	120.37	110.60	2	2
2	B	238	GLN	O-C-N	-5.43	113.97	123.20	3	1
1	A	334	PHE	CZ-CE2-CD2	-5.43	113.59	120.10	2	1
2	B	135	GLU	OE1-CD-OE2	-5.43	116.79	123.30	9	1
1	A	444	ALA	N-CA-CB	-5.43	102.50	110.10	11	1
1	A	484	TRP	CE2-CD2-CG	-5.42	102.96	107.30	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	388	TRP	CD1-CG-CD2	5.42	110.64	106.30	12	1
1	A	473	VAL	CA-CB-CG1	5.42	119.03	110.90	13	1
2	C	220	GLU	N-CA-CB	5.42	120.35	110.60	14	1
2	C	123	LEU	CB-CA-C	5.41	120.48	110.20	3	1
2	C	136	LEU	CB-CG-CD2	-5.41	101.80	111.00	4	1
2	B	90	LEU	CB-CG-CD2	5.41	120.19	111.00	10	1
2	C	186	ALA	N-CA-C	5.41	125.60	111.00	13	1
1	A	475	THR	CA-CB-CG2	5.41	119.97	112.40	7	1
2	B	170	MET	N-CA-CB	5.41	120.33	110.60	8	1
2	C	251	PHE	CG-CD1-CE1	-5.40	114.86	120.80	1	1
2	C	60	LEU	CB-CG-CD1	5.39	120.17	111.00	15	1
2	C	113	GLU	OE1-CD-OE2	-5.39	116.83	123.30	9	1
2	B	150	GLU	OE1-CD-OE2	-5.38	116.84	123.30	9	1
1	A	473	VAL	C-N-CA	5.38	135.15	121.70	2	1
2	C	147	GLU	OE1-CD-OE2	-5.38	116.84	123.30	2	2
2	B	214	TYR	CD1-CE1-CZ	-5.38	114.96	119.80	14	1
1	A	404	LYS	N-CA-CB	5.37	120.27	110.60	3	1
1	A	494	GLU	N-CA-CB	5.37	120.27	110.60	8	1
2	C	171	ARG	CG-CD-NE	-5.37	100.52	111.80	14	1
2	B	142	GLU	CB-CA-C	5.37	121.14	110.40	5	1
1	A	335	VAL	CA-CB-CG2	-5.37	102.84	110.90	2	1
1	A	342	TRP	CB-CA-C	-5.36	99.67	110.40	1	1
2	C	213	GLU	OE1-CD-OE2	-5.36	116.87	123.30	7	3
2	B	263	ASN	CB-CA-C	-5.36	99.68	110.40	8	1
2	C	73	ASP	CA-CB-CG	-5.35	101.62	113.40	3	1
1	A	384	GLY	O-C-N	-5.35	114.14	122.70	13	1
2	C	245	GLU	OE1-CD-OE2	-5.35	116.88	123.30	12	1
1	A	422	MET	CA-CB-CG	5.35	122.39	113.30	8	1
1	A	341	PHE	C-N-CA	5.34	135.06	121.70	6	1
1	A	453	ILE	CA-CB-CG1	5.34	121.14	111.00	3	1
2	B	145	ARG	NH1-CZ-NH2	-5.34	113.53	119.40	9	2
1	A	343	ARG	CG-CD-NE	-5.34	100.59	111.80	3	2
2	C	136	LEU	CB-CG-CD1	5.34	120.07	111.00	3	1
2	B	58	SER	O-C-N	-5.33	114.17	122.70	12	1
1	A	419	LEU	C-N-CA	5.33	135.03	121.70	14	1
2	B	152	ALA	N-CA-CB	-5.33	102.64	110.10	6	1
2	B	61	ARG	CD-NE-CZ	5.33	131.06	123.60	9	1
2	C	115	TYR	CD1-CG-CD2	5.33	123.76	117.90	12	2
1	A	476	TYR	CZ-CE2-CD2	5.33	124.60	119.80	2	2
1	A	478	TYR	CZ-CE2-CD2	-5.33	115.00	119.80	2	1
2	B	177	HIS	N-CA-CB	5.33	120.19	110.60	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	413	ASP	CB-CA-C	5.33	121.05	110.40	6	1
2	C	194	GLN	O-C-N	-5.32	114.18	122.70	5	1
2	B	67	VAL	CA-CB-CG1	5.32	118.88	110.90	13	2
2	B	60	LEU	CB-CG-CD2	5.32	120.04	111.00	12	1
1	A	383	LYS	CB-CA-C	-5.31	99.78	110.40	5	1
2	C	145	ARG	CD-NE-CZ	5.31	131.04	123.60	13	2
2	C	175	ARG	O-C-N	-5.31	114.20	122.70	14	1
2	B	221	HIS	CA-CB-CG	-5.31	104.57	113.60	9	1
2	C	141	VAL	CA-CB-CG1	-5.31	102.94	110.90	9	1
2	C	258	TYR	CD1-CE1-CZ	-5.31	115.02	119.80	14	1
2	C	138	ARG	NH1-CZ-NH2	5.31	125.24	119.40	1	1
1	A	432	GLY	CA-C-O	5.31	130.16	120.60	3	1
1	A	448	GLU	N-CA-CB	5.31	120.15	110.60	4	1
1	A	441	GLU	OE1-CD-OE2	-5.30	116.94	123.30	4	2
1	A	477	PHE	CG-CD1-CE1	5.30	126.63	120.80	6	1
2	B	79	THR	N-CA-CB	5.30	120.36	110.30	6	1
1	A	414	LYS	N-CA-CB	5.30	120.13	110.60	10	1
1	A	506	MET	CA-CB-CG	5.29	122.29	113.30	6	1
2	B	214	TYR	CZ-CE2-CD2	-5.29	115.04	119.80	14	1
2	C	245	GLU	N-CA-CB	-5.29	101.08	110.60	4	1
2	B	221	HIS	O-C-N	-5.29	114.24	122.70	12	1
1	A	325	THR	CA-CB-OG1	5.29	120.10	109.00	3	1
2	B	122	TYR	CD1-CE1-CZ	-5.28	115.05	119.80	3	1
2	C	181	LEU	CA-C-O	5.28	131.19	120.10	5	1
1	A	435	TYR	CZ-CE2-CD2	5.28	124.55	119.80	4	1
1	A	484	TRP	CG-CD2-CE3	5.28	138.65	133.90	10	2
2	C	222	LEU	CA-CB-CG	5.28	127.43	115.30	14	1
2	B	97	VAL	O-C-N	-5.27	114.26	122.70	4	1
1	A	421	TRP	CG-CD2-CE3	-5.27	129.15	133.90	11	1
2	B	224	THR	CA-CB-CG2	-5.27	105.02	112.40	5	1
2	C	200	LEU	CB-CG-CD1	5.27	119.96	111.00	15	1
2	B	172	ASP	CB-CA-C	5.27	120.93	110.40	7	1
1	A	449	TYR	CA-CB-CG	-5.27	103.40	113.40	5	1
2	B	68	THR	OG1-CB-CG2	-5.27	97.89	110.00	6	1
1	A	360	PHE	CD1-CG-CD2	-5.26	111.46	118.30	2	1
2	B	83	ARG	CD-NE-CZ	5.26	130.97	123.60	14	1
2	B	100	TYR	CG-CD2-CE2	-5.26	117.09	121.30	3	2
2	B	214	TYR	CG-CD1-CE1	-5.26	117.09	121.30	10	1
2	B	94	LYS	CB-CG-CD	5.25	125.26	111.60	4	1
2	B	251	PHE	CG-CD1-CE1	5.25	126.58	120.80	11	1
1	A	389	VAL	CA-CB-CG2	-5.25	103.02	110.90	15	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	71	PHE	CZ-CE2-CD2	-5.25	113.80	120.10	8	1
1	A	399	TYR	CD1-CE1-CZ	5.25	124.53	119.80	13	1
2	B	255	LEU	CB-CG-CD1	5.25	119.92	111.00	9	1
1	A	382	PHE	CD1-CE1-CZ	-5.25	113.80	120.10	10	1
1	A	336	PHE	CZ-CE2-CD2	-5.25	113.80	120.10	11	1
2	B	209	ALA	N-CA-CB	-5.25	102.75	110.10	4	1
1	A	444	ALA	CB-CA-C	-5.24	102.23	110.10	5	1
1	A	368	ILE	CB-CA-C	-5.24	101.11	111.60	14	1
1	A	429	PHE	CG-CD2-CE2	5.24	126.56	120.80	8	1
1	A	382	PHE	CG-CD1-CE1	5.23	126.56	120.80	10	1
2	C	206	ASN	N-CA-CB	5.23	120.02	110.60	10	1
2	C	234	GLU	CB-CA-C	5.23	120.86	110.40	1	1
2	C	217	LYS	N-CA-CB	5.23	120.02	110.60	14	1
2	B	130	TRP	CE2-CD2-CE3	5.23	124.97	118.70	13	1
2	B	153	ARG	O-C-N	-5.23	114.33	122.70	13	1
2	B	243	VAL	CG1-CB-CG2	-5.23	102.53	110.90	14	1
2	B	122	TYR	CG-CD2-CE2	5.23	125.48	121.30	8	1
1	A	419	LEU	CB-CG-CD2	-5.23	102.11	111.00	14	1
1	A	335	VAL	CA-CB-CG1	5.22	118.73	110.90	15	1
2	C	88	LYS	O-C-N	-5.22	114.35	122.70	4	1
1	A	449	TYR	N-CA-CB	5.22	119.99	110.60	8	1
2	C	95	ALA	O-C-N	-5.21	114.36	122.70	3	1
2	C	55	SER	O-C-N	-5.21	114.36	122.70	1	1
1	A	388	TRP	CG-CD2-CE3	-5.21	129.21	133.90	13	1
1	A	401	LYS	O-C-N	-5.21	114.37	122.70	3	2
2	B	115	TYR	CD1-CG-CD2	5.21	123.63	117.90	12	1
2	C	262	LEU	CB-CG-CD2	5.21	119.85	111.00	2	1
2	C	76	GLU	OE1-CD-OE2	5.21	129.55	123.30	15	1
2	C	129	LYS	CA-CB-CG	5.21	124.85	113.40	9	1
1	A	486	PHE	CG-CD1-CE1	5.20	126.52	120.80	4	1
1	A	466	SER	O-C-N	-5.20	114.38	122.70	12	1
1	A	340	TRP	CG-CD2-CE3	-5.20	129.22	133.90	1	1
1	A	330	ARG	CD-NE-CZ	5.20	130.88	123.60	9	1
1	A	368	ILE	CA-CB-CG2	-5.20	100.50	110.90	13	1
2	B	251	PHE	CB-CA-C	5.19	120.79	110.40	2	1
1	A	379	PHE	O-C-N	5.19	131.01	122.70	4	1
1	A	460	PRO	N-CD-CG	5.19	110.99	103.20	4	1
2	C	238	GLN	CA-CB-CG	5.19	124.83	113.40	9	1
1	A	390	PHE	CD1-CE1-CZ	5.19	126.33	120.10	5	1
2	C	204	LYS	CD-CE-NZ	-5.19	99.75	111.70	10	1
2	B	251	PHE	CD1-CE1-CZ	5.19	126.33	120.10	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	504	ASP	N-CA-CB	5.19	119.94	110.60	14	1
1	A	463	PRO	C-N-CA	5.19	134.67	121.70	12	1
1	A	338	GLU	OE1-CD-OE2	-5.19	117.08	123.30	10	1
2	B	178	VAL	C-N-CA	5.18	134.66	121.70	1	1
1	A	340	TRP	CB-CG-CD1	-5.18	120.26	127.00	11	1
2	B	199	ARG	N-CA-CB	-5.18	101.27	110.60	13	1
2	C	251	PHE	CD1-CG-CD2	5.18	125.04	118.30	1	1
2	C	97	VAL	O-C-N	-5.18	114.41	122.70	13	1
2	C	213	GLU	CB-CA-C	5.18	120.76	110.40	11	1
1	A	373	GLU	CG-CD-OE2	5.18	128.66	118.30	15	1
2	B	71	PHE	CG-CD1-CE1	-5.18	115.11	120.80	3	1
1	A	329	LEU	CB-CG-CD2	5.17	119.80	111.00	13	1
1	A	365	PRO	C-N-CA	5.17	134.63	121.70	13	1
2	C	126	PHE	CG-CD1-CE1	-5.17	115.11	120.80	13	1
1	A	342	TRP	CA-CB-CG	5.17	123.51	113.70	10	1
2	C	182	ARG	O-C-N	-5.16	114.44	122.70	10	1
1	A	478	TYR	CD1-CE1-CZ	-5.16	115.16	119.80	2	1
1	A	433	ASN	N-CA-CB	-5.16	101.32	110.60	12	1
2	C	120	GLU	OE1-CD-OE2	-5.16	117.11	123.30	3	1
2	C	105	GLN	N-CA-CB	-5.15	101.32	110.60	2	1
2	B	86	MET	O-C-N	-5.15	114.46	122.70	6	1
2	B	110	GLU	OE1-CD-OE2	-5.15	117.12	123.30	14	1
2	B	242	PRO	N-CD-CG	5.15	110.93	103.20	15	1
2	B	122	TYR	CA-CB-CG	-5.15	103.62	113.40	14	1
2	C	218	ALA	N-CA-CB	5.15	117.31	110.10	10	1
1	A	491	LEU	O-C-N	-5.14	114.47	122.70	4	1
1	A	405	GLU	O-C-N	-5.14	114.47	122.70	8	1
2	B	114	LEU	CB-CG-CD1	5.14	119.74	111.00	11	1
1	A	503	ARG	CD-NE-CZ	5.14	130.80	123.60	12	1
2	C	190	ASP	N-CA-CB	5.14	119.85	110.60	7	1
1	A	419	LEU	CB-CG-CD1	5.14	119.74	111.00	12	1
1	A	405	GLU	OE1-CD-OE2	-5.14	117.13	123.30	1	1
2	B	219	THR	OG1-CB-CG2	-5.13	98.19	110.00	2	1
2	B	101	LEU	CB-CG-CD1	-5.13	102.28	111.00	8	1
1	A	502	LEU	O-C-N	5.13	130.91	122.70	10	1
2	B	201	GLU	N-CA-CB	5.13	119.84	110.60	15	1
2	C	220	GLU	OE1-CD-OE2	-5.13	117.14	123.30	11	1
2	B	141	VAL	CA-CB-CG1	5.13	118.59	110.90	14	1
1	A	361	TRP	O-C-N	-5.12	114.50	122.70	4	1
2	B	88	LYS	O-C-N	-5.12	114.51	122.70	15	1
2	B	72	TRP	CE2-CD2-CG	-5.12	103.21	107.30	15	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	191	GLU	CA-CB-CG	5.12	124.66	113.40	12	1
2	B	113	GLU	CG-CD-OE2	5.12	128.53	118.30	15	1
2	B	241	LEU	N-CA-C	5.11	124.80	111.00	1	1
2	C	145	ARG	CG-CD-NE	-5.11	101.07	111.80	13	1
2	C	115	TYR	CB-CA-C	5.11	120.62	110.40	11	1
2	B	125	ASP	O-C-N	-5.10	114.54	122.70	3	1
1	A	430	PHE	CB-CA-C	-5.10	100.19	110.40	5	1
1	A	341	PHE	CG-CD1-CE1	5.10	126.41	120.80	8	1
1	A	464	ARG	O-C-N	-5.10	114.53	123.20	9	1
1	A	388	TRP	CE3-CZ3-CH2	-5.10	115.59	121.20	15	1
1	A	362	ARG	CG-CD-NE	-5.10	101.10	111.80	13	1
2	C	59	LYS	CD-CE-NZ	-5.09	99.98	111.70	9	1
2	B	249	VAL	O-C-N	-5.09	114.55	122.70	12	1
1	A	451	LYS	N-CA-CB	5.09	119.76	110.60	6	1
2	C	188	TYR	CB-CA-C	5.09	120.58	110.40	10	1
1	A	505	TRP	CE3-CZ3-CH2	-5.09	115.60	121.20	12	1
2	C	83	ARG	CD-NE-CZ	5.09	130.72	123.60	13	1
2	B	229	ALA	CB-CA-C	-5.08	102.47	110.10	2	1
2	C	224	THR	CA-CB-OG1	5.08	119.68	109.00	10	1
2	C	199	ARG	CD-NE-CZ	5.08	130.72	123.60	8	1
2	B	226	SER	O-C-N	-5.08	114.57	122.70	14	1
1	A	456	TRP	CH2-CZ2-CE2	-5.08	112.32	117.40	2	1
2	B	241	LEU	CA-C-N	5.08	131.32	117.10	6	1
2	B	104	PHE	CZ-CE2-CD2	-5.08	114.01	120.10	8	1
2	C	68	THR	O-C-N	-5.08	114.57	122.70	13	1
2	C	118	LYS	CA-CB-CG	5.08	124.56	113.40	10	1
2	B	206	ASN	N-CA-CB	5.07	119.73	110.60	3	1
1	A	437	ARG	CD-NE-CZ	5.07	130.70	123.60	4	1
2	B	72	TRP	CG-CD2-CE3	-5.07	129.34	133.90	3	1
2	B	233	LEU	O-C-N	-5.07	114.59	122.70	4	1
2	C	169	GLU	N-CA-CB	-5.07	101.48	110.60	6	1
2	C	173	ARG	CG-CD-NE	-5.07	101.15	111.80	9	1
2	C	188	TYR	CA-C-O	5.07	130.74	120.10	11	1
2	B	239	GLY	C-N-CA	5.07	134.37	121.70	13	1
2	C	203	LEU	CB-CG-CD2	5.07	119.61	111.00	3	1
2	B	88	LYS	N-CA-CB	5.07	119.72	110.60	7	1
2	C	126	PHE	CA-C-O	5.07	130.74	120.10	8	1
2	B	244	LEU	N-CA-CB	5.06	120.53	110.40	8	1
2	C	168	GLU	CG-CD-OE2	-5.06	108.17	118.30	12	1
1	A	359	GLN	N-CA-CB	5.06	119.71	110.60	13	1
2	C	238	GLN	CG-CD-OE1	-5.06	111.48	121.60	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	448	GLU	OE1-CD-OE2	-5.06	117.23	123.30	10	1
2	C	73	ASP	N-CA-CB	5.05	119.70	110.60	8	1
2	B	116	ARG	CB-CA-C	-5.05	100.29	110.40	11	1
2	B	156	LEU	CB-CG-CD1	5.05	119.59	111.00	15	2
1	A	376	ASP	C-N-CA	5.05	132.91	122.30	11	1
2	C	116	ARG	N-CA-CB	5.05	119.69	110.60	14	1
2	C	123	LEU	O-C-N	-5.05	114.62	122.70	7	1
1	A	479	LYS	CA-C-N	5.05	126.30	116.20	8	1
1	A	399	TYR	CZ-CE2-CD2	-5.05	115.25	119.80	14	1
2	C	61	ARG	CA-CB-CG	5.05	124.50	113.40	12	1
2	C	120	GLU	CB-CA-C	5.04	120.49	110.40	3	1
2	C	236	LEU	N-CA-CB	-5.04	100.31	110.40	10	2
2	B	199	ARG	CD-NE-CZ	5.04	130.66	123.60	13	1
2	C	142	GLU	N-CA-C	5.04	124.61	111.00	1	1
2	C	108	TRP	CD1-NE1-CE2	-5.04	104.46	109.00	8	1
2	B	124	ASP	CB-CA-C	5.04	120.48	110.40	3	1
1	A	421	TRP	CB-CA-C	5.04	120.48	110.40	4	1
2	C	260	LYS	O-C-N	-5.04	114.64	122.70	8	1
1	A	325	THR	O-C-N	-5.04	114.64	122.70	10	1
2	C	187	PRO	N-CA-CB	5.04	109.35	103.30	13	1
1	A	457	GLU	CA-C-O	5.04	130.68	120.10	4	1
2	C	80	GLU	N-CA-CB	-5.04	101.54	110.60	15	1
2	C	174	ALA	CB-CA-C	-5.03	102.55	110.10	2	1
1	A	457	GLU	O-C-N	-5.03	114.64	123.20	4	1
2	C	159	LEU	CB-CG-CD2	5.03	119.55	111.00	2	1
2	C	146	ALA	O-C-N	-5.03	114.65	122.70	5	1
1	A	392	GLU	CG-CD-OE1	5.03	128.36	118.30	6	1
1	A	434	LYS	CB-CA-C	5.03	120.46	110.40	6	1
2	B	58	SER	N-CA-CB	5.03	118.04	110.50	9	1
2	B	138	ARG	N-CA-CB	5.03	119.65	110.60	11	1
2	B	129	LYS	O-C-N	-5.03	114.66	122.70	12	1
2	C	170	MET	N-CA-CB	-5.02	101.56	110.60	6	1
1	A	456	TRP	CE2-CD2-CG	-5.02	103.28	107.30	12	1
2	C	185	LEU	O-C-N	-5.02	114.66	122.70	14	1
2	C	58	SER	CB-CA-C	-5.02	100.56	110.10	15	1
2	B	85	GLU	O-C-N	-5.02	114.67	122.70	8	1
2	B	146	ALA	N-CA-CB	-5.02	103.08	110.10	4	1
1	A	388	TRP	CB-CG-CD1	-5.02	120.48	127.00	7	1
1	A	393	ALA	O-C-N	-5.01	114.67	122.70	1	1
1	A	371	ALA	N-CA-CB	5.01	117.12	110.10	2	1
1	A	472	GLU	CG-CD-OE2	5.01	128.33	118.30	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	109	GLN	CB-CA-C	5.01	120.43	110.40	8	1
1	A	345	ARG	CD-NE-CZ	5.01	130.62	123.60	10	1
2	C	104	PHE	CB-CA-C	5.01	120.42	110.40	12	1
2	C	67	VAL	CA-CB-CG1	5.01	118.42	110.90	11	1
2	B	193	ARG	CG-CD-NE	-5.01	101.28	111.80	2	1
1	A	340	TRP	NE1-CE2-CZ2	5.01	135.91	130.40	9	1
2	C	63	GLN	CA-CB-CG	5.01	124.42	113.40	12	1
2	C	162	LYS	CB-CA-C	5.01	120.42	110.40	15	1
2	C	109	GLN	O-C-N	-5.01	114.69	122.70	8	1
1	A	448	GLU	C-N-CA	5.01	134.22	121.70	12	1
2	B	127	GLN	N-CA-CB	-5.01	101.59	110.60	15	1
2	C	158	GLU	OE1-CD-OE2	-5.00	117.30	123.30	5	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	478	TYR	Sidechain	11
1	A	503	ARG	Sidechain	10
2	B	100	TYR	Sidechain	8
1	A	476	TYR	Sidechain	7
2	C	115	TYR	Sidechain	7
2	B	145	ARG	Sidechain	7
1	A	374	ARG	Sidechain	7
1	A	428	TYR	Sidechain	6
2	C	100	TYR	Sidechain	6
1	A	483	TYR	Sidechain	6
2	B	137	TYR	Sidechain	6
2	B	237	ARG	Sidechain	6
2	B	214	TYR	Sidechain	6
2	B	115	TYR	Sidechain	6
2	C	116	ARG	Sidechain	6
1	A	362	ARG	Sidechain	5
2	C	199	ARG	Sidechain	5
2	C	122	TYR	Sidechain	5
1	A	399	TYR	Sidechain,Peptide	5
2	B	193	ARG	Sidechain	5
1	A	436	TYR	Sidechain	4
2	C	237	ARG	Sidechain	4
2	B	199	ARG	Sidechain	4

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	353	TYR	Sidechain	4
2	B	122	TYR	Sidechain	4
2	B	83	ARG	Sidechain	4
1	A	497	TYR	Sidechain	4
1	A	464	ARG	Sidechain	4
1	A	408	ARG	Sidechain	4
2	B	258	TYR	Sidechain	4
2	C	138	ARG	Sidechain	4
1	A	339	ARG	Sidechain	4
1	A	390	PHE	Sidechain	4
2	C	210	ARG	Sidechain	4
2	C	145	ARG	Sidechain	3
1	A	343	ARG	Sidechain	3
1	A	431	ARG	Sidechain	3
1	A	330	ARG	Sidechain	3
2	B	210	ARG	Sidechain	3
2	C	251	PHE	Sidechain	3
2	C	61	ARG	Sidechain	3
2	C	83	ARG	Sidechain	3
2	C	214	TYR	Sidechain	3
1	A	372	TYR	Sidechain	3
2	C	195	ARG	Sidechain	3
1	A	435	TYR	Sidechain	3
2	C	175	ARG	Sidechain	3
2	B	116	ARG	Sidechain	3
2	B	138	ARG	Sidechain	3
1	A	429	PHE	Sidechain	3
2	B	104	PHE	Sidechain	2
2	C	126	PHE	Sidechain	2
2	B	195	ARG	Sidechain	2
2	B	173	ARG	Sidechain	2
1	A	402	HIS	Sidechain	2
2	C	215	HIS	Sidechain	2
2	C	153	ARG	Sidechain	2
2	C	188	TYR	Sidechain	2
1	A	486	PHE	Sidechain	2
2	C	104	PHE	Sidechain	2
2	C	182	ARG	Sidechain	2
2	B	171	ARG	Sidechain	2
2	B	157	HIS	Sidechain	2
2	B	188	TYR	Sidechain	2
2	C	177	HIS	Sidechain	2

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	387	HIS	Sidechain	2
1	A	508	CYS	Peptide	2
1	A	437	ARG	Sidechain	2
1	A	420	PHE	Sidechain	2
2	B	153	ARG	Sidechain	2
1	A	443	ARG	Sidechain	2
2	B	182	ARG	Sidechain	2
2	B	175	ARG	Sidechain	2
2	B	263	ASN	Peptide	1
1	A	490	LYS	Peptide	1
2	C	235	ASP	Sidechain	1
1	A	474	PHE	Sidechain	1
2	B	251	PHE	Sidechain	1
2	C	137	TYR	Sidechain	1
2	C	57	PHE	Sidechain	1
1	A	381	PHE	Sidechain	1
2	C	71	PHE	Sidechain	1
2	B	184	HIS	Sidechain	1
2	B	215	HIS	Sidechain	1
1	A	345	ARG	Sidechain	1
2	C	171	ARG	Sidechain	1
2	B	61	ARG	Sidechain	1
2	C	157	HIS	Sidechain	1
1	A	341	PHE	Sidechain	1
2	B	126	PHE	Sidechain	1
2	C	73	ASP	Mainchain	1
1	A	469	GLY	Peptide	1
1	A	379	PHE	Sidechain	1
2	C	193	ARG	Sidechain	1
1	A	334	PHE	Sidechain	1
2	B	57	PHE	Sidechain	1
2	B	155	LYS	Mainchain	1
1	A	430	PHE	Sidechain	1
1	A	382	PHE	Sidechain	1
1	A	449	TYR	Sidechain	1
2	B	177	HIS	Sidechain	1
2	B	71	PHE	Sidechain	1
2	C	258	TYR	Sidechain	1

6.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in 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	1637	1565	1563	3±1
2	B	1753	1745	1742	2±1
2	C	1753	1745	1742	2±2
3	A	2208	3456	3456	32±5
3	B	4600	7200	7200	53±7
3	C	3220	5040	5040	35±5
All	All	227595	311265	311145	1695

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 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:618:PX4:H12	3:A:644:PX4:H13	0.80	1.50	9	1
3:A:627:PX4:O4	3:A:627:PX4:H3	0.78	1.77	3	2
3:C:363:PX4:H3	3:C:363:PX4:O4	0.74	1.82	11	1
3:B:356:PX4:H9	3:C:303:PX4:O2	0.72	1.84	11	2
3:A:610:PX4:H12	3:A:629:PX4:O6	0.72	1.83	14	1
3:C:333:PX4:O3	3:C:360:PX4:H4	0.72	1.84	14	6
3:B:398:PX4:H4	3:B:399:PX4:O8	0.72	1.85	6	4
3:A:620:PX4:O4	3:A:620:PX4:H3	0.71	1.86	15	3
3:C:326:PX4:O4	3:C:345:PX4:H3	0.71	1.85	8	1
3:B:379:PX4:H4	3:B:391:PX4:O4	0.70	1.86	8	5
3:A:601:PX4:H6	3:B:381:PX4:O4	0.70	1.85	11	1
3:B:332:PX4:H9	3:B:332:PX4:O3	0.69	1.88	6	1
3:C:326:PX4:H14	3:C:345:PX4:H3	0.69	1.63	11	1
3:A:619:PX4:H3	3:A:619:PX4:O4	0.68	1.88	2	1
3:A:608:PX4:O1	3:A:608:PX4:H4	0.68	1.86	15	1
2:C:55:SER:N	2:C:58:SER:HG	0.68	1.85	5	4
3:B:309:PX4:H3	3:B:335:PX4:O2	0.68	1.88	4	3
3:C:309:PX4:O2	3:C:344:PX4:H5	0.68	1.88	5	1
3:B:399:PX4:H8	3:C:356:PX4:C6	0.68	2.18	11	1
3:B:312:PX4:H52	3:B:317:PX4:H8	0.68	1.63	3	1
1:A:511:GLY:OXT	3:A:648:PX4:H11	0.67	1.90	1	3
3:B:398:PX4:O4	3:B:398:PX4:H3	0.67	1.90	8	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:329:PX4:H4	3:B:341:PX4:O2	0.66	1.90	3	1
3:B:356:PX4:O4	3:B:370:PX4:H3	0.66	1.90	7	2
1:A:494:GLU:OE1	3:A:646:PX4:H4	0.66	1.90	7	2
3:A:609:PX4:H7	3:A:609:PX4:O4	0.66	1.91	15	1
3:B:399:PX4:H4	3:C:336:PX4:O6	0.66	1.91	10	1
1:A:494:GLU:OE2	3:A:643:PX4:H6	0.65	1.91	3	3
3:A:620:PX4:H6	3:A:620:PX4:O6	0.65	1.92	3	3
3:C:309:PX4:O2	3:C:344:PX4:H4	0.65	1.92	7	1
3:B:379:PX4:O4	3:B:385:PX4:H13	0.65	1.92	11	2
3:C:364:PX4:O2	3:C:369:PX4:H4	0.65	1.91	5	1
3:A:634:PX4:H3	3:A:634:PX4:O1	0.65	1.91	7	1
3:B:391:PX4:O4	3:B:391:PX4:H3	0.65	1.91	4	1
3:A:608:PX4:H4	3:B:394:PX4:O3	0.65	1.92	9	2
3:A:618:PX4:C5	3:A:644:PX4:H13	0.65	2.22	9	1
3:B:330:PX4:O1	3:B:330:PX4:H3	0.65	1.92	11	3
3:B:303:PX4:H13	3:B:303:PX4:H17	0.64	1.69	13	1
3:B:382:PX4:H13	3:B:382:PX4:O2	0.64	1.92	10	1
1:A:490:LYS:O	3:A:635:PX4:H4	0.64	1.92	8	5
1:A:457:GLU:OE2	3:A:636:PX4:H10	0.64	1.93	2	1
3:B:391:PX4:O1	3:B:395:PX4:H13	0.64	1.93	15	2
3:A:636:PX4:O4	3:A:640:PX4:H4	0.64	1.92	1	2
3:A:644:PX4:O4	3:A:648:PX4:H3	0.64	1.91	14	5
3:A:631:PX4:H3	3:A:631:PX4:O1	0.64	1.93	9	2
3:C:306:PX4:H4	3:C:348:PX4:O2	0.64	1.92	11	2
3:C:317:PX4:O4	3:C:355:PX4:H3	0.63	1.93	7	8
3:A:610:PX4:H7	3:C:368:PX4:O6	0.63	1.92	7	1
3:B:338:PX4:H4	3:B:357:PX4:O8	0.63	1.93	8	1
3:A:619:PX4:H4	3:A:631:PX4:O3	0.63	1.92	14	1
3:C:321:PX4:H8	3:C:356:PX4:O2	0.63	1.93	14	1
3:B:368:PX4:O2	3:B:368:PX4:H7	0.63	1.92	9	1
3:A:612:PX4:C6	3:A:612:PX4:H3	0.63	2.23	10	1
3:B:335:PX4:O4	3:B:360:PX4:H8	0.63	1.93	10	1
3:B:327:PX4:H3	3:B:352:PX4:O2	0.63	1.94	3	3
3:C:333:PX4:H3	3:C:360:PX4:O3	0.63	1.93	12	3
3:B:338:PX4:O2	3:B:363:PX4:H3	0.63	1.93	4	2
3:B:324:PX4:O2	3:B:352:PX4:H4	0.63	1.93	12	4
3:A:611:PX4:H4	3:C:337:PX4:O1	0.63	1.93	8	2
3:C:364:PX4:O1	3:C:364:PX4:H3	0.63	1.93	7	1
3:A:610:PX4:H3	3:A:615:PX4:O8	0.63	1.94	15	2
3:C:369:PX4:H9	3:C:369:PX4:O1	0.63	1.93	6	1
3:B:390:PX4:O3	3:B:395:PX4:H9	0.63	1.94	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:390:PX4:O4	3:B:395:PX4:H4	0.63	1.93	14	7
3:C:319:PX4:O4	3:C:323:PX4:H8	0.63	1.94	6	1
3:A:620:PX4:H4	3:A:632:PX4:O4	0.63	1.94	7	1
3:A:619:PX4:H5	3:A:635:PX4:O3	0.63	1.93	14	1
3:B:337:PX4:O4	3:B:337:PX4:H3	0.62	1.93	15	1
3:B:356:PX4:H16	3:B:370:PX4:H3	0.62	1.69	1	1
3:B:309:PX4:O2	3:B:335:PX4:H9	0.62	1.94	12	1
3:B:315:PX4:H3	3:B:328:PX4:O2	0.62	1.95	2	3
3:B:356:PX4:H7	3:C:303:PX4:O3	0.62	1.94	2	1
3:B:391:PX4:H3	3:B:391:PX4:O1	0.62	1.94	5	2
3:C:316:PX4:H3	3:C:333:PX4:O1	0.61	1.95	2	1
3:B:351:PX4:H3	3:B:379:PX4:O1	0.61	1.95	7	1
3:C:342:PX4:O2	3:C:368:PX4:H5	0.61	1.95	7	1
3:B:396:PX4:O8	3:B:396:PX4:H4	0.61	1.95	2	1
3:B:341:PX4:C1	3:B:364:PX4:H13	0.61	2.24	13	1
2:B:72:TRP:CZ2	3:B:305:PX4:H9	0.61	2.30	14	1
3:A:615:PX4:O1	3:A:629:PX4:H3	0.61	1.95	15	1
2:B:55:SER:N	2:B:58:SER:HG	0.61	1.93	13	7
3:B:305:PX4:O3	3:B:305:PX4:H7	0.61	1.95	5	2
3:C:319:PX4:H7	3:C:334:PX4:O1	0.61	1.94	14	3
3:C:327:PX4:O3	3:C:327:PX4:H9	0.61	1.96	3	1
3:B:322:PX4:H3	3:B:332:PX4:O6	0.61	1.95	7	1
3:C:307:PX4:H9	3:C:307:PX4:O3	0.61	1.95	10	2
3:B:339:PX4:O2	3:B:339:PX4:H4	0.60	1.96	9	1
3:A:605:PX4:O1	3:A:607:PX4:H4	0.60	1.97	13	1
3:B:340:PX4:H4	3:B:340:PX4:O2	0.60	1.96	2	1
3:A:612:PX4:H4	3:C:358:PX4:O2	0.60	1.95	14	1
3:B:364:PX4:H45	3:B:382:PX4:H57	0.60	1.71	1	1
3:B:329:PX4:O1	3:B:329:PX4:H9	0.60	1.95	3	1
3:B:373:PX4:O4	3:B:373:PX4:H4	0.60	1.97	5	3
3:A:604:PX4:H11	3:B:384:PX4:O2	0.60	1.97	10	1
3:B:308:PX4:O2	3:C:302:PX4:H4	0.60	1.96	8	2
3:B:379:PX4:H9	3:B:391:PX4:O2	0.60	1.96	9	6
3:B:313:PX4:O1	3:B:313:PX4:H4	0.60	1.97	11	1
3:A:623:PX4:O2	3:A:630:PX4:H4	0.60	1.97	1	1
3:B:392:PX4:O2	3:B:393:PX4:H10	0.60	1.97	7	2
3:B:327:PX4:O3	3:B:327:PX4:H9	0.59	1.97	6	1
3:B:304:PX4:H4	3:C:301:PX4:O2	0.59	1.96	9	2
3:B:341:PX4:H4	3:B:364:PX4:O1	0.59	1.97	10	1
3:A:626:PX4:O4	3:C:365:PX4:H11	0.59	1.97	2	1
3:B:390:PX4:O2	3:B:395:PX4:H7	0.59	1.97	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:342:PX4:O1	3:B:360:PX4:H11	0.59	1.98	5	1
3:A:625:PX4:O2	3:A:636:PX4:H6	0.59	1.97	7	1
3:B:384:PX4:H3	3:B:384:PX4:O1	0.59	1.97	15	1
3:B:386:PX4:H4	3:B:392:PX4:O1	0.59	1.98	6	1
3:B:379:PX4:O2	3:B:379:PX4:H10	0.59	1.96	9	1
3:A:612:PX4:H9	3:C:351:PX4:O1	0.59	1.97	1	1
3:B:378:PX4:O4	3:C:305:PX4:H11	0.59	1.97	3	1
3:C:345:PX4:O2	3:C:364:PX4:H4	0.59	1.97	10	1
3:B:352:PX4:H11	3:B:369:PX4:O8	0.59	1.97	11	2
3:A:618:PX4:O1	3:A:618:PX4:H3	0.59	1.97	14	1
3:A:609:PX4:O1	3:A:609:PX4:H3	0.59	1.98	1	1
3:A:638:PX4:O6	3:A:648:PX4:H4	0.59	1.96	14	9
3:B:379:PX4:H3	3:B:391:PX4:O2	0.59	1.98	3	1
3:A:614:PX4:O2	3:C:340:PX4:H3	0.59	1.96	8	2
3:A:645:PX4:H7	3:A:645:PX4:O1	0.59	1.98	9	1
3:A:627:PX4:O1	3:A:632:PX4:H9	0.59	1.97	14	1
3:A:605:PX4:O8	3:A:607:PX4:H4	0.59	1.98	9	6
3:B:323:PX4:H3	3:B:323:PX4:O4	0.59	1.98	4	1
3:B:352:PX4:H4	3:B:369:PX4:O8	0.59	1.96	15	1
3:B:390:PX4:H9	3:B:390:PX4:O1	0.59	1.96	2	2
3:A:627:PX4:O3	3:A:632:PX4:H7	0.59	1.98	6	1
3:A:633:PX4:H5	3:C:370:PX4:O6	0.59	1.97	9	2
3:B:337:PX4:O1	3:B:362:PX4:H7	0.59	1.97	12	1
3:B:314:PX4:O2	3:B:334:PX4:H6	0.59	1.97	15	1
3:C:326:PX4:C6	3:C:345:PX4:H3	0.59	2.28	11	2
3:B:345:PX4:H4	3:B:345:PX4:O2	0.59	1.97	12	1
3:A:623:PX4:O2	3:A:639:PX4:H7	0.58	1.98	3	1
3:B:392:PX4:O3	3:B:393:PX4:H4	0.58	1.98	7	1
3:C:330:PX4:O2	3:C:330:PX4:H10	0.58	1.97	14	1
3:C:341:PX4:O1	3:C:362:PX4:H4	0.58	1.98	13	2
3:A:641:PX4:H3	3:A:646:PX4:O2	0.58	1.98	7	1
3:B:342:PX4:O6	3:B:342:PX4:H6	0.58	1.97	9	1
3:B:337:PX4:H4	3:B:342:PX4:O3	0.58	1.97	11	1
3:B:384:PX4:O1	3:B:384:PX4:H3	0.58	1.98	2	2
3:A:626:PX4:O4	3:A:626:PX4:H3	0.58	1.98	5	1
3:A:603:PX4:H13	3:A:603:PX4:O3	0.58	1.98	8	1
3:B:325:PX4:H13	3:B:331:PX4:O1	0.58	1.99	10	2
3:C:318:PX4:O2	3:C:342:PX4:H4	0.58	1.97	12	3
3:B:373:PX4:H4	3:B:373:PX4:O4	0.58	1.99	6	1
3:B:369:PX4:O4	3:B:373:PX4:H5	0.58	1.97	10	1
3:B:348:PX4:O1	3:B:364:PX4:H11	0.58	1.98	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:306:PX4:H4	3:C:348:PX4:O3	0.58	1.99	1	1
3:C:321:PX4:O4	3:C:356:PX4:H3	0.58	1.98	4	1
3:C:359:PX4:H3	3:C:366:PX4:O2	0.58	1.99	12	2
3:B:390:PX4:H7	3:B:395:PX4:O8	0.58	1.97	7	1
1:A:491:LEU:HB2	3:A:635:PX4:H10	0.58	1.73	8	1
3:A:643:PX4:H10	3:A:643:PX4:O2	0.58	1.99	10	1
3:B:390:PX4:H11	3:B:393:PX4:O1	0.58	1.99	10	1
3:B:345:PX4:O2	3:B:352:PX4:H9	0.58	1.99	11	1
3:A:610:PX4:H6	3:C:368:PX4:O6	0.58	1.98	3	1
3:B:356:PX4:H13	3:B:356:PX4:O2	0.58	1.98	13	2
3:A:628:PX4:O1	3:A:644:PX4:H5	0.58	1.99	1	1
3:B:356:PX4:O3	3:B:356:PX4:H6	0.58	1.99	5	3
3:A:615:PX4:O1	3:A:629:PX4:H13	0.58	1.99	10	1
3:A:620:PX4:H3	3:A:620:PX4:O4	0.58	1.99	1	1
3:B:324:PX4:O8	3:B:352:PX4:H7	0.58	1.99	3	1
3:C:321:PX4:H5	3:C:356:PX4:O4	0.58	1.98	12	1
3:C:310:PX4:H5	3:C:358:PX4:O3	0.57	1.98	9	2
3:A:626:PX4:H3	3:A:626:PX4:O2	0.57	1.99	1	1
3:A:608:PX4:H7	3:B:394:PX4:H2	0.57	1.76	5	2
3:B:324:PX4:H3	3:B:325:PX4:O2	0.57	1.99	6	2
3:C:302:PX4:O2	3:C:302:PX4:H3	0.57	1.99	9	1
3:B:341:PX4:H10	3:B:371:PX4:O1	0.57	1.99	1	2
3:A:621:PX4:O8	3:A:637:PX4:H7	0.57	2.00	3	1
3:A:604:PX4:H6	3:A:604:PX4:O3	0.57	1.99	7	1
3:A:633:PX4:H3	3:B:400:PX4:O2	0.57	1.97	13	2
2:B:179:ASP:OD2	3:B:318:PX4:H8	0.57	1.99	14	1
3:A:630:PX4:O2	3:A:630:PX4:H6	0.57	1.99	1	1
3:B:385:PX4:H3	3:B:385:PX4:O4	0.57	1.99	13	3
3:B:342:PX4:H13	3:B:342:PX4:O6	0.57	2.00	4	2
3:A:604:PX4:O8	3:B:394:PX4:H11	0.57	1.98	6	2
3:C:355:PX4:O1	3:C:367:PX4:H3	0.57	1.99	12	1
3:A:638:PX4:O4	3:A:648:PX4:H9	0.57	1.99	1	1
3:A:629:PX4:H4	3:A:629:PX4:O2	0.57	1.97	8	1
3:A:617:PX4:O2	3:C:365:PX4:H3	0.57	2.00	15	1
3:A:615:PX4:H4	3:C:360:PX4:O6	0.57	1.99	1	2
3:B:331:PX4:H3	3:B:331:PX4:O2	0.57	2.00	3	1
3:B:399:PX4:H10	3:C:321:PX4:O2	0.57	2.00	5	1
3:A:627:PX4:H12	3:A:627:PX4:O3	0.57	1.99	5	3
2:C:265:GLN:HA	3:C:336:PX4:H12	0.57	1.75	11	1
3:B:325:PX4:H4	3:B:331:PX4:O4	0.57	1.99	13	2
3:C:366:PX4:H4	3:C:366:PX4:O1	0.57	1.99	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:353:PX4:H4	3:B:353:PX4:O2	0.57	1.99	5	1
3:B:364:PX4:O6	3:B:382:PX4:H4	0.57	2.00	8	1
3:B:378:PX4:H4	3:B:390:PX4:O2	0.57	2.00	10	1
3:C:366:PX4:H13	3:C:369:PX4:O4	0.57	2.00	1	1
3:A:619:PX4:H4	3:A:635:PX4:O6	0.57	2.00	5	3
3:B:343:PX4:O3	3:B:343:PX4:H9	0.57	2.00	13	2
3:B:334:PX4:C6	3:B:334:PX4:H12	0.57	2.29	6	1
3:C:314:PX4:O8	3:C:349:PX4:H7	0.57	1.98	12	1
3:B:311:PX4:H4	3:B:311:PX4:O2	0.57	1.99	13	1
3:B:355:PX4:O1	3:B:367:PX4:H4	0.57	1.99	3	1
3:A:605:PX4:H10	3:A:605:PX4:O3	0.57	2.00	6	1
3:C:310:PX4:O4	3:C:310:PX4:H3	0.57	2.00	8	1
3:C:349:PX4:O8	3:C:349:PX4:H3	0.57	2.00	10	1
3:A:610:PX4:H11	3:A:631:PX4:O8	0.56	1.99	8	2
3:A:621:PX4:O1	3:A:621:PX4:H3	0.56	2.00	11	1
3:A:615:PX4:H6	3:A:615:PX4:O3	0.56	2.00	15	1
3:C:352:PX4:O8	3:C:364:PX4:H4	0.56	1.99	2	1
3:B:326:PX4:H4	3:B:326:PX4:O2	0.56	2.00	6	2
3:B:345:PX4:O2	3:B:352:PX4:H8	0.56	1.99	15	3
3:A:646:PX4:O3	3:A:646:PX4:H7	0.56	2.00	1	4
2:C:261:LYS:O	3:C:336:PX4:H4	0.56	2.00	6	1
3:B:354:PX4:O3	3:B:354:PX4:H13	0.56	2.00	10	1
3:B:316:PX4:O3	3:B:316:PX4:H13	0.56	1.99	13	1
2:B:73:ASP:OD2	3:B:312:PX4:H3	0.56	1.99	14	1
3:C:359:PX4:O3	3:C:366:PX4:H4	0.56	1.99	6	2
3:C:338:PX4:H3	3:C:338:PX4:O1	0.56	2.01	7	1
3:A:608:PX4:H11	3:B:394:PX4:O1	0.56	2.00	13	1
3:B:329:PX4:H13	3:B:341:PX4:O2	0.56	2.00	1	1
3:A:611:PX4:H4	3:A:611:PX4:O4	0.56	1.99	2	1
3:B:309:PX4:O4	3:B:333:PX4:H4	0.56	2.00	6	2
3:A:630:PX4:O3	3:A:630:PX4:H13	0.56	2.01	5	1
3:B:303:PX4:H10	3:B:303:PX4:O3	0.56	2.00	10	1
3:B:328:PX4:H3	3:B:328:PX4:O1	0.56	1.99	10	1
3:B:392:PX4:O3	3:B:393:PX4:H3	0.56	2.01	10	1
3:A:601:PX4:H11	3:B:389:PX4:O6	0.56	1.99	12	1
3:B:341:PX4:H4	3:B:364:PX4:O3	0.56	2.01	12	1
3:B:351:PX4:O2	3:B:351:PX4:H4	0.56	2.00	1	2
3:B:324:PX4:O3	3:B:324:PX4:H6	0.56	2.00	3	1
3:C:303:PX4:H12	3:C:303:PX4:O1	0.56	2.00	11	1
3:B:398:PX4:H6	3:B:399:PX4:O1	0.56	2.00	13	1
3:C:342:PX4:H10	3:C:342:PX4:O2	0.56	2.01	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:639:PX4:H7	3:A:640:PX4:O2	0.56	2.01	1	3
3:B:317:PX4:O3	3:B:317:PX4:H10	0.56	2.01	10	1
3:B:380:PX4:O4	3:B:380:PX4:H7	0.56	2.01	10	1
3:A:617:PX4:O3	3:A:617:PX4:H12	0.56	2.01	15	1
3:B:308:PX4:O3	3:B:308:PX4:H10	0.56	2.01	15	1
3:A:627:PX4:O3	3:A:627:PX4:H12	0.56	2.00	2	2
3:A:604:PX4:H4	3:A:605:PX4:O2	0.56	2.00	9	2
3:A:644:PX4:O1	3:A:648:PX4:H13	0.56	2.00	6	5
3:A:601:PX4:H8	3:B:381:PX4:O4	0.56	2.01	13	1
3:B:304:PX4:O2	3:B:311:PX4:H3	0.56	2.01	5	4
3:B:376:PX4:H3	3:B:389:PX4:O1	0.56	2.01	1	2
3:B:364:PX4:O3	3:B:364:PX4:H12	0.56	2.01	12	3
3:B:361:PX4:H4	3:B:361:PX4:O2	0.56	2.01	6	2
3:B:325:PX4:H60	3:B:331:PX4:H45	0.56	1.78	9	1
3:B:357:PX4:O3	3:B:372:PX4:H8	0.56	1.99	9	1
3:C:347:PX4:H3	3:C:354:PX4:O1	0.56	1.99	11	1
3:B:383:PX4:O8	3:B:386:PX4:H8	0.55	2.02	2	1
3:B:336:PX4:O2	3:B:336:PX4:H4	0.55	1.99	11	1
3:A:632:PX4:H11	3:C:369:PX4:O1	0.55	2.01	15	1
3:C:333:PX4:H3	3:C:360:PX4:O1	0.55	2.02	2	2
3:C:312:PX4:H6	3:C:325:PX4:O2	0.55	2.00	3	2
3:B:341:PX4:O3	3:B:364:PX4:H4	0.55	2.01	7	2
3:A:602:PX4:H11	3:B:382:PX4:O4	0.55	2.02	6	1
3:B:366:PX4:O1	3:B:385:PX4:H8	0.55	2.01	7	2
3:B:378:PX4:H4	3:B:390:PX4:O8	0.55	2.01	8	1
3:B:309:PX4:O2	3:B:335:PX4:H4	0.55	2.02	10	1
3:B:306:PX4:H6	3:B:346:PX4:O1	0.55	2.01	12	1
3:B:339:PX4:H4	3:B:339:PX4:O2	0.55	2.00	13	1
3:C:339:PX4:H13	3:C:346:PX4:O2	0.55	2.02	1	2
3:C:359:PX4:O2	3:C:359:PX4:H4	0.55	2.02	15	1
3:B:386:PX4:H3	3:B:386:PX4:O1	0.55	2.01	11	2
3:C:342:PX4:O1	3:C:342:PX4:H3	0.55	2.01	2	1
3:A:627:PX4:O1	3:A:632:PX4:H8	0.55	2.02	4	2
3:B:390:PX4:C6	3:B:395:PX4:H4	0.55	2.31	12	2
1:A:343:ARG:HB3	1:A:350:MET:SD	0.55	2.41	13	1
3:B:304:PX4:O1	3:B:311:PX4:H9	0.55	2.02	13	1
3:C:334:PX4:H4	3:C:334:PX4:O4	0.55	2.01	14	1
3:C:306:PX4:O2	3:C:348:PX4:H4	0.55	2.02	14	1
3:B:399:PX4:H9	3:C:336:PX4:O6	0.55	2.02	4	1
3:A:624:PX4:O4	3:A:624:PX4:H6	0.55	2.02	9	1
3:B:334:PX4:O2	3:B:334:PX4:H4	0.55	2.02	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:633:PX4:H7	3:B:400:PX4:O1	0.55	2.00	12	1
3:C:309:PX4:C23	3:C:344:PX4:H10	0.55	2.31	5	1
3:B:309:PX4:H10	3:B:342:PX4:H14	0.55	1.79	10	2
3:A:620:PX4:O1	3:A:628:PX4:H3	0.55	2.02	1	2
1:A:490:LYS:O	3:A:635:PX4:H9	0.55	2.01	5	1
3:B:375:PX4:O3	3:B:375:PX4:H13	0.55	2.02	9	2
3:A:641:PX4:H4	3:A:646:PX4:O2	0.55	2.01	15	1
3:C:355:PX4:H4	3:C:355:PX4:O2	0.55	2.01	6	2
3:A:643:PX4:H12	3:A:643:PX4:O3	0.55	2.01	8	2
3:B:329:PX4:O3	3:B:329:PX4:H7	0.55	2.01	9	1
3:B:310:PX4:H4	3:B:328:PX4:O6	0.55	2.02	7	1
3:A:614:PX4:H9	3:A:619:PX4:O2	0.55	2.02	10	1
3:C:353:PX4:H9	3:C:353:PX4:O3	0.55	2.01	12	1
3:C:348:PX4:O4	3:C:348:PX4:H3	0.55	2.01	13	1
3:B:314:PX4:H9	3:B:314:PX4:O3	0.54	2.03	5	1
3:B:349:PX4:H9	3:B:353:PX4:O2	0.54	2.01	7	1
3:B:338:PX4:H4	3:B:377:PX4:O2	0.54	2.02	14	1
3:A:604:PX4:O2	3:B:394:PX4:H13	0.54	2.02	15	1
3:B:329:PX4:O2	3:B:353:PX4:H3	0.54	2.02	7	1
3:C:362:PX4:H3	3:C:362:PX4:O4	0.54	2.02	8	1
3:C:367:PX4:H3	3:C:367:PX4:O4	0.54	2.02	9	1
3:B:345:PX4:O1	3:B:373:PX4:H3	0.54	2.01	15	1
3:B:305:PX4:H4	3:B:305:PX4:O2	0.54	2.02	8	2
3:C:333:PX4:O3	3:C:360:PX4:H12	0.54	2.03	7	1
3:B:359:PX4:H14	3:B:359:PX4:H9	0.54	1.79	12	1
3:A:602:PX4:O2	3:B:372:PX4:H5	0.54	2.01	4	1
3:C:347:PX4:H11	3:C:354:PX4:O3	0.54	2.02	4	1
3:B:336:PX4:O2	3:B:365:PX4:H10	0.54	2.03	1	1
3:C:305:PX4:H3	3:C:305:PX4:O4	0.54	2.02	2	1
3:B:349:PX4:O3	3:B:349:PX4:H13	0.54	2.02	11	3
3:A:624:PX4:H3	3:A:639:PX4:O1	0.54	2.02	8	1
3:A:616:PX4:H9	3:A:616:PX4:O3	0.54	2.02	15	3
3:B:328:PX4:O3	3:B:328:PX4:H10	0.54	2.03	12	1
3:B:338:PX4:H9	3:B:357:PX4:O1	0.54	2.03	14	2
3:A:639:PX4:H5	3:A:640:PX4:O2	0.54	2.03	3	1
3:B:305:PX4:H3	3:B:340:PX4:O1	0.54	2.03	3	1
3:B:377:PX4:H4	3:B:377:PX4:O2	0.54	2.03	4	1
3:B:334:PX4:H12	3:B:334:PX4:C6	0.54	2.32	5	1
3:C:307:PX4:H3	3:C:307:PX4:O1	0.54	2.03	1	1
3:B:349:PX4:O2	3:B:371:PX4:H4	0.54	2.01	8	2
3:B:340:PX4:O4	3:B:356:PX4:H11	0.54	2.03	6	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:627:PX4:O8	3:A:632:PX4:H4	0.54	2.03	8	2
3:B:383:PX4:H3	3:B:383:PX4:H14	0.54	1.79	8	1
3:B:329:PX4:O2	3:B:353:PX4:H7	0.54	2.02	12	1
3:B:372:PX4:H4	3:B:372:PX4:O1	0.54	2.03	14	2
3:A:602:PX4:O1	3:A:602:PX4:H9	0.54	2.03	1	1
3:A:637:PX4:O8	3:A:646:PX4:H10	0.54	2.03	1	3
3:C:363:PX4:H3	3:C:363:PX4:O2	0.54	2.03	8	1
3:B:304:PX4:O3	3:B:304:PX4:H9	0.54	2.02	9	1
3:B:399:PX4:H11	3:C:321:PX4:O6	0.54	2.02	12	1
3:C:325:PX4:H4	3:C:325:PX4:O2	0.54	2.03	12	1
3:A:632:PX4:H3	3:A:632:PX4:O4	0.54	2.03	14	1
3:C:367:PX4:O8	3:C:367:PX4:H3	0.54	2.03	1	1
3:A:618:PX4:H3	3:A:618:PX4:O2	0.54	2.04	2	1
3:B:304:PX4:O1	3:B:311:PX4:H10	0.54	2.03	3	1
3:A:624:PX4:H8	3:A:630:PX4:O4	0.54	2.03	4	3
3:B:369:PX4:O3	3:B:369:PX4:H7	0.54	2.03	12	3
3:B:349:PX4:H4	3:B:349:PX4:O2	0.54	2.02	15	1
3:A:617:PX4:H3	3:A:617:PX4:O1	0.53	2.03	4	1
3:B:353:PX4:O3	3:B:353:PX4:H7	0.53	2.03	6	1
3:A:624:PX4:H5	3:A:624:PX4:O8	0.53	2.02	9	1
3:A:604:PX4:H11	3:B:384:PX4:O4	0.53	2.03	2	1
2:C:262:LEU:O	3:C:336:PX4:H6	0.53	2.02	7	2
3:B:337:PX4:H7	3:B:337:PX4:O3	0.53	2.03	9	1
3:B:360:PX4:H9	3:B:362:PX4:O8	0.53	2.03	11	1
3:A:644:PX4:H7	3:A:644:PX4:O2	0.53	2.03	12	1
3:B:352:PX4:O8	3:B:352:PX4:H6	0.53	2.03	12	1
1:A:492:LYS:HG3	3:A:643:PX4:H11	0.53	1.79	3	1
3:B:320:PX4:O3	3:B:320:PX4:H13	0.53	2.03	7	1
3:B:399:PX4:H11	3:C:321:PX4:O3	0.53	2.03	8	1
3:C:366:PX4:O3	3:C:366:PX4:H12	0.53	2.03	9	1
3:A:624:PX4:O4	3:A:624:PX4:H4	0.53	2.03	1	1
3:B:367:PX4:O1	3:B:367:PX4:H3	0.53	2.03	9	1
3:B:358:PX4:O2	3:B:365:PX4:H11	0.53	2.04	1	1
3:A:615:PX4:O3	3:A:621:PX4:H9	0.53	2.03	9	1
3:C:337:PX4:H9	3:C:346:PX4:O1	0.53	2.04	11	1
3:B:356:PX4:O4	3:B:370:PX4:H4	0.53	2.03	1	1
3:C:360:PX4:H13	3:C:360:PX4:O3	0.53	2.04	5	3
3:A:633:PX4:H11	3:C:370:PX4:O4	0.53	2.03	12	2
3:C:334:PX4:H4	3:C:334:PX4:O2	0.53	2.04	10	1
3:A:615:PX4:H11	3:C:360:PX4:O4	0.53	2.03	10	1
3:B:338:PX4:H12	3:B:377:PX4:O4	0.53	2.03	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:634:PX4:O6	3:A:634:PX4:H13	0.53	2.03	1	1
3:C:315:PX4:H13	3:C:331:PX4:O2	0.53	2.04	5	1
3:B:391:PX4:H12	3:B:394:PX4:O4	0.53	2.04	10	1
3:A:644:PX4:O2	3:A:648:PX4:H6	0.53	2.03	13	4
3:B:329:PX4:O3	3:B:353:PX4:H3	0.53	2.04	13	1
3:C:334:PX4:H3	3:C:347:PX4:O1	0.53	2.03	13	1
3:C:358:PX4:O4	3:C:358:PX4:H3	0.53	2.04	14	1
3:A:630:PX4:H9	3:A:639:PX4:O3	0.53	2.04	2	1
3:B:358:PX4:O8	3:B:365:PX4:H4	0.53	2.04	12	1
3:C:319:PX4:H13	3:C:319:PX4:O1	0.53	2.04	12	1
3:B:339:PX4:O1	3:B:355:PX4:H12	0.53	2.04	14	2
3:C:333:PX4:H7	3:C:360:PX4:O1	0.53	2.03	14	2
3:B:334:PX4:O3	3:B:334:PX4:H10	0.53	2.04	14	1
3:A:615:PX4:H11	3:C:360:PX4:O2	0.53	2.04	8	3
3:C:310:PX4:O3	3:C:310:PX4:H9	0.53	2.03	13	2
3:B:399:PX4:H13	3:C:356:PX4:O3	0.53	2.04	8	1
2:C:164:SER:OG	3:C:325:PX4:H4	0.53	2.03	8	1
3:A:616:PX4:H13	3:C:362:PX4:O1	0.53	2.03	13	1
3:A:616:PX4:O1	3:A:616:PX4:H3	0.53	2.04	13	1
3:B:311:PX4:O1	3:B:311:PX4:H9	0.52	2.05	4	1
3:B:366:PX4:H3	3:B:366:PX4:O1	0.52	2.04	6	2
3:C:310:PX4:H12	3:C:358:PX4:O1	0.52	2.04	12	1
3:B:316:PX4:H13	3:B:316:PX4:O1	0.52	2.03	1	1
3:A:624:PX4:H7	3:C:361:PX4:O6	0.52	2.04	2	1
3:B:344:PX4:H53	3:C:335:PX4:H43	0.52	1.81	12	1
3:B:380:PX4:H9	3:B:380:PX4:O4	0.52	2.04	13	1
3:A:643:PX4:C6	3:A:643:PX4:H4	0.52	2.34	3	1
3:B:344:PX4:H9	3:B:344:PX4:H14	0.52	1.81	5	1
3:B:369:PX4:O1	3:B:383:PX4:H5	0.52	2.04	5	1
3:A:641:PX4:H7	3:A:641:PX4:O1	0.52	2.05	8	1
3:B:338:PX4:O2	3:B:338:PX4:H13	0.52	2.03	9	1
3:B:357:PX4:H3	3:B:357:PX4:O1	0.52	2.04	9	1
3:C:321:PX4:H11	3:C:356:PX4:O3	0.52	2.04	14	1
3:C:339:PX4:H4	3:C:339:PX4:O4	0.52	2.03	1	1
3:A:640:PX4:O4	3:A:640:PX4:H3	0.52	2.04	2	2
3:B:309:PX4:O2	3:B:309:PX4:H4	0.52	2.04	2	2
2:B:201:GLU:OE1	3:B:313:PX4:H4	0.52	2.05	5	1
3:B:376:PX4:O1	3:B:376:PX4:H10	0.52	2.05	5	1
3:C:322:PX4:H4	3:C:322:PX4:O2	0.52	2.05	6	1
3:C:347:PX4:H4	3:C:354:PX4:O6	0.52	2.04	8	1
3:A:604:PX4:O1	3:A:607:PX4:H6	0.52	2.05	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:318:PX4:O1	3:B:318:PX4:H10	0.52	2.04	8	2
3:B:364:PX4:H12	3:B:364:PX4:O2	0.52	2.04	10	1
3:A:604:PX4:H4	3:A:605:PX4:O4	0.52	2.05	13	1
3:B:395:PX4:H10	3:B:395:PX4:O3	0.52	2.05	1	1
3:C:318:PX4:O1	3:C:318:PX4:H3	0.52	2.05	4	2
3:C:338:PX4:H12	3:C:338:PX4:O3	0.52	2.04	5	3
3:A:639:PX4:O6	3:A:640:PX4:H13	0.52	2.04	15	1
3:B:378:PX4:H6	3:B:378:PX4:O1	0.52	2.05	5	1
3:C:343:PX4:H3	3:C:343:PX4:O1	0.52	2.05	9	2
3:B:379:PX4:H9	3:B:391:PX4:O1	0.52	2.05	11	1
3:A:622:PX4:H3	3:A:622:PX4:O1	0.52	2.05	12	1
3:C:347:PX4:O3	3:C:347:PX4:H10	0.52	2.05	13	1
3:B:394:PX4:H3	3:B:394:PX4:O2	0.52	2.04	10	2
3:B:341:PX4:O3	3:B:364:PX4:H7	0.52	2.05	6	1
3:B:387:PX4:O1	3:B:387:PX4:H3	0.52	2.05	6	1
3:C:364:PX4:H10	3:C:364:PX4:O2	0.52	2.05	1	1
3:A:619:PX4:H5	3:A:631:PX4:O7	0.52	2.05	2	1
3:B:398:PX4:H13	3:B:399:PX4:O6	0.52	2.03	3	1
3:C:312:PX4:H10	3:C:312:PX4:O3	0.52	2.05	7	1
3:C:360:PX4:H5	3:C:365:PX4:O8	0.52	2.05	7	1
3:B:324:PX4:O2	3:B:352:PX4:H9	0.52	2.04	8	1
3:B:388:PX4:H3	3:B:388:PX4:O1	0.52	2.05	10	1
3:B:378:PX4:H12	3:B:393:PX4:H14	0.52	1.81	3	1
3:A:637:PX4:O4	3:A:646:PX4:H12	0.52	2.05	4	2
3:B:342:PX4:O1	3:B:360:PX4:H5	0.52	2.05	4	1
3:B:304:PX4:O4	3:B:304:PX4:H7	0.52	2.05	6	1
3:A:636:PX4:H7	3:A:636:PX4:O4	0.52	2.05	8	1
3:B:311:PX4:H4	3:B:344:PX4:O4	0.52	2.05	8	1
3:A:620:PX4:H7	3:A:632:PX4:O8	0.52	2.05	11	3
3:B:388:PX4:O1	3:B:393:PX4:H11	0.52	2.05	12	2
3:A:606:PX4:H4	3:B:386:PX4:O4	0.51	2.05	1	2
3:B:311:PX4:H7	3:B:311:PX4:O3	0.51	2.05	1	4
3:A:636:PX4:H9	3:A:636:PX4:O3	0.51	2.05	7	2
3:B:336:PX4:H11	3:B:358:PX4:C1	0.51	2.34	4	1
3:A:607:PX4:H5	3:A:608:PX4:O1	0.51	2.04	7	1
2:B:60:LEU:HD11	2:C:243:VAL:HG22	0.51	1.82	10	1
3:B:379:PX4:O8	3:B:385:PX4:H4	0.51	2.05	11	2
3:A:635:PX4:H6	3:A:635:PX4:O1	0.51	2.05	11	1
3:C:320:PX4:H13	3:C:322:PX4:O1	0.51	2.06	4	2
3:C:301:PX4:O1	3:C:301:PX4:H3	0.51	2.06	3	1
3:B:309:PX4:O6	3:B:333:PX4:H9	0.51	2.05	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:399:PX4:H8	3:C:356:PX4:H14	0.51	1.82	11	1
3:B:350:PX4:H3	3:B:350:PX4:O1	0.51	2.05	1	2
3:B:378:PX4:H5	3:B:390:PX4:O1	0.51	2.06	1	1
3:A:632:PX4:H3	3:A:632:PX4:O1	0.51	2.05	4	1
3:C:317:PX4:O1	3:C:317:PX4:H3	0.51	2.05	4	2
3:B:308:PX4:O2	3:C:302:PX4:H9	0.51	2.05	7	1
3:A:644:PX4:O2	3:A:644:PX4:H9	0.51	2.06	11	1
3:B:318:PX4:H10	3:B:318:PX4:O2	0.51	2.06	12	1
3:B:327:PX4:H12	3:B:352:PX4:O1	0.51	2.04	12	2
2:C:84:GLN:OE1	3:C:314:PX4:H3	0.51	2.05	14	1
3:A:619:PX4:H9	3:A:635:PX4:H18	0.51	1.81	5	1
3:B:390:PX4:H3	3:B:395:PX4:H9	0.51	1.82	7	1
3:B:352:PX4:H6	3:B:352:PX4:O8	0.51	2.06	10	1
3:B:366:PX4:H6	3:B:366:PX4:O3	0.51	2.06	12	1
1:A:494:GLU:OE1	3:A:646:PX4:H6	0.51	2.05	14	2
3:C:328:PX4:H15	3:C:328:PX4:H9	0.51	1.82	2	1
3:B:364:PX4:O8	3:B:382:PX4:H12	0.51	2.06	4	1
3:C:319:PX4:O1	3:C:323:PX4:H11	0.51	2.05	5	1
3:A:607:PX4:H12	3:A:607:PX4:O3	0.51	2.06	6	1
3:B:342:PX4:O3	3:B:342:PX4:H7	0.51	2.06	10	2
3:B:380:PX4:O2	3:B:380:PX4:H4	0.51	2.04	8	1
3:B:340:PX4:O2	3:B:340:PX4:H4	0.51	2.06	9	1
3:B:364:PX4:O8	3:B:382:PX4:H4	0.51	2.06	1	1
3:B:366:PX4:H4	3:B:367:PX4:O1	0.51	2.06	5	1
3:B:385:PX4:O4	3:B:385:PX4:H3	0.51	2.05	10	3
3:C:357:PX4:O3	3:C:357:PX4:H6	0.51	2.06	13	1
3:B:304:PX4:H9	3:B:304:PX4:O4	0.51	2.06	15	1
3:B:395:PX4:O3	3:B:395:PX4:H10	0.51	2.05	5	2
3:A:614:PX4:O1	3:C:368:PX4:H5	0.51	2.06	5	1
3:C:367:PX4:O4	3:C:367:PX4:H3	0.51	2.05	7	4
3:B:349:PX4:C1	3:B:371:PX4:H12	0.51	2.35	7	1
2:B:73:ASP:OD2	3:B:312:PX4:H6	0.51	2.05	10	1
3:A:614:PX4:O1	3:C:340:PX4:H3	0.51	2.06	12	1
3:C:367:PX4:H7	3:C:367:PX4:O2	0.51	2.06	12	1
3:A:607:PX4:H9	3:A:607:PX4:O2	0.51	2.05	13	2
3:A:636:PX4:H11	3:A:645:PX4:O5	0.51	2.06	3	1
3:A:629:PX4:O2	3:A:637:PX4:H5	0.51	2.04	9	2
3:B:330:PX4:O3	3:B:330:PX4:H6	0.51	2.05	12	1
3:C:339:PX4:H7	3:C:339:PX4:O3	0.51	2.06	12	1
3:B:386:PX4:H10	3:B:392:PX4:O1	0.51	2.05	13	1
3:B:308:PX4:H72	3:C:345:PX4:H71	0.51	1.82	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:399:PX4:H12	3:C:321:PX4:O6	0.51	2.05	10	1
3:B:352:PX4:O3	3:B:352:PX4:H12	0.51	2.06	14	1
3:C:316:PX4:H4	3:C:316:PX4:O2	0.51	2.06	15	1
3:B:343:PX4:H3	3:B:343:PX4:O1	0.51	2.06	2	1
3:C:347:PX4:H3	3:C:347:PX4:O1	0.51	2.06	7	1
3:A:625:PX4:O3	3:A:625:PX4:H7	0.51	2.06	9	1
3:C:332:PX4:H10	3:C:332:PX4:O1	0.50	2.06	6	1
3:B:304:PX4:O1	3:B:304:PX4:H3	0.50	2.06	7	1
3:B:356:PX4:O4	3:B:370:PX4:H5	0.50	2.06	13	1
3:C:338:PX4:H9	3:C:347:PX4:O2	0.50	2.06	1	1
3:B:321:PX4:H3	3:B:321:PX4:O1	0.50	2.07	2	2
3:A:633:PX4:H8	3:C:370:PX4:O2	0.50	2.04	4	1
3:B:304:PX4:H9	3:B:304:PX4:O1	0.50	2.05	5	1
3:B:389:PX4:O3	3:B:389:PX4:H7	0.50	2.06	6	1
3:B:334:PX4:H4	3:B:334:PX4:O2	0.50	2.06	8	1
3:C:365:PX4:O3	3:C:365:PX4:H9	0.50	2.06	8	1
3:B:365:PX4:H6	3:B:365:PX4:O3	0.50	2.06	9	2
3:B:392:PX4:C6	3:B:393:PX4:H9	0.50	2.36	14	1
3:A:616:PX4:O1	3:C:367:PX4:H11	0.50	2.06	15	1
3:B:341:PX4:O1	3:B:364:PX4:H4	0.50	2.07	2	5
3:C:347:PX4:H4	3:C:366:PX4:O1	0.50	2.06	2	1
3:A:620:PX4:H4	3:A:632:PX4:C6	0.50	2.36	8	2
3:C:350:PX4:H9	3:C:367:PX4:O2	0.50	2.06	10	1
3:B:390:PX4:H14	3:B:395:PX4:H4	0.50	1.82	12	1
3:B:326:PX4:O3	3:B:326:PX4:H7	0.50	2.06	15	2
3:C:321:PX4:O1	3:C:321:PX4:H3	0.50	2.07	2	1
3:C:364:PX4:H12	3:C:364:PX4:O1	0.50	2.05	2	1
3:C:360:PX4:H8	3:C:365:PX4:O8	0.50	2.07	4	1
3:A:614:PX4:H6	3:C:368:PX4:O2	0.50	2.07	11	1
3:B:350:PX4:H12	3:B:350:PX4:O3	0.50	2.06	4	1
3:A:633:PX4:H10	3:B:400:PX4:O2	0.50	2.06	4	1
3:C:368:PX4:O3	3:C:368:PX4:H12	0.50	2.07	4	2
3:A:607:PX4:O3	3:A:607:PX4:H12	0.50	2.06	5	1
3:B:347:PX4:H9	3:B:374:PX4:O2	0.50	2.07	5	1
3:B:306:PX4:H3	3:B:346:PX4:O4	0.50	2.06	6	1
3:A:602:PX4:H11	3:B:382:PX4:O1	0.50	2.06	7	1
3:B:324:PX4:H9	3:B:325:PX4:O1	0.50	2.06	7	1
3:C:329:PX4:H3	3:C:329:PX4:O4	0.50	2.07	14	2
3:B:337:PX4:H8	3:B:342:PX4:O3	0.50	2.07	8	1
3:A:620:PX4:H5	3:C:359:PX4:O8	0.50	2.07	9	1
3:C:338:PX4:O4	3:C:363:PX4:H4	0.50	2.06	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:615:PX4:O4	3:A:629:PX4:H3	0.50	2.06	12	1
3:A:615:PX4:O2	3:A:621:PX4:H9	0.50	2.07	2	1
3:C:359:PX4:C1	3:C:366:PX4:H4	0.50	2.36	5	1
3:A:617:PX4:O4	3:A:617:PX4:H10	0.50	2.07	7	1
3:C:338:PX4:O4	3:C:363:PX4:H7	0.50	2.07	7	1
3:C:333:PX4:O1	3:C:360:PX4:H10	0.50	2.06	8	2
3:B:351:PX4:O3	3:B:351:PX4:H7	0.50	2.07	10	2
3:B:329:PX4:H12	3:B:332:PX4:O1	0.50	2.07	5	1
3:B:387:PX4:H9	3:B:393:PX4:O1	0.50	2.07	14	1
3:B:308:PX4:O6	3:C:302:PX4:H6	0.50	2.07	15	1
3:A:630:PX4:H8	3:A:639:PX4:O3	0.50	2.07	4	1
3:A:620:PX4:H9	3:A:632:PX4:O1	0.50	2.07	8	2
3:B:349:PX4:O3	3:B:371:PX4:H12	0.50	2.07	8	2
3:B:338:PX4:O3	3:B:338:PX4:H6	0.50	2.06	5	1
3:B:351:PX4:C3	3:B:361:PX4:H6	0.50	2.36	5	1
3:A:608:PX4:H9	3:B:394:PX4:O1	0.50	2.07	6	1
3:B:377:PX4:H4	3:B:377:PX4:O1	0.50	2.06	9	1
3:C:332:PX4:O4	3:C:332:PX4:H12	0.50	2.06	9	1
3:B:342:PX4:H6	3:B:342:PX4:O7	0.50	2.07	12	1
3:B:368:PX4:O2	3:B:368:PX4:H10	0.50	2.07	15	1
3:B:354:PX4:H13	3:B:354:PX4:O2	0.49	2.07	1	1
3:B:329:PX4:H7	3:B:329:PX4:O3	0.49	2.07	3	1
3:B:352:PX4:H3	3:B:352:PX4:O4	0.49	2.07	9	1
3:B:366:PX4:H4	3:B:367:PX4:O4	0.49	2.06	14	2
3:C:327:PX4:O1	3:C:327:PX4:H3	0.49	2.07	12	1
3:B:383:PX4:C1	3:B:386:PX4:H11	0.49	2.37	3	1
3:A:604:PX4:O2	3:B:394:PX4:H5	0.49	2.07	5	1
3:B:314:PX4:H7	3:B:314:PX4:O2	0.49	2.07	6	1
3:B:383:PX4:H3	3:B:383:PX4:C6	0.49	2.36	8	1
2:B:263:ASN:OD1	3:B:325:PX4:H5	0.49	2.07	11	1
3:C:323:PX4:H12	3:C:323:PX4:O3	0.49	2.08	11	1
3:A:611:PX4:H3	3:C:337:PX4:O1	0.49	2.08	4	1
3:B:336:PX4:O3	3:B:365:PX4:H10	0.49	2.06	5	1
3:B:338:PX4:H13	3:B:338:PX4:O4	0.49	2.06	7	2
3:B:371:PX4:H6	3:B:371:PX4:O3	0.49	2.07	10	1
3:C:326:PX4:H4	3:C:326:PX4:O1	0.49	2.08	11	1
3:A:637:PX4:O6	3:A:646:PX4:H8	0.49	2.07	13	1
3:A:604:PX4:H4	3:A:605:PX4:H14	0.49	1.82	15	1
3:A:619:PX4:H9	3:A:631:PX4:O4	0.49	2.08	15	1
3:A:647:PX4:H10	3:A:647:PX4:H14	0.49	1.84	1	1
3:C:370:PX4:O3	3:C:370:PX4:H10	0.49	2.07	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:614:PX4:H3	3:A:614:PX4:O1	0.49	2.07	9	1
3:B:356:PX4:O2	3:B:356:PX4:H13	0.49	2.07	10	1
2:C:84:GLN:OE1	3:C:314:PX4:H7	0.49	2.07	11	1
3:A:627:PX4:O2	3:A:642:PX4:H13	0.49	2.07	14	1
3:A:612:PX4:H3	3:C:351:PX4:O4	0.49	2.07	1	1
3:C:333:PX4:O3	3:C:333:PX4:H7	0.49	2.08	4	1
3:A:620:PX4:O4	3:A:620:PX4:C2	0.49	2.58	5	1
1:A:495:PRO:HD3	3:A:643:PX4:H7	0.49	1.83	6	1
3:A:610:PX4:H4	3:A:615:PX4:O8	0.49	2.07	7	1
3:A:611:PX4:O2	3:C:351:PX4:H10	0.49	2.07	12	1
3:B:341:PX4:O3	3:B:364:PX4:H6	0.49	2.07	14	1
3:C:362:PX4:O3	3:C:362:PX4:H12	0.49	2.07	6	2
3:A:611:PX4:H10	3:A:611:PX4:O3	0.49	2.08	5	1
3:C:347:PX4:H12	3:C:347:PX4:O3	0.49	2.07	10	2
3:C:309:PX4:O3	3:C:309:PX4:H7	0.49	2.08	9	1
3:B:368:PX4:H4	3:B:368:PX4:O2	0.49	2.07	1	1
3:B:374:PX4:O2	3:B:374:PX4:H4	0.49	2.07	1	1
2:B:73:ASP:CG	3:B:312:PX4:H3	0.49	2.27	2	1
3:A:607:PX4:O2	3:A:607:PX4:H12	0.49	2.07	4	1
3:A:621:PX4:O4	3:A:621:PX4:H3	0.49	2.08	4	1
3:A:609:PX4:H66	3:A:646:PX4:H42	0.49	1.84	7	1
3:C:328:PX4:H3	3:C:328:PX4:O2	0.49	2.07	8	1
3:C:307:PX4:H13	3:C:339:PX4:O3	0.49	2.08	9	1
3:C:317:PX4:O4	3:C:355:PX4:H13	0.49	2.08	12	3
3:C:364:PX4:O2	3:C:369:PX4:H3	0.49	2.07	10	1
2:C:153:ARG:HH11	2:C:157:HIS:CE1	0.49	2.25	11	1
2:C:262:LEU:O	3:C:336:PX4:H4	0.49	2.07	11	1
3:C:364:PX4:O1	3:C:369:PX4:H3	0.49	2.08	11	2
3:A:634:PX4:P1	3:A:644:PX4:H6	0.49	2.47	13	1
3:A:619:PX4:H4	3:A:631:PX4:H2	0.49	1.84	15	1
3:A:614:PX4:H4	3:A:619:PX4:O1	0.49	2.08	1	1
3:B:309:PX4:O1	3:B:333:PX4:H12	0.49	2.08	2	1
3:A:639:PX4:H11	3:A:640:PX4:O3	0.49	2.08	3	1
2:C:84:GLN:OE1	3:C:314:PX4:H13	0.49	2.07	4	2
3:C:316:PX4:H10	3:C:316:PX4:P1	0.49	2.47	5	1
3:C:333:PX4:H10	3:C:360:PX4:O4	0.49	2.08	11	1
3:C:328:PX4:H8	3:C:350:PX4:O2	0.49	2.08	11	1
3:B:338:PX4:H6	3:B:338:PX4:O4	0.49	2.08	13	1
3:C:311:PX4:H6	3:C:311:PX4:O3	0.49	2.08	4	3
3:C:323:PX4:H10	3:C:323:PX4:H14	0.49	1.84	6	1
3:A:644:PX4:O2	3:A:644:PX4:H3	0.49	2.08	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:338:PX4:H9	3:B:357:PX4:O2	0.49	2.08	8	1
3:B:330:PX4:O2	3:B:330:PX4:H3	0.49	2.07	13	1
3:C:362:PX4:H3	3:C:362:PX4:O1	0.49	2.07	15	1
3:C:340:PX4:H4	3:C:340:PX4:O2	0.49	2.08	9	1
3:B:310:PX4:O8	3:B:342:PX4:H11	0.49	2.08	10	2
3:A:604:PX4:H8	3:B:384:PX4:O2	0.49	2.07	12	1
3:B:354:PX4:H6	3:B:354:PX4:O4	0.49	2.08	13	1
3:A:615:PX4:O1	3:A:629:PX4:H9	0.49	2.07	14	1
3:C:360:PX4:H11	3:C:365:PX4:O8	0.48	2.07	1	1
3:B:396:PX4:H8	3:C:342:PX4:O4	0.48	2.08	2	1
3:B:342:PX4:H4	3:B:342:PX4:H17	0.48	1.85	3	1
3:A:624:PX4:H3	3:C:361:PX4:O6	0.48	2.07	5	1
3:B:329:PX4:H10	3:B:332:PX4:O3	0.48	2.08	5	1
3:B:335:PX4:O2	3:B:360:PX4:H8	0.48	2.08	6	1
3:A:642:PX4:O2	3:A:647:PX4:H4	0.48	2.08	8	1
3:B:327:PX4:O1	3:B:327:PX4:H4	0.48	2.08	11	1
3:B:339:PX4:O3	3:B:355:PX4:H12	0.48	2.08	13	1
3:C:360:PX4:H9	3:C:365:PX4:O1	0.48	2.07	8	2
3:A:647:PX4:H13	3:A:648:PX4:O8	0.48	2.08	11	1
3:A:601:PX4:H20	3:A:604:PX4:H7	0.48	1.83	12	1
3:A:606:PX4:H9	3:A:606:PX4:O3	0.48	2.07	13	1
3:A:617:PX4:H9	3:C:353:PX4:O3	0.48	2.07	13	1
3:B:326:PX4:O2	3:B:326:PX4:H4	0.48	2.07	13	1
3:B:349:PX4:O2	3:B:371:PX4:H12	0.48	2.08	15	1
3:A:611:PX4:O4	3:A:611:PX4:H9	0.48	2.06	1	1
3:B:339:PX4:H10	3:B:339:PX4:O3	0.48	2.08	3	2
3:A:614:PX4:O3	3:C:368:PX4:H8	0.48	2.07	5	1
3:B:369:PX4:O2	3:B:383:PX4:H10	0.48	2.08	7	1
3:C:310:PX4:H14	3:C:310:PX4:H10	0.48	1.85	7	1
3:C:348:PX4:O3	3:C:348:PX4:H12	0.48	2.08	9	2
3:B:346:PX4:O1	3:B:363:PX4:H12	0.48	2.07	14	1
3:C:306:PX4:O3	3:C:306:PX4:H6	0.48	2.08	2	1
3:B:308:PX4:H10	3:B:323:PX4:O2	0.48	2.09	6	1
3:C:353:PX4:C4	3:C:353:PX4:O3	0.48	2.60	12	1
3:B:370:PX4:H6	3:B:370:PX4:H47	0.48	1.84	14	1
3:A:604:PX4:O1	3:B:394:PX4:H8	0.48	2.08	4	1
3:B:357:PX4:H12	3:B:357:PX4:O3	0.48	2.09	5	2
2:C:86:MET:CG	3:C:314:PX4:H19	0.48	2.39	5	1
3:A:620:PX4:O2	3:A:638:PX4:H9	0.48	2.09	7	1
3:B:308:PX4:H3	3:B:308:PX4:O2	0.48	2.09	9	1
3:C:322:PX4:H10	3:C:322:PX4:O3	0.48	2.08	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:341:PX4:O4	3:B:364:PX4:H3	0.48	2.09	10	2
3:A:621:PX4:O2	3:A:637:PX4:H3	0.48	2.09	11	1
3:C:348:PX4:H6	3:C:370:PX4:O8	0.48	2.09	11	1
2:C:145:ARG:HG3	3:C:320:PX4:H10	0.48	1.84	12	1
3:A:640:PX4:H10	3:A:647:PX4:O2	0.48	2.09	13	1
3:B:332:PX4:O1	3:B:332:PX4:H3	0.48	2.08	13	1
3:C:349:PX4:O2	3:C:353:PX4:H4	0.48	2.08	2	1
3:B:318:PX4:O2	3:B:334:PX4:H3	0.48	2.08	3	2
3:C:369:PX4:H7	3:C:369:PX4:O3	0.48	2.08	5	1
3:C:346:PX4:H10	3:C:346:PX4:O3	0.48	2.09	6	2
3:C:310:PX4:H11	3:C:340:PX4:O2	0.48	2.09	12	1
3:A:605:PX4:O8	3:A:607:PX4:H13	0.48	2.09	15	1
3:B:398:PX4:O3	3:B:400:PX4:H4	0.48	2.08	15	1
3:B:324:PX4:H37	3:C:356:PX4:H70	0.48	1.85	2	1
3:B:305:PX4:H10	3:B:340:PX4:O4	0.48	2.09	3	1
3:B:306:PX4:H3	3:B:346:PX4:O1	0.48	2.09	4	1
3:B:336:PX4:H11	3:B:358:PX4:H2	0.48	1.85	4	1
3:A:604:PX4:H3	3:A:605:PX4:O2	0.48	2.09	5	1
3:A:621:PX4:H2	3:C:365:PX4:H9	0.48	1.84	10	1
3:B:388:PX4:O3	3:B:388:PX4:H9	0.48	2.09	13	2
3:B:303:PX4:C23	3:B:303:PX4:O5	0.48	2.61	14	1
3:C:326:PX4:O3	3:C:326:PX4:H7	0.48	2.09	15	1
3:C:357:PX4:H13	3:C:357:PX4:O2	0.48	2.08	15	1
3:A:636:PX4:H8	3:A:645:PX4:H22	0.48	1.85	1	1
3:C:314:PX4:H3	3:C:314:PX4:O4	0.48	2.08	2	1
3:B:360:PX4:H11	3:B:362:PX4:H3	0.48	1.86	3	1
3:C:310:PX4:H11	3:C:358:PX4:O2	0.48	2.09	9	2
3:A:627:PX4:O1	3:A:632:PX4:H4	0.48	2.08	6	1
3:B:309:PX4:O1	3:B:333:PX4:H10	0.48	2.08	6	1
3:B:372:PX4:O3	3:B:382:PX4:H11	0.48	2.09	9	1
3:B:335:PX4:O1	3:B:360:PX4:H11	0.48	2.09	10	1
3:A:604:PX4:H5	3:B:384:PX4:O2	0.48	2.09	13	2
3:B:319:PX4:O8	3:B:319:PX4:H7	0.48	2.08	2	1
3:A:614:PX4:H10	3:A:619:PX4:O2	0.48	2.09	9	1
3:B:332:PX4:H3	3:B:332:PX4:O1	0.48	2.08	14	1
3:B:336:PX4:O4	3:B:336:PX4:H4	0.48	2.08	2	1
3:A:632:PX4:O3	3:A:632:PX4:H12	0.48	2.08	3	1
3:B:318:PX4:H9	3:B:318:PX4:O3	0.48	2.09	4	1
3:B:323:PX4:O3	3:B:323:PX4:H12	0.48	2.08	11	2
3:C:339:PX4:O3	3:C:339:PX4:H7	0.48	2.09	11	1
3:B:351:PX4:H12	3:B:379:PX4:O1	0.48	2.07	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:400:PX4:O3	3:C:370:PX4:H6	0.47	2.09	1	1
3:B:363:PX4:O2	3:B:363:PX4:H4	0.47	2.09	4	1
3:A:611:PX4:O2	3:C:351:PX4:H4	0.47	2.08	9	2
3:A:625:PX4:H6	3:A:625:PX4:C6	0.47	2.39	8	1
3:C:342:PX4:O3	3:C:342:PX4:H12	0.47	2.08	9	2
3:B:390:PX4:O3	3:B:395:PX4:H7	0.47	2.09	10	1
3:A:630:PX4:O3	3:A:630:PX4:H6	0.47	2.09	11	2
3:B:392:PX4:O2	3:B:393:PX4:H9	0.47	2.09	11	1
3:C:326:PX4:O2	3:C:345:PX4:H6	0.47	2.08	11	1
3:C:340:PX4:H10	3:C:340:PX4:O3	0.47	2.09	13	1
2:B:73:ASP:OD1	3:B:312:PX4:H12	0.47	2.10	1	1
3:A:623:PX4:O4	3:A:623:PX4:H4	0.47	2.09	10	3
3:A:608:PX4:O1	3:A:608:PX4:H3	0.47	2.09	5	1
3:B:302:PX4:O1	3:B:307:PX4:H10	0.47	2.09	5	1
2:B:73:ASP:OD1	3:B:312:PX4:H3	0.47	2.08	5	1
3:B:336:PX4:H7	3:B:336:PX4:H14	0.47	1.87	8	1
3:C:357:PX4:O3	3:C:357:PX4:H13	0.47	2.10	8	1
3:A:601:PX4:O3	3:A:601:PX4:H9	0.47	2.09	9	2
3:C:355:PX4:H17	3:C:367:PX4:H4	0.47	1.86	14	1
3:C:329:PX4:H7	3:C:329:PX4:O1	0.47	2.09	2	1
3:C:340:PX4:O1	3:C:340:PX4:H10	0.47	2.09	5	1
3:B:349:PX4:H3	3:B:353:PX4:O1	0.47	2.09	9	1
3:B:318:PX4:O3	3:B:334:PX4:H13	0.47	2.10	10	1
3:C:351:PX4:H6	3:C:351:PX4:O1	0.47	2.09	12	1
3:B:374:PX4:O1	3:B:374:PX4:H3	0.47	2.08	13	1
3:B:376:PX4:O2	3:B:376:PX4:H12	0.47	2.10	13	1
3:B:330:PX4:O1	3:B:330:PX4:H4	0.47	2.09	14	1
3:B:378:PX4:H8	3:B:390:PX4:O2	0.47	2.09	1	1
3:A:624:PX4:H11	3:A:630:PX4:O2	0.47	2.10	3	1
3:B:312:PX4:O3	3:B:312:PX4:H7	0.47	2.09	5	1
3:B:356:PX4:O2	3:B:370:PX4:H9	0.47	2.10	6	1
3:B:388:PX4:O2	3:B:393:PX4:H11	0.47	2.09	9	1
3:B:388:PX4:O4	3:B:393:PX4:H5	0.47	2.09	12	2
3:C:330:PX4:O1	3:C:357:PX4:H10	0.47	2.08	15	1
2:C:153:ARG:O	2:C:157:HIS:CD2	0.47	2.67	5	2
3:B:347:PX4:O2	3:B:354:PX4:H5	0.47	2.09	5	1
3:C:369:PX4:H4	3:C:369:PX4:O2	0.47	2.09	11	2
1:A:493:VAL:O	3:A:643:PX4:H7	0.47	2.09	10	1
3:C:316:PX4:O1	3:C:316:PX4:H12	0.47	2.09	12	1
3:B:341:PX4:O3	3:B:341:PX4:H12	0.47	2.10	14	1
3:C:355:PX4:O5	3:C:367:PX4:H4	0.47	2.09	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:618:PX4:O1	3:B:400:PX4:H4	0.47	2.09	3	1
3:B:344:PX4:C6	3:B:344:PX4:H9	0.47	2.40	5	1
3:C:303:PX4:H10	3:C:303:PX4:O3	0.47	2.10	6	1
3:A:619:PX4:H3	3:A:631:PX4:H14	0.47	1.86	13	1
3:B:387:PX4:H9	3:B:387:PX4:O3	0.47	2.10	1	1
3:A:619:PX4:H10	3:A:635:PX4:O4	0.47	2.08	1	1
3:C:347:PX4:H6	3:C:354:PX4:O8	0.47	2.10	1	2
3:A:627:PX4:C6	3:A:627:PX4:H3	0.47	2.38	3	1
3:B:378:PX4:C6	3:C:305:PX4:H11	0.47	2.39	3	1
3:C:309:PX4:O2	3:C:309:PX4:H4	0.47	2.10	3	2
3:C:310:PX4:H9	3:C:310:PX4:O3	0.47	2.09	3	1
3:A:640:PX4:H6	3:A:640:PX4:O3	0.47	2.09	6	2
3:B:380:PX4:H4	3:B:380:PX4:O2	0.47	2.09	6	1
3:A:619:PX4:H9	3:A:635:PX4:O4	0.47	2.09	6	1
3:C:354:PX4:H3	3:C:354:PX4:O1	0.47	2.09	7	2
3:C:309:PX4:H13	3:C:312:PX4:O1	0.47	2.09	8	1
3:B:369:PX4:H7	3:B:369:PX4:O3	0.47	2.09	9	1
3:B:351:PX4:H11	3:B:361:PX4:H7	0.47	1.86	10	1
3:B:366:PX4:O1	3:B:366:PX4:H3	0.47	2.09	14	2
3:C:357:PX4:H6	3:C:357:PX4:O3	0.47	2.09	12	1
3:A:645:PX4:O1	3:A:645:PX4:H7	0.47	2.10	12	1
3:A:618:PX4:O1	3:B:400:PX4:H11	0.47	2.10	13	1
1:A:492:LYS:HB2	3:A:643:PX4:H8	0.47	1.87	14	1
3:C:314:PX4:H3	3:C:314:PX4:O1	0.47	2.10	3	1
3:C:306:PX4:H13	3:C:306:PX4:O2	0.47	2.10	5	1
3:C:337:PX4:H4	3:C:346:PX4:O3	0.47	2.10	6	1
3:A:606:PX4:H3	3:B:386:PX4:O1	0.47	2.09	8	1
3:C:336:PX4:H9	3:C:336:PX4:O3	0.47	2.09	14	1
3:B:336:PX4:H13	3:B:336:PX4:O3	0.47	2.10	15	1
3:C:315:PX4:O3	3:C:315:PX4:H7	0.47	2.10	3	1
3:C:309:PX4:O4	3:C:344:PX4:H8	0.47	2.09	5	1
3:B:308:PX4:O2	3:B:308:PX4:H12	0.47	2.09	6	1
3:B:308:PX4:H12	3:B:323:PX4:O2	0.47	2.10	10	1
3:B:334:PX4:H4	3:B:334:PX4:O4	0.47	2.10	15	1
3:B:388:PX4:O6	3:B:393:PX4:H5	0.47	2.10	1	1
3:C:325:PX4:O4	3:C:325:PX4:H4	0.47	2.10	5	1
3:B:316:PX4:O3	3:B:316:PX4:C5	0.47	2.63	13	1
3:B:397:PX4:H5	2:C:120:GLU:OE1	0.47	2.09	14	1
3:B:352:PX4:O4	3:B:352:PX4:H3	0.46	2.10	5	3
3:B:392:PX4:O1	3:B:392:PX4:H3	0.46	2.10	7	1
3:B:397:PX4:O1	3:B:397:PX4:H3	0.46	2.09	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:355:PX4:O2	3:C:355:PX4:H4	0.46	2.10	9	1
3:B:352:PX4:H14	3:B:352:PX4:H3	0.46	1.86	13	1
3:B:368:PX4:H71	3:C:345:PX4:H72	0.46	1.87	13	1
3:A:624:PX4:H3	3:A:624:PX4:O4	0.46	2.10	15	1
3:A:612:PX4:H3	3:C:351:PX4:O1	0.46	2.10	15	1
3:B:386:PX4:H4	3:B:392:PX4:O2	0.46	2.10	2	1
3:B:352:PX4:O4	3:B:352:PX4:H13	0.46	2.10	11	1
3:B:325:PX4:H8	3:B:331:PX4:O4	0.46	2.10	2	1
3:C:325:PX4:H10	3:C:325:PX4:O3	0.46	2.11	5	3
3:A:647:PX4:H11	3:A:648:PX4:O8	0.46	2.10	3	1
3:B:318:PX4:H12	3:B:318:PX4:O3	0.46	2.11	8	3
1:A:495:PRO:O	3:A:646:PX4:H5	0.46	2.10	7	1
3:C:341:PX4:O2	3:C:341:PX4:H4	0.46	2.10	7	1
3:A:629:PX4:O2	3:A:637:PX4:H11	0.46	2.11	8	1
3:B:370:PX4:H13	3:B:370:PX4:O3	0.46	2.10	8	1
3:B:306:PX4:H10	3:B:346:PX4:O1	0.46	2.09	9	1
3:B:379:PX4:O3	3:B:379:PX4:H12	0.46	2.09	9	2
3:B:396:PX4:O2	3:B:396:PX4:H4	0.46	2.11	9	1
3:C:318:PX4:H5	3:C:324:PX4:O1	0.46	2.11	11	1
3:C:330:PX4:H12	3:C:330:PX4:O3	0.46	2.10	11	1
3:B:370:PX4:O3	3:B:370:PX4:H13	0.46	2.11	14	2
3:B:320:PX4:H13	3:B:320:PX4:O3	0.46	2.10	15	2
3:C:338:PX4:O3	3:C:338:PX4:H9	0.46	2.10	15	1
3:B:340:PX4:H4	3:B:340:PX4:O4	0.46	2.09	1	1
3:A:642:PX4:H3	3:A:647:PX4:O2	0.46	2.10	3	1
3:A:625:PX4:H9	3:A:625:PX4:O1	0.46	2.10	4	1
3:B:322:PX4:O1	3:B:322:PX4:H7	0.46	2.10	8	1
3:A:608:PX4:H9	3:B:395:PX4:O2	0.46	2.10	12	1
3:B:392:PX4:H3	3:B:392:PX4:O1	0.46	2.11	14	1
3:C:310:PX4:C6	3:C:310:PX4:H3	0.46	2.40	14	1
3:B:379:PX4:O4	3:B:385:PX4:H4	0.46	2.11	15	1
3:B:314:PX4:H3	3:B:314:PX4:O1	0.46	2.10	1	1
3:B:362:PX4:O3	3:B:362:PX4:H12	0.46	2.11	3	2
3:B:351:PX4:H7	3:B:351:PX4:O3	0.46	2.11	5	1
2:C:86:MET:HG3	3:C:314:PX4:H19	0.46	1.88	5	1
3:B:332:PX4:O2	3:B:332:PX4:H7	0.46	2.10	6	1
3:B:337:PX4:H15	3:B:339:PX4:H3	0.46	1.86	6	1
3:B:318:PX4:O4	3:B:334:PX4:H3	0.46	2.11	2	1
3:B:372:PX4:O1	3:B:372:PX4:H4	0.46	2.10	9	1
3:C:355:PX4:O1	3:C:367:PX4:H11	0.46	2.10	9	1
3:B:341:PX4:C2	3:B:364:PX4:O3	0.46	2.64	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:119:VAL:HG13	2:B:120:GLU:N	0.46	2.25	13	1
3:B:315:PX4:O3	3:B:315:PX4:H13	0.46	2.10	2	2
3:C:356:PX4:H10	3:C:356:PX4:O3	0.46	2.10	2	1
3:A:639:PX4:H8	3:A:640:PX4:O4	0.46	2.11	3	1
3:C:315:PX4:H4	3:C:331:PX4:O1	0.46	2.10	5	2
3:A:645:PX4:H13	3:A:647:PX4:O1	0.46	2.11	5	1
3:B:345:PX4:O2	3:B:345:PX4:H4	0.46	2.10	7	1
1:A:386:LYS:HD2	1:A:402:HIS:CE1	0.46	2.45	9	1
3:B:345:PX4:O8	3:B:373:PX4:H3	0.46	2.10	9	1
3:C:360:PX4:H13	3:C:360:PX4:C6	0.46	2.41	9	1
3:A:643:PX4:O3	3:A:643:PX4:H12	0.46	2.10	11	1
3:A:633:PX4:H3	3:B:400:PX4:O1	0.46	2.11	11	1
3:C:316:PX4:H10	3:C:316:PX4:O3	0.46	2.10	12	1
3:C:345:PX4:O3	3:C:345:PX4:H10	0.46	2.11	13	1
3:B:324:PX4:O3	3:B:324:PX4:C3	0.46	2.64	3	1
3:A:648:PX4:O2	3:A:648:PX4:H10	0.46	2.10	4	1
3:A:631:PX4:H6	3:A:631:PX4:O3	0.46	2.09	7	1
3:B:360:PX4:H4	3:B:360:PX4:O1	0.46	2.11	9	1
3:C:366:PX4:O4	3:C:366:PX4:H3	0.46	2.11	11	1
3:C:367:PX4:O3	3:C:367:PX4:H9	0.46	2.11	13	1
3:B:400:PX4:O1	3:C:370:PX4:H3	0.46	2.10	2	1
3:B:310:PX4:H9	3:B:310:PX4:O3	0.46	2.11	4	2
3:A:604:PX4:H16	3:B:394:PX4:H8	0.46	1.86	7	1
3:C:362:PX4:C6	3:C:362:PX4:H3	0.46	2.41	8	1
3:B:302:PX4:O3	3:B:302:PX4:H7	0.46	2.10	9	1
3:A:610:PX4:H5	3:C:368:PX4:O6	0.46	2.11	11	1
3:C:335:PX4:O2	3:C:335:PX4:H4	0.46	2.10	12	1
3:B:332:PX4:O3	3:B:332:PX4:H6	0.46	2.11	15	1
3:B:319:PX4:H8	3:B:320:PX4:O1	0.46	2.11	2	1
3:C:343:PX4:O3	3:C:343:PX4:H12	0.46	2.10	2	1
3:A:610:PX4:O2	3:A:610:PX4:H9	0.46	2.10	4	1
3:B:341:PX4:H12	3:B:364:PX4:H15	0.46	1.87	11	1
3:B:371:PX4:O2	3:B:375:PX4:H7	0.46	2.11	12	1
3:B:338:PX4:H3	3:B:357:PX4:H1	0.46	1.86	13	1
3:B:341:PX4:H1	3:B:364:PX4:H13	0.46	1.87	13	1
3:C:305:PX4:O3	3:C:305:PX4:H9	0.46	2.11	13	2
3:A:641:PX4:O3	3:A:641:PX4:H9	0.46	2.11	15	1
3:C:363:PX4:O2	3:C:363:PX4:H10	0.46	2.10	15	1
2:B:69:GLN:OE1	3:B:317:PX4:H5	0.45	2.11	1	1
3:B:351:PX4:H43	3:C:361:PX4:H41	0.45	1.88	1	1
3:A:602:PX4:H6	3:B:382:PX4:O2	0.45	2.11	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:326:PX4:H3	3:C:326:PX4:O1	0.45	2.11	2	1
3:B:350:PX4:H40	3:C:340:PX4:H43	0.45	1.88	6	1
3:B:400:PX4:O3	3:B:400:PX4:H6	0.45	2.11	6	2
3:A:621:PX4:C23	3:A:621:PX4:O4	0.45	2.64	8	1
3:C:306:PX4:H9	3:C:348:PX4:O2	0.45	2.12	9	1
3:C:309:PX4:O3	3:C:309:PX4:H9	0.45	2.11	15	1
3:C:368:PX4:H3	3:C:368:PX4:O4	0.45	2.11	15	1
3:C:306:PX4:O4	3:C:306:PX4:H3	0.45	2.11	1	1
3:B:360:PX4:H12	3:B:362:PX4:O3	0.45	2.11	3	1
3:A:619:PX4:O3	3:A:619:PX4:H12	0.45	2.11	4	1
3:B:391:PX4:H8	3:B:394:PX4:O1	0.45	2.12	4	1
3:B:349:PX4:O3	3:B:371:PX4:H4	0.45	2.11	5	1
3:B:332:PX4:H3	3:B:332:PX4:O8	0.45	2.12	9	1
3:A:638:PX4:H13	3:A:638:PX4:O3	0.45	2.10	15	1
3:C:302:PX4:H3	3:C:302:PX4:O1	0.45	2.11	15	1
3:A:637:PX4:O3	3:A:637:PX4:H13	0.45	2.11	1	1
3:A:614:PX4:H4	3:A:614:PX4:O8	0.45	2.11	3	1
3:C:323:PX4:O3	3:C:323:PX4:H10	0.45	2.12	6	2
3:B:320:PX4:O3	3:B:320:PX4:C5	0.45	2.64	7	1
3:B:321:PX4:H12	3:B:330:PX4:C6	0.45	2.40	10	1
3:A:602:PX4:H4	3:B:382:PX4:O2	0.45	2.10	12	1
3:B:400:PX4:O4	3:B:400:PX4:H3	0.45	2.11	1	1
3:B:377:PX4:O3	3:B:377:PX4:H7	0.45	2.11	3	2
3:C:329:PX4:H8	3:C:347:PX4:O8	0.45	2.12	8	1
3:C:359:PX4:H3	3:C:366:PX4:O4	0.45	2.11	8	1
3:A:604:PX4:O1	3:B:394:PX4:H7	0.45	2.11	9	1
3:B:399:PX4:H5	3:C:321:PX4:O6	0.45	2.11	13	2
3:B:385:PX4:O1	3:B:385:PX4:H9	0.45	2.12	14	1
3:A:643:PX4:O4	3:A:643:PX4:H10	0.45	2.11	6	1
3:A:626:PX4:H6	3:A:626:PX4:O3	0.45	2.12	8	2
3:B:376:PX4:H4	3:B:381:PX4:P1	0.45	2.52	7	1
3:B:356:PX4:O4	3:B:370:PX4:H7	0.45	2.11	8	1
3:C:326:PX4:O1	3:C:345:PX4:H6	0.45	2.12	12	1
3:A:625:PX4:H7	3:A:625:PX4:O3	0.45	2.11	13	1
3:A:617:PX4:O2	3:C:365:PX4:H12	0.45	2.12	13	1
3:B:308:PX4:H12	3:B:308:PX4:O3	0.45	2.11	3	1
3:B:394:PX4:O3	3:B:394:PX4:H12	0.45	2.11	3	1
1:A:487:ASN:CB	3:A:643:PX4:H6	0.45	2.42	4	1
3:B:398:PX4:H17	3:B:398:PX4:H12	0.45	1.89	5	1
3:C:353:PX4:O1	3:C:353:PX4:H3	0.45	2.12	8	1
3:B:342:PX4:O6	3:B:342:PX4:H13	0.45	2.11	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:644:PX4:H10	3:A:644:PX4:O6	0.45	2.11	14	1
3:A:608:PX4:H4	3:B:394:PX4:O6	0.45	2.12	7	1
3:A:633:PX4:H7	3:B:400:PX4:H16	0.45	1.88	8	1
3:B:378:PX4:O2	3:C:305:PX4:H11	0.45	2.11	8	1
3:C:317:PX4:H12	3:C:317:PX4:O3	0.45	2.12	10	2
3:B:340:PX4:O8	3:B:356:PX4:H12	0.45	2.11	11	1
3:B:392:PX4:H15	3:B:393:PX4:H9	0.45	1.89	14	1
3:A:608:PX4:H10	3:B:394:PX4:O1	0.45	2.11	2	1
3:B:378:PX4:H9	3:B:378:PX4:O3	0.45	2.12	3	1
3:B:378:PX4:H12	3:B:390:PX4:O2	0.45	2.12	5	1
3:A:616:PX4:O8	3:A:616:PX4:H13	0.45	2.12	7	1
3:B:377:PX4:H14	3:B:377:PX4:H7	0.45	1.88	12	1
3:C:321:PX4:O1	3:C:321:PX4:H4	0.45	2.12	13	1
3:C:365:PX4:H6	3:C:365:PX4:O1	0.45	2.11	14	1
3:A:604:PX4:H4	3:A:605:PX4:C6	0.45	2.41	15	1
3:C:347:PX4:H12	3:C:347:PX4:O1	0.45	2.11	15	1
3:B:392:PX4:O8	3:B:393:PX4:H3	0.45	2.10	4	2
3:B:325:PX4:H5	3:B:331:PX4:O3	0.45	2.12	4	1
3:B:336:PX4:H8	3:B:358:PX4:O3	0.45	2.12	4	1
3:C:333:PX4:H12	3:C:360:PX4:O1	0.45	2.12	6	1
3:C:327:PX4:H8	3:C:332:PX4:O3	0.45	2.12	8	1
2:B:115:TYR:O	2:B:119:VAL:HG12	0.45	2.12	12	1
2:C:104:PHE:CE1	3:C:324:PX4:H28	0.45	2.47	15	1
3:A:602:PX4:O5	3:A:603:PX4:H7	0.45	2.11	2	1
3:C:355:PX4:O3	3:C:367:PX4:H8	0.45	2.12	2	1
2:C:101:LEU:HD11	3:C:324:PX4:C8	0.45	2.42	9	1
3:C:366:PX4:O6	3:C:366:PX4:H6	0.45	2.12	9	1
3:A:638:PX4:H4	3:A:638:PX4:O4	0.45	2.11	11	1
1:A:474:PHE:CE2	1:A:485:LYS:HE2	0.45	2.47	12	1
2:B:171:ARG:NH1	3:B:307:PX4:H3	0.45	2.27	12	1
1:A:503:ARG:NH2	3:A:644:PX4:O1	0.45	2.51	13	1
3:C:368:PX4:H3	3:C:368:PX4:O8	0.45	2.12	13	1
3:B:333:PX4:C6	3:B:333:PX4:C1	0.45	2.95	14	1
3:B:369:PX4:H7	3:B:369:PX4:O2	0.45	2.11	14	1
3:B:339:PX4:O3	3:B:339:PX4:H10	0.44	2.11	1	1
3:A:620:PX4:H8	3:C:359:PX4:O1	0.44	2.12	1	1
3:A:613:PX4:H42	3:A:622:PX4:H44	0.44	1.87	2	1
3:B:349:PX4:O2	3:B:371:PX4:H3	0.44	2.12	6	1
3:C:333:PX4:O4	3:C:360:PX4:H10	0.44	2.12	6	1
3:B:312:PX4:H4	3:B:312:PX4:O2	0.44	2.12	7	2
3:B:322:PX4:H3	3:B:322:PX4:O4	0.44	2.12	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:397:PX4:H5	2:C:120:GLU:OE2	0.44	2.12	11	1
3:C:344:PX4:H3	3:C:344:PX4:O1	0.44	2.12	11	1
3:B:388:PX4:O2	3:B:393:PX4:H8	0.44	2.12	12	1
3:B:366:PX4:H12	3:B:367:PX4:O1	0.44	2.12	13	1
3:C:334:PX4:H7	3:C:347:PX4:O6	0.44	2.11	14	1
3:C:301:PX4:H3	3:C:301:PX4:O4	0.44	2.12	1	1
3:A:615:PX4:O4	3:A:615:PX4:H3	0.44	2.12	2	1
3:C:330:PX4:H3	3:C:330:PX4:O1	0.44	2.13	2	1
3:B:378:PX4:H3	3:B:378:PX4:O4	0.44	2.13	4	1
3:C:309:PX4:O1	3:C:344:PX4:H7	0.44	2.13	4	1
3:A:620:PX4:O3	3:A:620:PX4:H12	0.44	2.12	6	1
3:A:639:PX4:H14	3:A:640:PX4:H6	0.44	1.90	6	1
3:B:347:PX4:P1	3:B:354:PX4:H11	0.44	2.51	6	1
3:B:321:PX4:O3	3:B:321:PX4:H9	0.44	2.12	8	1
3:C:309:PX4:O1	3:C:309:PX4:H9	0.44	2.12	9	1
3:C:362:PX4:H12	3:C:362:PX4:O3	0.44	2.11	13	1
3:C:333:PX4:O1	3:C:360:PX4:H4	0.44	2.13	5	1
3:A:642:PX4:O4	3:A:647:PX4:H10	0.44	2.13	14	2
3:A:602:PX4:O6	3:A:603:PX4:H3	0.44	2.11	7	1
3:C:320:PX4:O1	3:C:320:PX4:H4	0.44	2.11	7	1
3:B:366:PX4:H45	3:C:367:PX4:C22	0.44	2.43	8	1
3:B:336:PX4:O3	3:B:350:PX4:H7	0.44	2.12	7	1
3:B:338:PX4:H10	3:B:377:PX4:O2	0.44	2.11	13	1
3:B:393:PX4:O3	3:B:393:PX4:H13	0.44	2.12	14	2
3:C:359:PX4:O3	3:C:359:PX4:H10	0.44	2.12	1	1
3:A:617:PX4:O8	3:A:617:PX4:H10	0.44	2.13	6	1
3:B:340:PX4:H13	3:B:370:PX4:H2	0.44	1.89	10	1
3:B:396:PX4:H6	3:B:396:PX4:O1	0.44	2.12	12	1
3:B:359:PX4:H9	3:B:359:PX4:O3	0.44	2.12	13	1
3:B:384:PX4:O3	3:B:384:PX4:H12	0.44	2.13	13	1
3:B:302:PX4:H4	3:B:302:PX4:C6	0.44	2.42	1	1
3:A:648:PX4:H12	3:A:648:PX4:O3	0.44	2.13	3	1
1:A:457:GLU:OE2	3:A:636:PX4:H13	0.44	2.12	4	1
3:C:314:PX4:O1	3:C:314:PX4:H3	0.44	2.13	4	1
3:B:314:PX4:O2	3:B:334:PX4:H8	0.44	2.12	6	1
3:A:625:PX4:H6	3:A:625:PX4:H15	0.44	1.89	8	1
3:A:618:PX4:H12	3:A:644:PX4:C5	0.44	2.34	9	1
3:B:301:PX4:O1	3:B:301:PX4:H4	0.44	2.13	10	1
3:A:643:PX4:O2	3:A:643:PX4:H10	0.44	2.12	12	1
3:B:347:PX4:H9	3:B:347:PX4:O3	0.44	2.13	13	1
3:C:348:PX4:H12	3:C:348:PX4:O3	0.44	2.13	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:345:PX4:O2	3:C:364:PX4:H3	0.44	2.13	4	2
1:A:493:VAL:O	3:A:643:PX4:H5	0.44	2.12	7	1
3:C:341:PX4:H7	3:C:341:PX4:O3	0.44	2.13	1	1
3:A:639:PX4:H12	3:A:639:PX4:O2	0.44	2.12	4	1
3:B:336:PX4:O1	3:B:350:PX4:H8	0.44	2.12	8	1
3:B:341:PX4:O1	3:B:341:PX4:H3	0.44	2.13	9	1
3:A:633:PX4:H4	3:A:633:PX4:O2	0.44	2.13	12	1
3:B:354:PX4:H18	3:B:354:PX4:O8	0.44	2.13	15	1
3:A:611:PX4:O3	3:C:351:PX4:H12	0.44	2.13	2	1
3:C:302:PX4:O3	3:C:302:PX4:H6	0.44	2.13	3	1
3:C:305:PX4:O2	3:C:305:PX4:H3	0.44	2.13	4	1
3:C:344:PX4:O2	3:C:344:PX4:H4	0.44	2.13	4	1
3:B:396:PX4:O1	3:B:397:PX4:H10	0.44	2.12	7	1
3:B:307:PX4:O1	3:B:307:PX4:H3	0.44	2.13	8	2
3:C:315:PX4:H7	3:C:315:PX4:O3	0.44	2.13	8	1
3:A:647:PX4:H7	3:A:647:PX4:H15	0.44	1.88	14	1
3:B:345:PX4:H2	3:B:373:PX4:H13	0.44	1.90	15	1
3:B:382:PX4:O2	3:B:382:PX4:H13	0.43	2.13	5	1
3:A:625:PX4:O2	3:A:636:PX4:H4	0.43	2.13	6	3
3:A:644:PX4:H6	3:A:644:PX4:O3	0.43	2.13	6	1
3:B:368:PX4:O3	3:B:368:PX4:H9	0.43	2.13	9	1
2:B:217:LYS:O	2:B:221:HIS:CD2	0.43	2.71	12	1
3:B:321:PX4:H4	3:B:330:PX4:O2	0.43	2.13	14	1
3:A:627:PX4:O4	3:A:627:PX4:C2	0.43	2.57	3	1
3:A:601:PX4:H5	3:B:381:PX4:O1	0.43	2.12	4	2
3:C:344:PX4:H7	3:C:344:PX4:O2	0.43	2.13	7	1
3:C:337:PX4:H12	3:C:346:PX4:O7	0.43	2.13	8	1
3:C:301:PX4:O2	3:C:301:PX4:H10	0.43	2.13	10	1
3:C:366:PX4:H7	3:C:369:PX4:O1	0.43	2.12	10	1
3:B:372:PX4:O2	3:B:382:PX4:H4	0.43	2.14	11	1
3:B:376:PX4:O1	3:B:376:PX4:H12	0.43	2.13	12	1
1:A:494:GLU:OE1	3:A:646:PX4:H13	0.43	2.13	13	1
3:C:349:PX4:O3	3:C:349:PX4:H13	0.43	2.13	13	1
3:A:639:PX4:H7	3:A:639:PX4:O3	0.43	2.12	15	1
3:A:621:PX4:H33	3:C:360:PX4:H45	0.43	1.89	2	1
3:A:605:PX4:O8	3:A:607:PX4:H3	0.43	2.12	3	1
3:A:614:PX4:H7	3:A:619:PX4:H14	0.43	1.90	3	1
3:A:601:PX4:H13	3:B:389:PX4:O2	0.43	2.13	7	1
3:A:633:PX4:H7	3:B:400:PX4:C6	0.43	2.43	7	1
1:A:493:VAL:HG13	3:A:645:PX4:H9	0.43	1.90	8	1
3:C:334:PX4:H10	3:C:334:PX4:O3	0.43	2.13	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:312:PX4:H8	3:C:325:PX4:O4	0.43	2.13	10	1
3:A:629:PX4:O2	3:A:629:PX4:H4	0.43	2.13	13	1
3:B:399:PX4:H13	3:C:336:PX4:O6	0.43	2.13	13	1
3:C:352:PX4:H8	3:C:361:PX4:O4	0.43	2.14	14	1
3:A:602:PX4:C8	3:A:603:PX4:H7	0.43	2.44	2	1
3:A:619:PX4:O3	3:A:635:PX4:H7	0.43	2.14	2	1
3:A:613:PX4:O2	3:C:346:PX4:H6	0.43	2.12	2	1
3:B:342:PX4:H4	3:B:342:PX4:O4	0.43	2.13	3	2
3:C:347:PX4:H5	3:C:354:PX4:O4	0.43	2.13	3	1
3:B:336:PX4:H7	3:B:336:PX4:O3	0.43	2.13	4	1
3:C:324:PX4:O4	3:C:324:PX4:H3	0.43	2.13	6	1
3:C:321:PX4:H4	3:C:356:PX4:O2	0.43	2.13	10	2
3:A:644:PX4:O1	3:A:648:PX4:H6	0.43	2.14	9	1
3:B:319:PX4:H4	3:B:319:PX4:O1	0.43	2.14	9	1
3:C:359:PX4:H13	3:C:359:PX4:O3	0.43	2.13	12	1
3:B:341:PX4:O3	3:B:364:PX4:H13	0.43	2.13	13	1
3:B:340:PX4:H9	3:B:340:PX4:O3	0.43	2.13	14	1
1:A:456:TRP:CE3	1:A:459:ILE:HD11	0.43	2.48	15	1
3:A:646:PX4:C3	3:A:646:PX4:O3	0.43	2.66	1	1
3:B:399:PX4:O2	3:C:356:PX4:H12	0.43	2.13	2	1
3:A:606:PX4:H3	3:A:606:PX4:O1	0.43	2.13	4	2
3:B:360:PX4:H13	3:B:362:PX4:O8	0.43	2.13	4	1
3:B:390:PX4:O3	3:B:390:PX4:H7	0.43	2.13	4	1
3:B:379:PX4:H3	3:B:391:PX4:O4	0.43	2.12	5	1
3:B:332:PX4:C4	3:B:332:PX4:O3	0.43	2.64	6	1
3:A:636:PX4:H9	3:A:636:PX4:O2	0.43	2.14	8	1
3:C:333:PX4:H10	3:C:360:PX4:P1	0.43	2.53	11	1
3:A:617:PX4:H6	3:C:349:PX4:O2	0.43	2.13	13	1
3:C:344:PX4:O4	3:C:344:PX4:H3	0.43	2.14	14	1
3:A:622:PX4:H6	3:A:622:PX4:O3	0.43	2.14	2	1
3:B:302:PX4:O1	3:B:307:PX4:H4	0.43	2.14	3	2
3:B:309:PX4:H8	3:B:342:PX4:O1	0.43	2.14	7	1
3:C:365:PX4:H3	3:C:365:PX4:O1	0.43	2.13	13	1
3:B:365:PX4:O6	3:B:365:PX4:H7	0.43	2.14	14	1
3:B:303:PX4:H3	3:B:303:PX4:O4	0.43	2.14	15	1
3:C:359:PX4:O3	3:C:366:PX4:H9	0.43	2.14	2	1
3:C:329:PX4:H10	3:C:347:PX4:O2	0.43	2.14	3	1
3:C:333:PX4:H9	3:C:333:PX4:O1	0.43	2.14	4	1
3:B:341:PX4:O4	3:B:364:PX4:H9	0.43	2.14	6	1
3:C:318:PX4:H6	3:C:318:PX4:O3	0.43	2.14	6	1
3:C:343:PX4:H12	3:C:343:PX4:O3	0.43	2.13	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:321:GLY:HA2	1:A:323:PHE:CZ	0.43	2.49	7	1
3:A:603:PX4:C5	3:A:603:PX4:O3	0.43	2.67	8	1
3:C:352:PX4:H9	3:C:361:PX4:O1	0.43	2.14	12	1
3:B:331:PX4:O2	3:B:331:PX4:H6	0.43	2.14	2	1
3:B:336:PX4:O1	3:B:350:PX4:H9	0.43	2.14	4	1
3:B:302:PX4:H4	3:B:302:PX4:O4	0.43	2.14	5	1
3:A:618:PX4:O3	3:A:618:PX4:H6	0.43	2.14	7	2
3:B:319:PX4:H5	3:B:320:PX4:O4	0.43	2.13	7	1
3:B:311:PX4:O3	3:B:311:PX4:H7	0.43	2.14	9	1
3:B:387:PX4:H6	3:B:387:PX4:O3	0.43	2.14	11	1
3:C:318:PX4:O3	3:C:318:PX4:H6	0.43	2.13	11	1
3:C:369:PX4:O2	3:C:369:PX4:H7	0.43	2.13	1	1
2:C:211:LEU:HD12	2:C:215:HIS:CD2	0.43	2.49	3	1
3:A:611:PX4:H15	3:A:613:PX4:H11	0.43	1.90	7	1
3:B:357:PX4:O3	3:B:357:PX4:C5	0.43	2.67	7	1
3:A:610:PX4:H13	3:A:629:PX4:O6	0.43	2.14	8	2
3:C:361:PX4:O3	3:C:361:PX4:H12	0.43	2.13	9	1
3:C:313:PX4:O8	3:C:337:PX4:H3	0.43	2.14	11	1
3:B:356:PX4:H16	3:B:370:PX4:C2	0.43	2.43	1	1
3:C:305:PX4:H18	3:C:305:PX4:O8	0.43	2.13	1	1
3:C:352:PX4:O8	3:C:364:PX4:H7	0.43	2.14	1	1
3:C:344:PX4:H9	3:C:344:PX4:O3	0.43	2.13	6	1
1:A:486:PHE:CZ	1:A:491:LEU:HA	0.43	2.49	7	1
3:B:359:PX4:H3	3:B:359:PX4:O1	0.43	2.14	7	1
3:B:332:PX4:O2	3:B:332:PX4:H9	0.43	2.14	8	1
3:C:321:PX4:H12	3:C:321:PX4:O3	0.42	2.14	1	1
3:B:365:PX4:O1	3:B:365:PX4:H3	0.42	2.14	4	1
3:C:309:PX4:H2	3:C:344:PX4:H11	0.42	1.90	5	1
1:A:430:PHE:CD1	1:A:435:TYR:HB3	0.42	2.49	7	1
3:A:633:PX4:H9	3:B:400:PX4:O4	0.42	2.13	8	1
3:A:627:PX4:H5	3:C:361:PX4:H7	0.42	1.91	9	1
3:C:335:PX4:C28	3:C:335:PX4:H47	0.42	2.44	10	1
3:B:341:PX4:H3	3:B:341:PX4:O1	0.42	2.14	12	1
3:B:338:PX4:H3	3:B:357:PX4:O1	0.42	2.14	15	2
3:A:639:PX4:O2	3:A:640:PX4:H11	0.42	2.14	13	1
3:B:394:PX4:H9	3:B:394:PX4:O2	0.42	2.13	13	1
3:A:642:PX4:O1	3:A:647:PX4:H3	0.42	2.13	15	1
3:B:373:PX4:O1	3:B:388:PX4:H8	0.42	2.14	15	1
3:A:619:PX4:H9	3:A:635:PX4:O6	0.42	2.13	3	1
3:A:601:PX4:O3	3:A:601:PX4:H7	0.42	2.14	5	1
3:B:378:PX4:O2	3:C:305:PX4:H10	0.42	2.14	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:358:PX4:H3	3:C:358:PX4:O4	0.42	2.14	9	1
3:A:634:PX4:O4	3:A:644:PX4:H6	0.42	2.14	10	1
3:C:319:PX4:H13	3:C:319:PX4:O3	0.42	2.14	11	1
3:C:326:PX4:C9	3:C:328:PX4:H24	0.42	2.45	13	1
1:A:457:GLU:OE1	3:A:636:PX4:H12	0.42	2.14	1	1
3:B:377:PX4:O2	3:B:377:PX4:H4	0.42	2.14	1	1
3:C:337:PX4:H6	3:C:337:PX4:O3	0.42	2.14	3	1
3:B:356:PX4:O8	3:B:370:PX4:H10	0.42	2.14	4	1
3:B:358:PX4:O2	3:B:365:PX4:H13	0.42	2.13	7	1
3:A:615:PX4:H8	3:C:360:PX4:O2	0.42	2.14	7	1
3:B:325:PX4:H9	3:B:325:PX4:O3	0.42	2.14	15	3
3:B:352:PX4:O3	3:B:369:PX4:H10	0.42	2.14	9	1
3:C:329:PX4:O3	3:C:329:PX4:H6	0.42	2.14	10	1
2:B:184:HIS:CE1	2:C:123:LEU:HA	0.42	2.49	12	1
3:B:383:PX4:H3	3:B:383:PX4:O1	0.42	2.15	12	1
3:B:379:PX4:O2	3:B:385:PX4:H6	0.42	2.14	12	1
3:B:386:PX4:H3	3:B:386:PX4:O2	0.42	2.14	15	1
3:C:305:PX4:C8	3:C:305:PX4:O8	0.42	2.67	1	1
3:A:605:PX4:O4	3:A:607:PX4:H3	0.42	2.15	9	2
3:B:307:PX4:O3	3:B:307:PX4:H6	0.42	2.15	2	1
3:C:352:PX4:H10	3:C:352:PX4:O3	0.42	2.14	2	1
3:B:376:PX4:H10	3:B:376:PX4:O3	0.42	2.14	9	2
3:A:619:PX4:O4	3:A:619:PX4:H3	0.42	2.15	7	2
3:B:399:PX4:H3	3:B:399:PX4:O1	0.42	2.14	9	1
3:C:323:PX4:H10	3:C:323:PX4:C6	0.42	2.44	9	1
3:A:612:PX4:O4	3:A:612:PX4:H3	0.42	2.12	10	1
3:B:321:PX4:H9	3:B:321:PX4:O3	0.42	2.15	10	2
3:A:646:PX4:H7	3:A:646:PX4:O3	0.42	2.14	11	1
3:A:640:PX4:O3	3:A:640:PX4:H6	0.42	2.15	12	1
3:B:371:PX4:O3	3:B:371:PX4:H6	0.42	2.15	12	1
3:B:382:PX4:H6	3:B:382:PX4:O3	0.42	2.14	14	2
3:B:334:PX4:O1	3:B:346:PX4:H7	0.42	2.14	15	1
3:A:620:PX4:C2	3:A:620:PX4:O4	0.42	2.66	1	1
3:B:304:PX4:H7	3:B:304:PX4:O3	0.42	2.15	3	1
3:B:313:PX4:O3	3:B:313:PX4:H9	0.42	2.14	5	1
3:A:634:PX4:H4	3:A:641:PX4:O1	0.42	2.13	8	1
3:C:329:PX4:H6	3:C:329:PX4:O3	0.42	2.13	8	1
3:B:399:PX4:O3	3:C:356:PX4:H3	0.42	2.13	9	1
3:A:633:PX4:H6	3:C:370:PX4:H47	0.42	1.91	11	1
3:A:628:PX4:O1	3:A:644:PX4:H11	0.42	2.14	11	1
3:C:351:PX4:H13	3:C:351:PX4:O3	0.42	2.14	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:624:PX4:O3	3:A:624:PX4:H13	0.42	2.15	13	3
3:B:385:PX4:H22	3:B:389:PX4:H48	0.42	1.92	2	1
3:B:312:PX4:C27	3:B:317:PX4:H8	0.42	2.38	3	1
2:C:193:ARG:NH2	3:C:311:PX4:O1	0.42	2.53	5	1
3:B:315:PX4:H13	3:B:315:PX4:O3	0.42	2.13	8	1
3:B:328:PX4:O3	3:B:328:PX4:H12	0.42	2.14	9	1
3:B:320:PX4:P1	3:B:320:PX4:H13	0.42	2.54	11	1
3:C:306:PX4:O1	3:C:306:PX4:H3	0.42	2.14	11	1
3:C:364:PX4:O3	3:C:364:PX4:H12	0.42	2.14	12	1
3:C:370:PX4:H10	3:C:370:PX4:O3	0.42	2.14	12	1
3:A:633:PX4:H9	3:C:370:PX4:O6	0.42	2.15	1	1
1:A:490:LYS:HB2	3:A:643:PX4:H12	0.42	1.91	2	1
3:A:623:PX4:H10	3:A:623:PX4:O6	0.42	2.13	5	1
3:C:329:PX4:H14	3:C:329:PX4:H7	0.42	1.91	7	1
3:B:303:PX4:O2	3:B:303:PX4:H4	0.42	2.15	8	1
3:C:348:PX4:O3	3:C:370:PX4:H12	0.42	2.15	8	1
3:B:386:PX4:O3	3:B:386:PX4:H12	0.42	2.14	9	1
3:B:309:PX4:O6	3:B:315:PX4:H4	0.42	2.15	10	1
3:B:331:PX4:H3	3:B:331:PX4:O1	0.42	2.15	10	1
3:B:378:PX4:C6	3:B:378:PX4:H1	0.42	2.44	10	1
3:B:367:PX4:H6	3:B:367:PX4:O3	0.42	2.13	11	1
3:B:378:PX4:O2	3:B:387:PX4:H4	0.42	2.13	13	1
3:B:392:PX4:O8	3:B:393:PX4:H7	0.42	2.14	14	2
3:A:642:PX4:O3	3:A:642:PX4:H10	0.42	2.14	3	1
3:C:365:PX4:C6	3:C:365:PX4:H4	0.42	2.45	4	1
3:A:615:PX4:H7	3:A:615:PX4:O6	0.42	2.15	6	1
3:B:349:PX4:O3	3:B:371:PX4:H9	0.42	2.15	6	1
3:C:337:PX4:H4	3:C:346:PX4:P1	0.42	2.54	6	1
3:C:348:PX4:H9	3:C:348:PX4:O3	0.42	2.15	6	1
3:B:326:PX4:H70	3:C:327:PX4:H71	0.42	1.92	8	1
3:C:333:PX4:H4	3:C:360:PX4:O3	0.42	2.14	9	1
3:A:635:PX4:H6	3:A:635:PX4:O3	0.42	2.13	10	1
3:C:312:PX4:H5	3:C:325:PX4:O2	0.42	2.15	12	1
3:C:359:PX4:H6	3:C:363:PX4:O2	0.42	2.15	12	1
3:A:642:PX4:O6	3:A:647:PX4:H9	0.42	2.15	15	1
1:A:457:GLU:OE2	3:A:636:PX4:H3	0.42	2.14	3	1
3:A:621:PX4:O8	3:A:637:PX4:H6	0.42	2.15	4	1
3:B:323:PX4:O3	3:B:323:PX4:H9	0.42	2.14	5	1
3:B:360:PX4:O2	3:B:381:PX4:H6	0.42	2.13	7	1
3:C:331:PX4:H3	3:C:331:PX4:O1	0.42	2.15	7	1
3:A:647:PX4:O4	3:A:647:PX4:H9	0.42	2.14	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:341:PX4:P1	3:C:362:PX4:H9	0.42	2.54	11	1
3:B:321:PX4:H5	3:B:330:PX4:O2	0.42	2.15	12	1
3:B:381:PX4:H71	3:B:394:PX4:H35	0.42	1.91	14	1
3:C:305:PX4:O4	3:C:305:PX4:H3	0.42	2.14	1	1
3:C:312:PX4:O2	3:C:312:PX4:H4	0.42	2.14	1	1
3:A:642:PX4:C4	3:A:642:PX4:O3	0.42	2.67	3	1
3:B:345:PX4:O3	3:B:345:PX4:H10	0.42	2.15	3	1
3:B:349:PX4:H13	3:B:349:PX4:O3	0.42	2.15	3	1
3:A:639:PX4:H10	3:A:639:PX4:O3	0.42	2.15	4	1
3:B:331:PX4:H6	3:B:331:PX4:H14	0.42	1.91	6	1
3:A:601:PX4:H9	3:A:601:PX4:O3	0.42	2.14	13	2
3:C:324:PX4:O2	3:C:324:PX4:H3	0.42	2.15	11	2
3:B:349:PX4:H7	3:B:353:PX4:O2	0.42	2.15	9	1
3:C:321:PX4:O4	3:C:321:PX4:H3	0.42	2.15	10	1
3:B:314:PX4:O2	3:B:314:PX4:H7	0.42	2.15	13	1
3:B:312:PX4:H54	3:B:317:PX4:H10	0.42	1.90	13	1
3:A:613:PX4:H13	3:A:613:PX4:O4	0.42	2.15	14	1
3:A:610:PX4:H4	3:C:368:PX4:O6	0.42	2.13	15	1
3:B:308:PX4:H17	3:C:302:PX4:H13	0.42	1.91	15	1
3:C:315:PX4:O4	3:C:315:PX4:H4	0.41	2.14	6	1
3:C:366:PX4:H6	3:C:369:PX4:O4	0.41	2.14	7	1
1:A:504:ASP:OD2	3:A:641:PX4:H11	0.41	2.15	10	1
3:B:330:PX4:C3	3:B:330:PX4:O3	0.41	2.68	12	1
3:A:614:PX4:O3	3:A:614:PX4:H12	0.41	2.14	14	1
3:A:623:PX4:H13	3:A:623:PX4:O3	0.41	2.15	2	1
3:B:339:PX4:H4	3:B:339:PX4:O4	0.41	2.15	2	1
3:B:388:PX4:O3	3:B:388:PX4:H7	0.41	2.15	6	1
3:B:359:PX4:H8	3:B:363:PX4:O2	0.41	2.16	8	1
3:B:362:PX4:O2	3:B:362:PX4:H12	0.41	2.15	9	1
3:A:617:PX4:O1	3:A:617:PX4:H3	0.41	2.15	11	1
2:B:100:TYR:CD2	2:C:209:ALA:HB2	0.41	2.50	11	1
2:B:126:PHE:HB2	2:C:184:HIS:CE1	0.41	2.50	11	1
3:C:366:PX4:H3	3:C:366:PX4:O4	0.41	2.14	12	1
3:A:615:PX4:O3	3:A:615:PX4:H6	0.41	2.14	14	1
3:C:341:PX4:H4	3:C:341:PX4:O2	0.41	2.16	14	1
3:A:626:PX4:O8	3:C:365:PX4:H5	0.41	2.16	3	1
3:C:350:PX4:H12	3:C:352:PX4:O1	0.41	2.15	3	1
3:B:361:PX4:O2	3:B:361:PX4:H4	0.41	2.14	5	1
3:B:358:PX4:O1	3:B:365:PX4:H11	0.41	2.15	5	1
3:A:635:PX4:O2	3:A:635:PX4:H3	0.41	2.15	6	1
3:B:334:PX4:H10	3:B:334:PX4:O3	0.41	2.15	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:309:PX4:H4	3:C:309:PX4:C6	0.41	2.45	6	1
3:B:397:PX4:O3	3:B:397:PX4:H9	0.41	2.15	11	1
3:A:639:PX4:H4	3:A:639:PX4:O1	0.41	2.15	12	1
3:B:334:PX4:O2	3:B:346:PX4:H9	0.41	2.15	12	1
3:B:367:PX4:O3	3:B:367:PX4:H6	0.41	2.15	12	1
3:A:615:PX4:H12	3:C:360:PX4:O1	0.41	2.15	13	1
3:B:361:PX4:O3	3:B:361:PX4:H7	0.41	2.16	14	1
1:A:483:TYR:CD2	1:A:505:TRP:CZ2	0.41	3.08	2	1
3:A:613:PX4:O3	3:A:613:PX4:H6	0.41	2.16	9	2
3:B:321:PX4:O1	3:B:321:PX4:H3	0.41	2.15	6	1
3:C:319:PX4:O1	3:C:323:PX4:H5	0.41	2.15	6	1
3:B:305:PX4:H7	3:B:305:PX4:O3	0.41	2.14	7	2
3:A:638:PX4:H4	3:A:638:PX4:C6	0.41	2.45	10	1
3:C:355:PX4:H10	3:C:367:PX4:O3	0.41	2.15	13	1
3:B:358:PX4:H10	3:B:360:PX4:O1	0.41	2.14	1	1
3:A:635:PX4:H34	3:C:358:PX4:H68	0.41	1.93	7	1
3:B:337:PX4:O1	3:B:362:PX4:H4	0.41	2.15	8	1
3:B:366:PX4:O3	3:B:366:PX4:H6	0.41	2.15	8	1
3:B:346:PX4:H6	3:B:346:PX4:O3	0.41	2.15	9	1
3:B:312:PX4:O8	3:C:304:PX4:H10	0.41	2.16	12	1
3:C:311:PX4:O3	3:C:311:PX4:H6	0.41	2.15	12	1
3:B:309:PX4:O4	3:B:335:PX4:H7	0.41	2.16	14	1
3:B:347:PX4:O1	3:B:374:PX4:H10	0.41	2.15	14	1
3:A:633:PX4:H11	3:B:400:PX4:O2	0.41	2.16	2	1
3:C:350:PX4:H7	3:C:350:PX4:O3	0.41	2.16	4	1
3:C:342:PX4:H9	3:C:342:PX4:O3	0.41	2.16	5	1
3:C:349:PX4:O1	3:C:349:PX4:H13	0.41	2.15	7	1
1:A:476:TYR:CE1	1:A:485:LYS:HG3	0.41	2.51	9	1
3:A:601:PX4:O5	3:A:604:PX4:H9	0.41	2.16	12	1
3:A:633:PX4:H5	3:C:370:PX4:O4	0.41	2.16	14	1
3:B:392:PX4:H12	3:B:393:PX4:O6	0.41	2.15	15	1
3:A:635:PX4:O3	3:A:635:PX4:H6	0.41	2.16	2	1
3:A:642:PX4:O2	3:A:642:PX4:H4	0.41	2.15	10	2
3:C:348:PX4:O3	3:C:348:PX4:H9	0.41	2.16	5	1
3:A:613:PX4:O1	3:C:346:PX4:H6	0.41	2.15	7	1
3:A:601:PX4:H3	3:A:601:PX4:O8	0.41	2.15	8	1
3:C:306:PX4:H6	3:C:306:PX4:O3	0.41	2.16	9	1
3:A:630:PX4:H13	3:A:630:PX4:O2	0.41	2.16	11	1
3:B:373:PX4:H10	3:B:373:PX4:O3	0.41	2.15	11	1
3:C:304:PX4:H3	3:C:304:PX4:O2	0.41	2.16	11	1
3:B:355:PX4:H6	3:B:355:PX4:O3	0.41	2.16	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:359:PX4:H9	3:C:359:PX4:H15	0.41	1.92	2	1
3:B:380:PX4:H10	3:B:380:PX4:O3	0.41	2.15	4	1
3:C:360:PX4:C5	3:C:360:PX4:O3	0.41	2.68	5	1
3:B:349:PX4:H30	3:B:353:PX4:H48	0.41	1.91	6	1
3:B:370:PX4:O3	3:C:305:PX4:H13	0.41	2.15	6	1
2:B:86:MET:CE	3:B:308:PX4:H10	0.41	2.46	7	1
3:A:604:PX4:H8	3:B:384:PX4:C6	0.41	2.46	7	1
3:C:309:PX4:H7	3:C:309:PX4:O3	0.41	2.16	7	1
3:B:345:PX4:O1	3:B:373:PX4:H13	0.41	2.15	8	1
3:B:400:PX4:C3	3:B:400:PX4:O3	0.41	2.69	10	1
3:C:335:PX4:H54	3:C:335:PX4:H47	0.41	1.92	10	1
3:A:620:PX4:H54	3:A:628:PX4:H27	0.41	1.92	11	1
3:B:320:PX4:O1	3:B:320:PX4:H6	0.41	2.15	11	1
3:B:356:PX4:H1	3:B:356:PX4:H14	0.41	1.93	15	1
3:C:350:PX4:H3	3:C:352:PX4:O1	0.41	2.16	15	1
3:C:365:PX4:O3	3:C:365:PX4:H13	0.41	2.16	15	1
3:C:332:PX4:H10	3:C:332:PX4:O3	0.41	2.16	1	1
3:A:621:PX4:O2	3:C:365:PX4:H10	0.41	2.16	1	1
3:C:328:PX4:O3	3:C:328:PX4:H9	0.41	2.16	1	1
3:C:363:PX4:H12	3:C:363:PX4:O3	0.41	2.15	1	1
2:B:112:MET:HE1	3:B:304:PX4:H50	0.41	1.91	2	1
3:B:326:PX4:H42	3:C:327:PX4:H45	0.41	1.93	3	1
3:B:304:PX4:H3	3:C:301:PX4:O1	0.41	2.16	4	1
3:A:605:PX4:O3	3:A:605:PX4:H10	0.41	2.16	5	1
3:B:396:PX4:O4	3:B:396:PX4:H4	0.41	2.16	5	1
3:C:347:PX4:H7	3:C:366:PX4:O1	0.41	2.16	5	1
3:C:323:PX4:C6	3:C:323:PX4:H10	0.41	2.46	6	1
2:C:130:TRP:HA	2:C:130:TRP:CE3	0.41	2.50	7	1
3:A:627:PX4:H3	3:A:627:PX4:O4	0.41	2.16	7	1
3:C:305:PX4:H6	3:C:305:PX4:O3	0.41	2.16	9	1
3:A:602:PX4:H14	3:A:602:PX4:H9	0.41	1.93	9	1
3:B:347:PX4:H45	3:C:363:PX4:H42	0.41	1.93	10	1
3:B:358:PX4:O3	3:B:358:PX4:H7	0.41	2.15	10	1
3:B:390:PX4:O1	3:B:390:PX4:H4	0.41	2.16	15	1
3:C:335:PX4:H12	3:C:335:PX4:O2	0.41	2.15	15	1
3:A:608:PX4:H3	3:A:608:PX4:O1	0.41	2.16	4	2
3:B:340:PX4:H7	3:B:340:PX4:O3	0.41	2.15	4	1
3:B:337:PX4:C6	3:B:339:PX4:H3	0.41	2.46	6	1
3:C:309:PX4:H4	3:C:309:PX4:O4	0.41	2.16	6	1
3:B:302:PX4:O2	3:B:307:PX4:H7	0.41	2.17	8	1
3:B:336:PX4:H7	3:B:336:PX4:C6	0.41	2.46	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:368:PX4:H9	3:B:368:PX4:O3	0.41	2.16	10	1
3:C:333:PX4:H4	3:C:360:PX4:C1	0.41	2.46	10	1
3:B:359:PX4:C4	3:B:359:PX4:O3	0.41	2.67	12	1
3:A:607:PX4:H10	3:A:608:PX4:O1	0.41	2.16	13	1
3:A:608:PX4:O8	3:B:390:PX4:H11	0.41	2.16	13	1
3:B:349:PX4:H15	3:B:349:PX4:C1	0.41	2.45	14	1
3:B:397:PX4:H67	3:C:318:PX4:H69	0.41	1.92	14	1
3:A:628:PX4:O3	3:A:628:PX4:H10	0.41	2.16	15	1
3:B:338:PX4:H10	3:B:357:PX4:O1	0.40	2.15	1	1
3:B:366:PX4:O1	3:B:385:PX4:H5	0.40	2.16	1	1
3:B:355:PX4:H7	3:B:376:PX4:O2	0.40	2.16	2	1
3:A:633:PX4:O1	3:A:633:PX4:H13	0.40	2.15	5	1
3:C:357:PX4:C25	3:C:363:PX4:H11	0.40	2.45	6	1
3:B:327:PX4:O1	3:B:327:PX4:H3	0.40	2.16	7	1
3:B:388:PX4:O6	3:B:393:PX4:H9	0.40	2.16	7	1
3:A:612:PX4:H3	3:C:351:PX4:H18	0.40	1.92	8	1
2:B:128:LYS:HA	3:B:320:PX4:H8	0.40	1.92	9	1
3:B:324:PX4:H4	3:B:327:PX4:O2	0.40	2.16	11	1
3:B:311:PX4:H3	3:B:344:PX4:O2	0.40	2.16	11	1
3:C:351:PX4:O3	3:C:351:PX4:H13	0.40	2.16	11	1
3:C:352:PX4:H7	3:C:361:PX4:O3	0.40	2.16	12	1
3:A:602:PX4:H7	3:A:602:PX4:H14	0.40	1.92	6	1
3:B:369:PX4:O1	3:B:373:PX4:H11	0.40	2.16	10	1
3:A:641:PX4:H22	3:A:646:PX4:H20	0.40	1.93	12	1
3:C:334:PX4:O3	3:C:334:PX4:H10	0.40	2.16	12	1
2:C:244:LEU:HD22	3:C:331:PX4:H31	0.40	1.92	14	1
3:B:376:PX4:O3	3:B:376:PX4:H10	0.40	2.17	15	1
3:C:313:PX4:H72	3:C:346:PX4:H68	0.40	1.92	2	1
3:C:361:PX4:H12	3:C:361:PX4:O3	0.40	2.15	3	1
3:B:353:PX4:O4	3:B:371:PX4:H4	0.40	2.16	6	1
3:B:391:PX4:H6	3:B:391:PX4:O3	0.40	2.16	6	1
3:B:370:PX4:O2	3:B:370:PX4:H4	0.40	2.16	7	1
3:B:377:PX4:H7	3:B:377:PX4:O3	0.40	2.15	7	1
3:B:366:PX4:C3	3:B:366:PX4:O3	0.40	2.69	8	1
3:A:608:PX4:H4	3:B:394:PX4:C1	0.40	2.46	9	1
3:B:324:PX4:O1	3:B:352:PX4:H9	0.40	2.17	9	1
3:C:307:PX4:H20	3:C:313:PX4:H14	0.40	1.92	10	1
3:A:638:PX4:O3	3:A:638:PX4:H13	0.40	2.16	12	1
2:C:84:GLN:HE21	2:C:88:LYS:HG3	0.40	1.77	15	1
3:B:301:PX4:O2	3:B:301:PX4:H4	0.40	2.16	2	1
3:C:337:PX4:O3	3:C:346:PX4:H12	0.40	2.16	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:358:PX4:H9	3:B:358:PX4:O3	0.40	2.16	5	1
3:C:322:PX4:O3	3:C:322:PX4:H10	0.40	2.17	5	1
3:C:359:PX4:O3	3:C:366:PX4:C2	0.40	2.70	6	1
3:A:638:PX4:H18	3:A:648:PX4:H9	0.40	1.93	8	1
3:B:325:PX4:O3	3:B:325:PX4:H9	0.40	2.17	10	1
3:B:310:PX4:O1	3:B:342:PX4:H10	0.40	2.16	10	1
3:C:347:PX4:C5	3:C:347:PX4:O3	0.40	2.68	10	1
3:C:352:PX4:O3	3:C:352:PX4:H10	0.40	2.17	10	1
3:C:361:PX4:H3	3:C:361:PX4:O2	0.40	2.16	14	1
3:C:315:PX4:O2	3:C:315:PX4:H9	0.40	2.16	4	1
3:C:354:PX4:O2	3:C:354:PX4:H3	0.40	2.16	4	1
3:C:350:PX4:O3	3:C:350:PX4:H7	0.40	2.17	5	1
3:A:620:PX4:O2	3:A:638:PX4:H3	0.40	2.17	8	1
3:B:387:PX4:H13	3:B:387:PX4:O3	0.40	2.16	9	1
3:A:604:PX4:H13	3:A:605:PX4:O4	0.40	2.16	11	1
3:C:305:PX4:H9	3:C:305:PX4:O3	0.40	2.17	12	1
3:C:311:PX4:O8	3:C:317:PX4:H7	0.40	2.17	15	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	194/196 (99%)	176±3 (91±2%)	15±3 (8±2%)	3±2 (1±1%)	14	59
2	B	209/211 (99%)	204±1 (98±1%)	4±1 (2±1%)	0±0 (0±0%)	50	82
2	C	209/211 (99%)	205±1 (98±0%)	4±1 (2±1%)	0±0 (0±0%)	50	82
All	All	9180/9270 (99%)	8779 (96%)	344 (4%)	57 (1%)	29	74

All 27 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	392	GLU	9
2	C	231	PRO	6

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Mol	Chain	Res	Type	Models (Total)
1	A	393	ALA	4
1	A	448	GLU	4
2	B	143	PRO	3
1	A	375	LYS	3
1	A	354	PRO	3
1	A	472	GLU	2
1	A	510	SER	2
1	A	411	PRO	2
1	A	397	PRO	2
2	B	142	GLU	2
1	A	400	PRO	1
2	C	104	PHE	1
1	A	503	ARG	1
1	A	479	LYS	1
1	A	491	LEU	1
1	A	322	ASN	1
2	B	187	PRO	1
1	A	362	ARG	1
1	A	432	GLY	1
1	A	367	SER	1
2	B	119	VAL	1
1	A	498	PRO	1
1	A	338	GLU	1
1	A	414	LYS	1
1	A	323	PHE	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	169/169 (100%)	164±2 (97±1%)	5±2 (3±1%)	44 89
2	B	187/187 (100%)	183±2 (98±1%)	4±2 (2±1%)	57 93
2	C	187/187 (100%)	182±3 (97±1%)	5±3 (3±1%)	45 89
All	All	8145/8145 (100%)	7932 (97%)	213 (3%)	49 91

All 112 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)
2	B	210	ARG	14
2	C	210	ARG	14
1	A	372	TYR	10
2	B	86	MET	7
1	A	435	TYR	5
1	A	342	TRP	4
1	A	411	PRO	4
1	A	365	PRO	4
2	C	63	GLN	4
2	C	204	LYS	4
2	C	56	THR	4
1	A	422	MET	3
1	A	368	ILE	3
2	C	139	GLN	3
1	A	375	LYS	3
2	B	123	LEU	3
2	C	219	THR	3
1	A	404	LYS	3
2	B	237	ARG	3
2	C	71	PHE	3
2	C	119	VAL	3
1	A	348	GLN	2
1	A	478	TYR	2
1	A	397	PRO	2
2	B	127	GLN	2
2	C	183	THR	2
2	B	106	LYS	2
2	C	242	PRO	2
2	C	195	ARG	2
2	C	58	SER	2
2	B	119	VAL	2
1	A	414	LYS	2
1	A	433	ASN	2
2	B	66	PRO	2
2	C	116	ARG	2
1	A	470	SER	2
1	A	340	TRP	2
2	C	236	LEU	2
1	A	436	TYR	2
2	B	255	LEU	1
1	A	388	TRP	1
2	C	206	ASN	1
2	C	97	VAL	1

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Mol	Chain	Res	Type	Models (Total)
2	C	154	GLN	1
2	B	140	LYS	1
2	C	246	SER	1
2	C	170	MET	1
1	A	341	PHE	1
1	A	316	PRO	1
2	C	199	ARG	1
2	B	99	PRO	1
2	C	192	LEU	1
2	C	75	LEU	1
1	A	484	TRP	1
2	C	160	GLN	1
2	C	211	LEU	1
2	C	252	LEU	1
2	C	100	TYR	1
2	B	93	VAL	1
1	A	445	VAL	1
2	B	166	LEU	1
1	A	419	LEU	1
2	C	247	PHE	1
1	A	492	LYS	1
2	C	166	LEU	1
2	B	165	PRO	1
2	B	136	LEU	1
1	A	408	ARG	1
1	A	412	THR	1
1	A	382	PHE	1
2	C	177	HIS	1
2	B	139	GLN	1
2	C	127	GLN	1
2	B	121	PRO	1
2	C	93	VAL	1
2	C	175	ARG	1
2	B	90	LEU	1
2	B	181	LEU	1
2	C	102	ASP	1
2	C	147	GLU	1
2	C	162	LYS	1
2	B	264	THR	1
1	A	346	ASN	1
2	B	128	LYS	1
1	A	374	ARG	1

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Mol	Chain	Res	Type	Models (Total)
2	C	238	GLN	1
1	A	468	MET	1
2	B	242	PRO	1
2	C	118	LYS	1
2	B	224	THR	1
2	B	215	HIS	1
2	C	112	MET	1
1	A	509	PRO	1
2	C	104	PHE	1
2	C	224	THR	1
2	C	128	LYS	1
2	C	57	PHE	1
1	A	491	LEU	1
2	B	187	PRO	1
2	C	143	PRO	1
1	A	378	LYS	1
1	A	455	VAL	1
2	B	84	GLN	1
2	B	194	GLN	1
1	A	430	PHE	1
2	B	56	THR	1
2	B	67	VAL	1
1	A	443	ARG	1
2	B	92	GLU	1
1	A	370	THR	1
2	C	77	LYS	1
2	C	165	PRO	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 (i)

Of 220 ligands modelled in this entry, 2 are monoatomic - leaving 218 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
3	PX4	B	367	-	45,45,45	1.14±0.00	0±0 (0±0%)
3	PX4	B	330	-	45,45,45	1.03±0.00	0±0 (0±0%)
3	PX4	B	382	-	45,45,45	0.90±0.00	0±0 (0±0%)
3	PX4	C	327	-	45,45,45	1.01±0.00	0±0 (0±0%)
3	PX4	C	315	-	45,45,45	1.10±0.00	0±0 (0±0%)
3	PX4	C	322	-	45,45,45	1.22±0.00	0±0 (0±0%)
3	PX4	C	348	-	45,45,45	1.14±0.00	0±0 (0±0%)
3	PX4	B	347	-	45,45,45	1.07±0.00	0±0 (0±0%)
3	PX4	C	352	-	45,45,45	1.01±0.00	0±0 (0±0%)
3	PX4	C	346	-	45,45,45	1.07±0.00	0±0 (0±0%)
3	PX4	A	620	-	45,45,45	1.03±0.00	0±0 (0±0%)
3	PX4	A	611	-	45,45,45	1.03±0.00	0±0 (0±0%)
3	PX4	C	318	-	45,45,45	0.92±0.00	0±0 (0±0%)
3	PX4	A	608	-	45,45,45	0.95±0.00	0±0 (0±0%)
3	PX4	C	356	-	45,45,45	1.20±0.00	0±0 (0±0%)
3	PX4	C	335	-	45,45,45	1.06±0.00	0±0 (0±0%)
3	PX4	C	313	-	45,45,45	0.97±0.00	0±0 (0±0%)
3	PX4	C	344	-	45,45,45	1.09±0.00	0±0 (0±0%)
3	PX4	C	351	-	45,45,45	1.02±0.00	0±0 (0±0%)
3	PX4	C	303	-	45,45,45	1.06±0.00	0±0 (0±0%)
3	PX4	B	345	-	45,45,45	1.03±0.00	0±0 (0±0%)
3	PX4	C	349	-	45,45,45	0.88±0.00	0±0 (0±0%)
3	PX4	C	321	-	45,45,45	1.00±0.00	0±0 (0±0%)
3	PX4	A	602	-	45,45,45	1.02±0.00	0±0 (0±0%)
3	PX4	C	309	-	45,45,45	1.06±0.00	0±0 (0±0%)
3	PX4	B	374	-	45,45,45	0.89±0.00	0±0 (0±0%)
3	PX4	B	326	-	45,45,45	0.95±0.00	0±0 (0±0%)
3	PX4	C	340	-	45,45,45	1.13±0.00	0±0 (0±0%)
3	PX4	B	333	-	45,45,45	1.07±0.00	0±0 (0±0%)
3	PX4	A	606	-	45,45,45	1.05±0.00	0±0 (0±0%)
3	PX4	A	639	-	45,45,45	1.01±0.00	0±0 (0±0%)
3	PX4	B	389	-	45,45,45	1.17±0.00	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	PX4	A	601	-	45,45,45	0.91±0.00	0±0 (0±0%)
3	PX4	C	310	-	45,45,45	0.97±0.00	0±0 (0±0%)
3	PX4	B	348	-	45,45,45	1.03±0.00	0±0 (0±0%)
3	PX4	B	341	-	45,45,45	1.22±0.00	0±0 (0±0%)
3	PX4	B	363	-	45,45,45	1.04±0.00	0±0 (0±0%)
3	PX4	B	303	-	45,45,45	0.98±0.00	0±0 (0±0%)
3	PX4	B	356	-	45,45,45	1.15±0.00	0±0 (0±0%)
3	PX4	B	302	-	45,45,45	0.99±0.00	0±0 (0±0%)
3	PX4	C	370	-	45,45,45	1.26±0.00	0±0 (0±0%)
3	PX4	B	350	-	45,45,45	1.67±0.00	1±0 (2±0%)
3	PX4	C	339	-	45,45,45	0.96±0.00	0±0 (0±0%)
3	PX4	B	355	-	45,45,45	1.02±0.00	0±0 (0±0%)
3	PX4	B	352	-	45,45,45	1.03±0.00	0±0 (0±0%)
3	PX4	C	326	-	45,45,45	1.11±0.00	0±0 (0±0%)
3	PX4	A	634	-	45,45,45	1.01±0.00	0±0 (0±0%)
3	PX4	A	622	-	45,45,45	0.93±0.00	0±0 (0±0%)
3	PX4	B	400	-	45,45,45	0.85±0.00	0±0 (0±0%)
3	PX4	A	632	-	45,45,45	1.08±0.00	0±0 (0±0%)
3	PX4	A	623	-	45,45,45	1.01±0.00	0±0 (0±0%)
3	PX4	B	337	-	45,45,45	0.99±0.00	0±0 (0±0%)
3	PX4	A	614	-	45,45,45	0.99±0.00	0±0 (0±0%)
3	PX4	C	336	-	45,45,45	1.17±0.00	0±0 (0±0%)
3	PX4	A	615	-	45,45,45	0.82±0.00	0±0 (0±0%)
3	PX4	A	621	-	45,45,45	0.82±0.00	0±0 (0±0%)
3	PX4	C	319	-	45,45,45	1.02±0.00	0±0 (0±0%)
3	PX4	A	648	-	45,45,45	0.94±0.00	0±0 (0±0%)
3	PX4	A	605	-	45,45,45	0.92±0.00	0±0 (0±0%)
3	PX4	B	323	-	45,45,45	0.95±0.00	0±0 (0±0%)
3	PX4	C	304	-	45,45,45	1.10±0.00	0±0 (0±0%)
3	PX4	B	309	-	45,45,45	1.13±0.00	0±0 (0±0%)
3	PX4	C	334	-	45,45,45	0.96±0.00	0±0 (0±0%)
3	PX4	B	324	-	45,45,45	1.08±0.00	0±0 (0±0%)
3	PX4	B	362	-	45,45,45	0.99±0.00	0±0 (0±0%)
3	PX4	C	361	-	45,45,45	0.96±0.00	0±0 (0±0%)
3	PX4	B	306	-	45,45,45	1.00±0.00	0±0 (0±0%)
3	PX4	C	308	-	45,45,45	1.15±0.00	0±0 (0±0%)
3	PX4	B	304	-	45,45,45	1.27±0.00	0±0 (0±0%)
3	PX4	C	305	-	45,45,45	0.97±0.00	0±0 (0±0%)
3	PX4	C	337	-	45,45,45	1.05±0.00	0±0 (0±0%)
3	PX4	B	364	-	45,45,45	1.05±0.00	0±0 (0±0%)
3	PX4	B	329	-	45,45,45	1.21±0.00	0±0 (0±0%)
3	PX4	A	646	-	45,45,45	1.07±0.00	0±0 (0±0%)
3	PX4	B	328	-	45,45,45	0.90±0.00	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	PX4	B	344	-	45,45,45	0.94±0.00	0±0 (0±0%)
3	PX4	C	330	-	45,45,45	1.02±0.00	0±0 (0±0%)
3	PX4	C	306	-	45,45,45	1.04±0.00	0±0 (0±0%)
3	PX4	B	305	-	45,45,45	1.13±0.00	0±0 (0±0%)
3	PX4	C	345	-	45,45,45	1.14±0.00	0±0 (0±0%)
3	PX4	C	317	-	45,45,45	0.92±0.00	0±0 (0±0%)
3	PX4	B	343	-	45,45,45	0.93±0.00	0±0 (0±0%)
3	PX4	C	311	-	45,45,45	1.06±0.00	0±0 (0±0%)
3	PX4	A	607	-	45,45,45	1.08±0.00	0±0 (0±0%)
3	PX4	A	644	-	45,45,45	1.29±0.00	0±0 (0±0%)
3	PX4	B	375	-	45,45,45	0.84±0.00	0±0 (0±0%)
3	PX4	B	361	-	45,45,45	1.11±0.00	0±0 (0±0%)
3	PX4	A	628	-	45,45,45	0.96±0.00	0±0 (0±0%)
3	PX4	A	619	-	45,45,45	0.98±0.00	0±0 (0±0%)
3	PX4	B	301	-	45,45,45	1.07±0.00	0±0 (0±0%)
3	PX4	B	396	-	45,45,45	1.13±0.00	0±0 (0±0%)
3	PX4	A	610	-	45,45,45	1.09±0.00	0±0 (0±0%)
3	PX4	C	316	-	45,45,45	1.25±0.00	0±0 (0±0%)
3	PX4	B	360	-	45,45,45	1.12±0.00	0±0 (0±0%)
3	PX4	A	626	-	45,45,45	1.05±0.00	0±0 (0±0%)
3	PX4	C	329	-	45,45,45	1.14±0.00	0±0 (0±0%)
3	PX4	C	365	-	45,45,45	1.10±0.00	0±0 (0±0%)
3	PX4	A	624	-	45,45,45	1.08±0.00	0±0 (0±0%)
3	PX4	B	378	-	45,45,45	0.99±0.00	0±0 (0±0%)
3	PX4	B	380	-	45,45,45	1.30±0.00	0±0 (0±0%)
3	PX4	A	613	-	45,45,45	0.99±0.00	0±0 (0±0%)
3	PX4	C	368	-	45,45,45	1.23±0.00	0±0 (0±0%)
3	PX4	B	321	-	45,45,45	1.17±0.00	0±0 (0±0%)
3	PX4	A	637	-	45,45,45	0.92±0.00	0±0 (0±0%)
3	PX4	B	354	-	45,45,45	1.02±0.00	0±0 (0±0%)
3	PX4	B	319	-	45,45,45	1.11±0.00	0±0 (0±0%)
3	PX4	B	314	-	45,45,45	1.10±0.00	0±0 (0±0%)
3	PX4	A	616	-	45,45,45	0.95±0.00	0±0 (0±0%)
3	PX4	B	398	-	45,45,45	1.08±0.00	0±0 (0±0%)
3	PX4	B	393	-	45,45,45	1.09±0.00	0±0 (0±0%)
3	PX4	B	385	-	45,45,45	1.33±0.00	0±0 (0±0%)
3	PX4	C	369	-	45,45,45	0.98±0.00	0±0 (0±0%)
3	PX4	B	379	-	45,45,45	0.88±0.00	0±0 (0±0%)
3	PX4	A	642	-	45,45,45	1.14±0.00	0±0 (0±0%)
3	PX4	B	399	-	45,45,45	1.11±0.00	0±0 (0±0%)
3	PX4	B	358	-	45,45,45	1.01±0.00	0±0 (0±0%)
3	PX4	B	331	-	45,45,45	0.95±0.00	0±0 (0±0%)
3	PX4	A	603	-	45,45,45	1.24±0.00	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	PX4	C	338	-	45,45,45	1.05±0.00	0±0 (0±0%)
3	PX4	C	333	-	45,45,45	0.95±0.00	0±0 (0±0%)
3	PX4	B	316	-	45,45,45	1.14±0.00	0±0 (0±0%)
3	PX4	B	359	-	45,45,45	1.08±0.00	0±0 (0±0%)
3	PX4	C	323	-	45,45,45	1.17±0.00	0±0 (0±0%)
3	PX4	A	604	-	45,45,45	1.00±0.00	0±0 (0±0%)
3	PX4	A	618	-	45,45,45	0.85±0.00	0±0 (0±0%)
3	PX4	B	317	-	45,45,45	0.96±0.00	0±0 (0±0%)
3	PX4	B	377	-	45,45,45	1.11±0.00	0±0 (0±0%)
3	PX4	B	391	-	45,45,45	1.17±0.00	0±0 (0±0%)
3	PX4	A	629	-	45,45,45	1.09±0.00	0±0 (0±0%)
3	PX4	A	609	-	45,45,45	1.27±0.00	0±0 (0±0%)
3	PX4	B	312	-	45,45,45	1.34±0.00	0±0 (0±0%)
3	PX4	A	633	-	45,45,45	1.41±0.00	0±0 (0±0%)
3	PX4	C	301	-	45,45,45	1.09±0.00	0±0 (0±0%)
3	PX4	B	353	-	45,45,45	0.86±0.00	0±0 (0±0%)
3	PX4	A	638	-	45,45,45	0.89±0.00	0±0 (0±0%)
3	PX4	B	346	-	45,45,45	1.03±0.00	0±0 (0±0%)
3	PX4	C	332	-	45,45,45	1.06±0.00	0±0 (0±0%)
3	PX4	C	342	-	45,45,45	1.04±0.00	0±0 (0±0%)
3	PX4	B	387	-	45,45,45	1.23±0.00	0±0 (0±0%)
3	PX4	C	366	-	45,45,45	0.94±0.00	0±0 (0±0%)
3	PX4	A	640	-	45,45,45	0.91±0.00	0±0 (0±0%)
3	PX4	A	631	-	45,45,45	1.21±0.00	0±0 (0±0%)
3	PX4	B	338	-	45,45,45	0.89±0.00	0±0 (0±0%)
3	PX4	A	641	-	45,45,45	1.03±0.00	0±0 (0±0%)
3	PX4	B	390	-	45,45,45	1.21±0.00	0±0 (0±0%)
3	PX4	B	373	-	45,45,45	1.17±0.00	0±0 (0±0%)
3	PX4	C	358	-	45,45,45	0.97±0.00	0±0 (0±0%)
3	PX4	B	368	-	45,45,45	1.07±0.00	0±0 (0±0%)
3	PX4	B	340	-	45,45,45	1.20±0.00	0±0 (0±0%)
3	PX4	B	349	-	45,45,45	0.93±0.00	0±0 (0±0%)
3	PX4	A	643	-	45,45,45	1.07±0.00	0±0 (0±0%)
3	PX4	B	311	-	45,45,45	1.15±0.00	0±0 (0±0%)
3	PX4	B	395	-	45,45,45	0.86±0.00	0±0 (0±0%)
3	PX4	A	645	-	45,45,45	1.23±0.00	0±0 (0±0%)
3	PX4	C	314	-	45,45,45	0.94±0.00	0±0 (0±0%)
3	PX4	C	347	-	45,45,45	1.24±0.00	0±0 (0±0%)
3	PX4	B	394	-	45,45,45	1.09±0.00	0±0 (0±0%)
3	PX4	B	313	-	45,45,45	0.91±0.00	0±0 (0±0%)
3	PX4	B	332	-	45,45,45	0.90±0.00	0±0 (0±0%)
3	PX4	C	331	-	45,45,45	0.81±0.00	0±0 (0±0%)
3	PX4	C	324	-	45,45,45	1.07±0.00	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	PX4	B	322	-	45,45,45	0.98±0.00	0±0 (0±0%)
3	PX4	C	312	-	45,45,45	1.02±0.00	0±0 (0±0%)
3	PX4	B	318	-	45,45,45	0.97±0.00	0±0 (0±0%)
3	PX4	C	325	-	45,45,45	0.96±0.00	0±0 (0±0%)
3	PX4	C	363	-	45,45,45	0.99±0.00	0±0 (0±0%)
3	PX4	B	369	-	45,45,45	0.91±0.00	0±0 (0±0%)
3	PX4	B	325	-	45,45,45	1.01±0.00	0±0 (0±0%)
3	PX4	B	336	-	45,45,45	1.04±0.00	0±0 (0±0%)
3	PX4	B	366	-	45,45,45	1.06±0.00	0±0 (0±0%)
3	PX4	C	353	-	45,45,45	1.04±0.00	0±0 (0±0%)
3	PX4	B	381	-	45,45,45	1.19±0.00	0±0 (0±0%)
3	PX4	C	343	-	45,45,45	1.16±0.00	0±0 (0±0%)
3	PX4	B	327	-	45,45,45	1.13±0.00	0±0 (0±0%)
3	PX4	C	367	-	45,45,45	1.07±0.00	0±0 (0±0%)
3	PX4	A	625	-	45,45,45	0.98±0.00	0±0 (0±0%)
3	PX4	B	334	-	45,45,45	0.90±0.00	0±0 (0±0%)
3	PX4	B	371	-	45,45,45	1.09±0.00	0±0 (0±0%)
3	PX4	B	383	-	45,45,45	0.97±0.00	0±0 (0±0%)
3	PX4	B	386	-	45,45,45	1.03±0.00	0±0 (0±0%)
3	PX4	B	370	-	45,45,45	1.05±0.00	0±0 (0±0%)
3	PX4	C	350	-	45,45,45	1.41±0.00	0±0 (0±0%)
3	PX4	A	635	-	45,45,45	1.00±0.00	0±0 (0±0%)
3	PX4	C	364	-	45,45,45	1.16±0.00	0±0 (0±0%)
3	PX4	B	392	-	45,45,45	0.97±0.00	0±0 (0±0%)
3	PX4	A	617	-	45,45,45	1.20±0.00	0±0 (0±0%)
3	PX4	C	362	-	45,45,45	1.04±0.00	0±0 (0±0%)
3	PX4	A	636	-	45,45,45	1.02±0.00	0±0 (0±0%)
3	PX4	B	308	-	45,45,45	0.98±0.00	0±0 (0±0%)
3	PX4	B	320	-	45,45,45	1.05±0.00	0±0 (0±0%)
3	PX4	A	612	-	45,45,45	0.99±0.00	0±0 (0±0%)
3	PX4	B	315	-	45,45,45	1.02±0.00	0±0 (0±0%)
3	PX4	B	310	-	45,45,45	1.06±0.00	0±0 (0±0%)
3	PX4	C	355	-	45,45,45	1.08±0.00	0±0 (0±0%)
3	PX4	B	307	-	45,45,45	1.20±0.00	0±0 (0±0%)
3	PX4	B	384	-	45,45,45	0.90±0.00	0±0 (0±0%)
3	PX4	C	341	-	45,45,45	0.98±0.00	0±0 (0±0%)
3	PX4	C	359	-	45,45,45	1.32±0.00	0±0 (0±0%)
3	PX4	C	360	-	45,45,45	1.14±0.00	0±0 (0±0%)
3	PX4	B	351	-	45,45,45	1.01±0.00	0±0 (0±0%)
3	PX4	C	328	-	45,45,45	0.76±0.00	0±0 (0±0%)
3	PX4	B	357	-	45,45,45	0.92±0.00	0±0 (0±0%)
3	PX4	C	354	-	45,45,45	1.15±0.00	0±0 (0±0%)
3	PX4	B	376	-	45,45,45	1.17±0.00	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	PX4	B	388	-	45,45,45	1.15±0.00	0±0 (0±0%)
3	PX4	C	357	-	45,45,45	0.88±0.00	0±0 (0±0%)
3	PX4	A	627	-	45,45,45	1.04±0.00	0±0 (0±0%)
3	PX4	C	307	-	45,45,45	1.10±0.00	0±0 (0±0%)
3	PX4	B	339	-	45,45,45	0.78±0.00	0±0 (0±0%)
3	PX4	B	372	-	45,45,45	1.04±0.00	0±0 (0±0%)
3	PX4	B	365	-	45,45,45	0.86±0.00	0±0 (0±0%)
3	PX4	B	335	-	45,45,45	1.07±0.00	0±0 (0±0%)
3	PX4	B	342	-	45,45,45	0.98±0.00	0±0 (0±0%)
3	PX4	A	647	-	45,45,45	1.08±0.00	0±0 (0±0%)
3	PX4	B	397	-	45,45,45	0.96±0.00	0±0 (0±0%)
3	PX4	A	630	-	45,45,45	0.86±0.00	0±0 (0±0%)
3	PX4	C	320	-	45,45,45	1.17±0.00	0±0 (0±0%)
3	PX4	C	302	-	45,45,45	0.97±0.00	0±0 (0±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
3	PX4	B	367	-	51,53,53	0.95±0.00	0±0 (0±0%)
3	PX4	B	330	-	51,53,53	0.79±0.00	0±0 (0±0%)
3	PX4	B	382	-	51,53,53	0.88±0.00	0±0 (0±0%)
3	PX4	C	327	-	51,53,53	0.83±0.00	0±0 (0±0%)
3	PX4	C	315	-	51,53,53	0.85±0.00	0±0 (0±0%)
3	PX4	C	322	-	51,53,53	1.03±0.00	0±0 (0±0%)
3	PX4	C	348	-	51,53,53	0.89±0.00	0±0 (0±0%)
3	PX4	B	347	-	51,53,53	0.97±0.00	0±0 (0±0%)
3	PX4	C	352	-	51,53,53	0.94±0.00	0±0 (0±0%)
3	PX4	C	346	-	51,53,53	1.05±0.00	0±0 (0±0%)
3	PX4	A	620	-	51,53,53	0.97±0.00	0±0 (0±0%)
3	PX4	A	611	-	51,53,53	0.89±0.00	0±0 (0±0%)
3	PX4	C	318	-	51,53,53	0.93±0.00	0±0 (0±0%)
3	PX4	A	608	-	51,53,53	1.09±0.00	0±0 (0±0%)
3	PX4	C	356	-	51,53,53	0.80±0.00	0±0 (0±0%)
3	PX4	C	335	-	51,53,53	0.96±0.00	0±0 (0±0%)
3	PX4	C	313	-	51,53,53	0.90±0.00	0±0 (0±0%)
3	PX4	C	344	-	51,53,53	0.87±0.00	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	PX4	C	351	-	51,53,53	1.11±0.00	0±0 (0±0%)
3	PX4	C	303	-	51,53,53	1.08±0.00	0±0 (0±0%)
3	PX4	B	345	-	51,53,53	1.01±0.00	0±0 (0±0%)
3	PX4	C	349	-	51,53,53	0.73±0.00	0±0 (0±0%)
3	PX4	C	321	-	51,53,53	0.92±0.00	0±0 (0±0%)
3	PX4	A	602	-	51,53,53	1.02±0.00	0±0 (0±0%)
3	PX4	C	309	-	51,53,53	1.10±0.00	0±0 (0±0%)
3	PX4	B	374	-	51,53,53	1.07±0.00	0±0 (0±0%)
3	PX4	B	326	-	51,53,53	0.91±0.00	0±0 (0±0%)
3	PX4	C	340	-	51,53,53	0.87±0.00	0±0 (0±0%)
3	PX4	B	333	-	51,53,53	1.13±0.00	0±0 (0±0%)
3	PX4	A	606	-	51,53,53	0.95±0.00	0±0 (0±0%)
3	PX4	A	639	-	51,53,53	0.83±0.00	0±0 (0±0%)
3	PX4	B	389	-	51,53,53	0.99±0.00	0±0 (0±0%)
3	PX4	A	601	-	51,53,53	0.95±0.00	0±0 (0±0%)
3	PX4	C	310	-	51,53,53	1.06±0.00	0±0 (0±0%)
3	PX4	B	348	-	51,53,53	0.97±0.00	0±0 (0±0%)
3	PX4	B	341	-	51,53,53	1.01±0.00	0±0 (0±0%)
3	PX4	B	363	-	51,53,53	0.87±0.00	0±0 (0±0%)
3	PX4	B	303	-	51,53,53	0.95±0.00	0±0 (0±0%)
3	PX4	B	356	-	51,53,53	0.88±0.00	0±0 (0±0%)
3	PX4	B	302	-	51,53,53	1.00±0.00	0±0 (0±0%)
3	PX4	C	370	-	51,53,53	1.05±0.00	0±0 (0±0%)
3	PX4	B	350	-	51,53,53	0.91±0.00	0±0 (0±0%)
3	PX4	C	339	-	51,53,53	0.99±0.00	0±0 (0±0%)
3	PX4	B	355	-	51,53,53	0.87±0.00	0±0 (0±0%)
3	PX4	B	352	-	51,53,53	0.98±0.00	0±0 (0±0%)
3	PX4	C	326	-	51,53,53	0.77±0.00	0±0 (0±0%)
3	PX4	A	634	-	51,53,53	0.89±0.00	0±0 (0±0%)
3	PX4	A	622	-	51,53,53	1.13±0.00	0±0 (0±0%)
3	PX4	B	400	-	51,53,53	1.02±0.00	0±0 (0±0%)
3	PX4	A	632	-	51,53,53	0.95±0.00	0±0 (0±0%)
3	PX4	A	623	-	51,53,53	0.88±0.00	0±0 (0±0%)
3	PX4	B	337	-	51,53,53	1.02±0.00	0±0 (0±0%)
3	PX4	A	614	-	51,53,53	0.69±0.00	0±0 (0±0%)
3	PX4	C	336	-	51,53,53	0.82±0.00	0±0 (0±0%)
3	PX4	A	615	-	51,53,53	0.93±0.00	0±0 (0±0%)
3	PX4	A	621	-	51,53,53	0.97±0.00	0±0 (0±0%)
3	PX4	C	319	-	51,53,53	0.94±0.00	0±0 (0±0%)
3	PX4	A	648	-	51,53,53	1.02±0.00	0±0 (0±0%)
3	PX4	A	605	-	51,53,53	0.89±0.00	0±0 (0±0%)
3	PX4	B	323	-	51,53,53	0.81±0.00	0±0 (0±0%)
3	PX4	C	304	-	51,53,53	0.93±0.00	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	PX4	B	309	-	51,53,53	0.99±0.00	0±0 (0±0%)
3	PX4	C	334	-	51,53,53	0.83±0.00	0±0 (0±0%)
3	PX4	B	324	-	51,53,53	1.07±0.00	0±0 (0±0%)
3	PX4	B	362	-	51,53,53	0.72±0.00	0±0 (0±0%)
3	PX4	C	361	-	51,53,53	0.98±0.00	0±0 (0±0%)
3	PX4	B	306	-	51,53,53	0.98±0.00	0±0 (0±0%)
3	PX4	C	308	-	51,53,53	0.84±0.00	0±0 (0±0%)
3	PX4	B	304	-	51,53,53	0.97±0.00	0±0 (0±0%)
3	PX4	C	305	-	51,53,53	0.82±0.00	0±0 (0±0%)
3	PX4	C	337	-	51,53,53	1.26±0.00	0±0 (0±0%)
3	PX4	B	364	-	51,53,53	1.05±0.00	0±0 (0±0%)
3	PX4	B	329	-	51,53,53	1.04±0.00	0±0 (0±0%)
3	PX4	A	646	-	51,53,53	0.93±0.00	0±0 (0±0%)
3	PX4	B	328	-	51,53,53	0.99±0.00	0±0 (0±0%)
3	PX4	B	344	-	51,53,53	1.09±0.00	0±0 (0±0%)
3	PX4	C	330	-	51,53,53	1.00±0.00	0±0 (0±0%)
3	PX4	C	306	-	51,53,53	0.89±0.00	0±0 (0±0%)
3	PX4	B	305	-	51,53,53	0.88±0.00	0±0 (0±0%)
3	PX4	C	345	-	51,53,53	1.09±0.00	0±0 (0±0%)
3	PX4	C	317	-	51,53,53	0.93±0.00	0±0 (0±0%)
3	PX4	B	343	-	51,53,53	1.03±0.00	0±0 (0±0%)
3	PX4	C	311	-	51,53,53	0.91±0.00	0±0 (0±0%)
3	PX4	A	607	-	51,53,53	0.92±0.00	0±0 (0±0%)
3	PX4	A	644	-	51,53,53	0.97±0.00	0±0 (0±0%)
3	PX4	B	375	-	51,53,53	1.01±0.00	0±0 (0±0%)
3	PX4	B	361	-	51,53,53	0.91±0.00	0±0 (0±0%)
3	PX4	A	628	-	51,53,53	0.94±0.00	0±0 (0±0%)
3	PX4	A	619	-	51,53,53	0.87±0.00	0±0 (0±0%)
3	PX4	B	301	-	51,53,53	0.97±0.00	0±0 (0±0%)
3	PX4	B	396	-	51,53,53	0.86±0.00	0±0 (0±0%)
3	PX4	A	610	-	51,53,53	1.12±0.00	0±0 (0±0%)
3	PX4	C	316	-	51,53,53	0.84±0.00	0±0 (0±0%)
3	PX4	B	360	-	51,53,53	1.08±0.00	0±0 (0±0%)
3	PX4	A	626	-	51,53,53	0.89±0.00	0±0 (0±0%)
3	PX4	C	329	-	51,53,53	0.94±0.00	0±0 (0±0%)
3	PX4	C	365	-	51,53,53	0.92±0.00	0±0 (0±0%)
3	PX4	A	624	-	51,53,53	0.90±0.00	0±0 (0±0%)
3	PX4	B	378	-	51,53,53	1.11±0.00	0±0 (0±0%)
3	PX4	B	380	-	51,53,53	0.99±0.00	0±0 (0±0%)
3	PX4	A	613	-	51,53,53	1.08±0.00	0±0 (0±0%)
3	PX4	C	368	-	51,53,53	1.00±0.00	0±0 (0±0%)
3	PX4	B	321	-	51,53,53	0.80±0.00	0±0 (0±0%)
3	PX4	A	637	-	51,53,53	1.07±0.00	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	PX4	B	354	-	51,53,53	0.87±0.00	0±0 (0±0%)
3	PX4	B	319	-	51,53,53	0.95±0.00	0±0 (0±0%)
3	PX4	B	314	-	51,53,53	1.00±0.00	0±0 (0±0%)
3	PX4	A	616	-	51,53,53	0.72±0.00	0±0 (0±0%)
3	PX4	B	398	-	51,53,53	0.98±0.00	0±0 (0±0%)
3	PX4	B	393	-	51,53,53	0.91±0.00	0±0 (0±0%)
3	PX4	B	385	-	51,53,53	0.81±0.00	0±0 (0±0%)
3	PX4	C	369	-	51,53,53	0.86±0.00	0±0 (0±0%)
3	PX4	B	379	-	51,53,53	0.98±0.00	0±0 (0±0%)
3	PX4	A	642	-	51,53,53	0.84±0.00	0±0 (0±0%)
3	PX4	B	399	-	51,53,53	0.88±0.00	0±0 (0±0%)
3	PX4	B	358	-	51,53,53	1.10±0.00	0±0 (0±0%)
3	PX4	B	331	-	51,53,53	0.94±0.00	0±0 (0±0%)
3	PX4	A	603	-	51,53,53	0.93±0.00	0±0 (0±0%)
3	PX4	C	338	-	51,53,53	0.88±0.00	0±0 (0±0%)
3	PX4	C	333	-	51,53,53	1.11±0.00	0±0 (0±0%)
3	PX4	B	316	-	51,53,53	0.91±0.00	0±0 (0±0%)
3	PX4	B	359	-	51,53,53	1.03±0.00	0±0 (0±0%)
3	PX4	C	323	-	51,53,53	0.94±0.00	0±0 (0±0%)
3	PX4	A	604	-	51,53,53	0.93±0.00	0±0 (0±0%)
3	PX4	A	618	-	51,53,53	1.07±0.00	0±0 (0±0%)
3	PX4	B	317	-	51,53,53	0.96±0.00	0±0 (0±0%)
3	PX4	B	377	-	51,53,53	1.05±0.00	0±0 (0±0%)
3	PX4	B	391	-	51,53,53	1.11±0.00	0±0 (0±0%)
3	PX4	A	629	-	51,53,53	0.72±0.00	0±0 (0±0%)
3	PX4	A	609	-	51,53,53	1.03±0.00	0±0 (0±0%)
3	PX4	B	312	-	51,53,53	1.00±0.00	0±0 (0±0%)
3	PX4	A	633	-	51,53,53	0.99±0.00	0±0 (0±0%)
3	PX4	C	301	-	51,53,53	0.81±0.00	0±0 (0±0%)
3	PX4	B	353	-	51,53,53	0.99±0.00	0±0 (0±0%)
3	PX4	A	638	-	51,53,53	0.81±0.00	0±0 (0±0%)
3	PX4	B	346	-	51,53,53	1.03±0.00	0±0 (0±0%)
3	PX4	C	332	-	51,53,53	1.11±0.00	0±0 (0±0%)
3	PX4	C	342	-	51,53,53	0.90±0.00	0±0 (0±0%)
3	PX4	B	387	-	51,53,53	0.96±0.00	0±0 (0±0%)
3	PX4	C	366	-	51,53,53	0.85±0.00	0±0 (0±0%)
3	PX4	A	640	-	51,53,53	0.85±0.00	0±0 (0±0%)
3	PX4	A	631	-	51,53,53	0.84±0.00	0±0 (0±0%)
3	PX4	B	338	-	51,53,53	0.90±0.00	0±0 (0±0%)
3	PX4	A	641	-	51,53,53	1.08±0.00	0±0 (0±0%)
3	PX4	B	390	-	51,53,53	1.14±0.00	0±0 (0±0%)
3	PX4	B	373	-	51,53,53	0.96±0.00	0±0 (0±0%)
3	PX4	C	358	-	51,53,53	0.75±0.00	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	PX4	B	368	-	51,53,53	0.96±0.00	0±0 (0±0%)
3	PX4	B	340	-	51,53,53	0.94±0.00	0±0 (0±0%)
3	PX4	B	349	-	51,53,53	0.86±0.00	0±0 (0±0%)
3	PX4	A	643	-	51,53,53	1.02±0.00	0±0 (0±0%)
3	PX4	B	311	-	51,53,53	0.86±0.00	0±0 (0±0%)
3	PX4	B	395	-	51,53,53	0.87±0.00	0±0 (0±0%)
3	PX4	A	645	-	51,53,53	0.90±0.00	0±0 (0±0%)
3	PX4	C	314	-	51,53,53	0.89±0.00	0±0 (0±0%)
3	PX4	C	347	-	51,53,53	0.99±0.00	0±0 (0±0%)
3	PX4	B	394	-	51,53,53	0.86±0.00	0±0 (0±0%)
3	PX4	B	313	-	51,53,53	1.10±0.00	0±0 (0±0%)
3	PX4	B	332	-	51,53,53	0.91±0.00	0±0 (0±0%)
3	PX4	C	331	-	51,53,53	0.94±0.00	0±0 (0±0%)
3	PX4	C	324	-	51,53,53	1.13±0.00	0±0 (0±0%)
3	PX4	B	322	-	51,53,53	0.95±0.00	0±0 (0±0%)
3	PX4	C	312	-	51,53,53	1.11±0.00	0±0 (0±0%)
3	PX4	B	318	-	51,53,53	0.93±0.00	0±0 (0±0%)
3	PX4	C	325	-	51,53,53	0.83±0.00	0±0 (0±0%)
3	PX4	C	363	-	51,53,53	0.94±0.00	0±0 (0±0%)
3	PX4	B	369	-	51,53,53	1.03±0.00	0±0 (0±0%)
3	PX4	B	325	-	51,53,53	1.00±0.00	0±0 (0±0%)
3	PX4	B	336	-	51,53,53	1.03±0.00	0±0 (0±0%)
3	PX4	B	366	-	51,53,53	1.04±0.00	0±0 (0±0%)
3	PX4	C	353	-	51,53,53	0.90±0.00	0±0 (0±0%)
3	PX4	B	381	-	51,53,53	0.96±0.00	0±0 (0±0%)
3	PX4	C	343	-	51,53,53	1.07±0.00	0±0 (0±0%)
3	PX4	B	327	-	51,53,53	1.27±0.00	1±0 (1±0%)
3	PX4	C	367	-	51,53,53	0.87±0.00	0±0 (0±0%)
3	PX4	A	625	-	51,53,53	0.82±0.00	0±0 (0±0%)
3	PX4	B	334	-	51,53,53	0.74±0.00	0±0 (0±0%)
3	PX4	B	371	-	51,53,53	0.84±0.00	0±0 (0±0%)
3	PX4	B	383	-	51,53,53	0.94±0.00	0±0 (0±0%)
3	PX4	B	386	-	51,53,53	0.90±0.00	0±0 (0±0%)
3	PX4	B	370	-	51,53,53	1.01±0.00	0±0 (0±0%)
3	PX4	C	350	-	51,53,53	1.04±0.00	0±0 (0±0%)
3	PX4	A	635	-	51,53,53	0.88±0.00	0±0 (0±0%)
3	PX4	C	364	-	51,53,53	0.98±0.00	0±0 (0±0%)
3	PX4	B	392	-	51,53,53	0.90±0.00	0±0 (0±0%)
3	PX4	A	617	-	51,53,53	1.01±0.00	0±0 (0±0%)
3	PX4	C	362	-	51,53,53	0.88±0.00	0±0 (0±0%)
3	PX4	A	636	-	51,53,53	1.03±0.00	0±0 (0±0%)
3	PX4	B	308	-	51,53,53	0.66±0.00	0±0 (0±0%)
3	PX4	B	320	-	51,53,53	0.82±0.00	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	PX4	A	612	-	51,53,53	0.99±0.00	0±0 (0±0%)
3	PX4	B	315	-	51,53,53	1.11±0.00	0±0 (0±0%)
3	PX4	B	310	-	51,53,53	0.92±0.00	0±0 (0±0%)
3	PX4	C	355	-	51,53,53	1.03±0.00	0±0 (0±0%)
3	PX4	B	307	-	51,53,53	0.88±0.00	0±0 (0±0%)
3	PX4	B	384	-	51,53,53	0.86±0.00	0±0 (0±0%)
3	PX4	C	341	-	51,53,53	0.92±0.00	0±0 (0±0%)
3	PX4	C	359	-	51,53,53	0.90±0.00	0±0 (0±0%)
3	PX4	C	360	-	51,53,53	0.92±0.00	0±0 (0±0%)
3	PX4	B	351	-	51,53,53	1.08±0.00	0±0 (0±0%)
3	PX4	C	328	-	51,53,53	0.99±0.00	0±0 (0±0%)
3	PX4	B	357	-	51,53,53	0.86±0.00	0±0 (0±0%)
3	PX4	C	354	-	51,53,53	0.72±0.00	0±0 (0±0%)
3	PX4	B	376	-	51,53,53	0.96±0.00	0±0 (0±0%)
3	PX4	B	388	-	51,53,53	0.87±0.00	0±0 (0±0%)
3	PX4	C	357	-	51,53,53	1.12±0.00	0±0 (0±0%)
3	PX4	A	627	-	51,53,53	1.05±0.00	0±0 (0±0%)
3	PX4	C	307	-	51,53,53	0.94±0.00	0±0 (0±0%)
3	PX4	B	339	-	51,53,53	0.94±0.00	0±0 (0±0%)
3	PX4	B	372	-	51,53,53	0.94±0.00	0±0 (0±0%)
3	PX4	B	365	-	51,53,53	1.09±0.00	0±0 (0±0%)
3	PX4	B	335	-	51,53,53	0.81±0.00	0±0 (0±0%)
3	PX4	B	342	-	51,53,53	0.89±0.00	0±0 (0±0%)
3	PX4	A	647	-	51,53,53	1.06±0.00	0±0 (0±0%)
3	PX4	B	397	-	51,53,53	0.77±0.00	0±0 (0±0%)
3	PX4	A	630	-	51,53,53	0.94±0.00	0±0 (0±0%)
3	PX4	C	320	-	51,53,53	1.07±0.00	0±0 (0±0%)
3	PX4	C	302	-	51,53,53	0.92±0.00	0±0 (0±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	PX4	B	367	-	-	0±0,49,49,49	-
3	PX4	A	611	-	-	0±0,49,49,49	-
3	PX4	A	623	-	-	0±0,49,49,49	-
3	PX4	B	305	-	-	0±0,49,49,49	-
3	PX4	C	317	-	-	0±0,49,49,49	-
3	PX4	A	607	-	-	0±0,49,49,49	-
3	PX4	B	375	-	-	0±0,49,49,49	-
3	PX4	B	321	-	-	0±0,49,49,49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PX4	B	329	-	-	0±0,49,49,49	-
3	PX4	A	633	-	-	0±0,49,49,49	-
3	PX4	A	603	-	-	0±0,49,49,49	-
3	PX4	B	360	-	-	0±0,49,49,49	-
3	PX4	B	344	-	-	0±0,49,49,49	-
3	PX4	B	337	-	-	0±0,49,49,49	-
3	PX4	C	347	-	-	0±0,49,49,49	-
3	PX4	A	622	-	-	0±0,49,49,49	-
3	PX4	B	322	-	-	0±0,49,49,49	-
3	PX4	B	361	-	-	0±0,49,49,49	-
3	PX4	A	604	-	-	0±0,49,49,49	-
3	PX4	B	353	-	-	0±0,49,49,49	-
3	PX4	C	331	-	-	0±0,49,49,49	-
3	PX4	C	356	-	-	0±0,49,49,49	-
3	PX4	A	625	-	-	0±0,49,49,49	-
3	PX4	B	370	-	-	0±0,49,49,49	-
3	PX4	A	617	-	-	0±0,49,49,49	-
3	PX4	B	303	-	-	0±0,49,49,49	-
3	PX4	A	634	-	-	0±0,49,49,49	-
3	PX4	A	624	-	-	0±0,49,49,49	-
3	PX4	A	614	-	-	0±0,49,49,49	-
3	PX4	C	308	-	-	0±0,49,49,49	-
3	PX4	C	344	-	-	0±0,49,49,49	-
3	PX4	C	328	-	-	0±0,49,49,49	-
3	PX4	B	326	-	-	0±0,49,49,49	-
3	PX4	B	393	-	-	0±0,49,49,49	-
3	PX4	C	360	-	-	0±0,49,49,49	-
3	PX4	C	354	-	-	0±0,49,49,49	-
3	PX4	C	319	-	-	0±0,49,49,49	-
3	PX4	C	312	-	-	0±0,49,49,49	-
3	PX4	B	339	-	-	0±0,49,49,49	-
3	PX4	B	350	-	-	0±0,49,49,49	-
3	PX4	B	346	-	-	0±0,49,49,49	-
3	PX4	C	335	-	-	0±0,49,49,49	-
3	PX4	C	314	-	-	0±0,49,49,49	-
3	PX4	B	376	-	-	0±0,49,49,49	-
3	PX4	B	383	-	-	0±0,49,49,49	-
3	PX4	B	304	-	-	0±0,49,49,49	-
3	PX4	B	355	-	-	0±0,49,49,49	-
3	PX4	C	343	-	-	0±0,49,49,49	-
3	PX4	B	388	-	-	0±0,49,49,49	-
3	PX4	B	382	-	-	0±0,49,49,49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PX4	C	359	-	-	0±0,49,49,49	-
3	PX4	A	631	-	-	0±0,49,49,49	-
3	PX4	C	340	-	-	0±0,49,49,49	-
3	PX4	B	332	-	-	0±0,49,49,49	-
3	PX4	C	369	-	-	0±0,49,49,49	-
3	PX4	C	330	-	-	0±0,49,49,49	-
3	PX4	B	358	-	-	0±0,49,49,49	-
3	PX4	B	323	-	-	0±0,49,49,49	-
3	PX4	A	601	-	-	0±0,49,49,49	-
3	PX4	A	608	-	-	0±0,49,49,49	-
3	PX4	C	311	-	-	0±0,49,49,49	-
3	PX4	A	613	-	-	0±0,49,49,49	-
3	PX4	C	366	-	-	0±0,49,49,49	-
3	PX4	B	336	-	-	0±0,49,49,49	-
3	PX4	B	357	-	-	0±0,49,49,49	-
3	PX4	B	380	-	-	0±0,49,49,49	-
3	PX4	B	342	-	-	0±0,49,49,49	-
3	PX4	B	364	-	-	0±0,49,49,49	-
3	PX4	B	363	-	-	0±0,49,49,49	-
3	PX4	A	636	-	-	0±0,49,49,49	-
3	PX4	A	644	-	-	0±0,49,49,49	-
3	PX4	A	618	-	-	0±0,49,49,49	-
3	PX4	C	350	-	-	0±0,49,49,49	-
3	PX4	C	309	-	-	0±0,49,49,49	-
3	PX4	B	387	-	-	0±0,49,49,49	-
3	PX4	C	305	-	-	0±0,49,49,49	-
3	PX4	B	394	-	-	0±0,49,49,49	-
3	PX4	B	372	-	-	0±0,49,49,49	-
3	PX4	B	384	-	-	0±0,49,49,49	-
3	PX4	A	629	-	-	0±0,49,49,49	-
3	PX4	A	619	-	-	0±0,49,49,49	-
3	PX4	C	306	-	-	0±0,49,49,49	-
3	PX4	B	365	-	-	0±0,49,49,49	-
3	PX4	C	320	-	-	0±0,49,49,49	-
3	PX4	B	338	-	-	0±0,49,49,49	-
3	PX4	B	395	-	-	0±0,49,49,49	-
3	PX4	B	347	-	-	0±0,49,49,49	-
3	PX4	B	334	-	-	0±0,49,49,49	-
3	PX4	C	367	-	-	0±0,49,49,49	-
3	PX4	B	316	-	-	0±0,49,49,49	-
3	PX4	A	635	-	-	0±0,49,49,49	-
3	PX4	A	642	-	-	0±0,49,49,49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PX4	C	333	-	-	0±0,49,49,49	-
3	PX4	A	605	-	-	0±0,49,49,49	-
3	PX4	C	336	-	-	0±0,49,49,49	-
3	PX4	C	368	-	-	0±0,49,49,49	-
3	PX4	A	638	-	-	0±0,49,49,49	-
3	PX4	B	314	-	-	0±0,49,49,49	-
3	PX4	B	333	-	-	0±0,49,49,49	-
3	PX4	C	349	-	-	0±0,49,49,49	-
3	PX4	B	385	-	-	0±0,49,49,49	-
3	PX4	A	645	-	-	0±0,49,49,49	-
3	PX4	A	609	-	-	0±0,49,49,49	-
3	PX4	B	345	-	-	0±0,49,49,49	-
3	PX4	B	354	-	-	0±0,49,49,49	-
3	PX4	A	620	-	-	0±0,49,49,49	-
3	PX4	B	374	-	-	0±0,49,49,49	-
3	PX4	A	640	-	-	0±0,49,49,49	-
3	PX4	B	352	-	-	0±0,49,49,49	-
3	PX4	C	303	-	-	0±0,49,49,49	-
3	PX4	B	343	-	-	0±0,49,49,49	-
3	PX4	C	322	-	-	0±0,49,49,49	-
3	PX4	A	630	-	-	0±0,49,49,49	-
3	PX4	B	340	-	-	0±0,49,49,49	-
3	PX4	B	328	-	-	0±0,49,49,49	-
3	PX4	B	308	-	-	0±0,49,49,49	-
3	PX4	B	325	-	-	0±0,49,49,49	-
3	PX4	C	323	-	-	0±0,49,49,49	-
3	PX4	A	626	-	-	0±0,49,49,49	-
3	PX4	C	341	-	-	0±0,49,49,49	-
3	PX4	C	363	-	-	0±0,49,49,49	-
3	PX4	C	301	-	-	0±0,49,49,49	-
3	PX4	C	351	-	-	0±0,49,49,49	-
3	PX4	C	364	-	-	0±0,49,49,49	-
3	PX4	C	302	-	-	0±0,49,49,49	-
3	PX4	B	335	-	-	0±0,49,49,49	-
3	PX4	C	355	-	-	0±0,49,49,49	-
3	PX4	C	321	-	-	0±0,49,49,49	-
3	PX4	C	362	-	-	0±0,49,49,49	-
3	PX4	B	389	-	-	0±0,49,49,49	-
3	PX4	B	349	-	-	0±0,49,49,49	-
3	PX4	A	612	-	-	0±0,49,49,49	-
3	PX4	A	602	-	-	0±0,49,49,49	-
3	PX4	C	339	-	-	0±0,49,49,49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PX4	B	379	-	-	0±0,49,49,49	-
3	PX4	C	338	-	-	0±0,49,49,49	-
3	PX4	C	342	-	-	0±0,49,49,49	-
3	PX4	B	386	-	-	0±0,49,49,49	-
3	PX4	B	307	-	-	0±0,49,49,49	-
3	PX4	B	362	-	-	0±0,49,49,49	-
3	PX4	C	353	-	-	0±0,49,49,49	-
3	PX4	A	627	-	-	0±0,49,49,49	-
3	PX4	C	332	-	-	0±0,49,49,49	-
3	PX4	C	325	-	-	0±0,49,49,49	-
3	PX4	B	377	-	-	0±0,49,49,49	-
3	PX4	B	398	-	-	0±0,49,49,49	-
3	PX4	B	391	-	-	0±0,49,49,49	-
3	PX4	B	311	-	-	0±0,49,49,49	-
3	PX4	B	390	-	-	0±0,49,49,49	-
3	PX4	C	370	-	-	0±0,49,49,49	-
3	PX4	B	319	-	-	0±0,49,49,49	-
3	PX4	A	641	-	-	0±0,49,49,49	-
3	PX4	A	628	-	-	0±0,49,49,49	-
3	PX4	C	337	-	-	0±0,49,49,49	-
3	PX4	B	331	-	-	0±0,49,49,49	-
3	PX4	B	301	-	-	0±0,49,49,49	-
3	PX4	C	327	-	-	0±0,49,49,49	-
3	PX4	B	341	-	-	0±0,49,49,49	-
3	PX4	B	373	-	-	0±0,49,49,49	-
3	PX4	C	313	-	-	0±0,49,49,49	-
3	PX4	B	317	-	-	0±0,49,49,49	-
3	PX4	B	369	-	-	0±0,49,49,49	-
3	PX4	B	306	-	-	0±0,49,49,49	-
3	PX4	B	313	-	-	0±0,49,49,49	-
3	PX4	A	621	-	-	0±0,49,49,49	-
3	PX4	A	639	-	-	0±0,49,49,49	-
3	PX4	A	648	-	-	0±0,49,49,49	-
3	PX4	B	320	-	-	0±0,49,49,49	-
3	PX4	B	330	-	-	0±0,49,49,49	-
3	PX4	C	315	-	-	0±0,49,49,49	-
3	PX4	C	316	-	-	0±0,49,49,49	-
3	PX4	C	357	-	-	0±0,49,49,49	-
3	PX4	C	318	-	-	0±0,49,49,49	-
3	PX4	B	378	-	-	0±0,49,49,49	-
3	PX4	C	329	-	-	0±0,49,49,49	-
3	PX4	B	356	-	-	0±0,49,49,49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PX4	C	358	-	-	0±0,49,49,49	-
3	PX4	B	348	-	-	0±0,49,49,49	-
3	PX4	B	368	-	-	0±0,49,49,49	-
3	PX4	B	318	-	-	0±0,49,49,49	-
3	PX4	C	365	-	-	0±0,49,49,49	-
3	PX4	C	346	-	-	0±0,49,49,49	-
3	PX4	C	326	-	-	0±0,49,49,49	-
3	PX4	B	327	-	-	0±0,49,49,49	-
3	PX4	B	399	-	-	0±0,49,49,49	-
3	PX4	B	359	-	-	0±0,49,49,49	-
3	PX4	A	637	-	-	0±0,49,49,49	-
3	PX4	B	396	-	-	0±0,49,49,49	-
3	PX4	C	348	-	-	0±0,49,49,49	-
3	PX4	C	334	-	-	0±0,49,49,49	-
3	PX4	B	397	-	-	0±0,49,49,49	-
3	PX4	B	366	-	-	0±0,49,49,49	-
3	PX4	B	312	-	-	0±0,49,49,49	-
3	PX4	B	324	-	-	0±0,49,49,49	-
3	PX4	A	643	-	-	0±0,49,49,49	-
3	PX4	A	616	-	-	0±0,49,49,49	-
3	PX4	A	632	-	-	0±0,49,49,49	-
3	PX4	B	371	-	-	0±0,49,49,49	-
3	PX4	B	310	-	-	0±0,49,49,49	-
3	PX4	A	610	-	-	0±0,49,49,49	-
3	PX4	C	345	-	-	0±0,49,49,49	-
3	PX4	C	307	-	-	0±0,49,49,49	-
3	PX4	C	310	-	-	0±0,49,49,49	-
3	PX4	A	615	-	-	0±0,49,49,49	-
3	PX4	C	352	-	-	0±0,49,49,49	-
3	PX4	C	304	-	-	0±0,49,49,49	-
3	PX4	A	606	-	-	0±0,49,49,49	-
3	PX4	B	400	-	-	0±0,49,49,49	-
3	PX4	B	309	-	-	0±0,49,49,49	-
3	PX4	C	361	-	-	0±0,49,49,49	-
3	PX4	B	302	-	-	0±0,49,49,49	-
3	PX4	B	392	-	-	0±0,49,49,49	-
3	PX4	B	381	-	-	0±0,49,49,49	-
3	PX4	A	647	-	-	0±0,49,49,49	-
3	PX4	B	351	-	-	0±0,49,49,49	-
3	PX4	B	315	-	-	0±0,49,49,49	-
3	PX4	A	646	-	-	0±0,49,49,49	-
3	PX4	C	324	-	-	0±0,49,49,49	-

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	350	PX4	C8-C7	5.07	1.66	1.50	4	15

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	327	PX4	C7-O7-C23	5.48	104.30	117.79	3	15

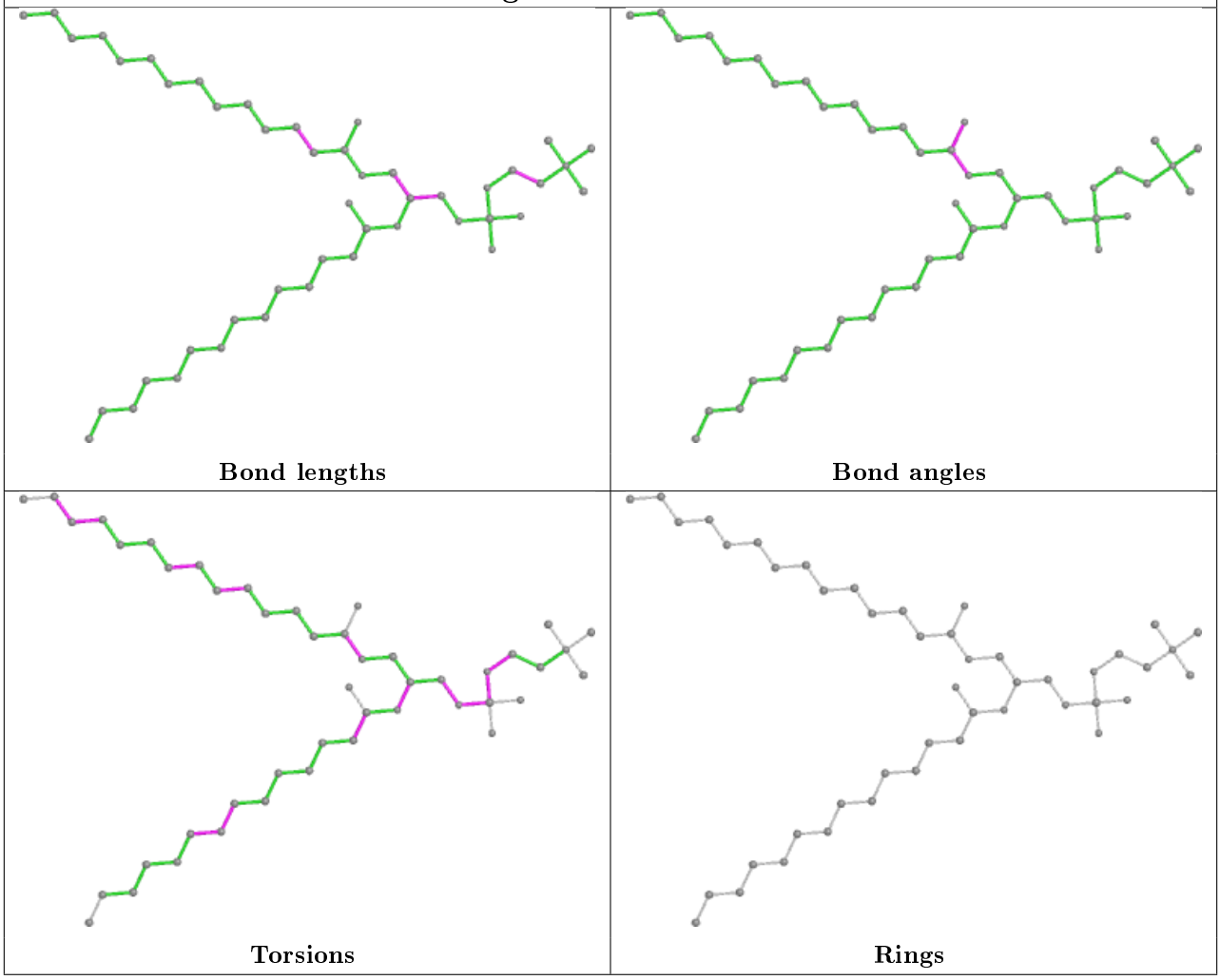
There are no chirality outliers.

There are no torsion outliers.

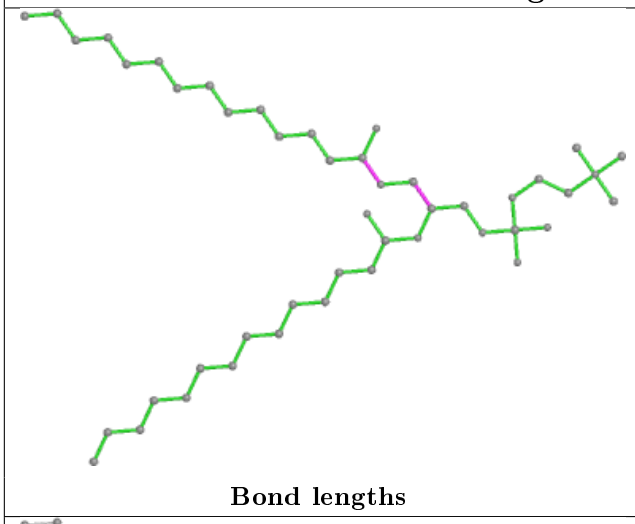
There are no ring outliers.

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.

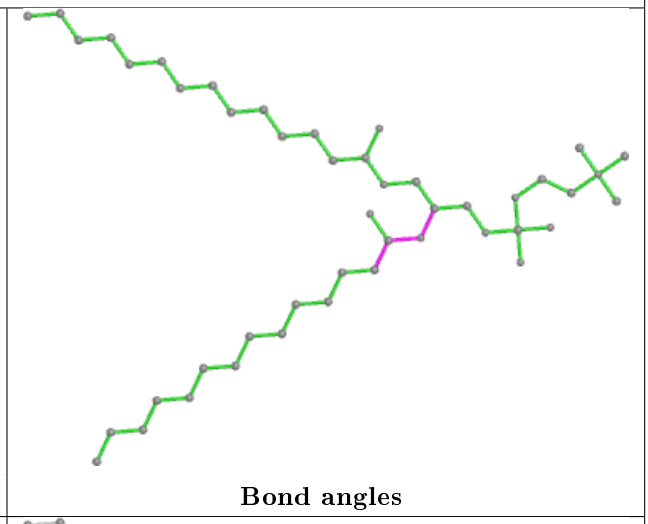
Ligand PX4 B 367



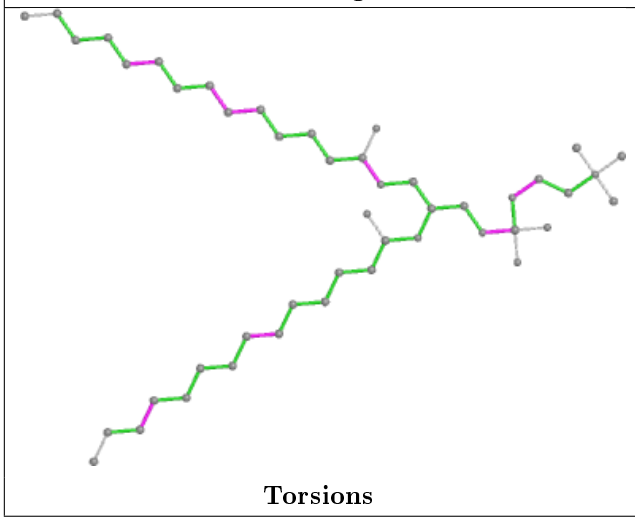
Ligand PX4 A 611



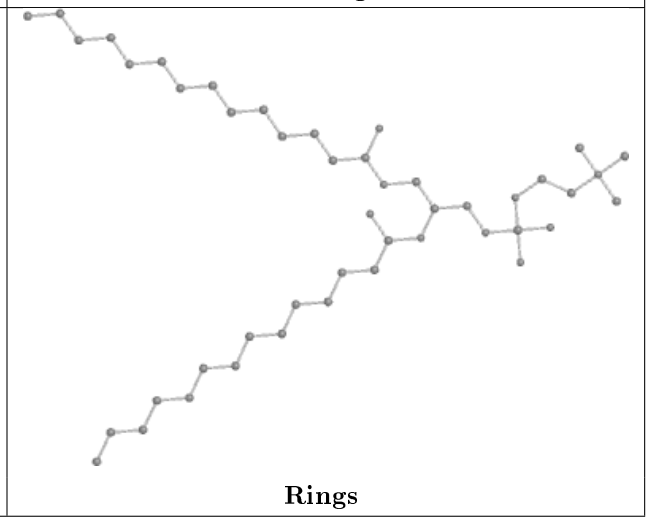
Bond lengths



Bond angles

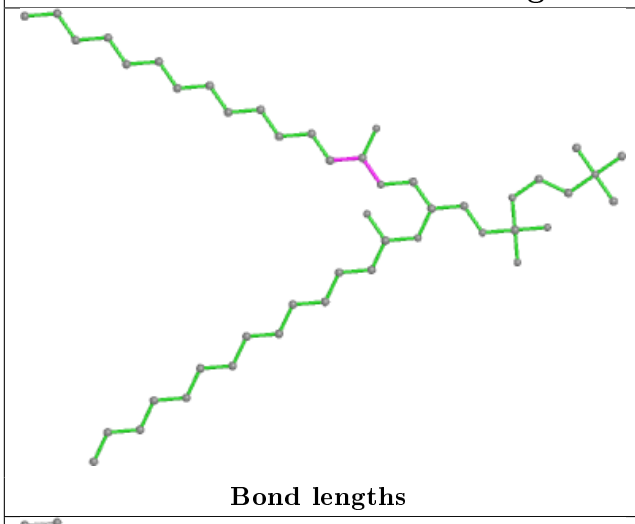


Torsions

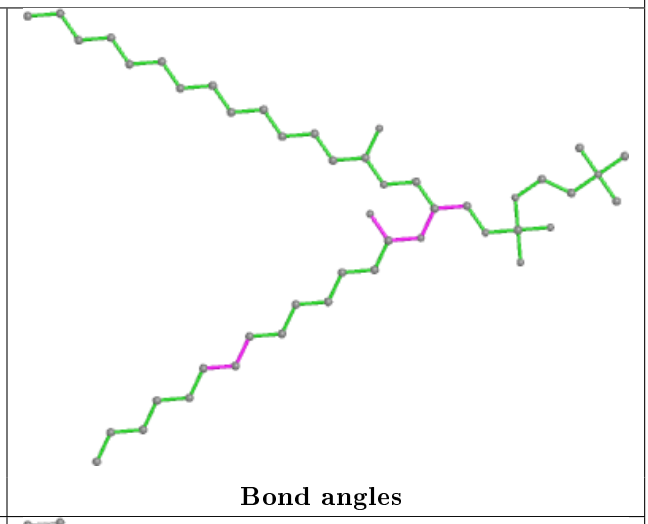


Rings

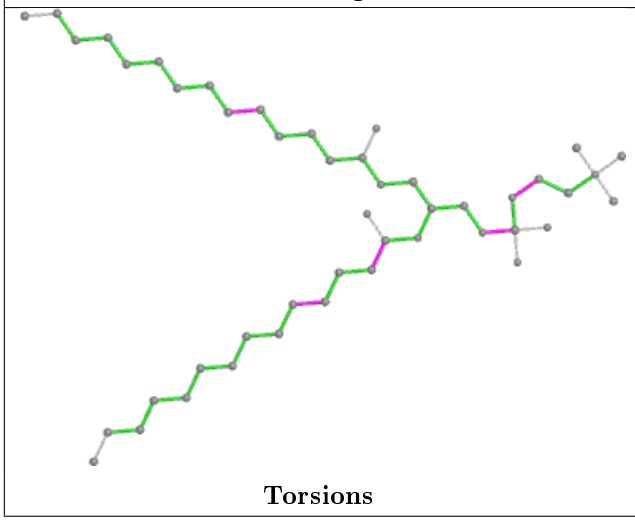
Ligand PX4 A 623



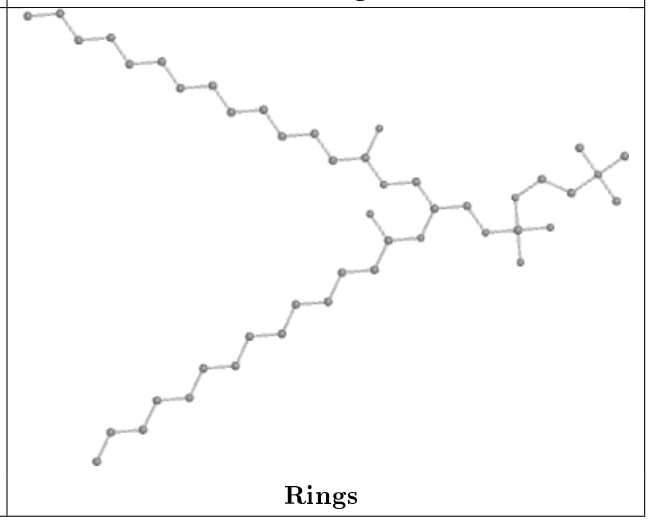
Bond lengths



Bond angles

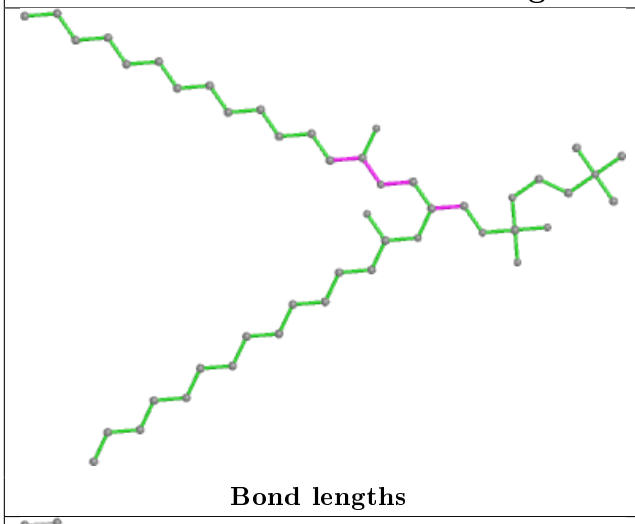


Torsions

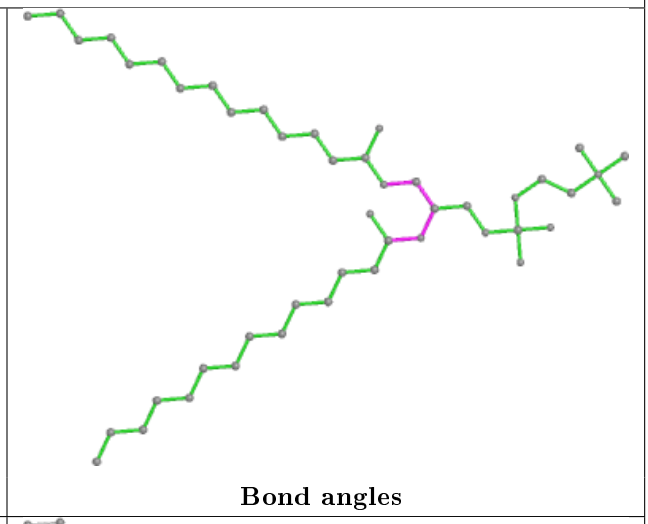


Rings

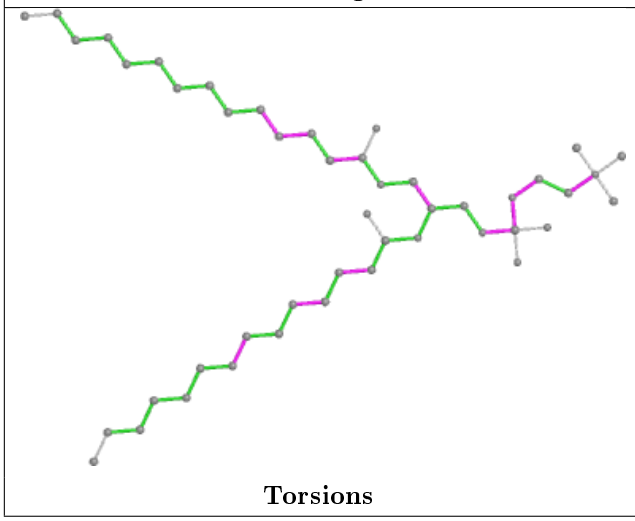
Ligand PX4 B 305



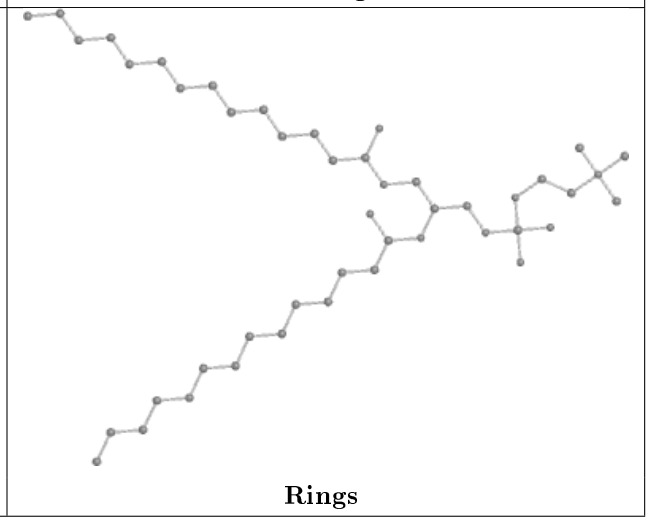
Bond lengths



Bond angles

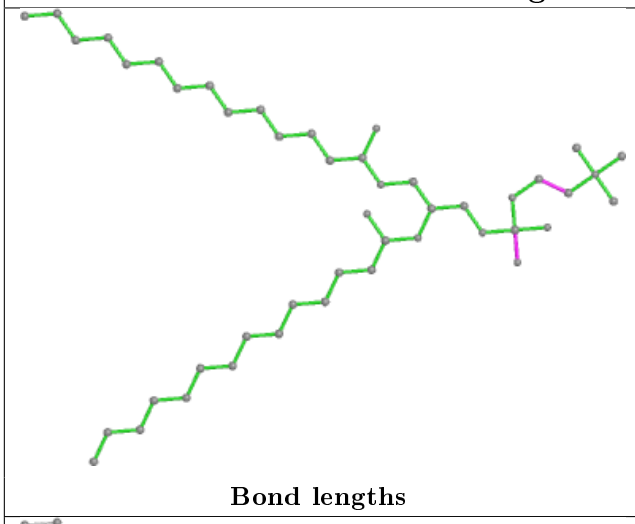


Torsions

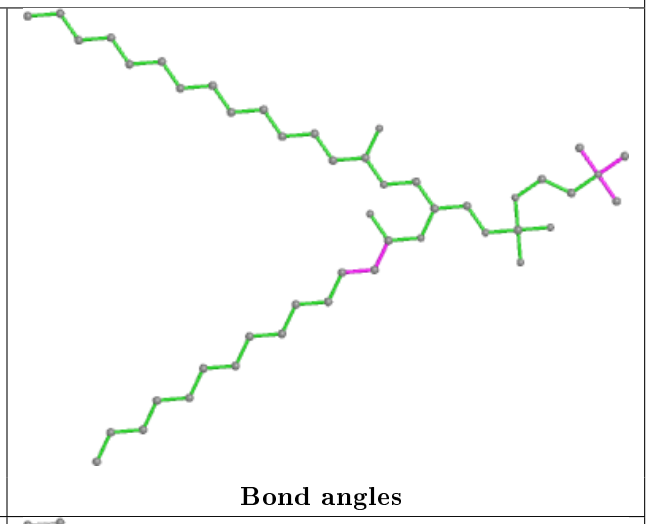


Rings

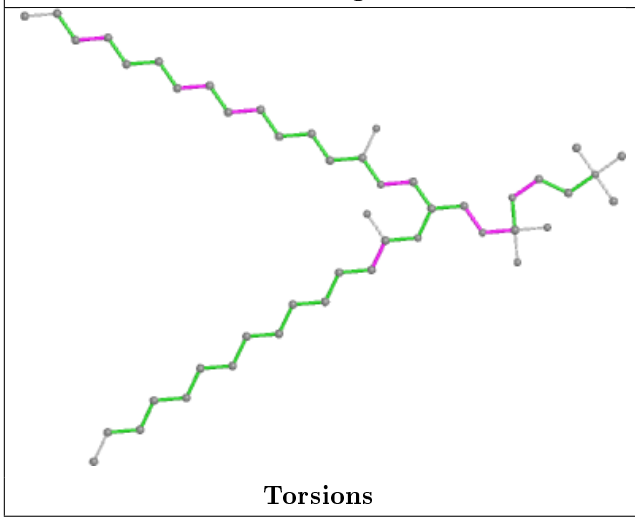
Ligand PX4 C 317



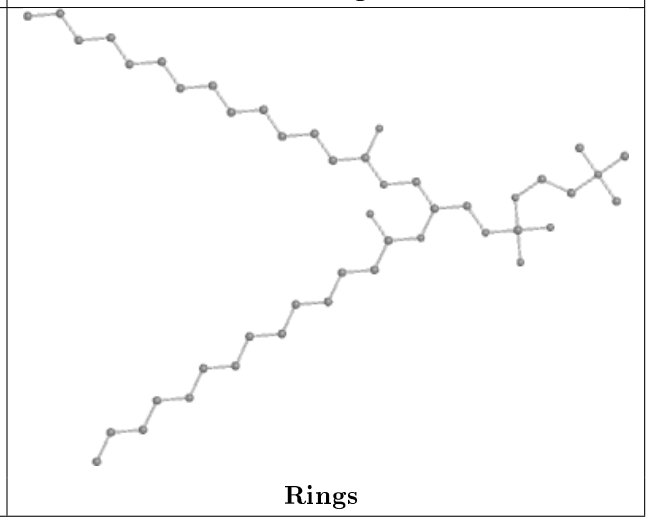
Bond lengths



Bond angles

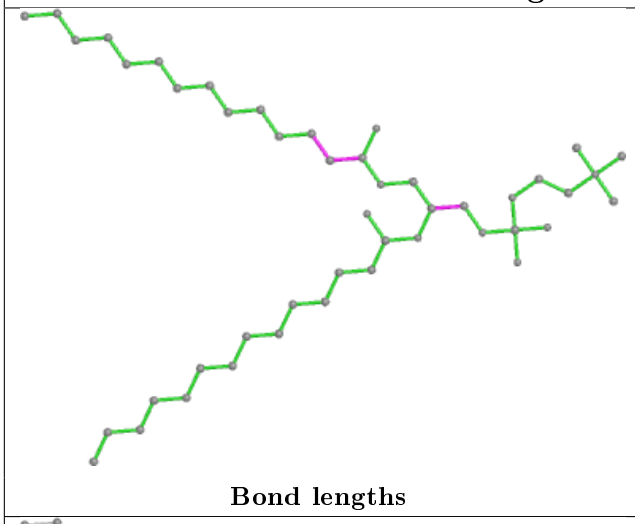


Torsions

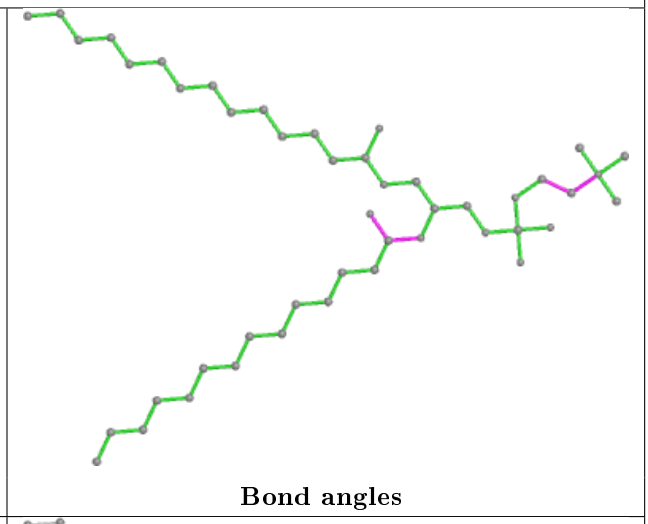


Rings

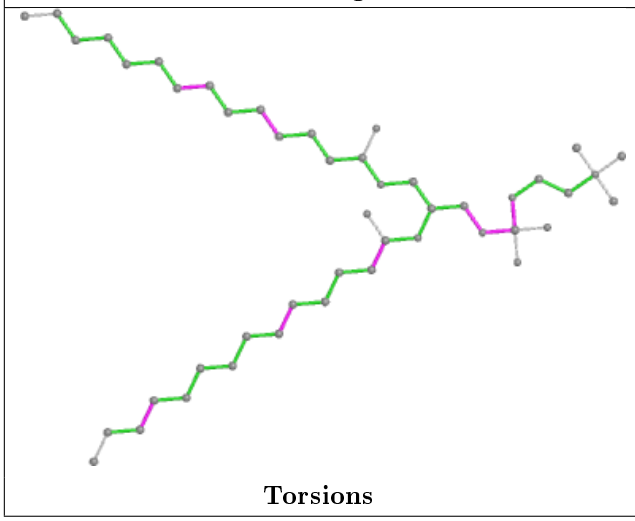
Ligand PX4 A 607



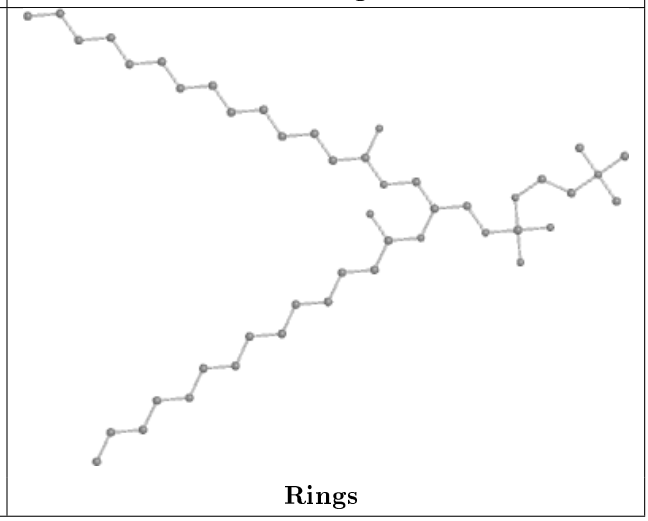
Bond lengths



Bond angles

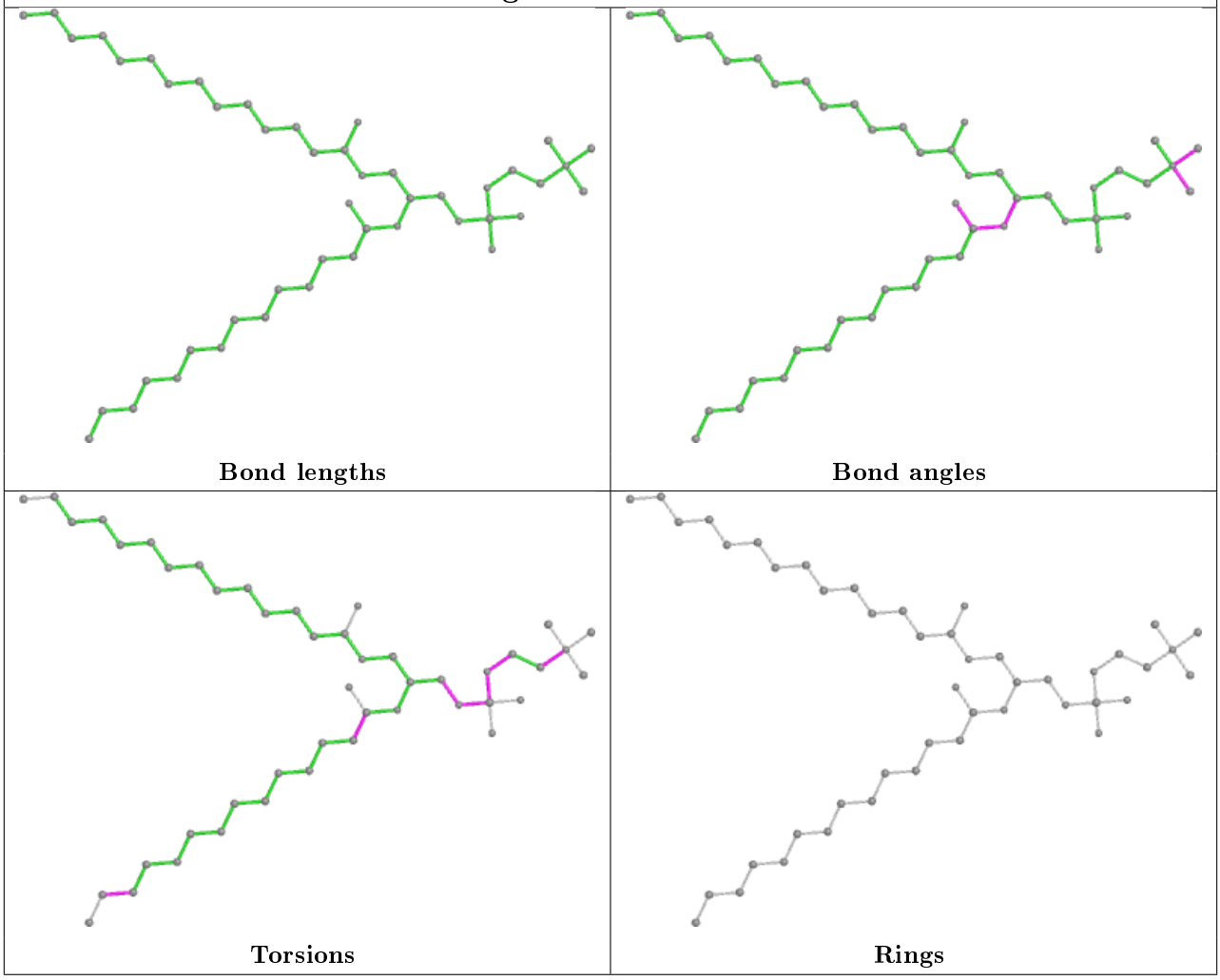


Torsions

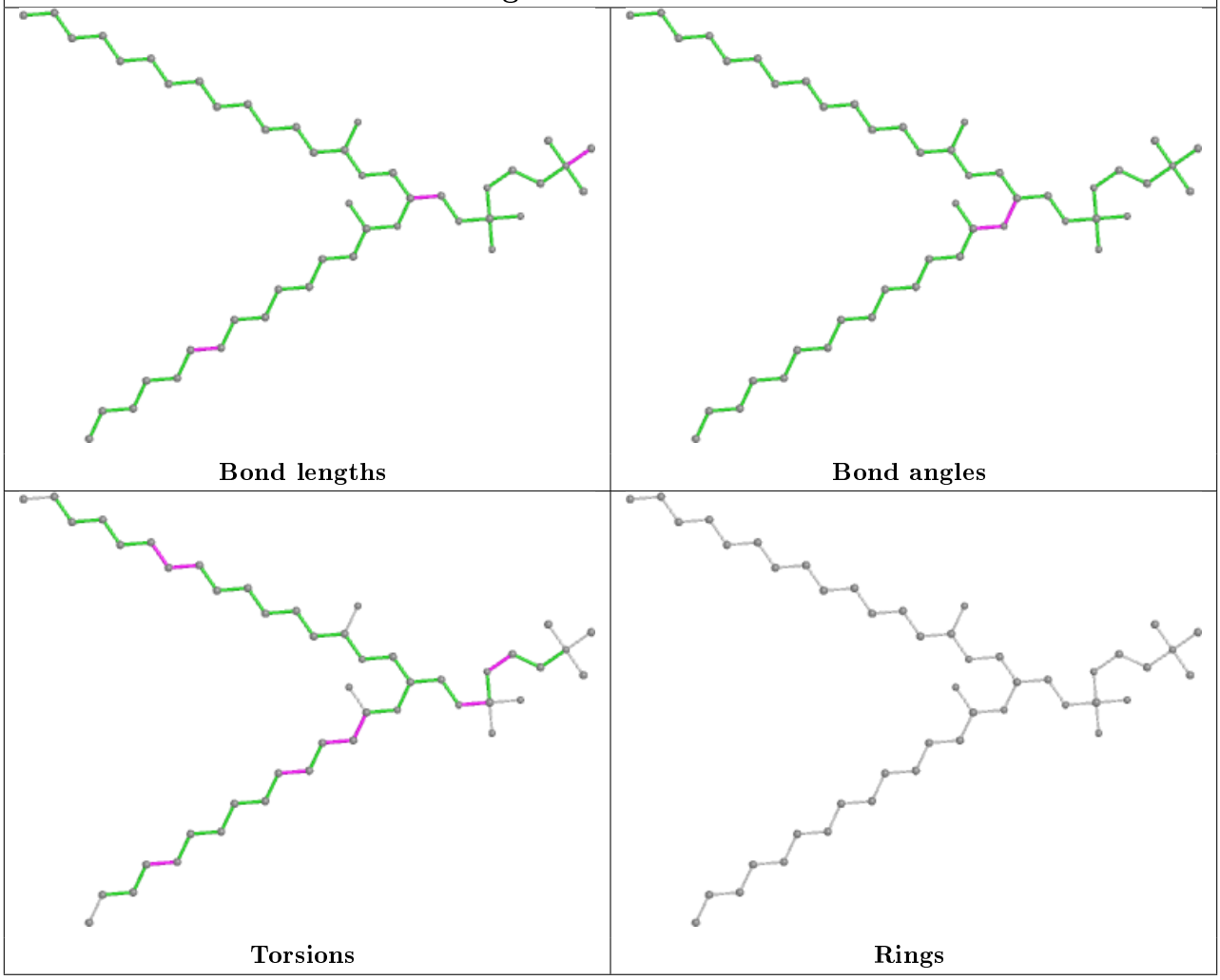


Rings

Ligand PX4 B 375



Ligand PX4 B 321



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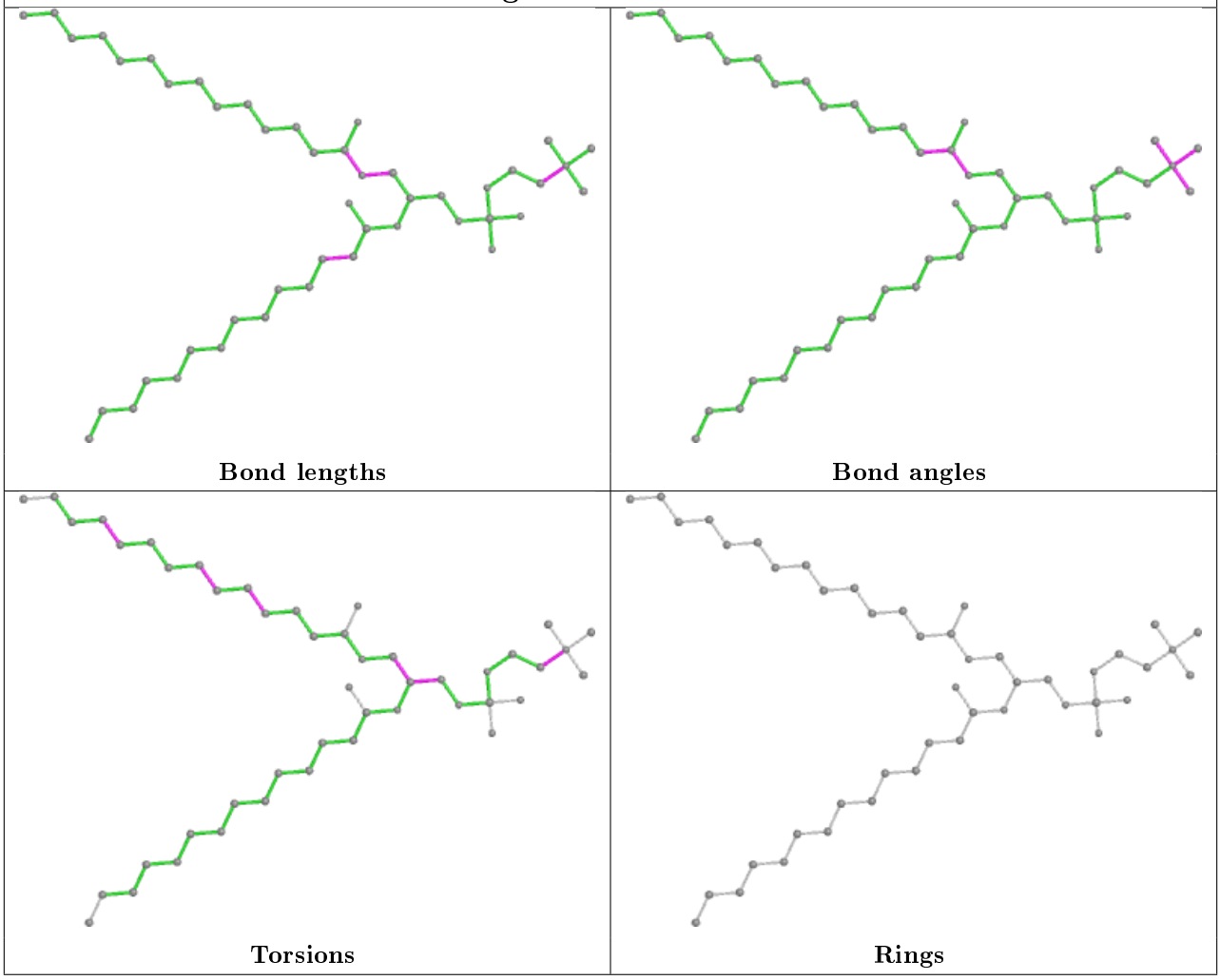
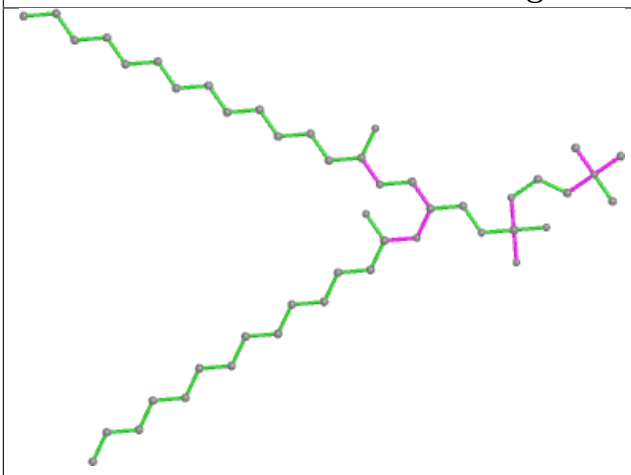
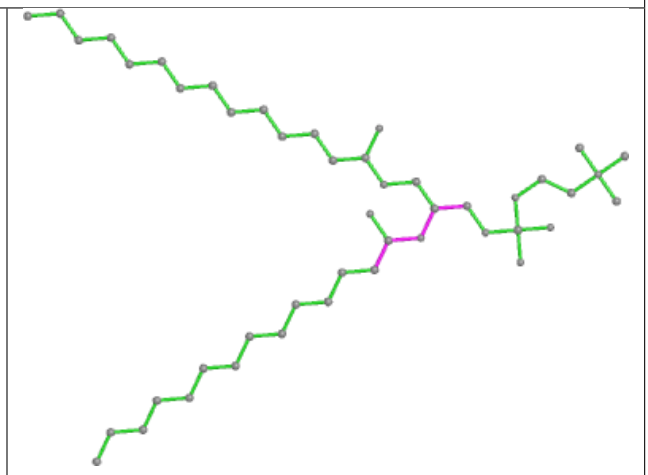


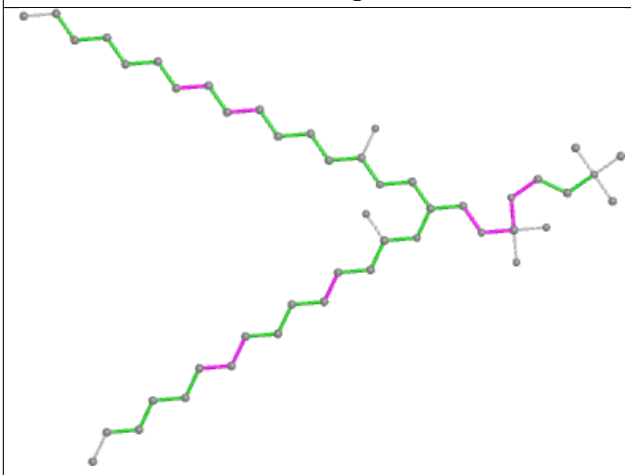
Ligand PX4 A 633



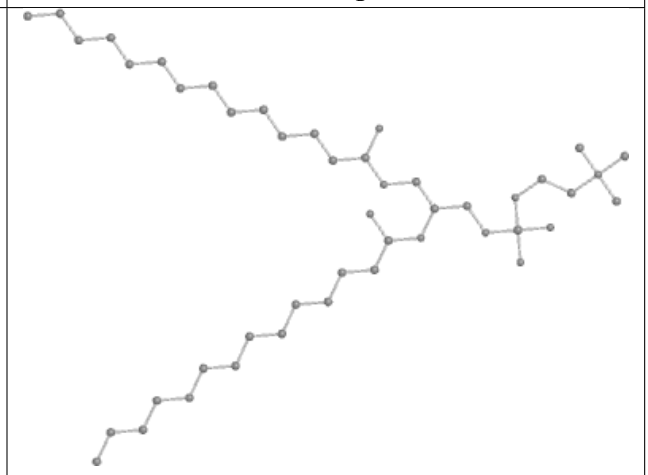
Bond lengths



Bond angles

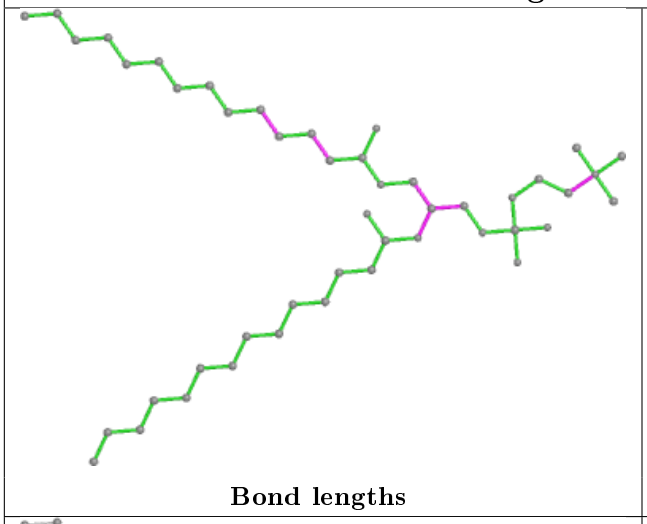


Torsions

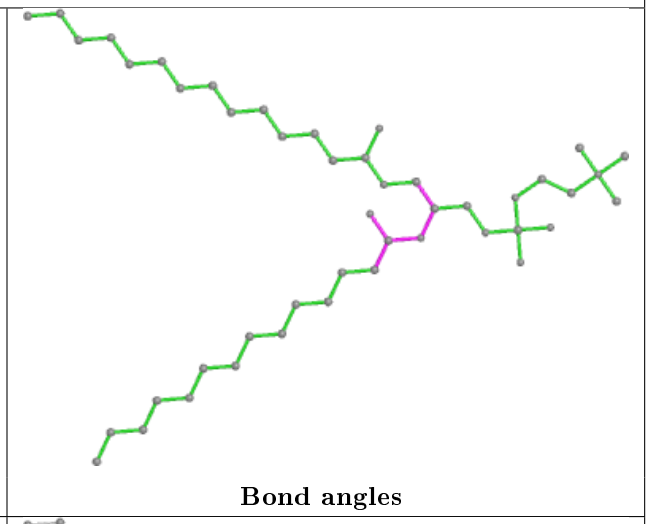


Rings

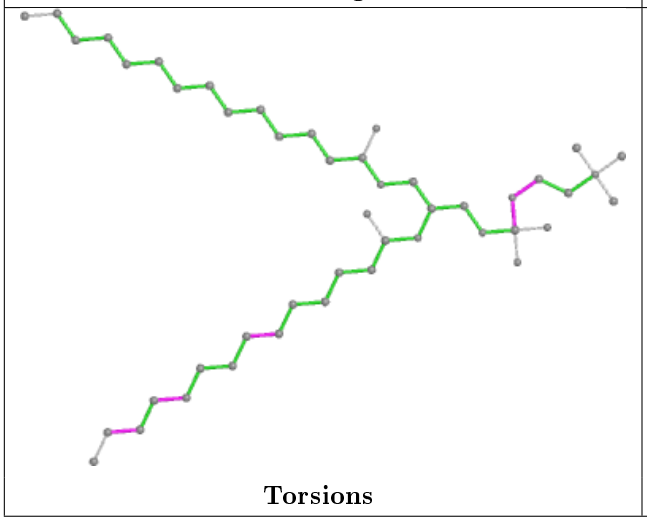
Ligand PX4 A 603



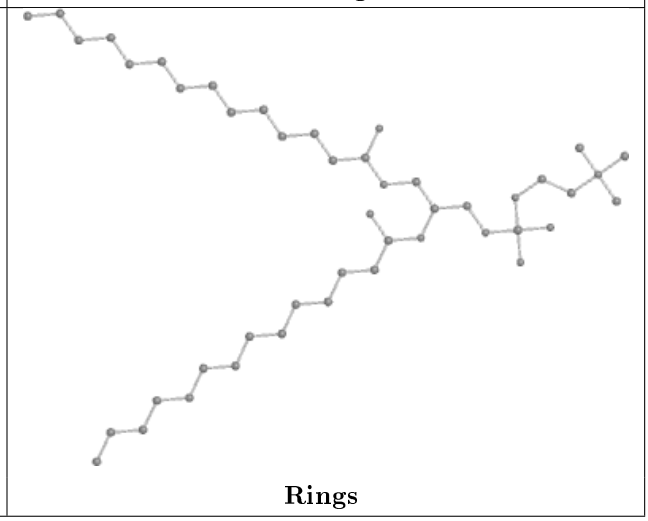
Bond lengths



Bond angles

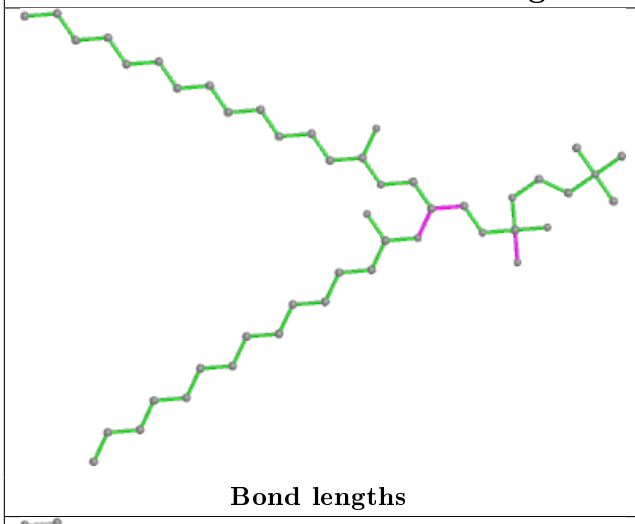


Torsions

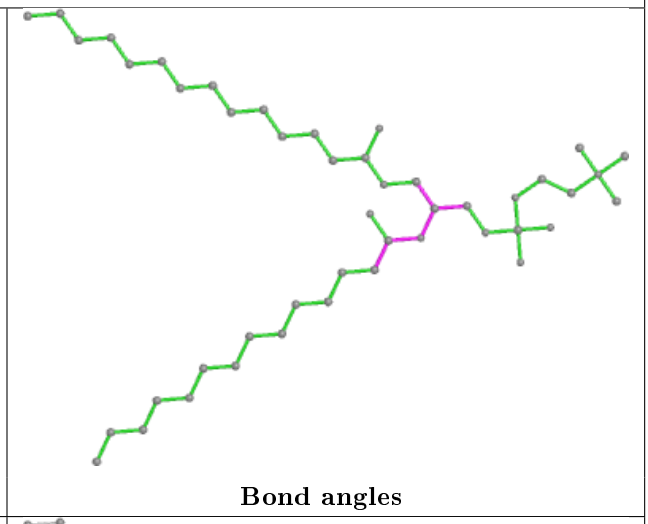


Rings

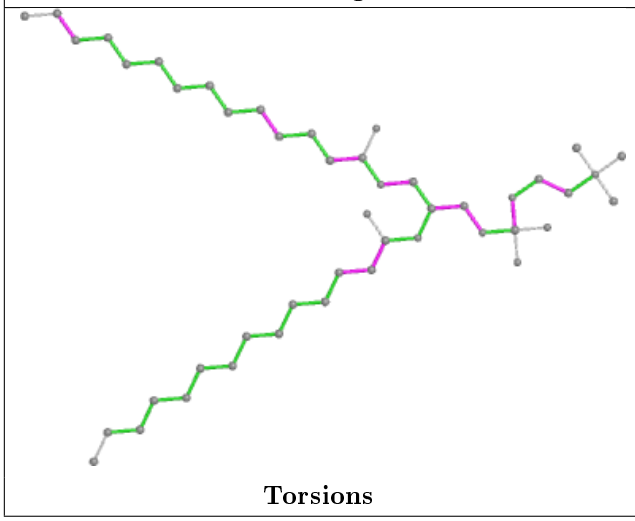
Ligand PX4 B 360



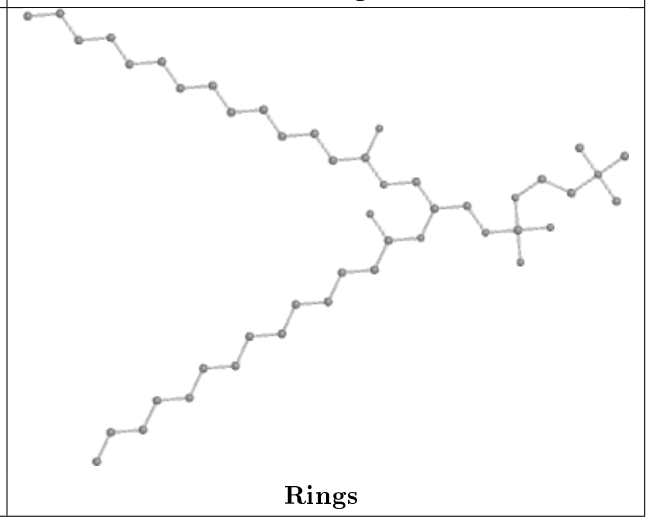
Bond lengths



Bond angles

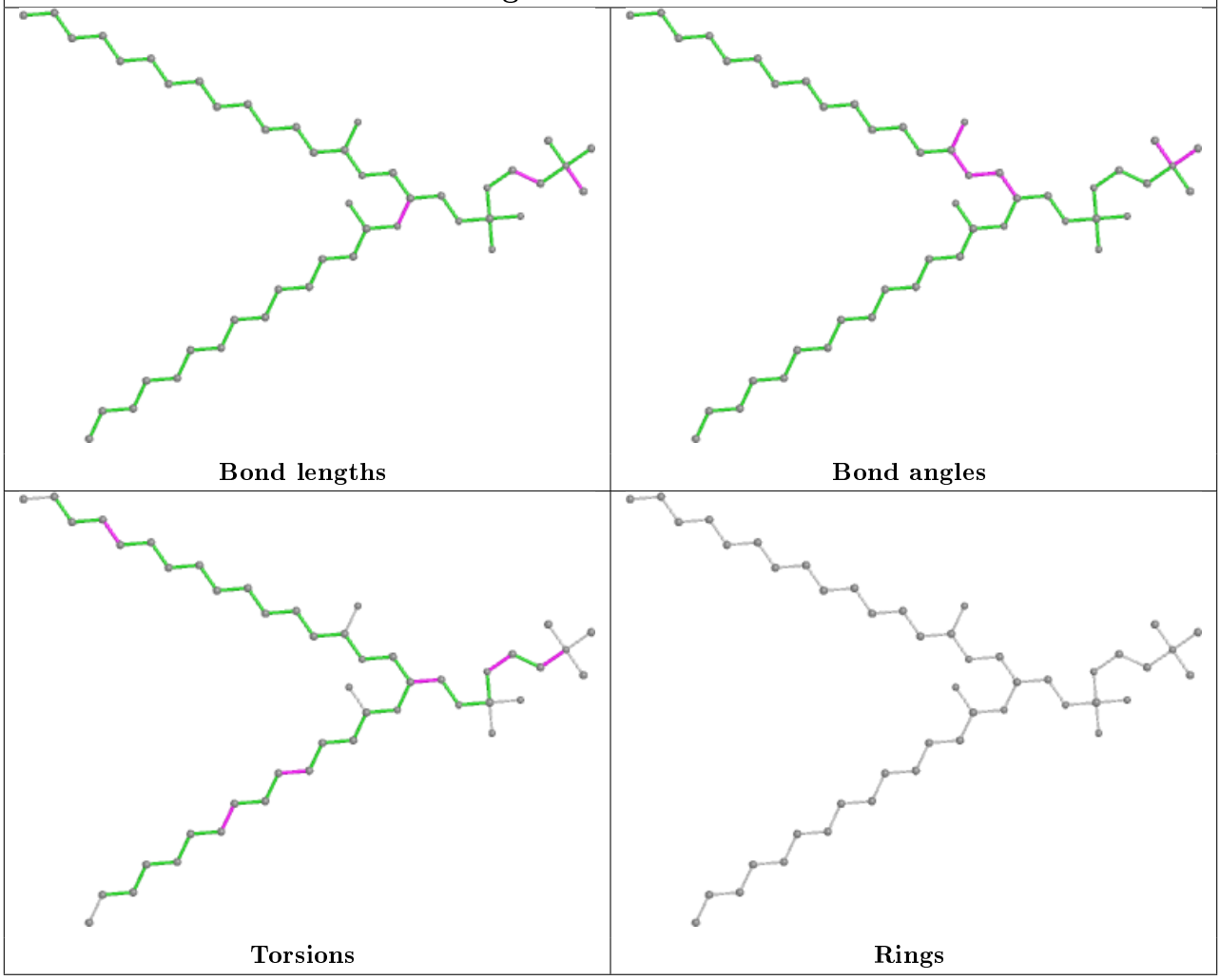


Torsions

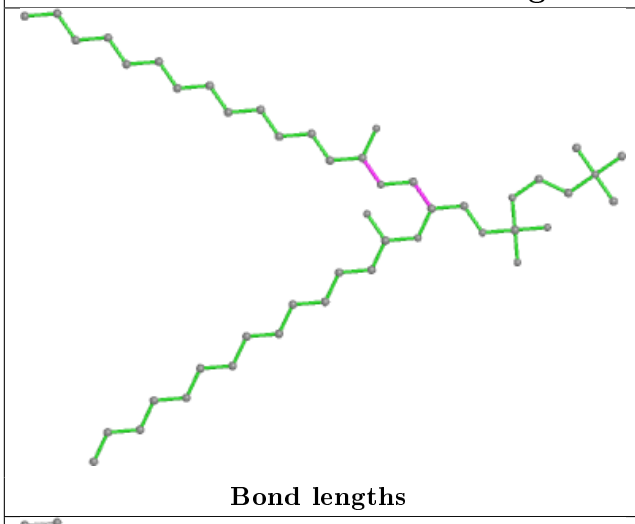


Rings

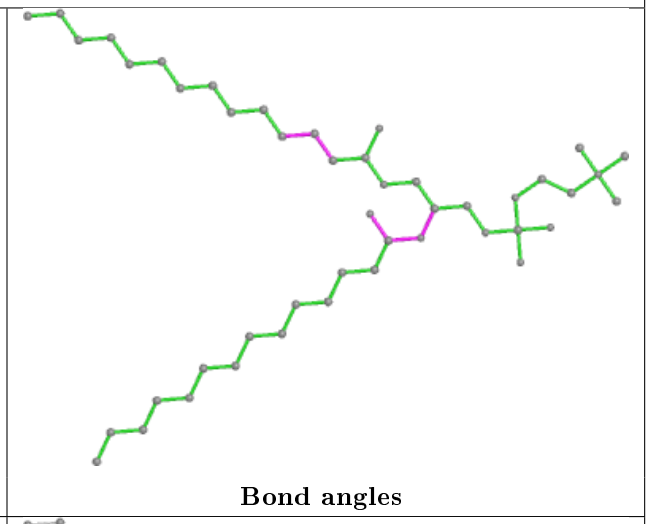
Ligand PX4 B 344



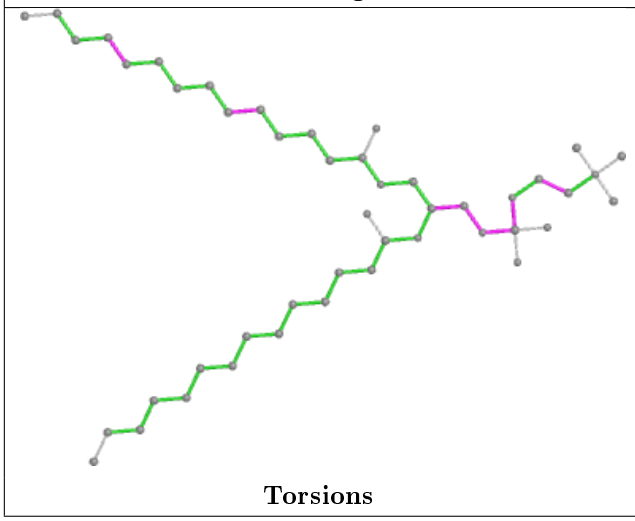
Ligand PX4 B 337



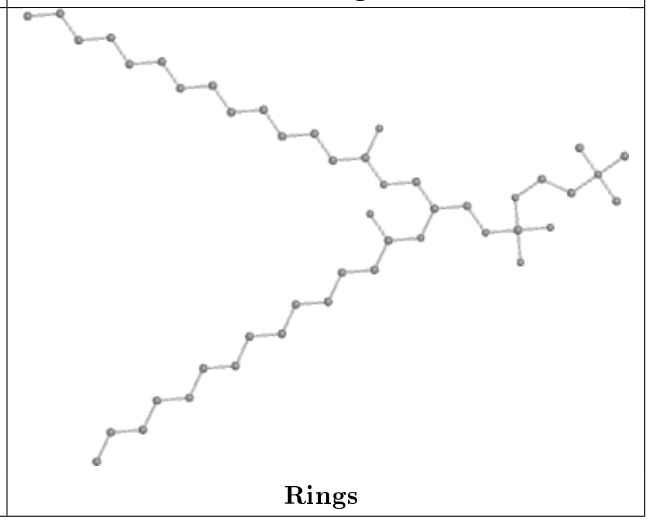
Bond lengths



Bond angles

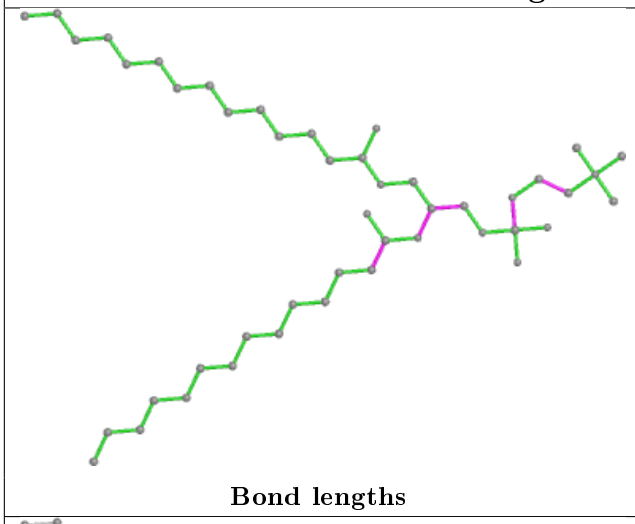


Torsions

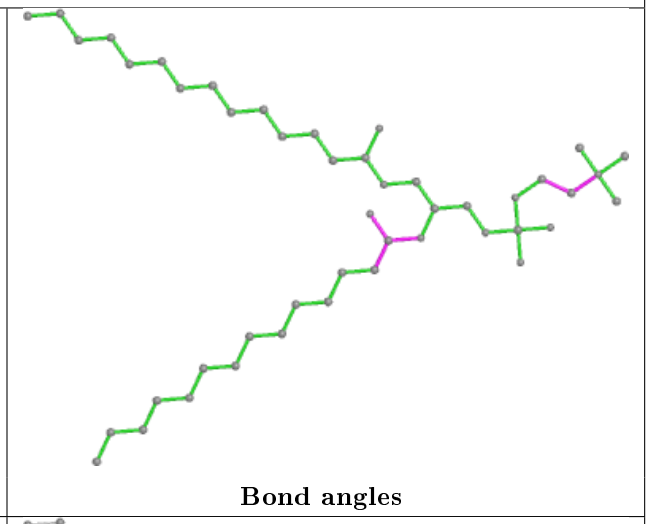


Rings

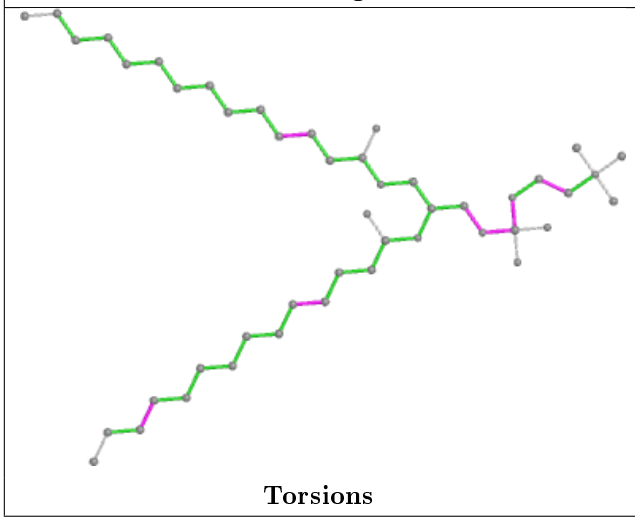
Ligand PX4 C 347



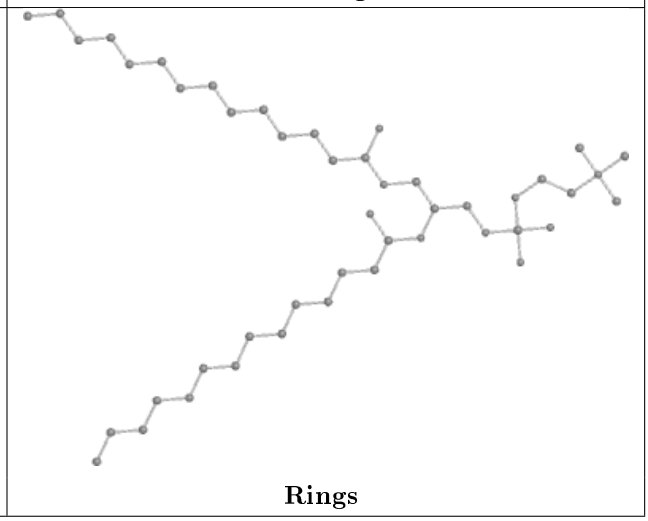
Bond lengths



Bond angles

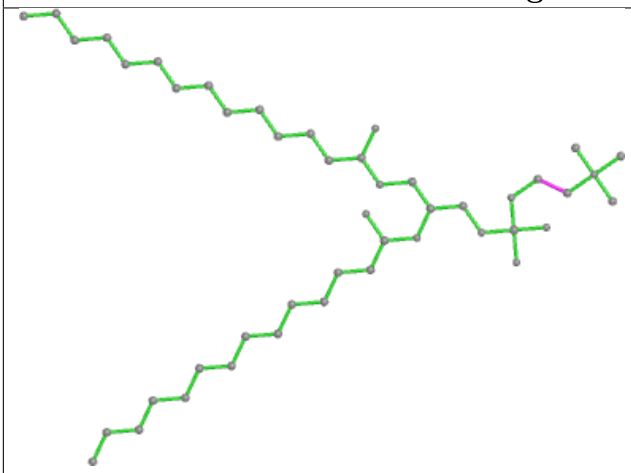


Torsions

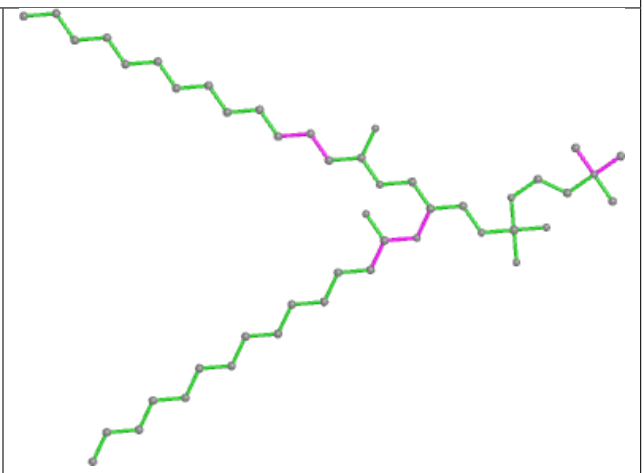


Rings

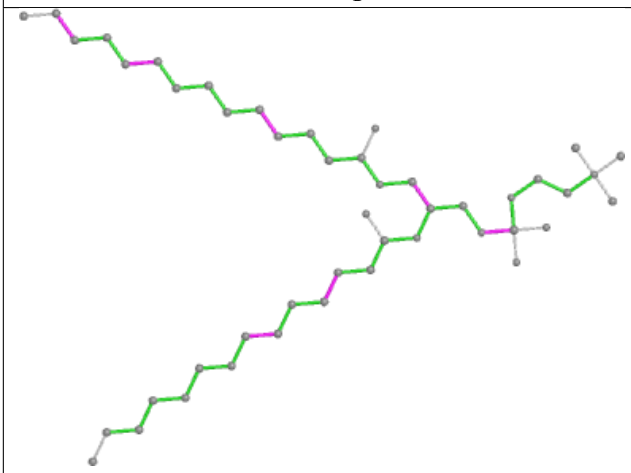
Ligand PX4 A 622



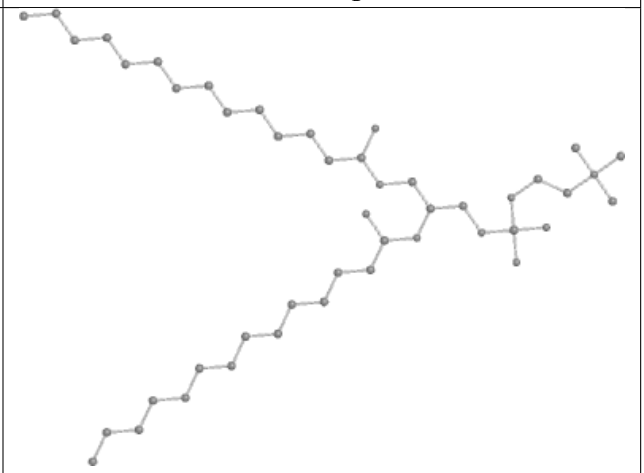
Bond lengths



Bond angles

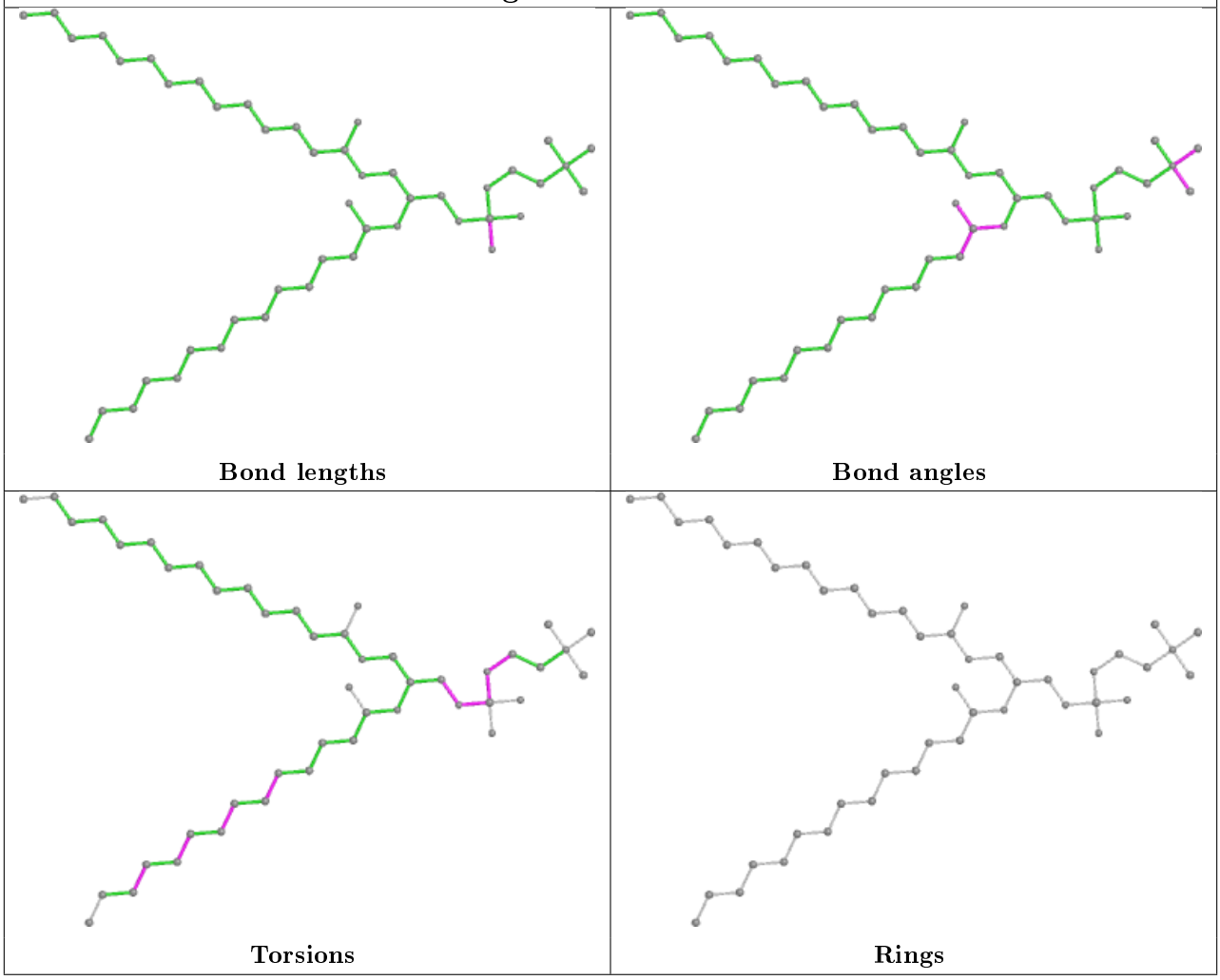


Torsions

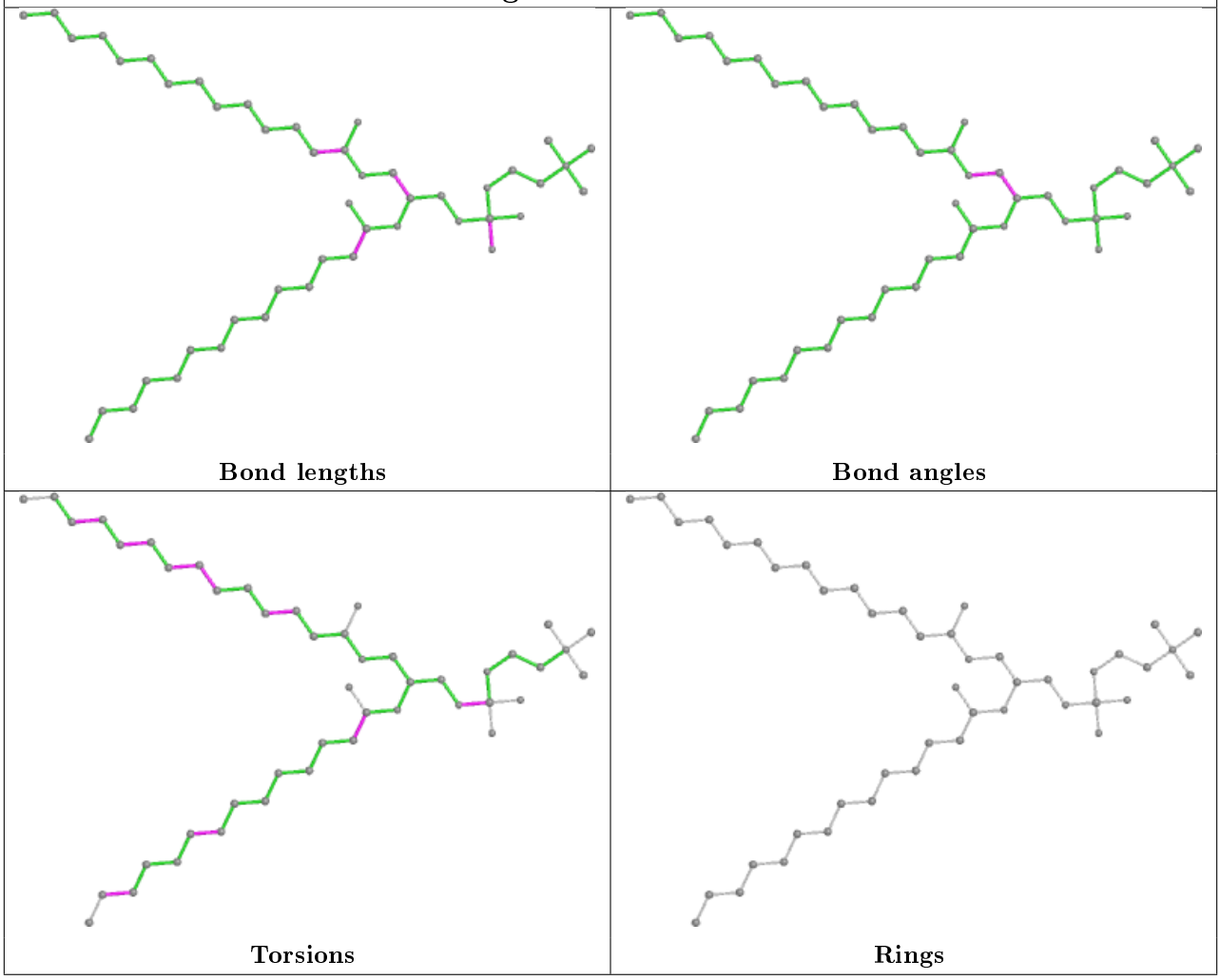


Rings

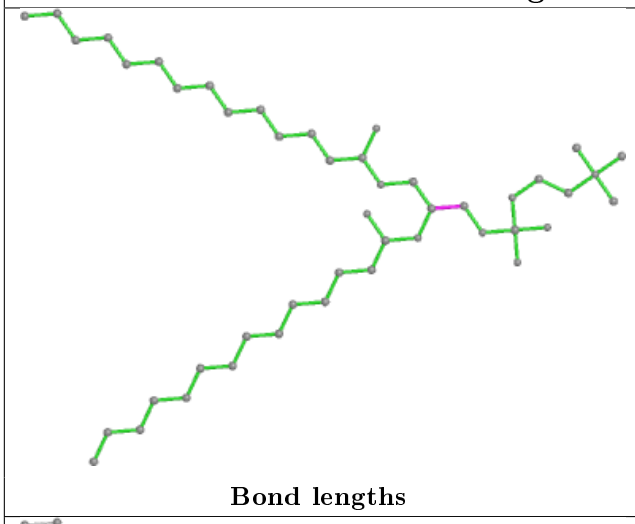
Ligand PX4 B 322



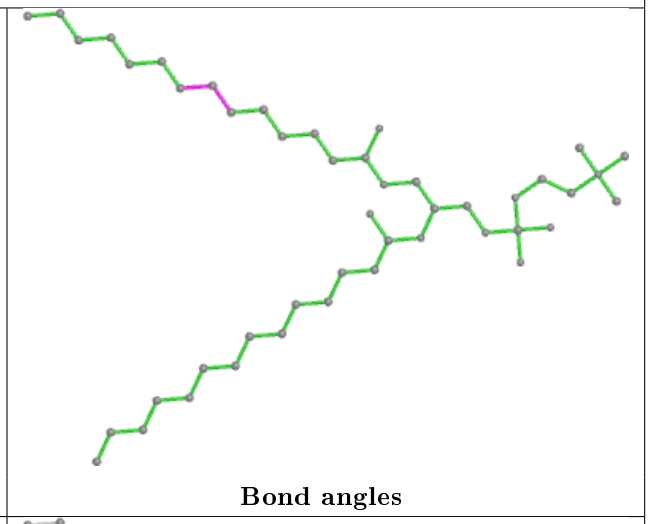
Ligand PX4 B 361



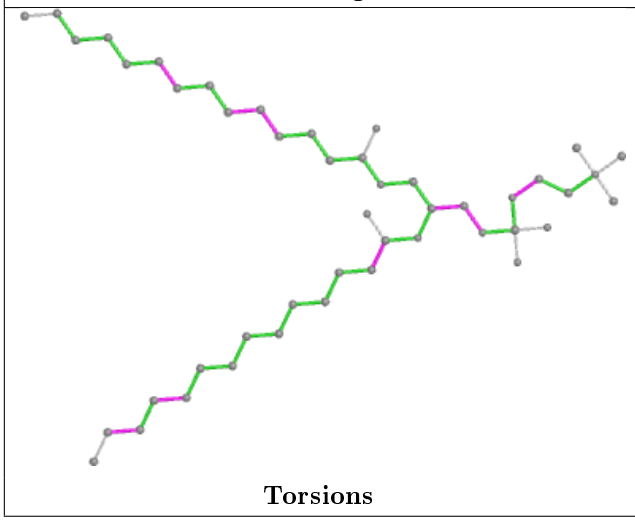
Ligand PX4 A 604



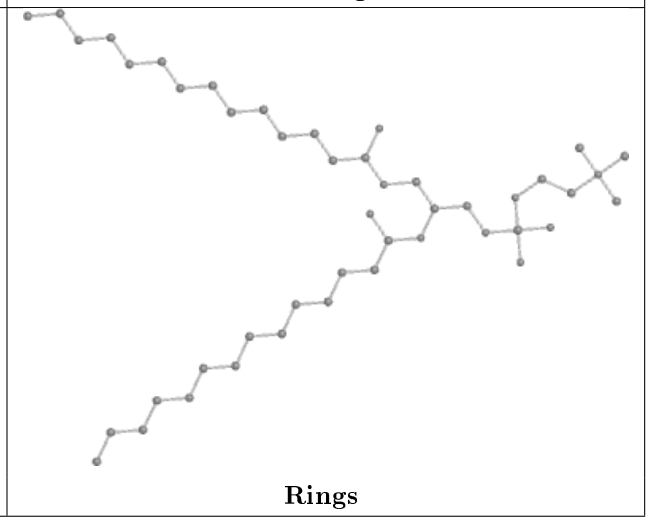
Bond lengths



Bond angles

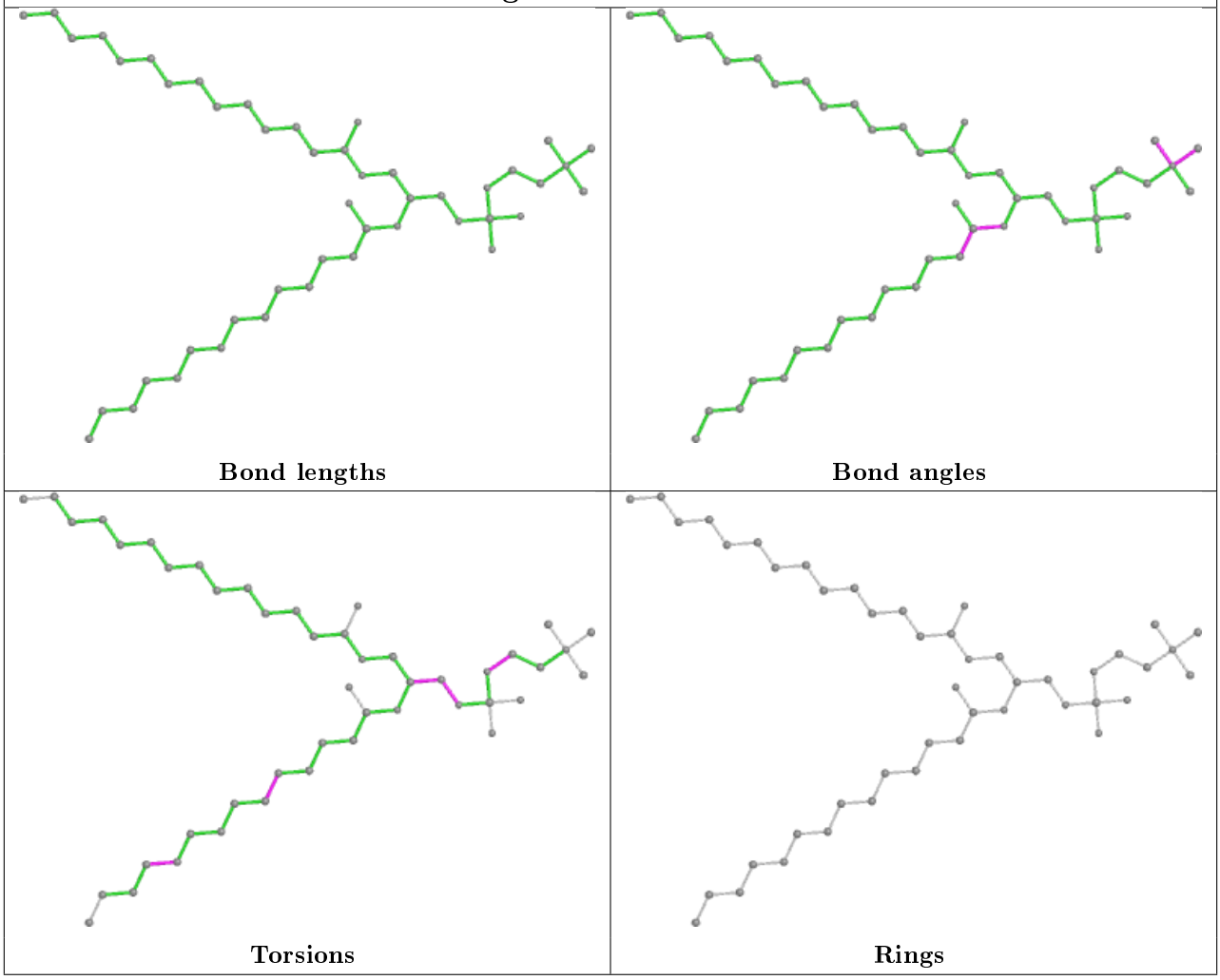


Torsions

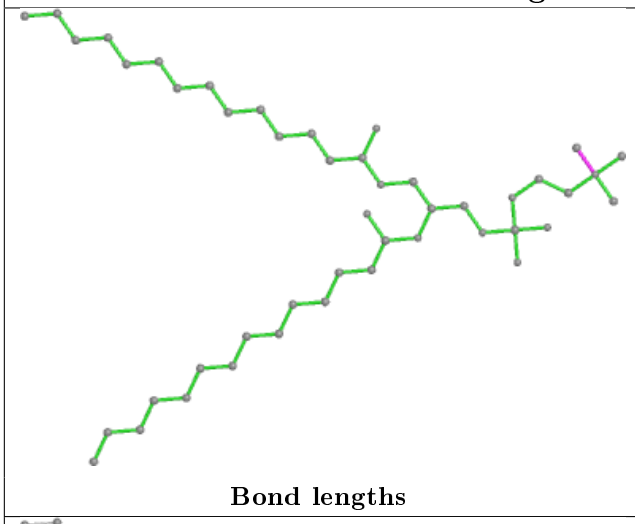


Rings

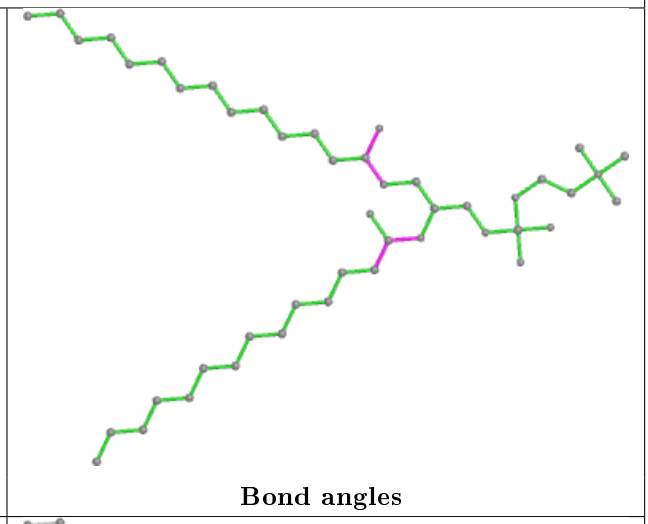
Ligand PX4 B 353



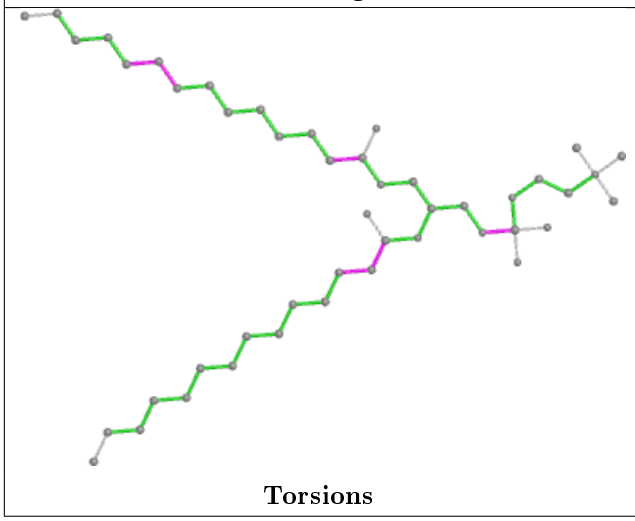
Ligand PX4 C 331



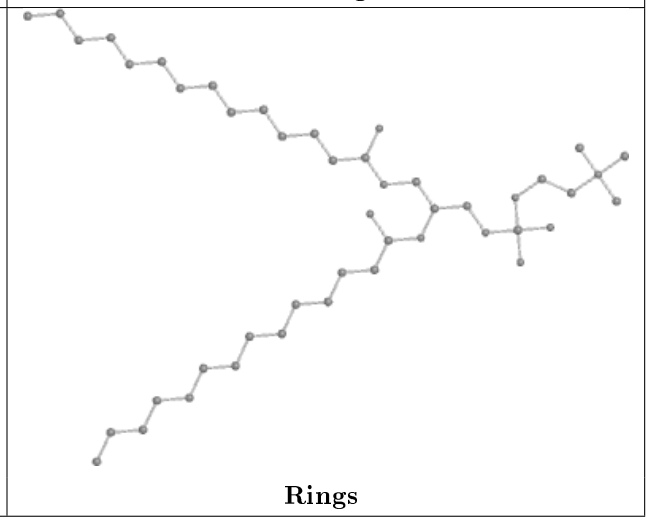
Bond lengths



Bond angles

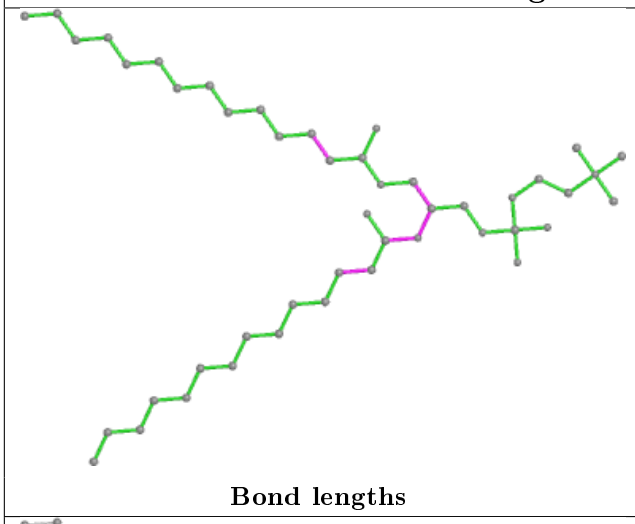


Torsions

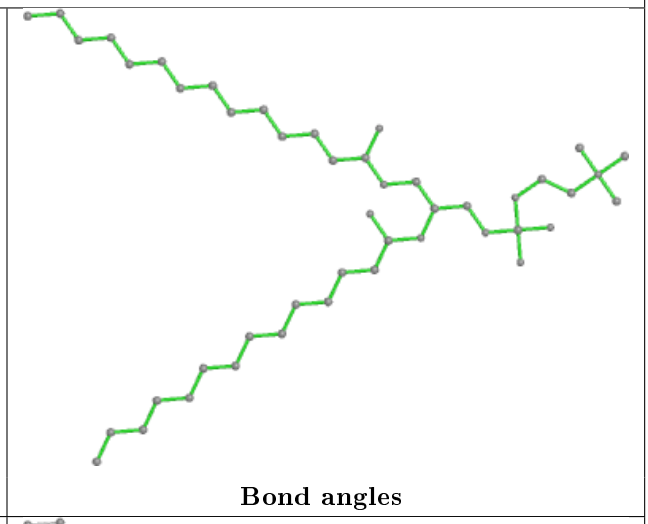


Rings

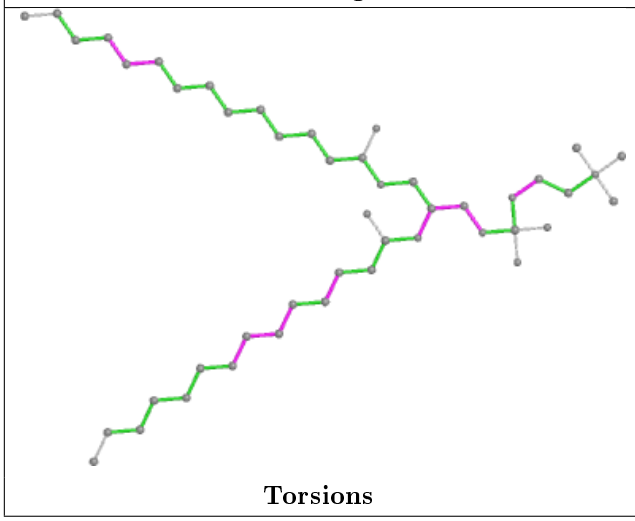
Ligand PX4 C 356



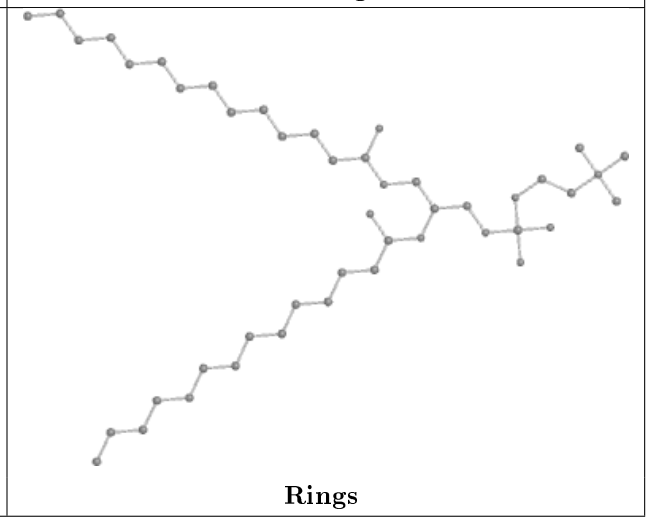
Bond lengths



Bond angles

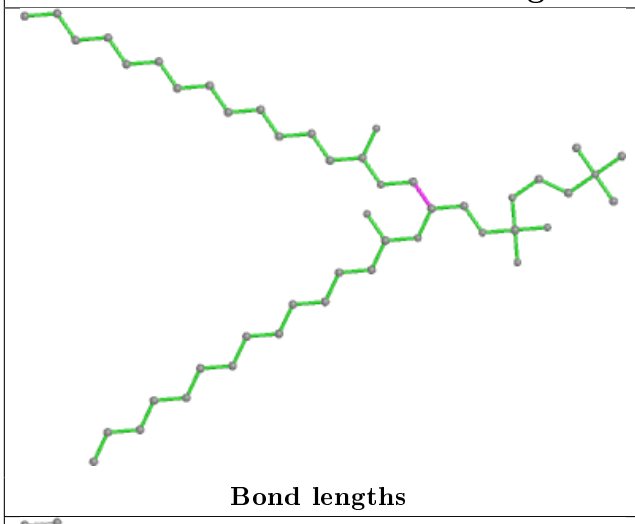


Torsions

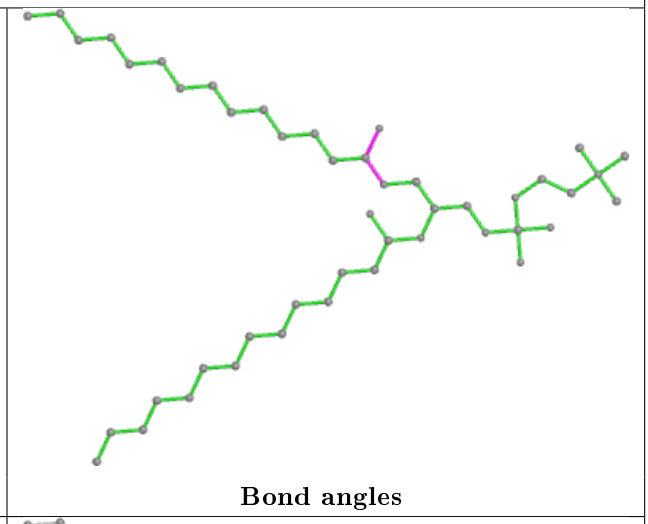


Rings

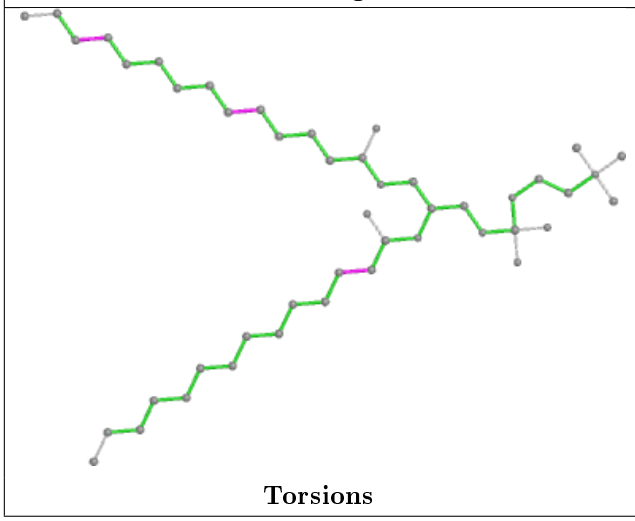
Ligand PX4 A 625



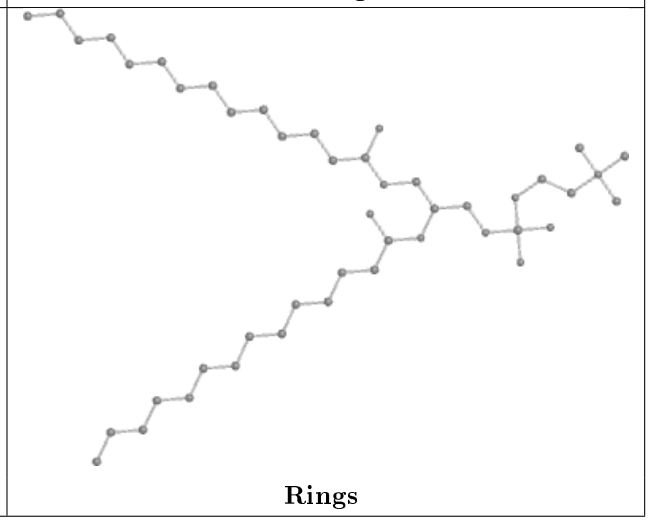
Bond lengths



Bond angles

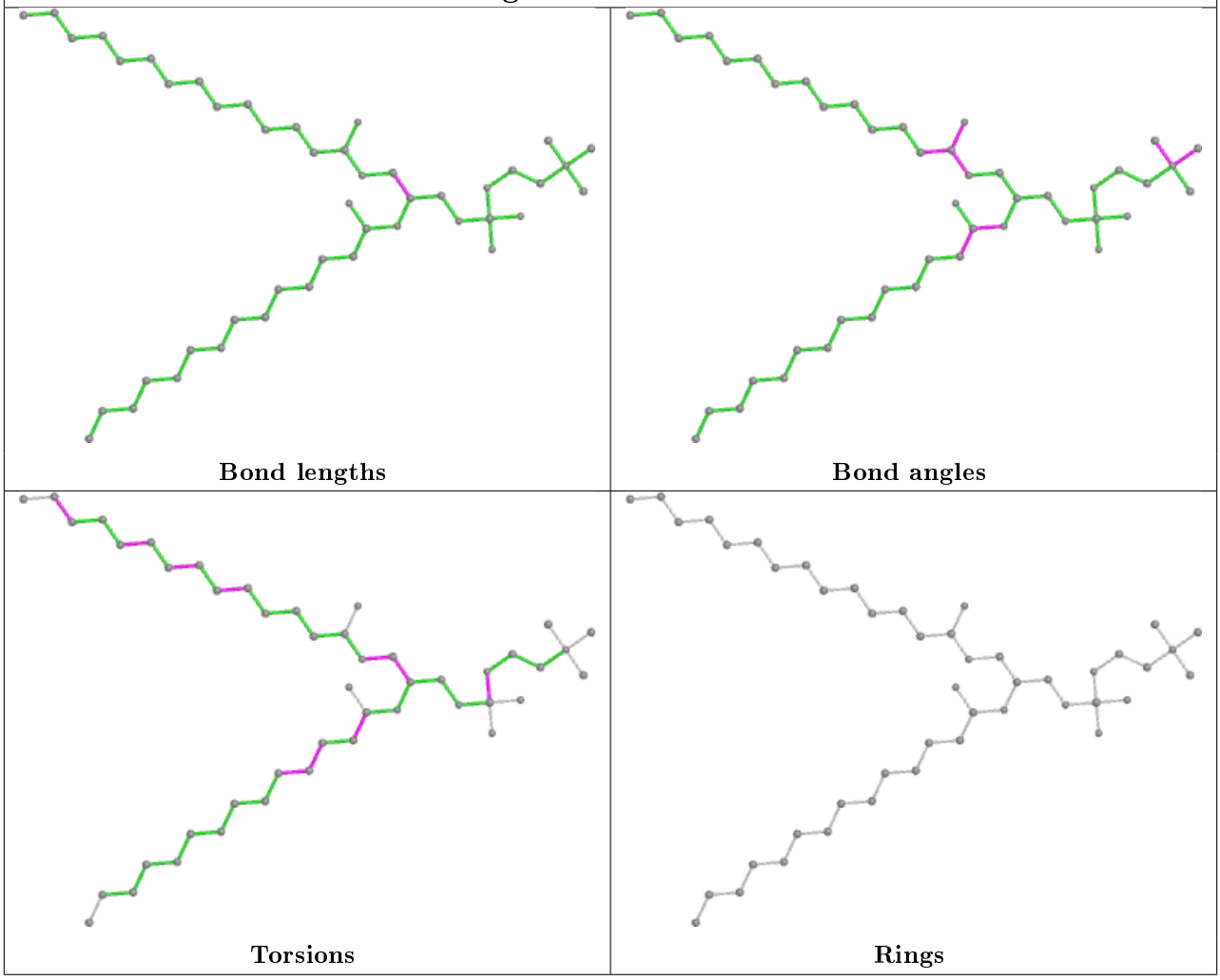


Torsions

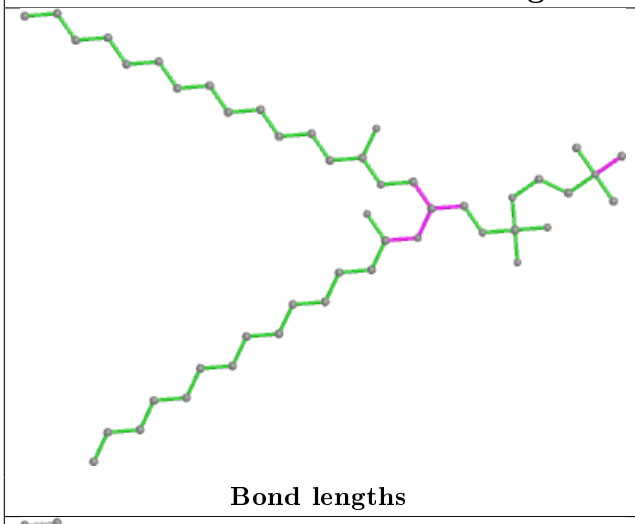


Rings

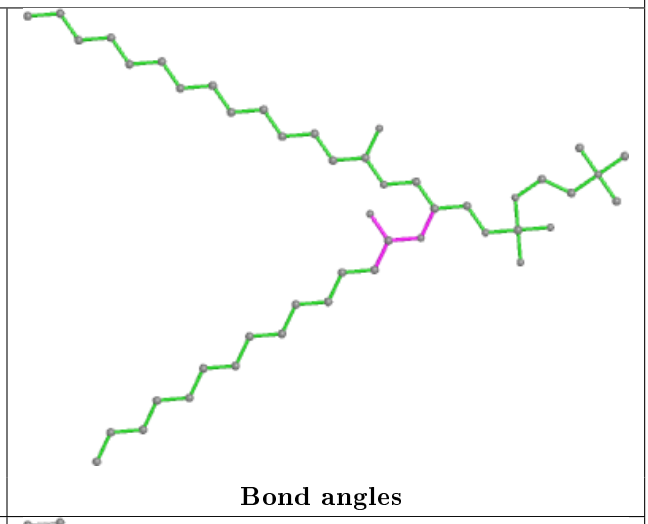
Ligand PX4 B 370



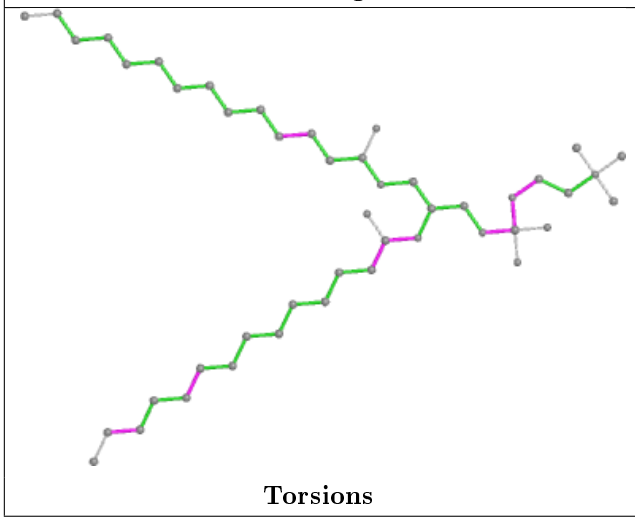
Ligand PX4 A 617



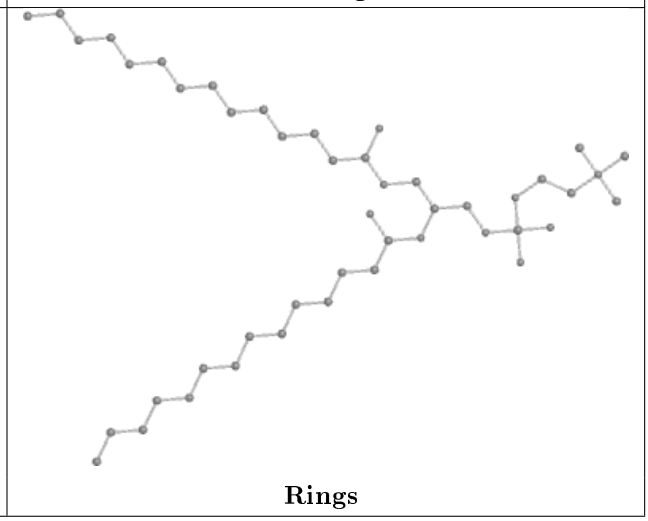
Bond lengths



Bond angles

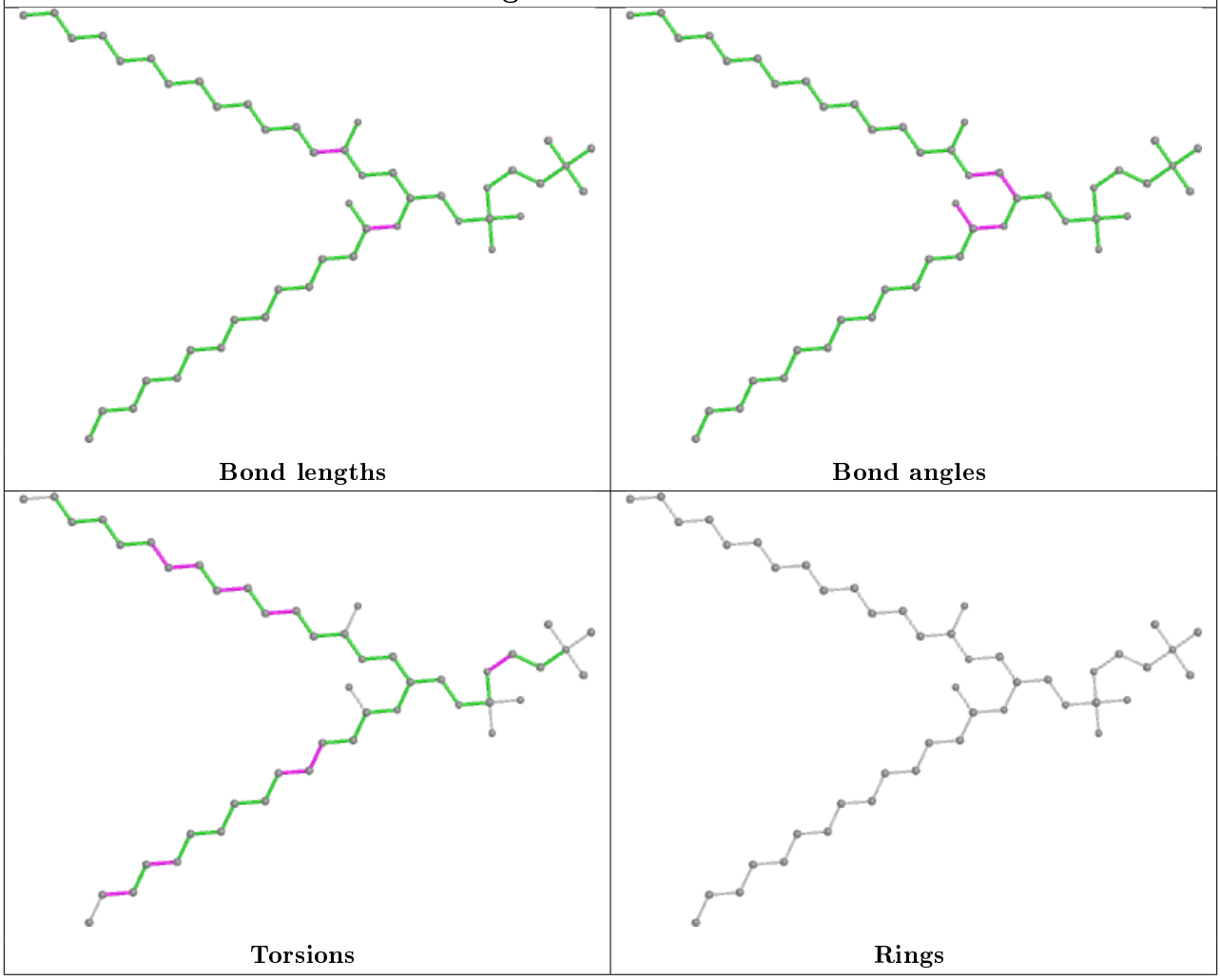


Torsions

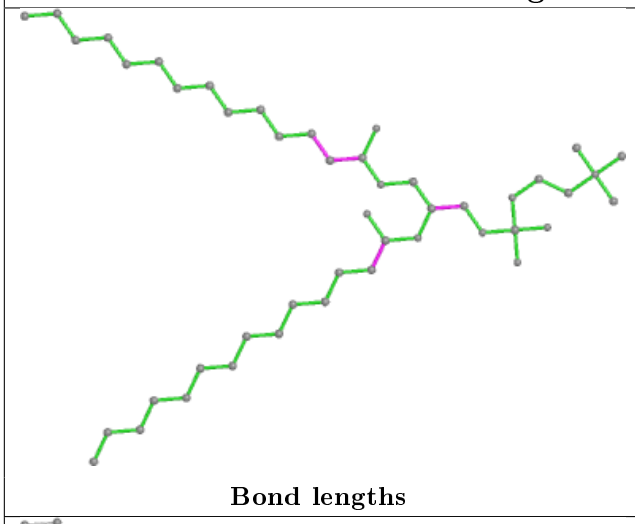


Rings

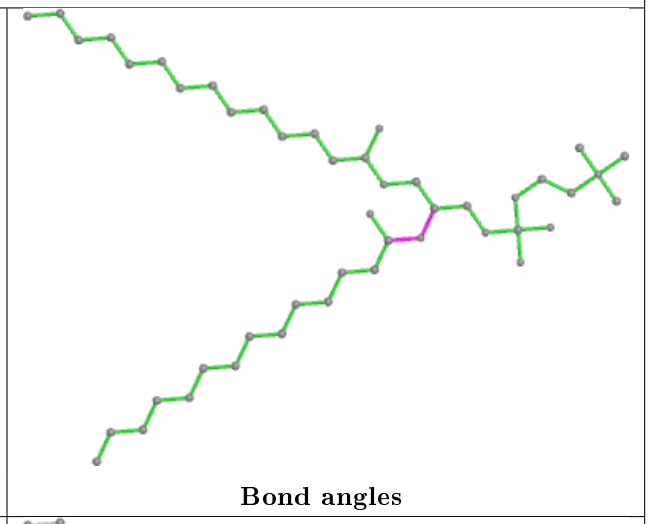
Ligand PX4 B 303



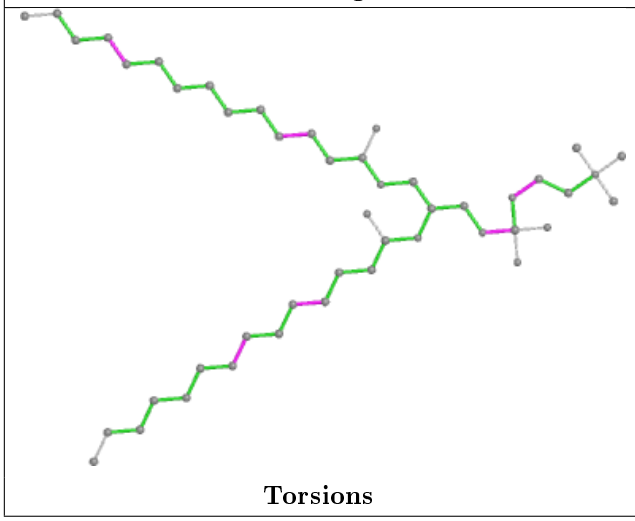
Ligand PX4 A 634



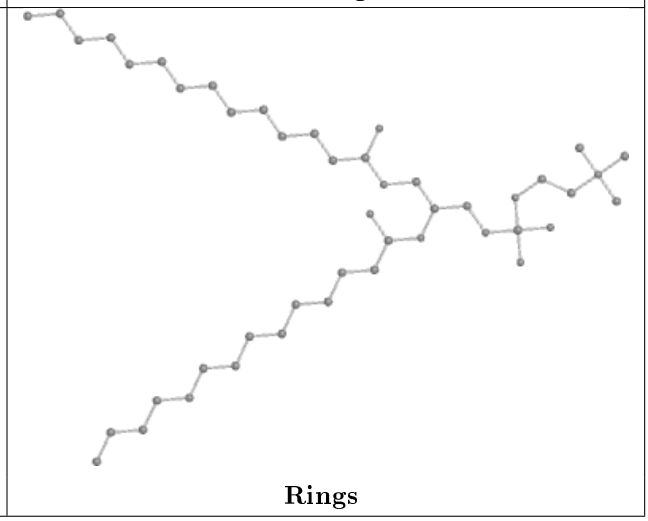
Bond lengths



Bond angles

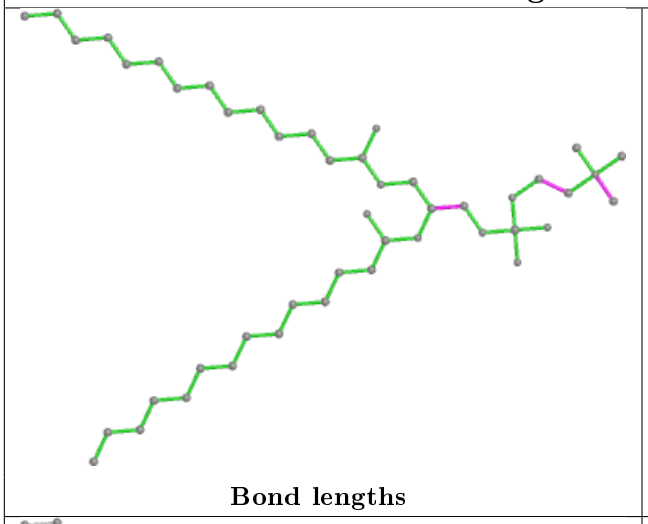


Torsions

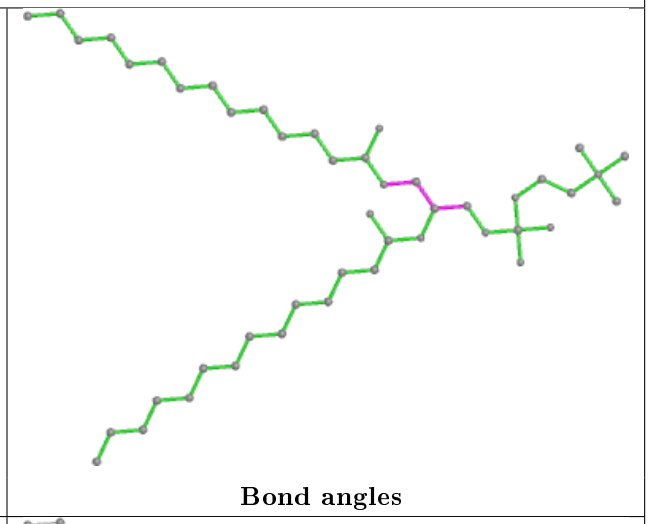


Rings

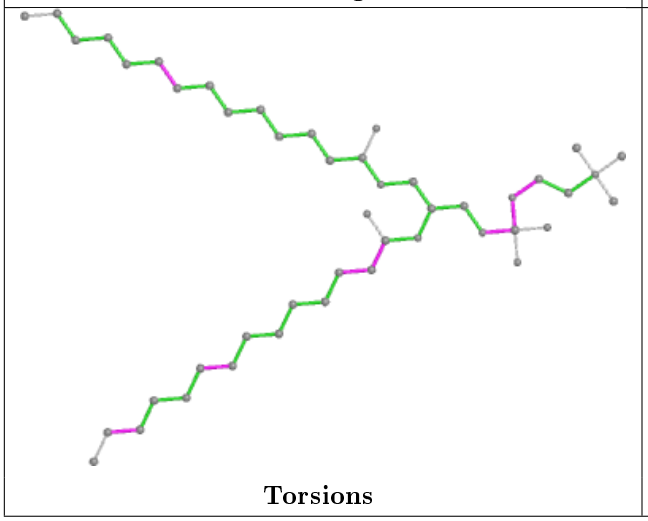
Ligand PX4 A 624



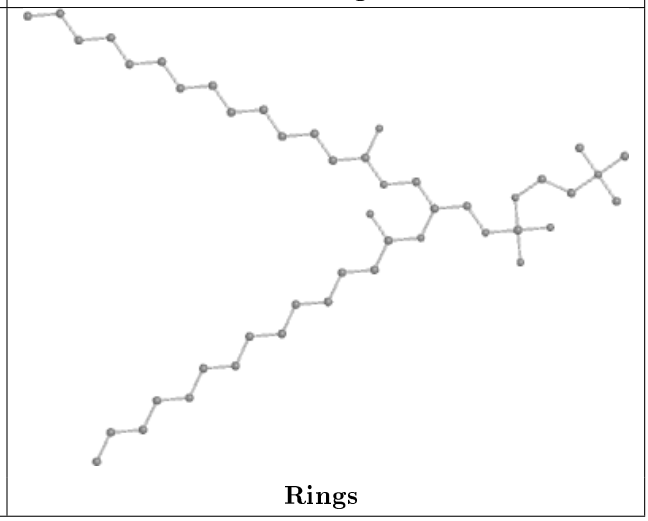
Bond lengths



Bond angles

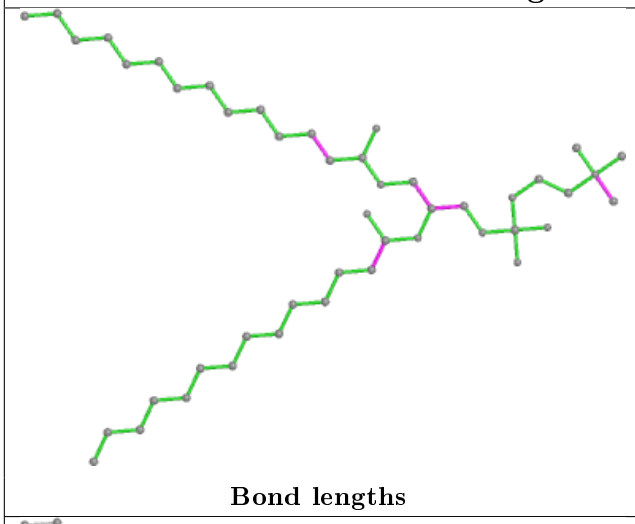


Torsions

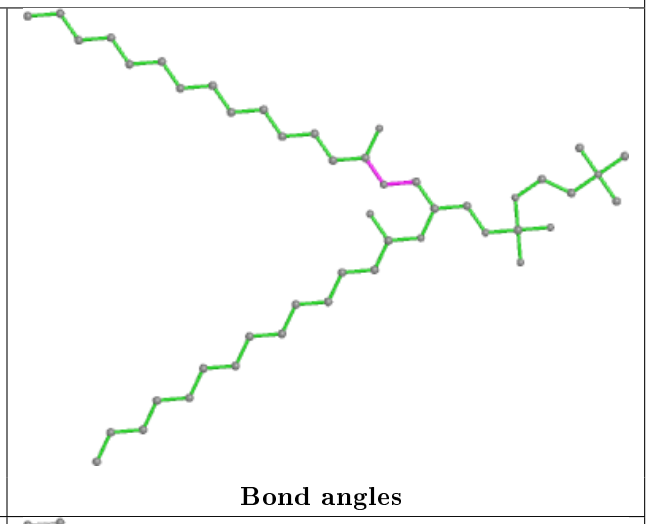


Rings

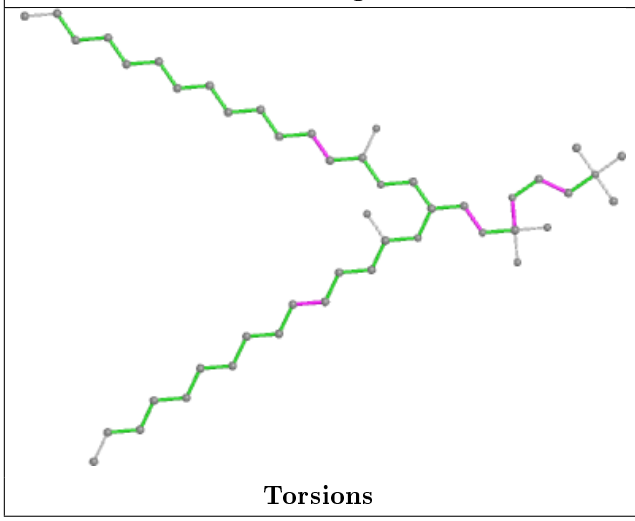
Ligand PX4 A 614



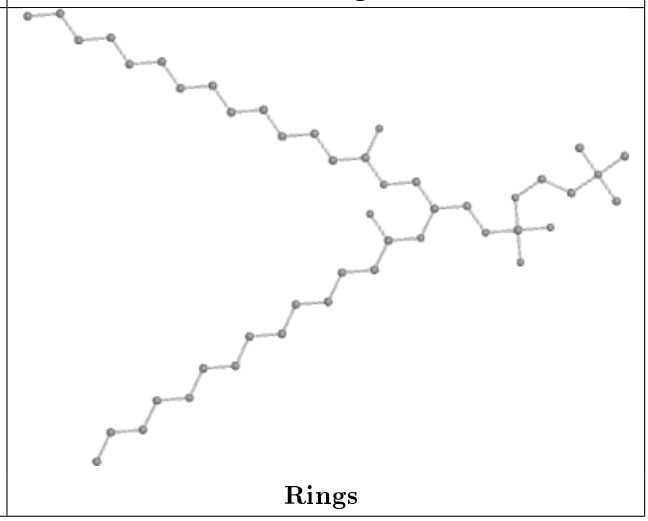
Bond lengths



Bond angles

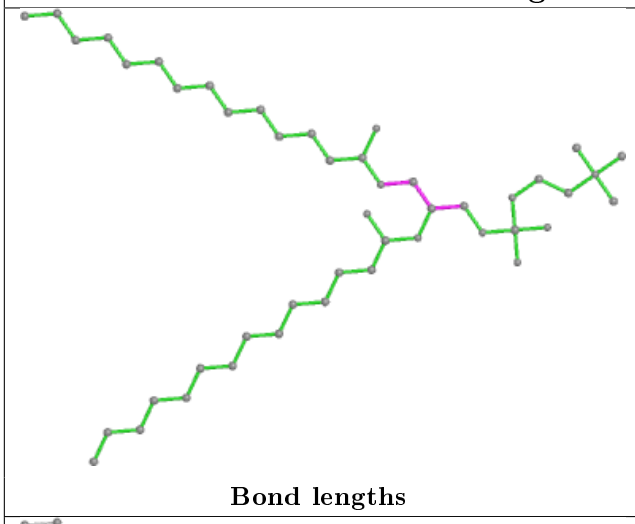


Torsions

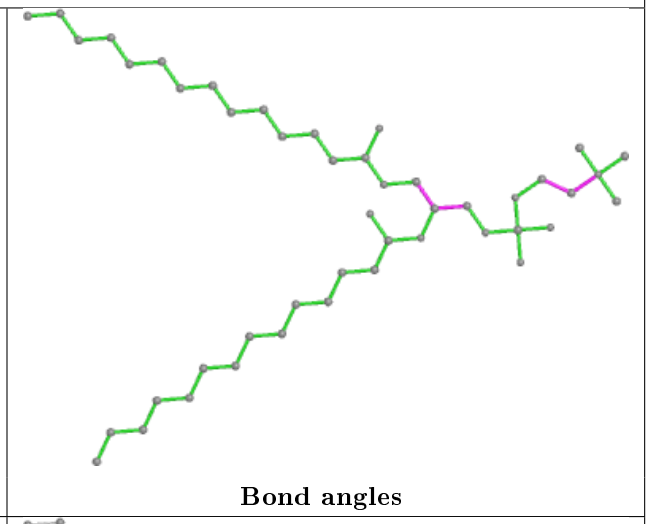


Rings

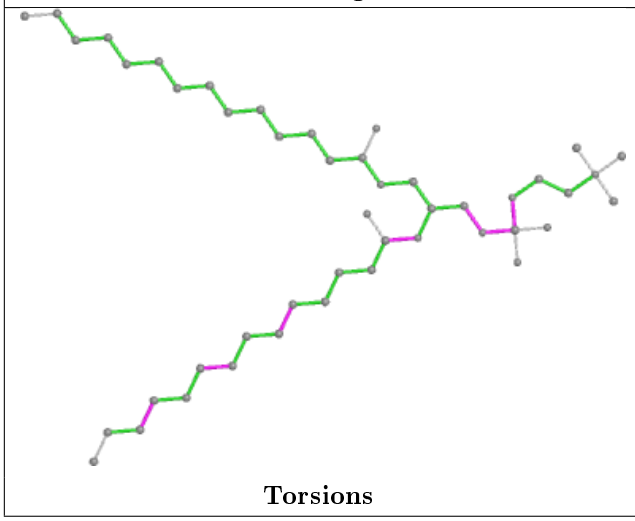
Ligand PX4 C 308



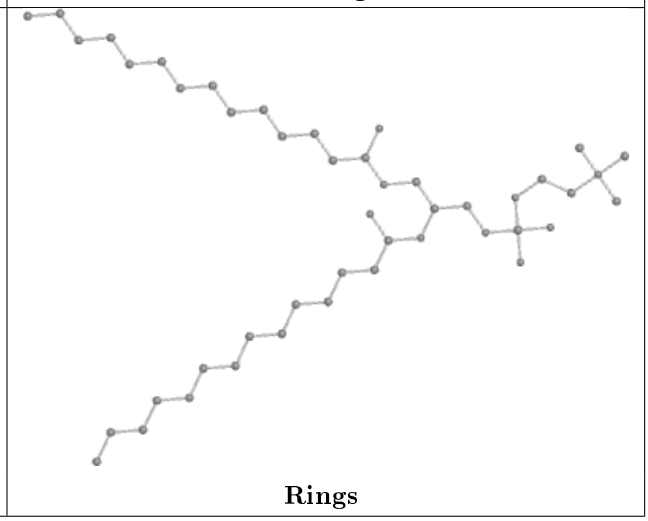
Bond lengths



Bond angles

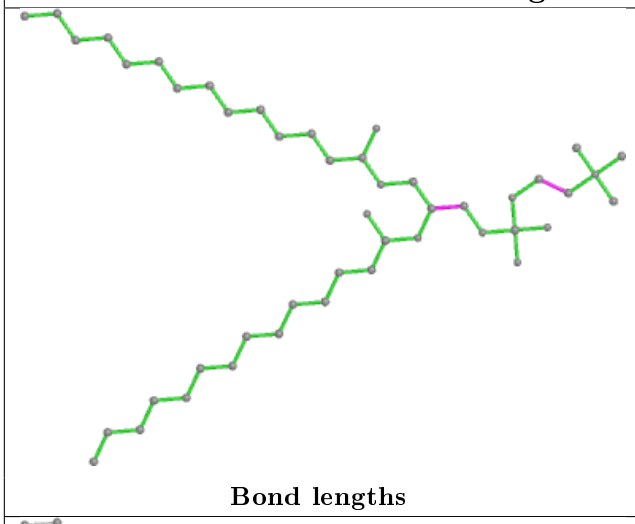


Torsions

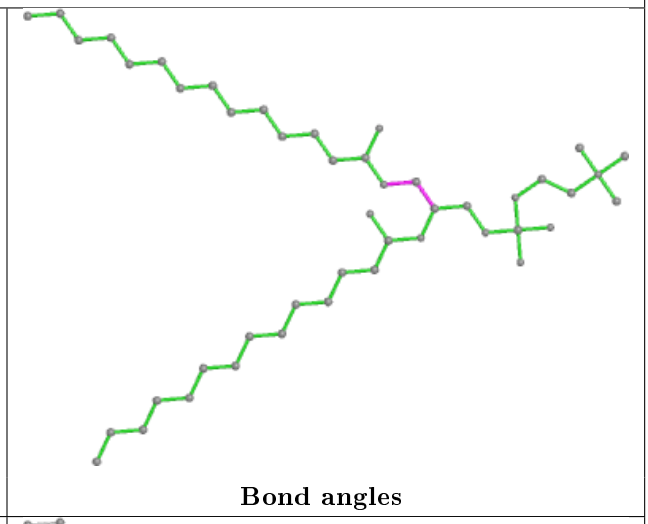


Rings

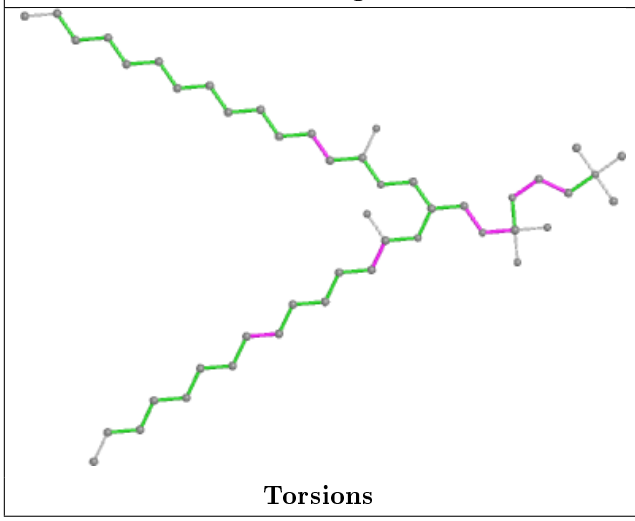
Ligand PX4 C 344



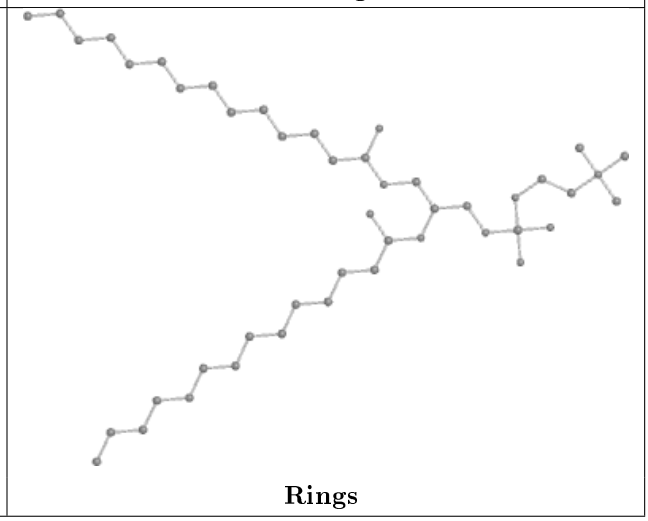
Bond lengths



Bond angles

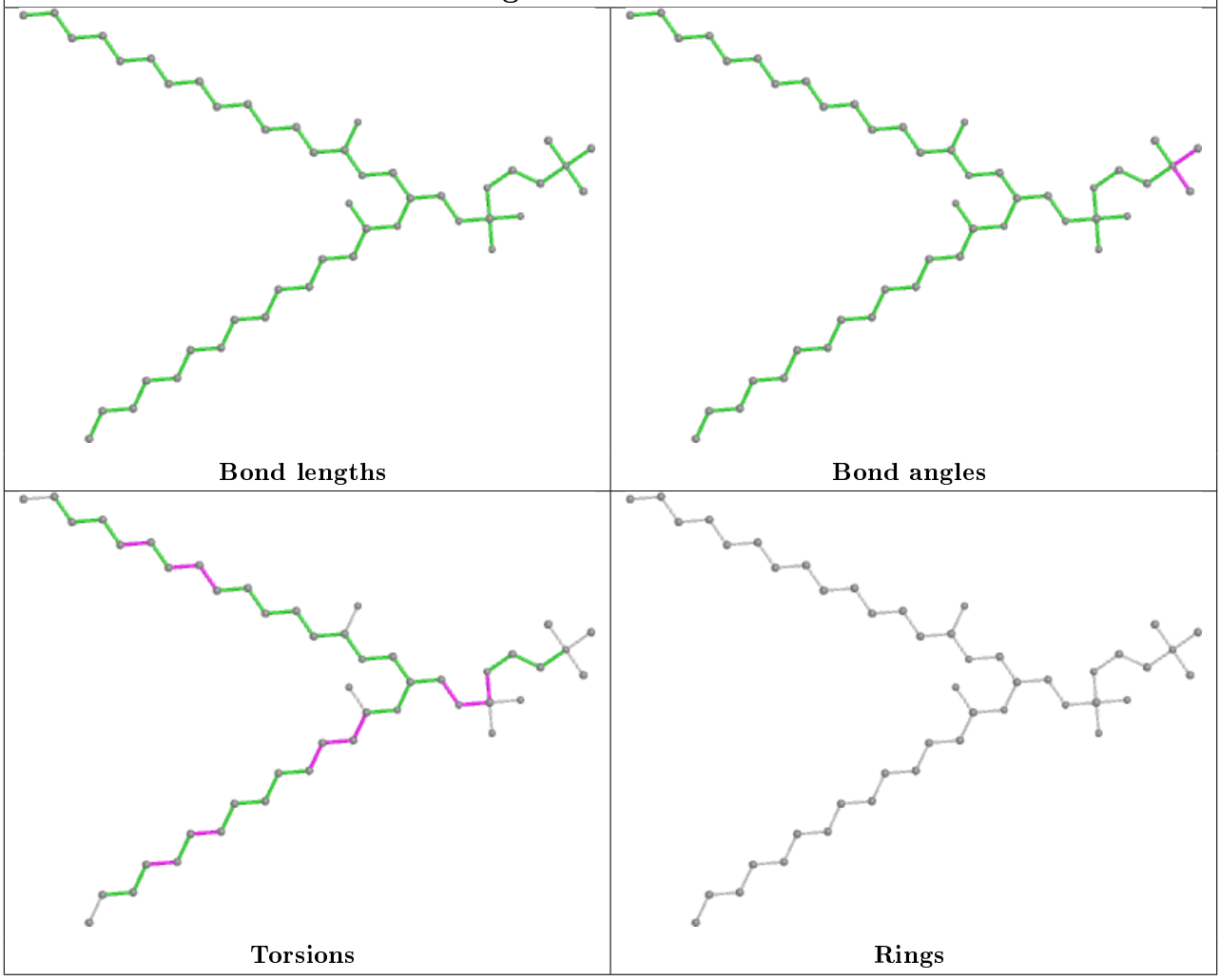


Torsions

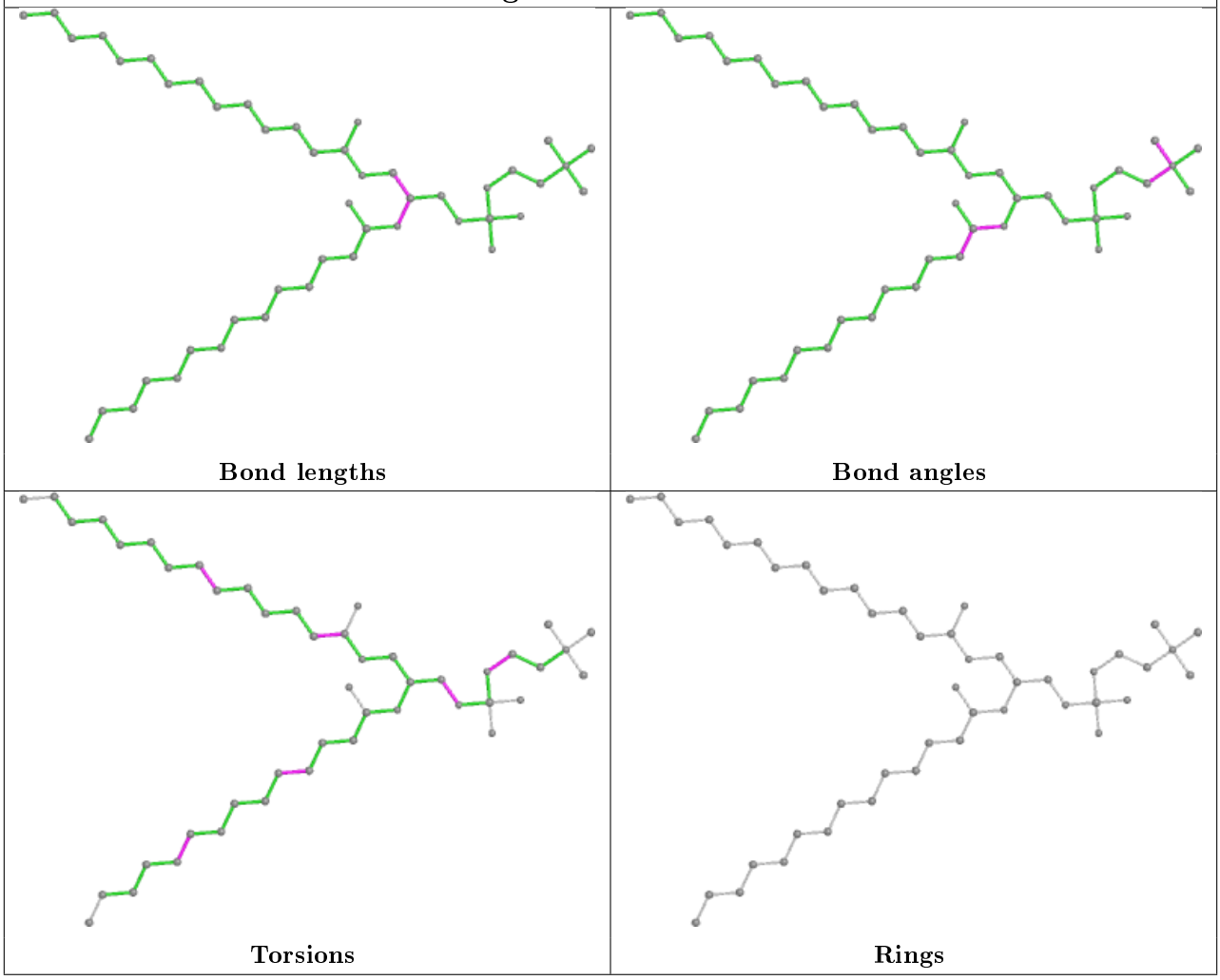


Rings

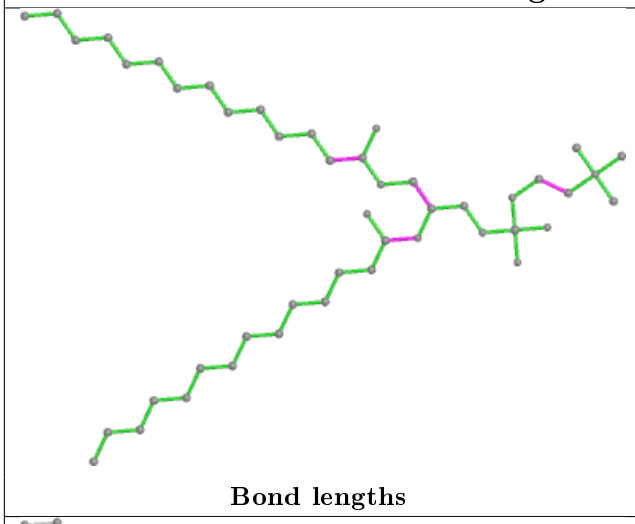
Ligand PX4 C 328



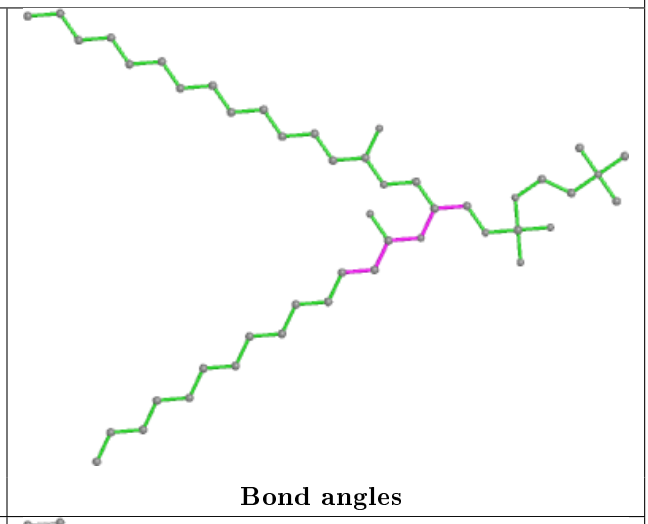
Ligand PX4 B 326



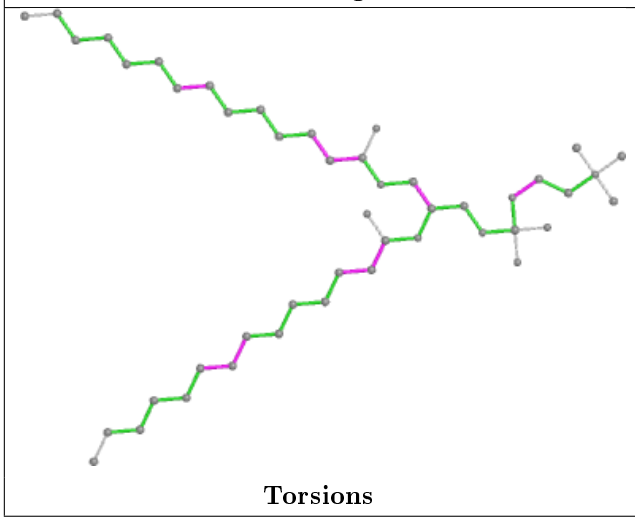
Ligand PX4 B 393



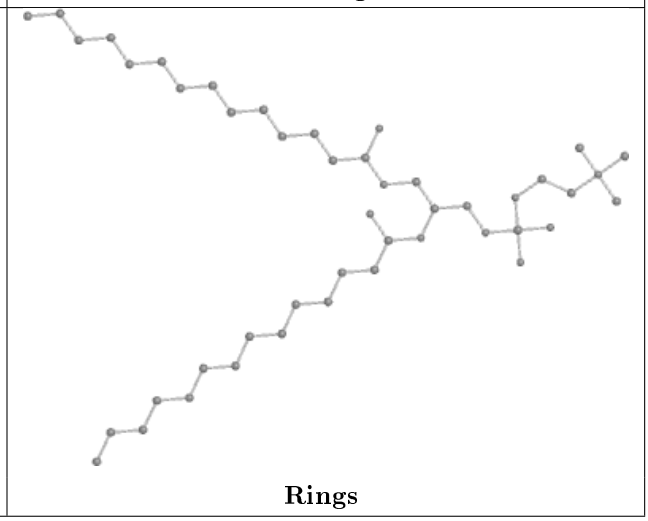
Bond lengths



Bond angles

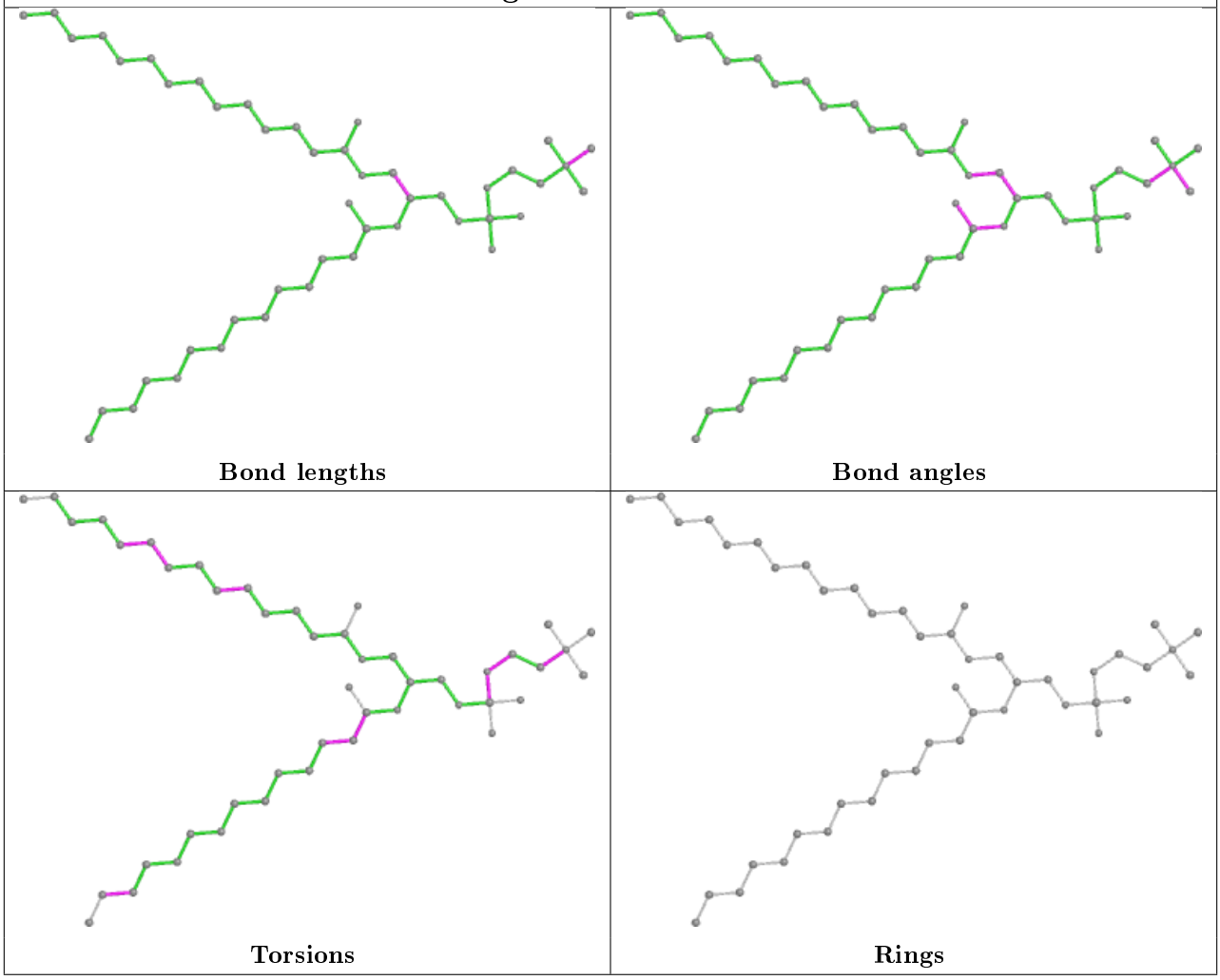


Torsions

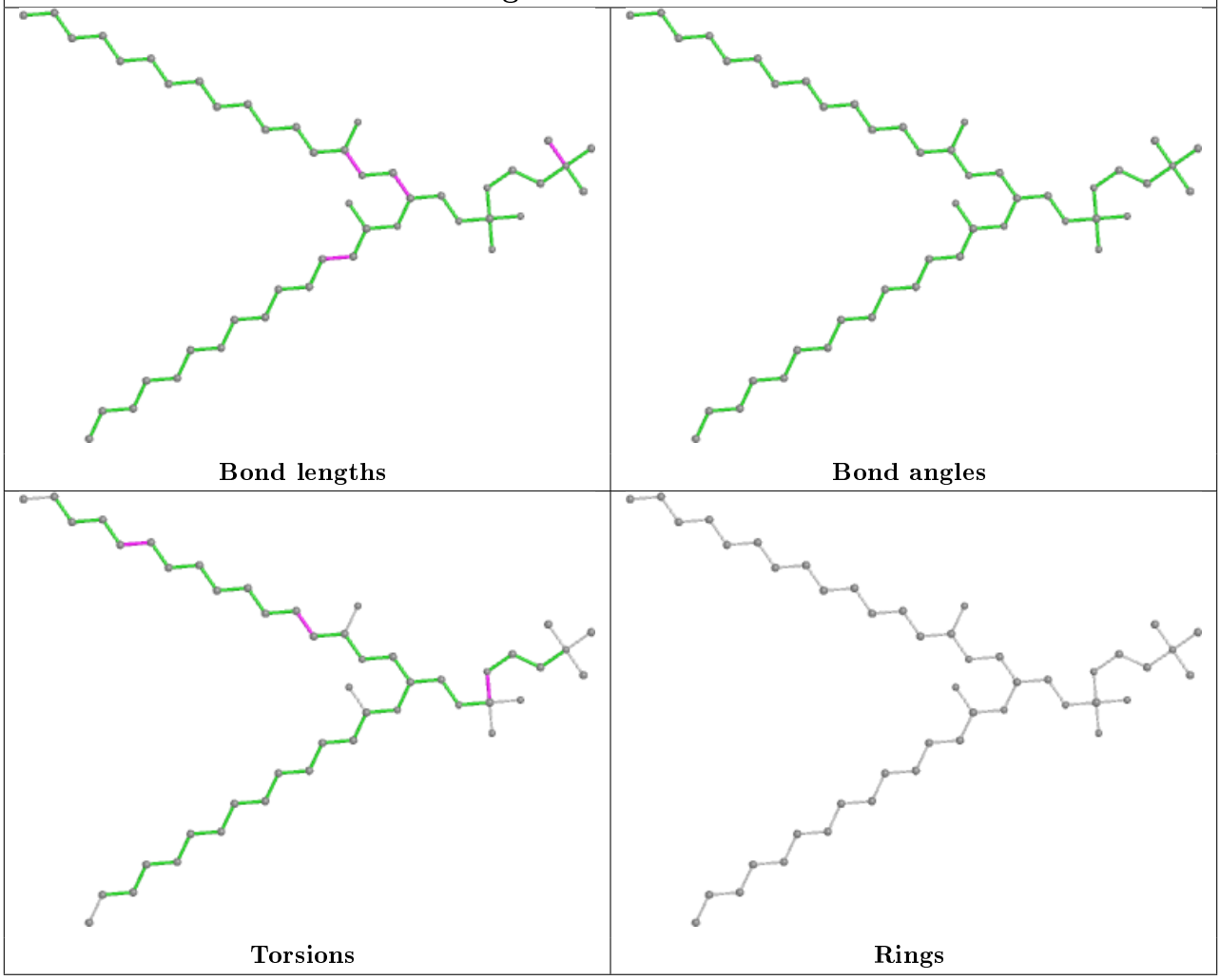


Rings

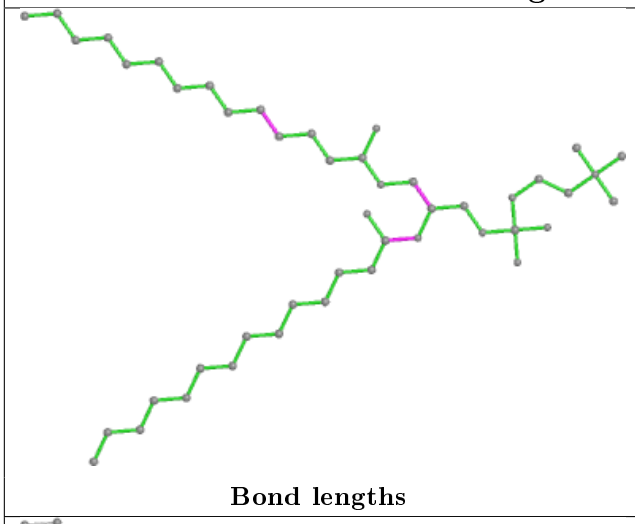
Ligand PX4 C 360



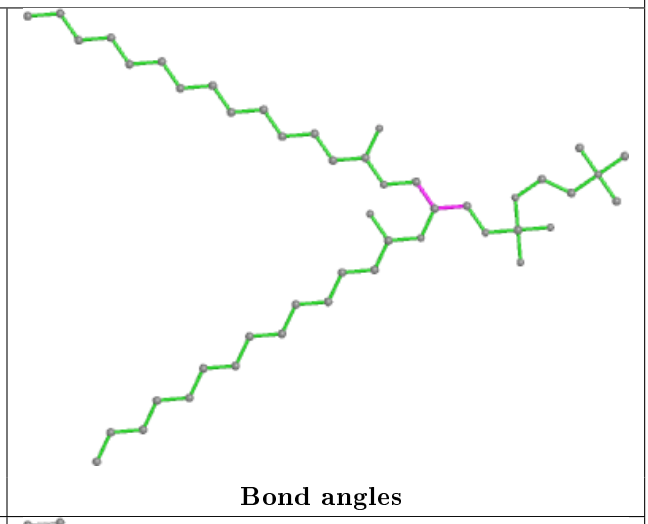
Ligand PX4 C 354



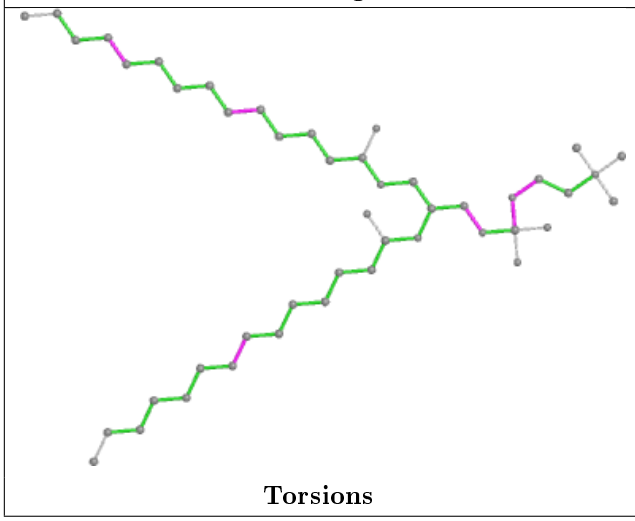
Ligand PX4 C 319



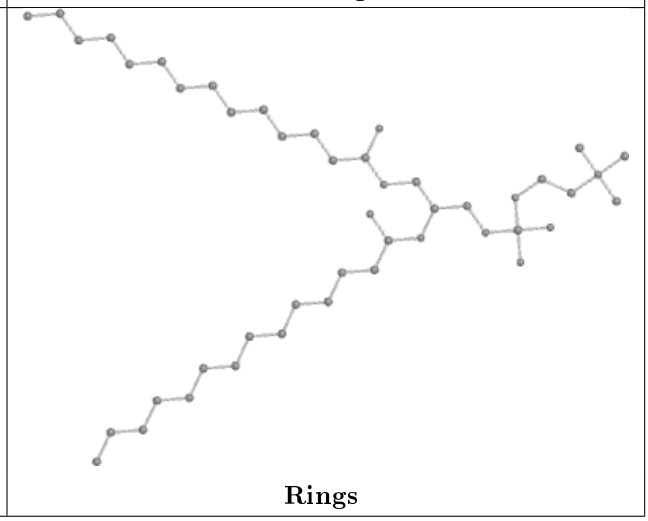
Bond lengths



Bond angles

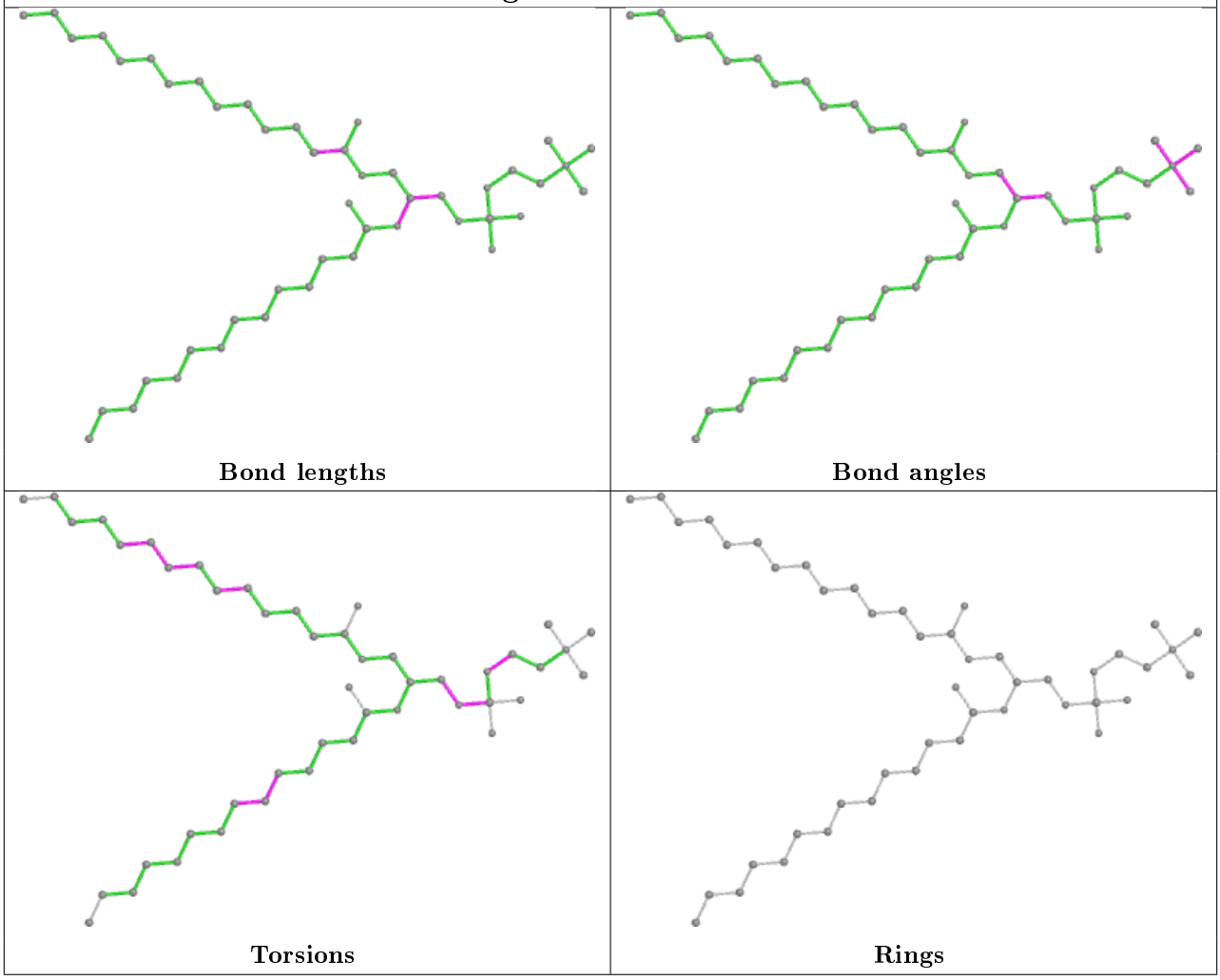


Torsions

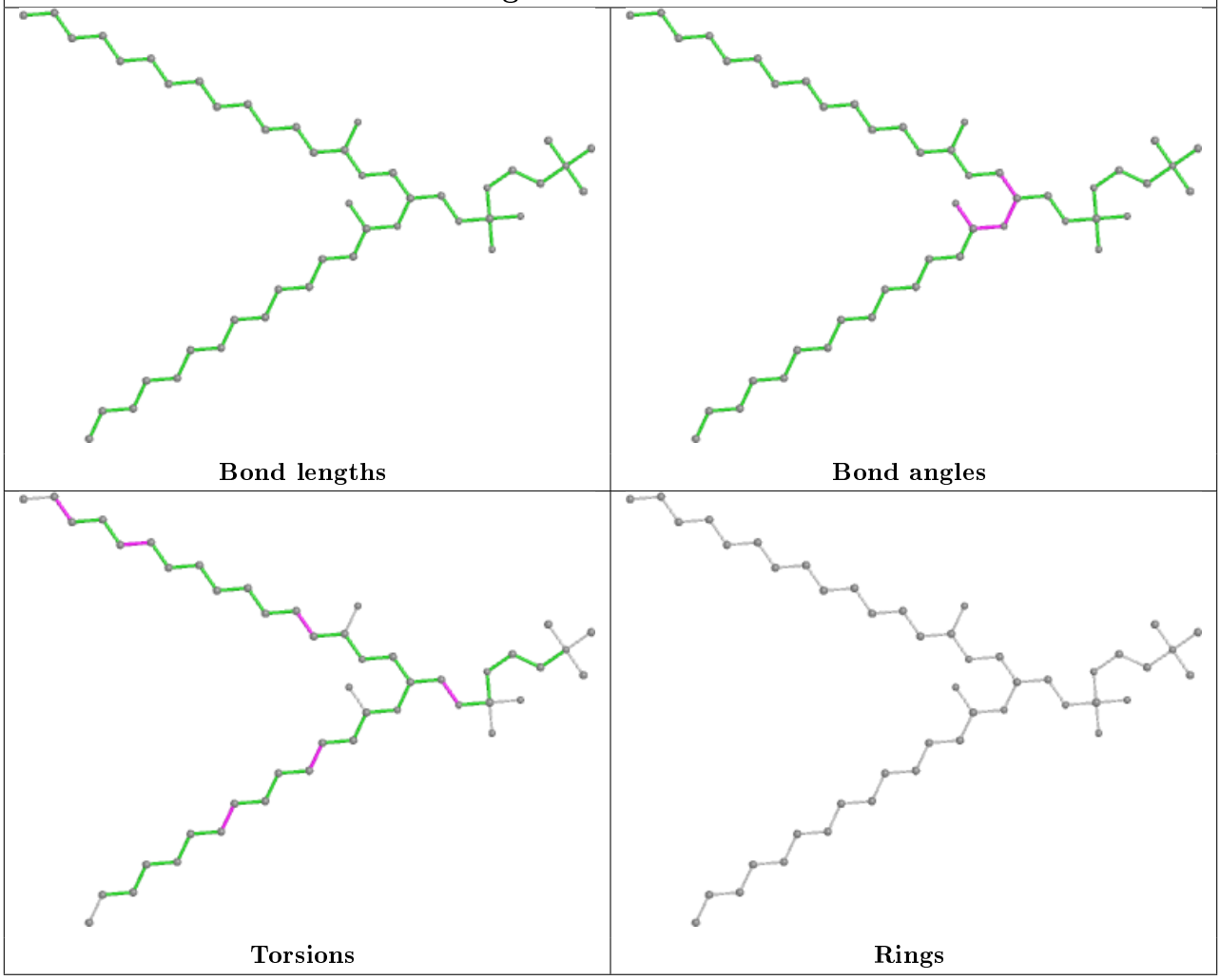


Rings

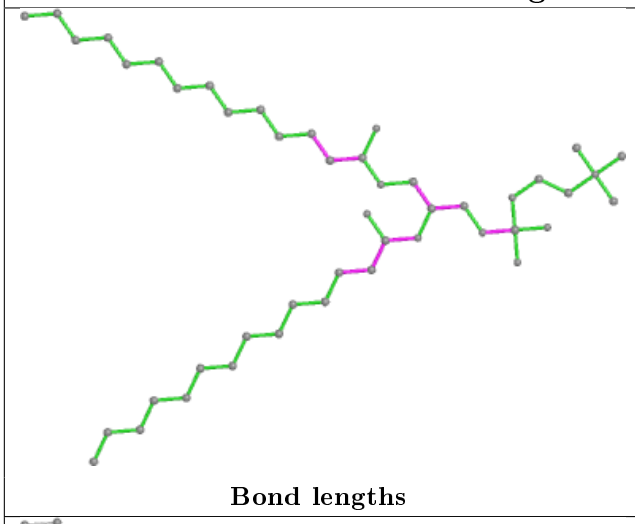
Ligand PX4 C 312



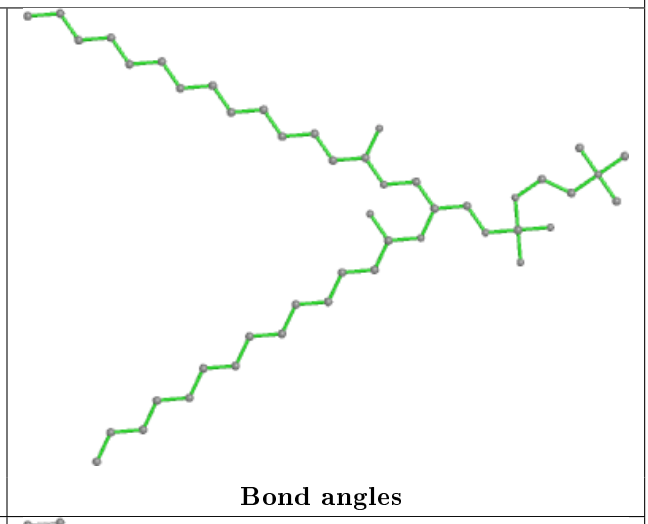
Ligand PX4 B 339



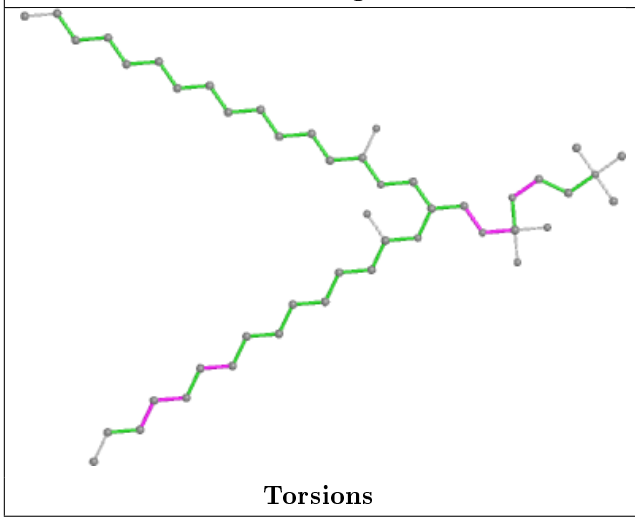
Ligand PX4 B 350



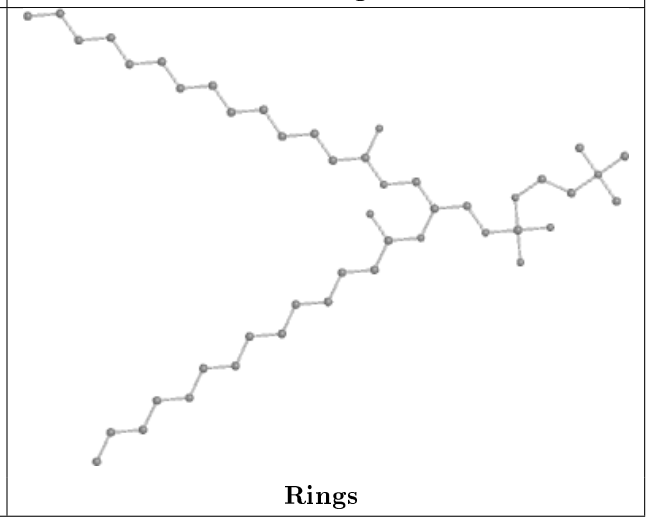
Bond lengths



Bond angles

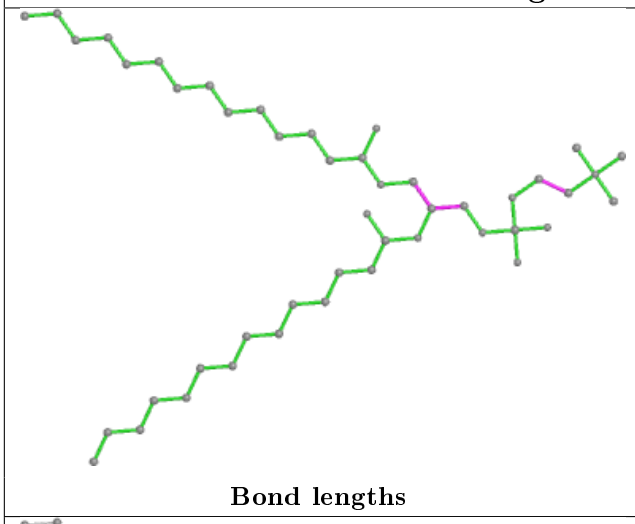


Torsions

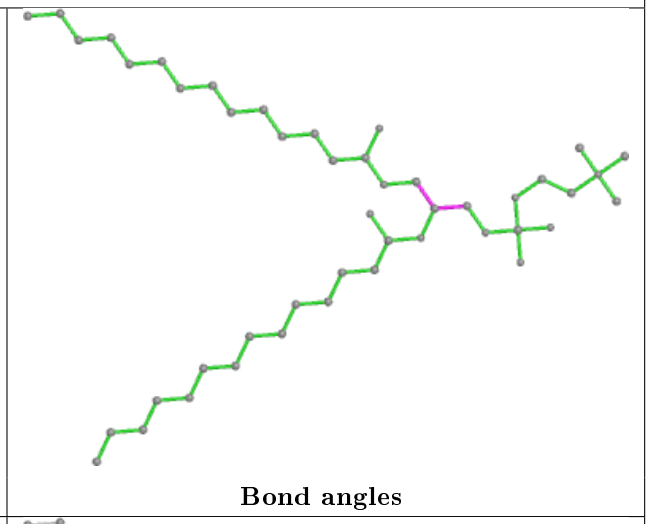


Rings

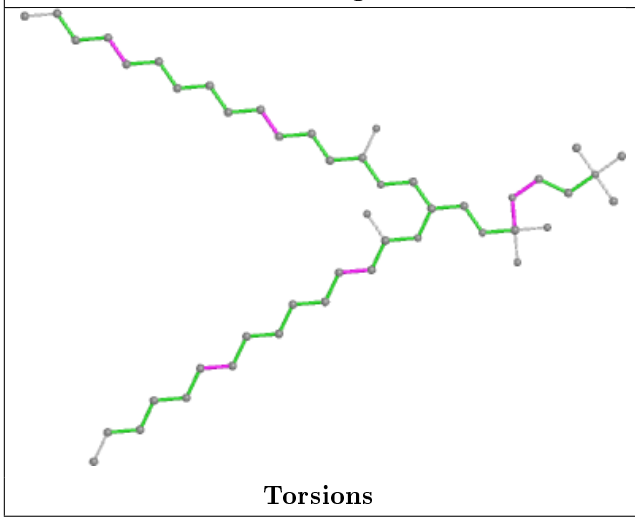
Ligand PX4 B 346



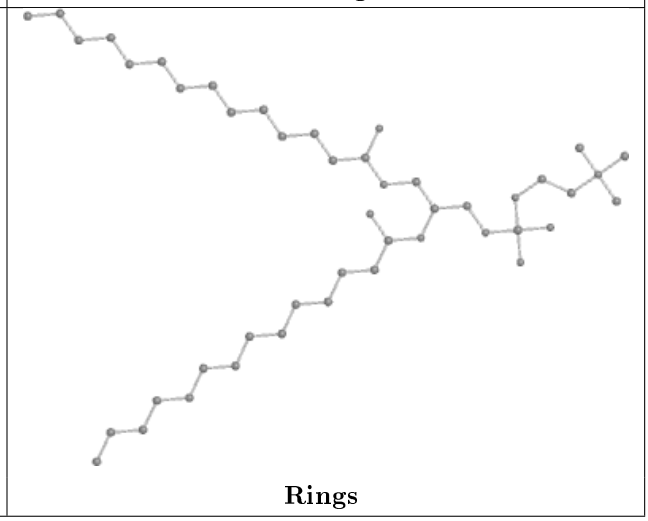
Bond lengths



Bond angles

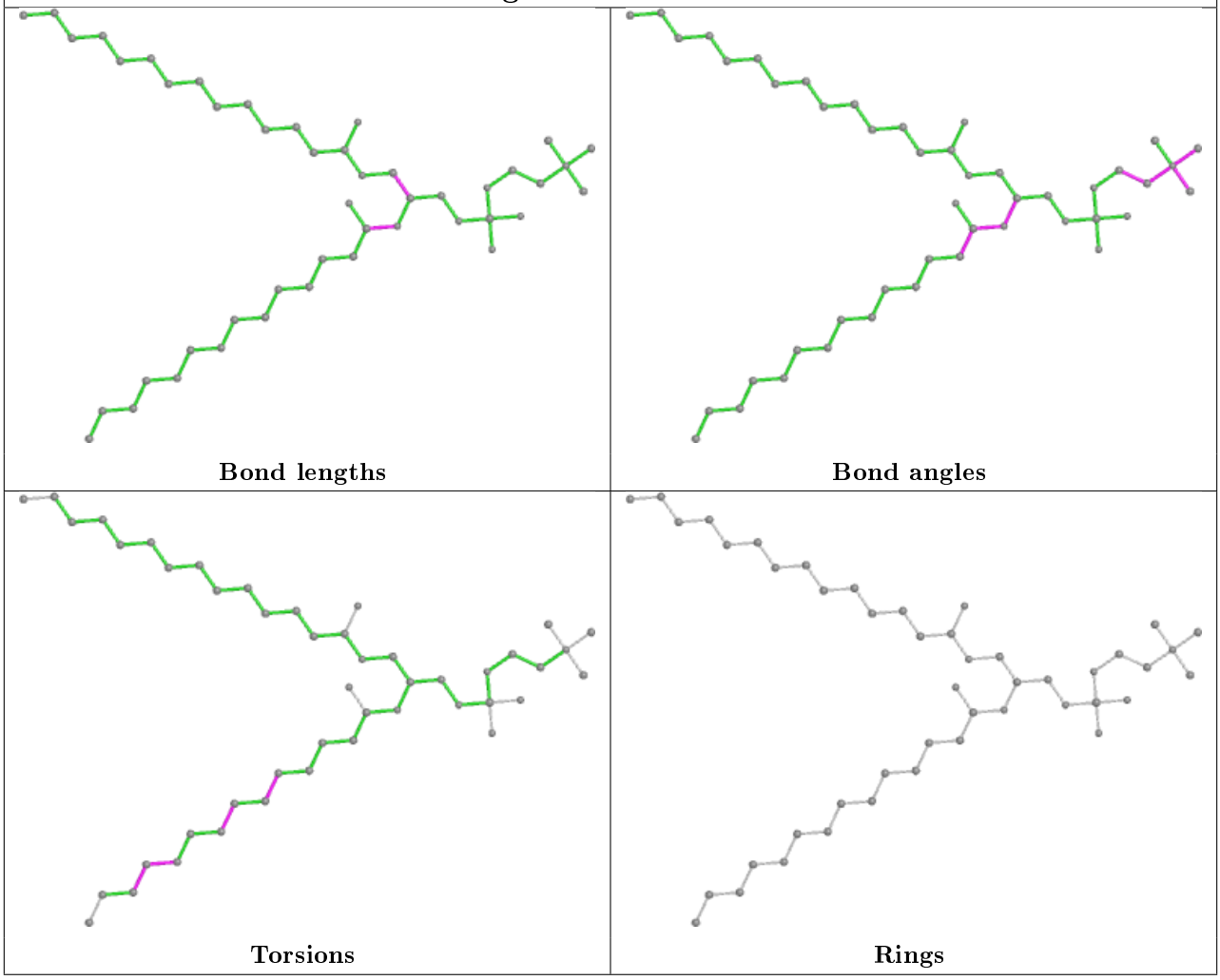


Torsions

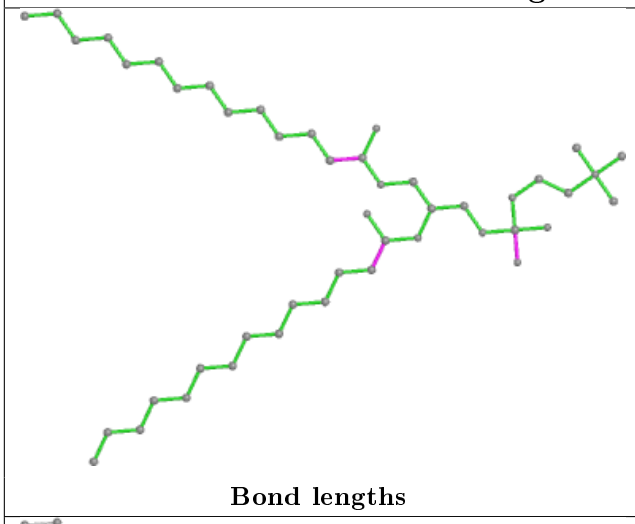


Rings

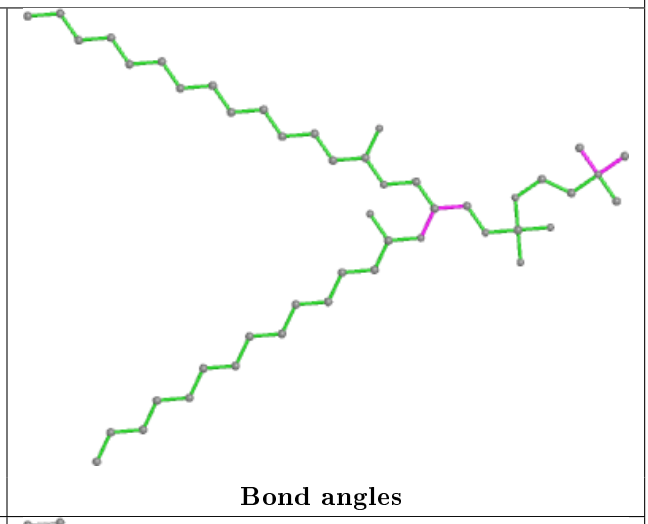
Ligand PX4 C 335



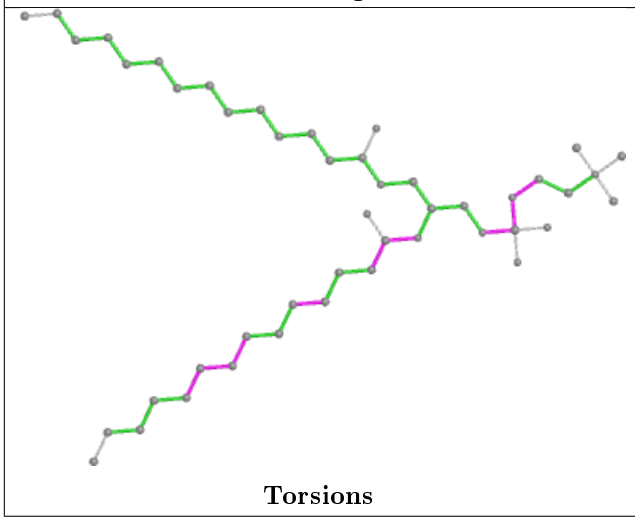
Ligand PX4 C 314



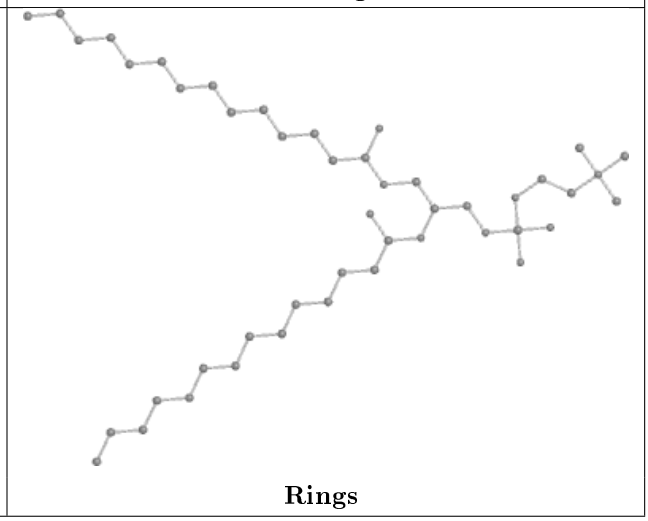
Bond lengths



Bond angles

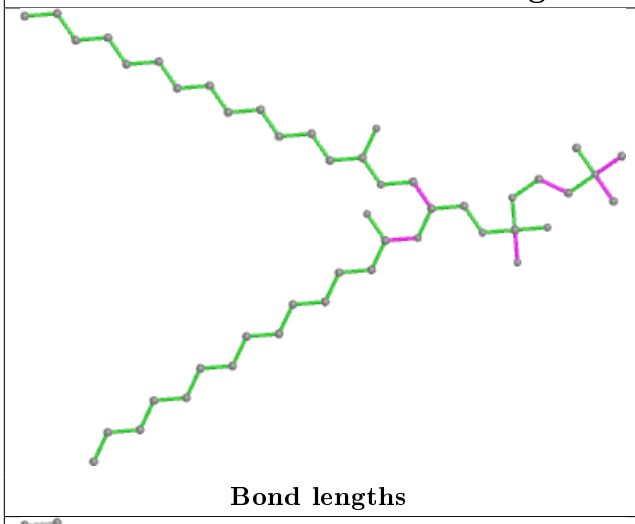


Torsions

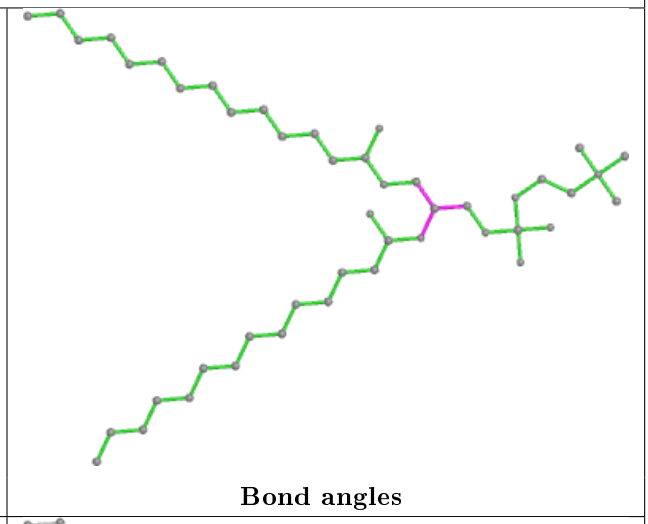


Rings

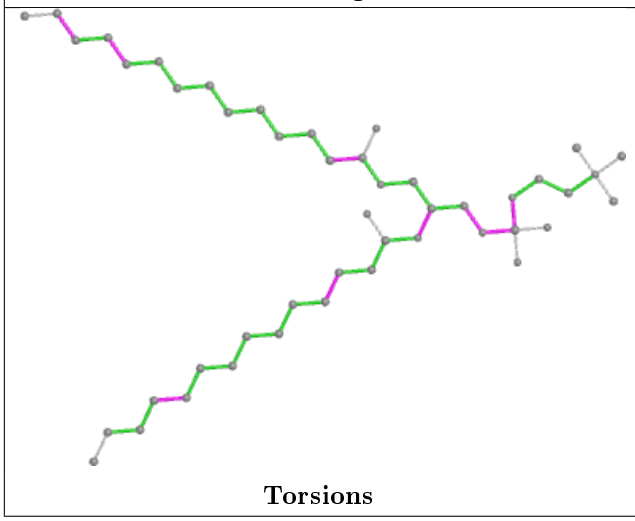
Ligand PX4 B 376



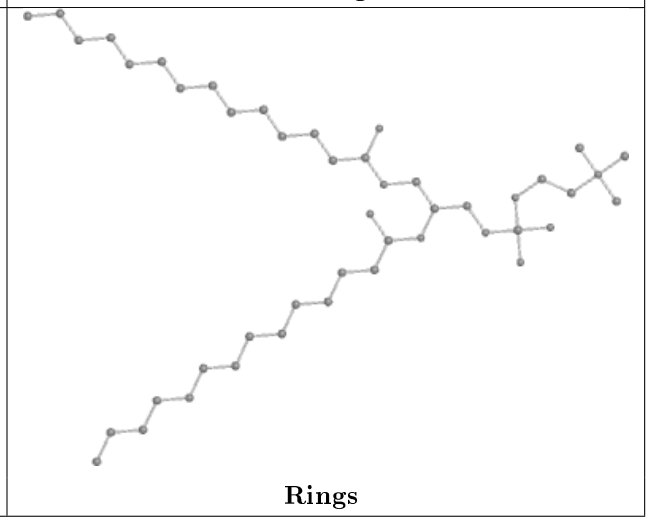
Bond lengths



Bond angles

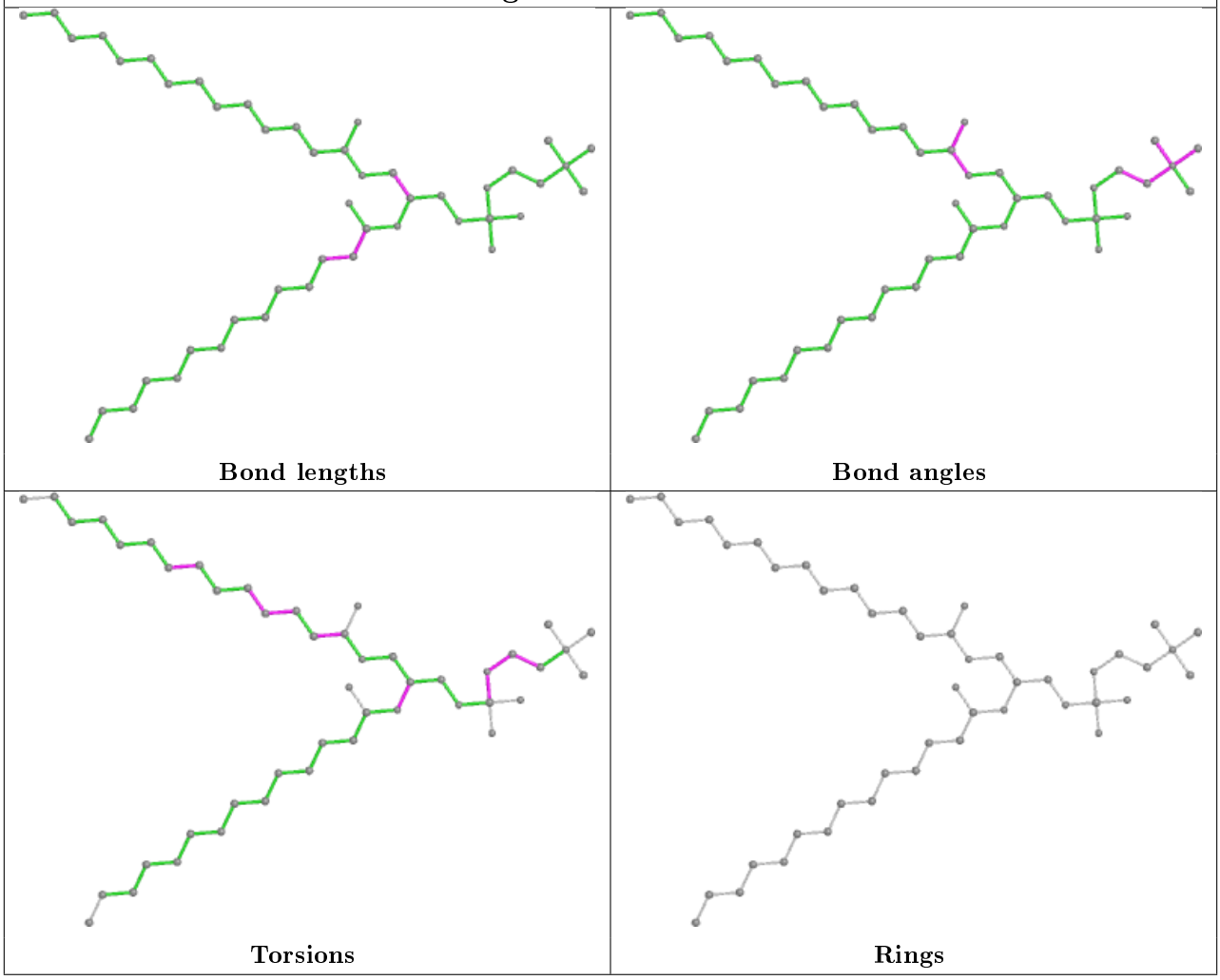


Torsions

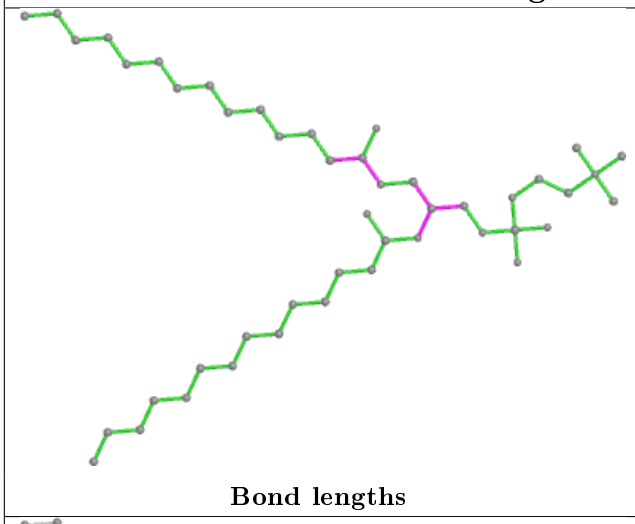


Rings

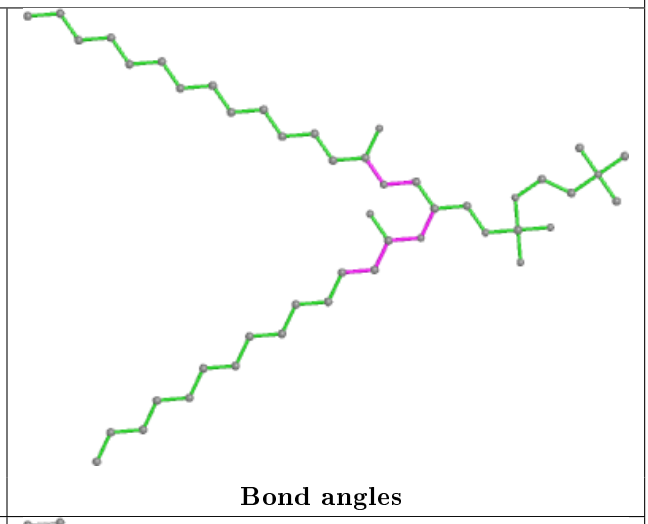
Ligand PX4 B 383



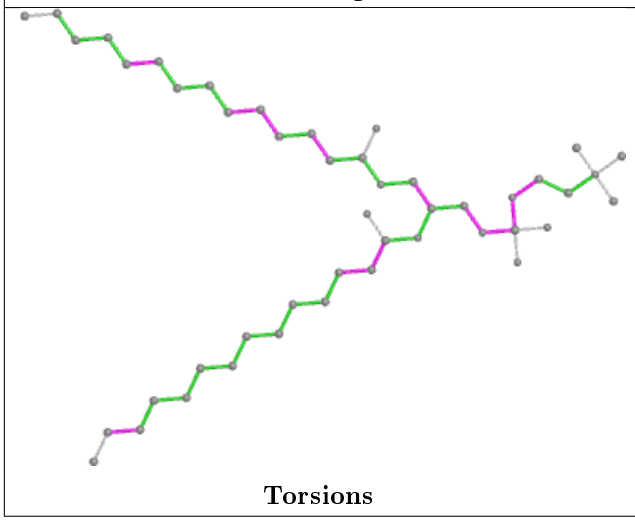
Ligand PX4 B 304



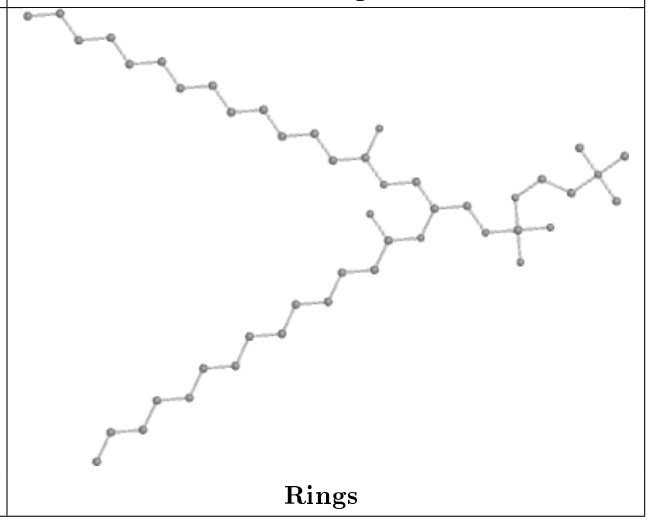
Bond lengths



Bond angles

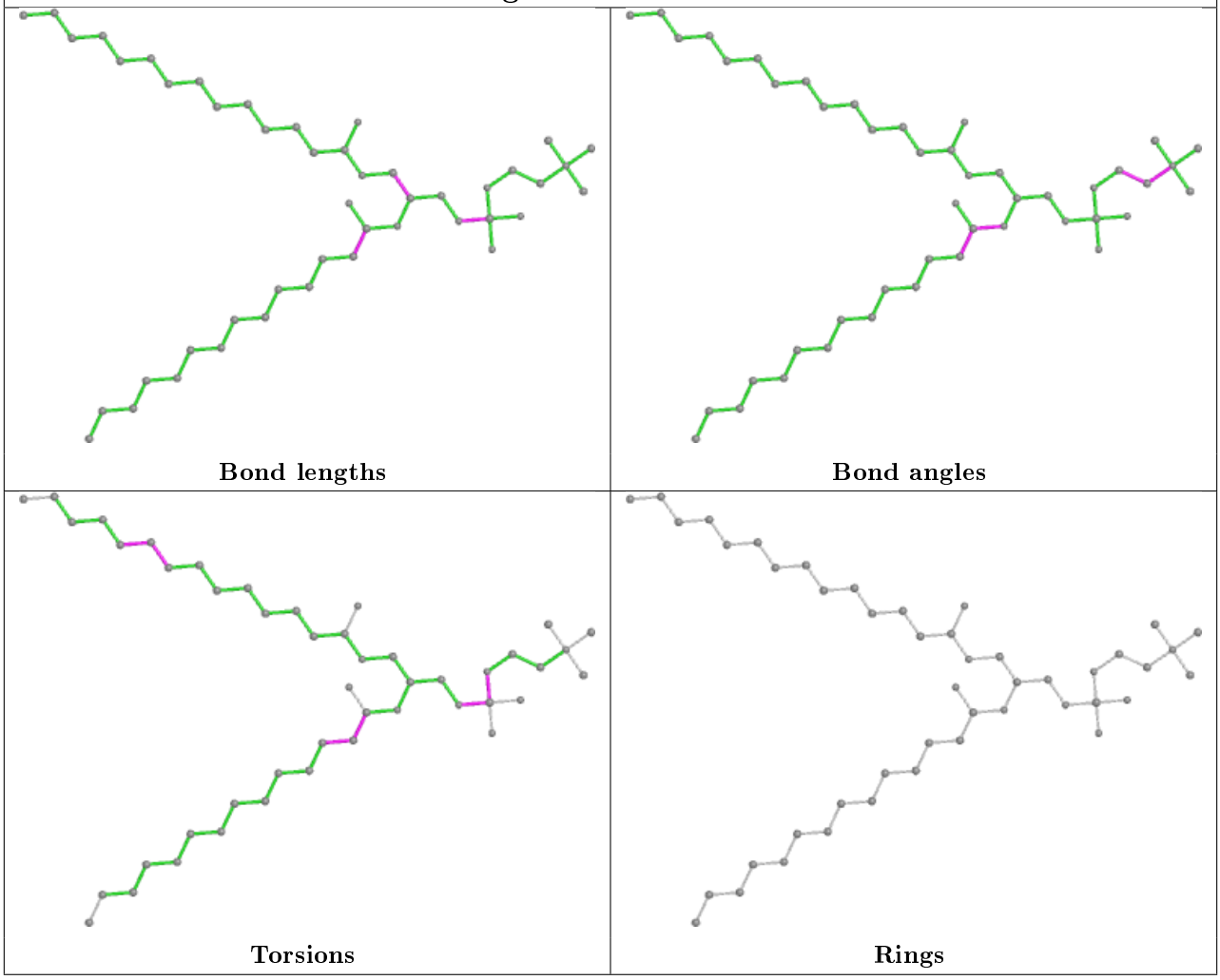


Torsions

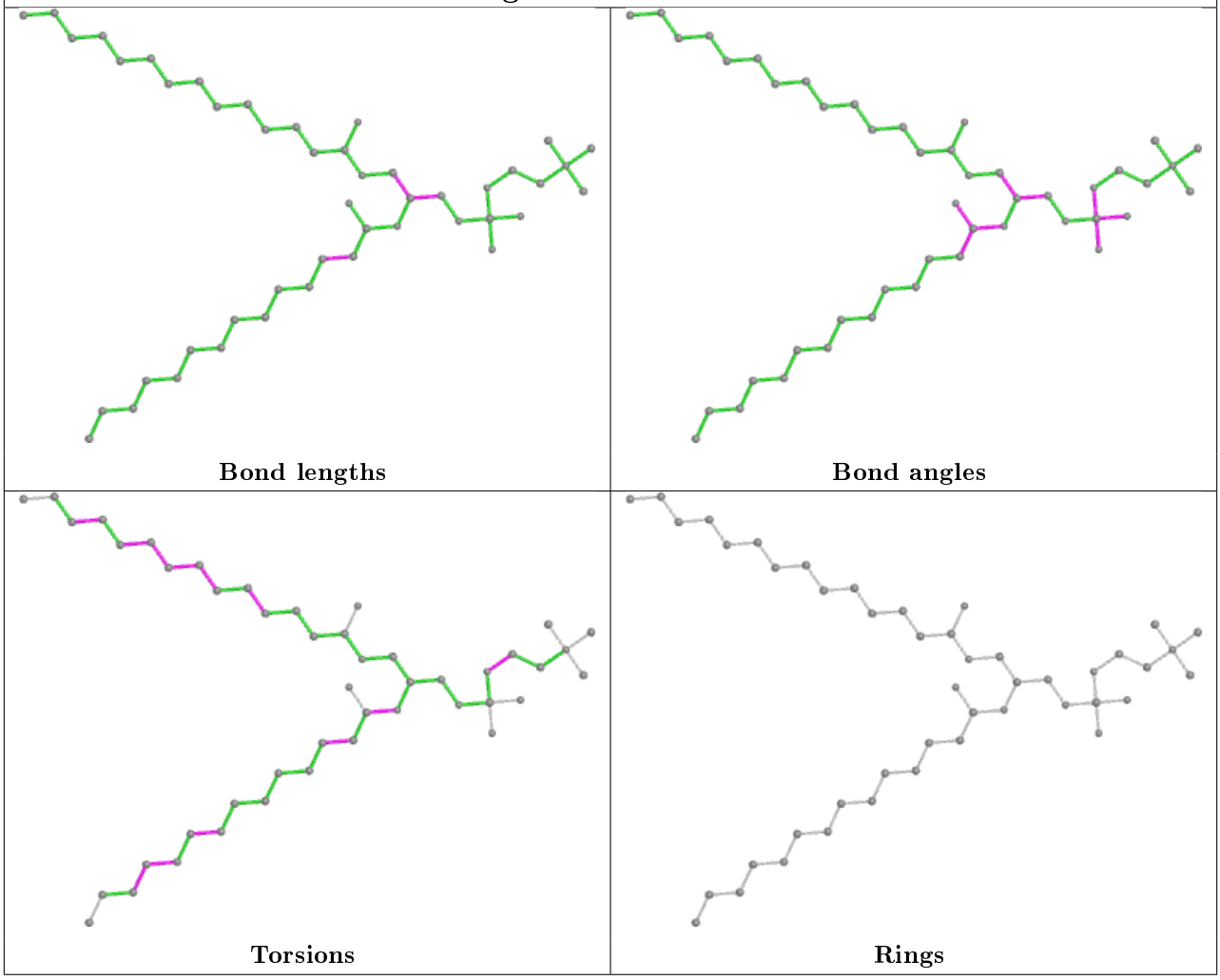


Rings

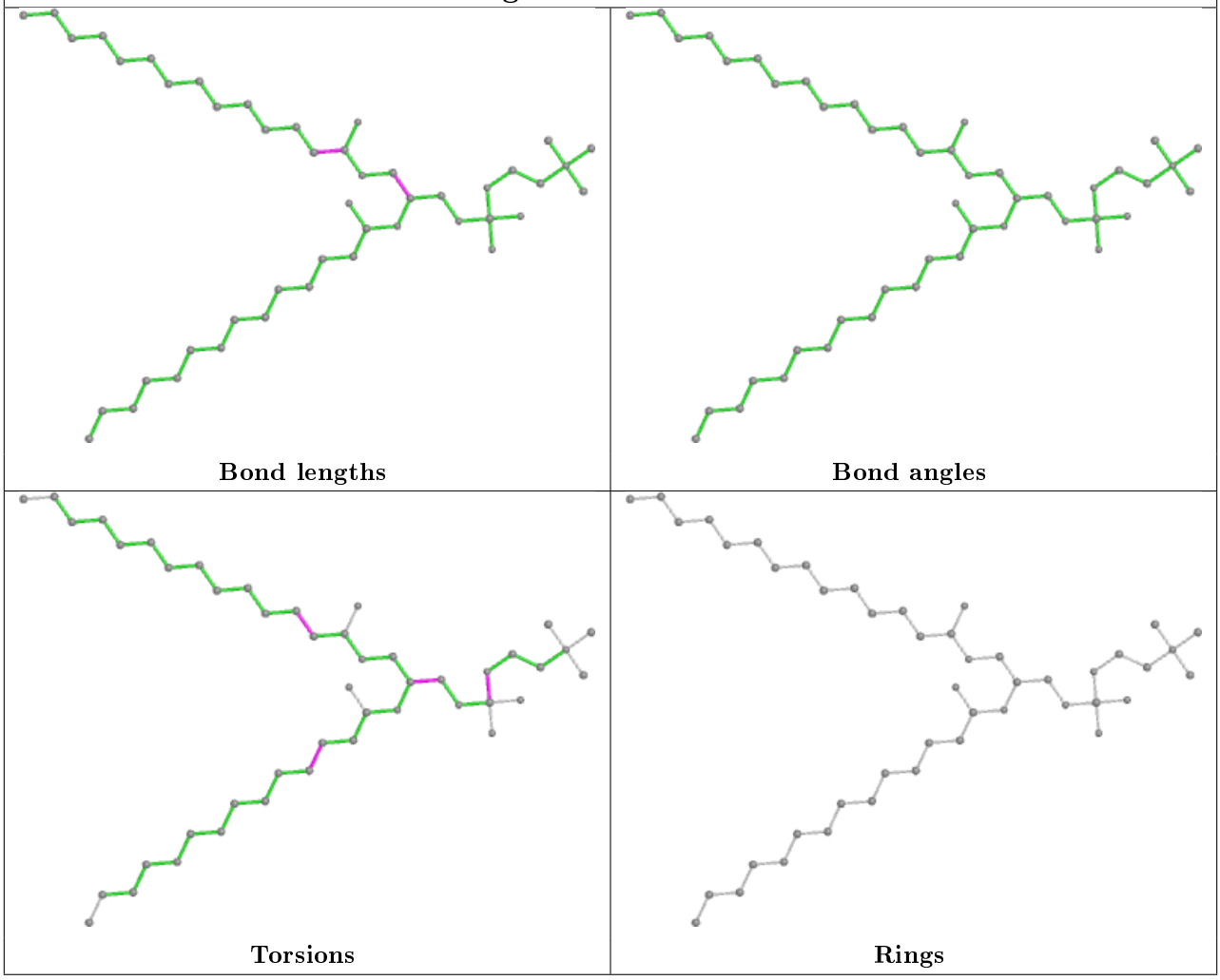
Ligand PX4 B 355



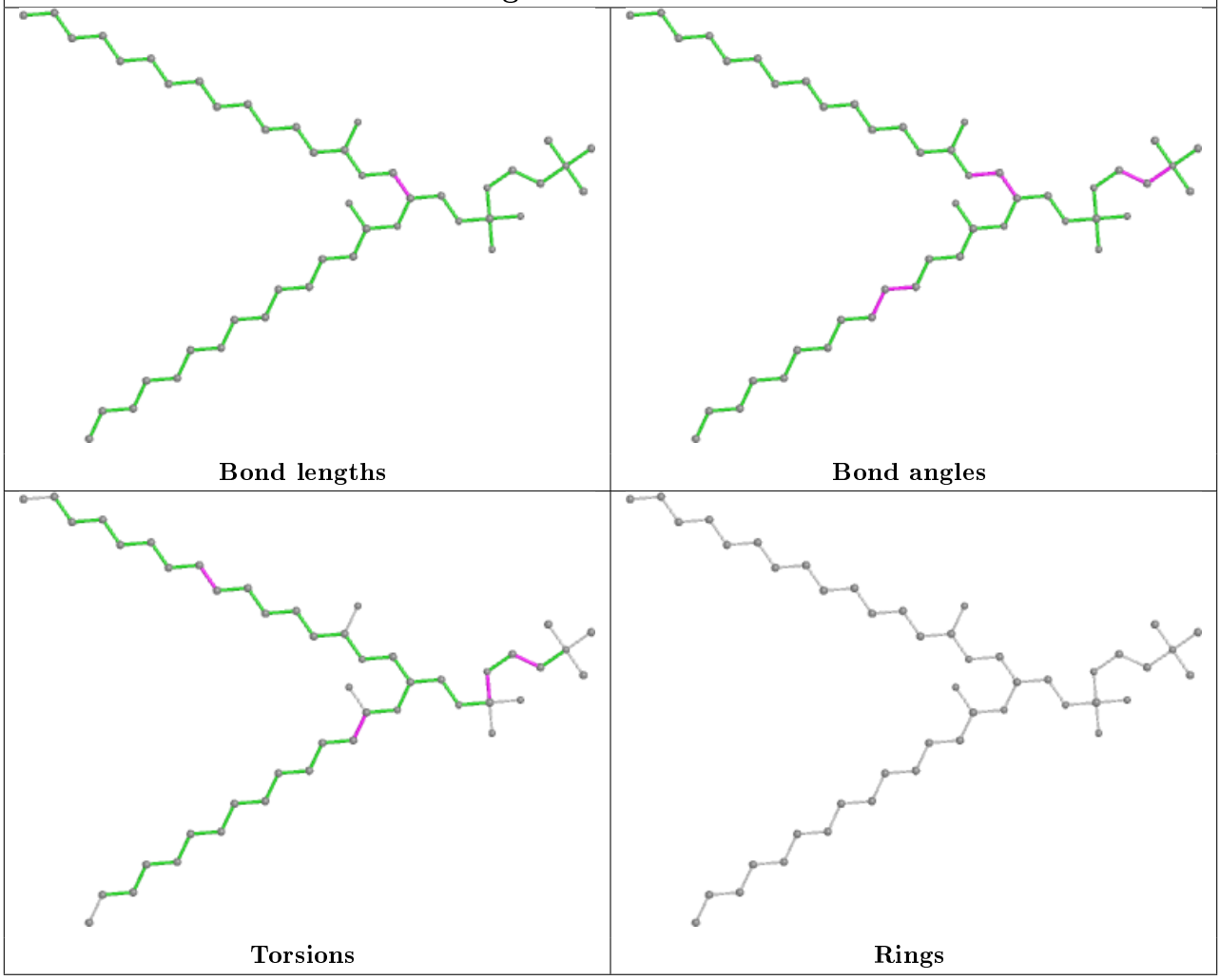
Ligand PX4 C 343



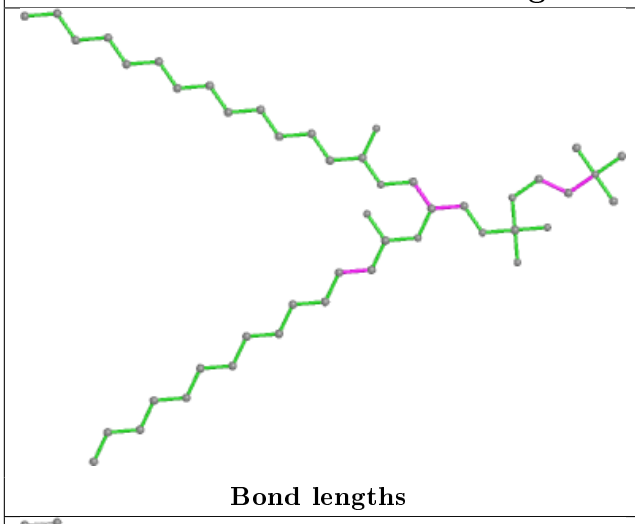
Ligand PX4 B 388



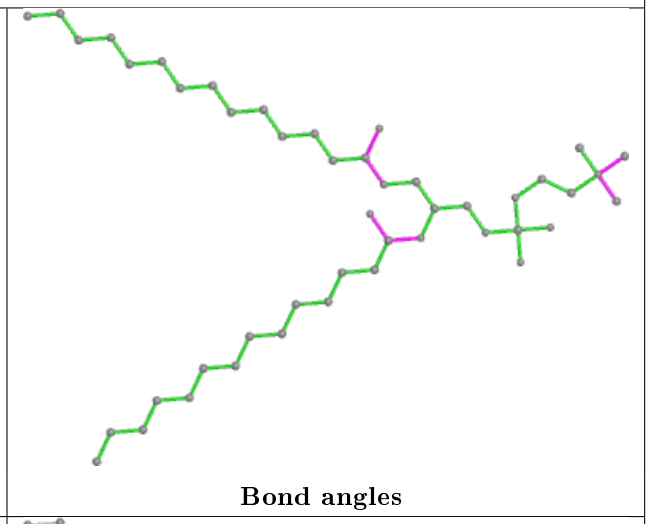
Ligand PX4 B 382



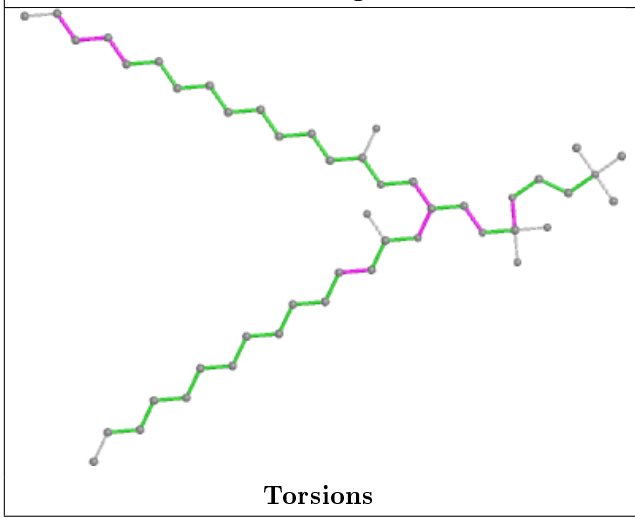
Ligand PX4 C 359



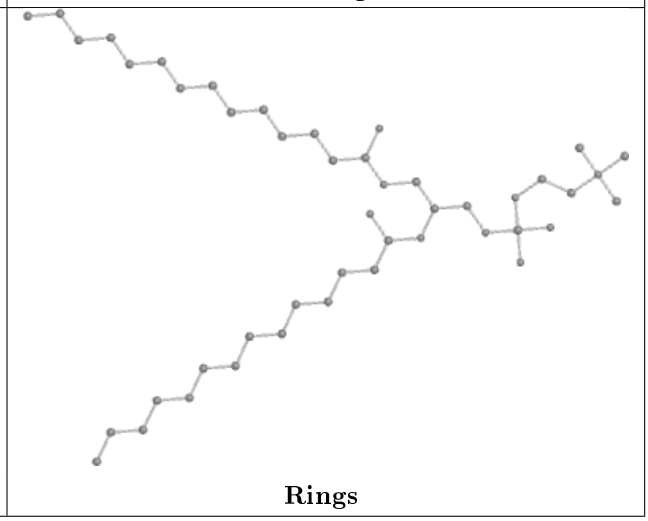
Bond lengths



Bond angles

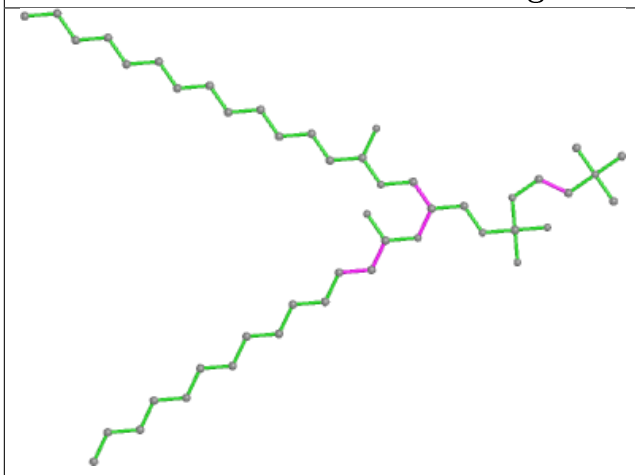


Torsions

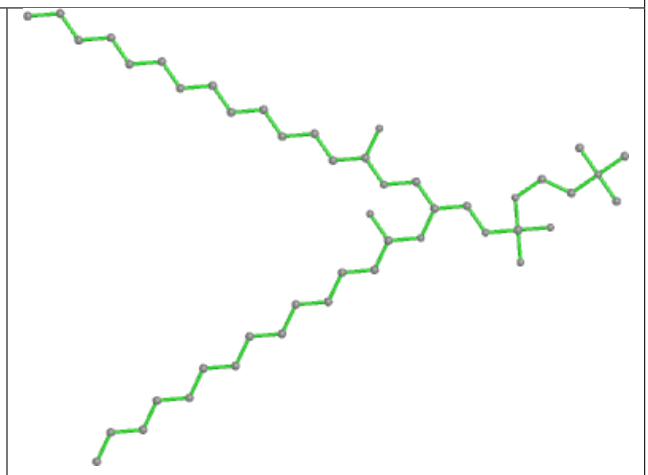


Rings

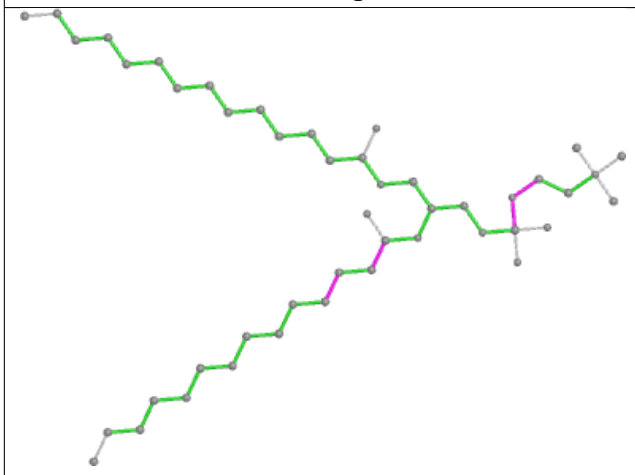
Ligand PX4 A 631



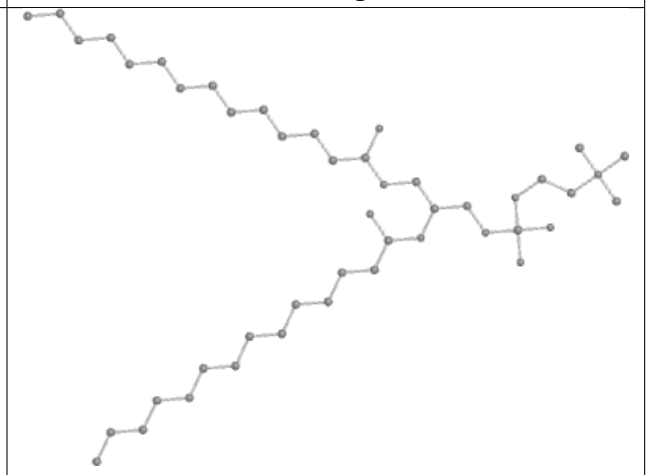
Bond lengths



Bond angles

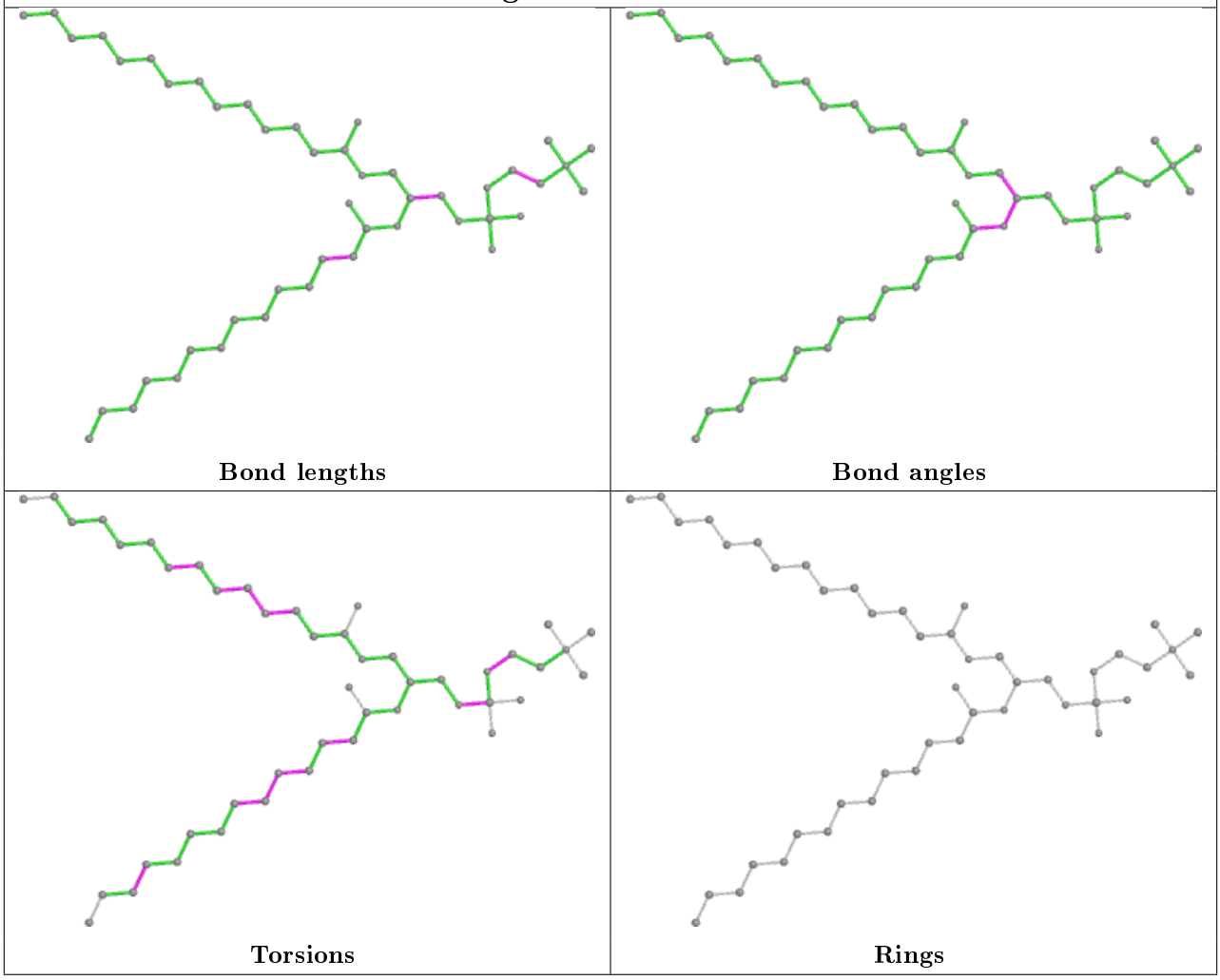


Torsions

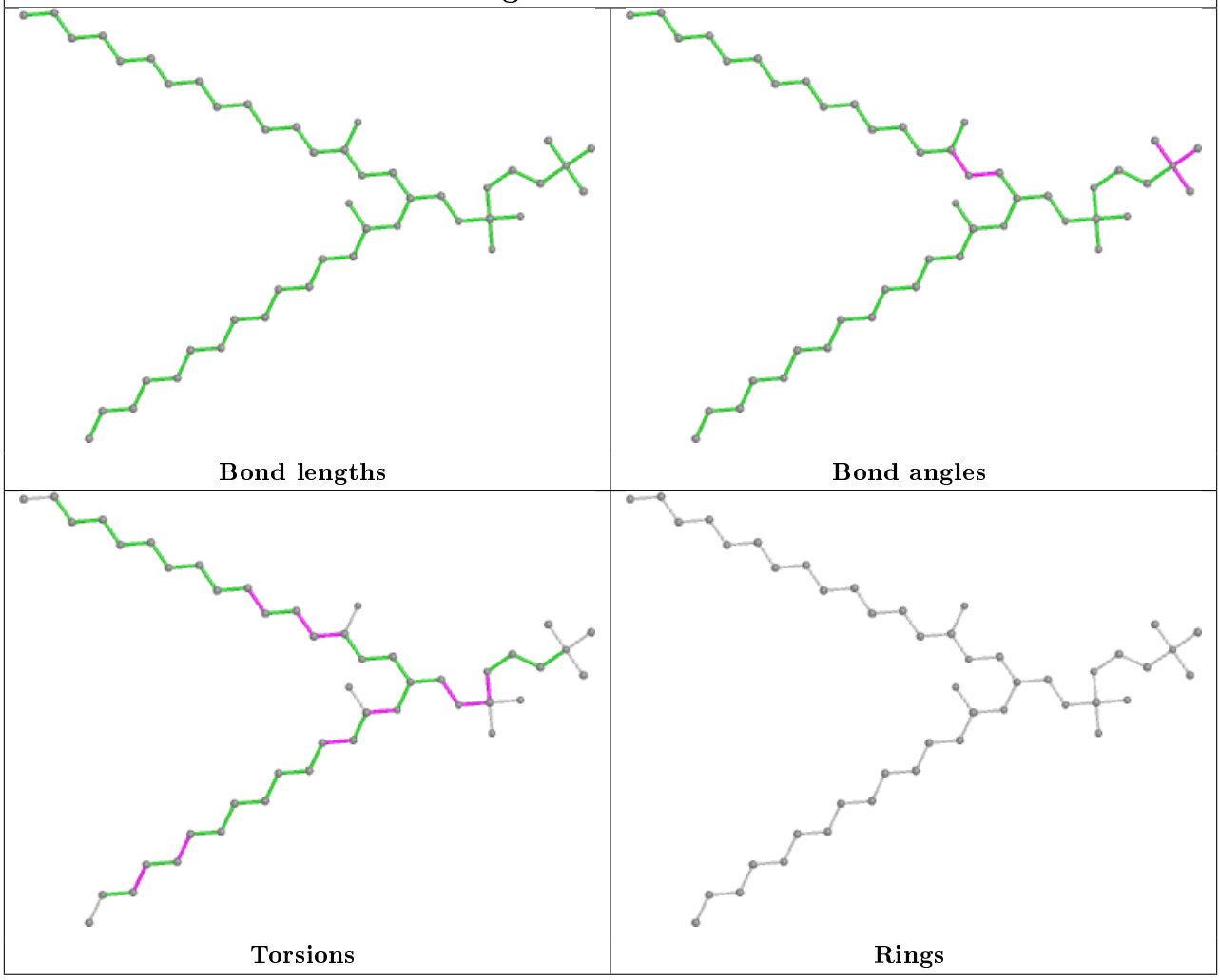


Rings

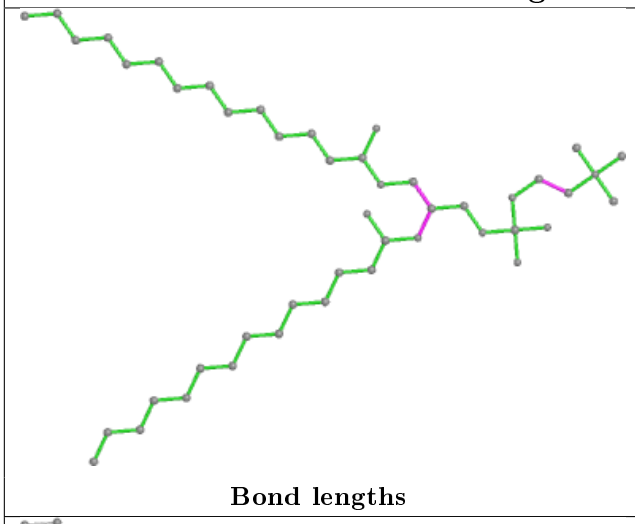
Ligand PX4 C 340



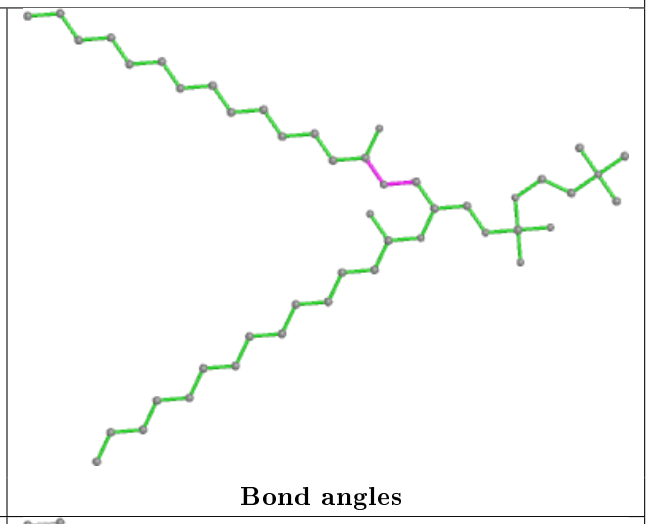
Ligand PX4 B 332



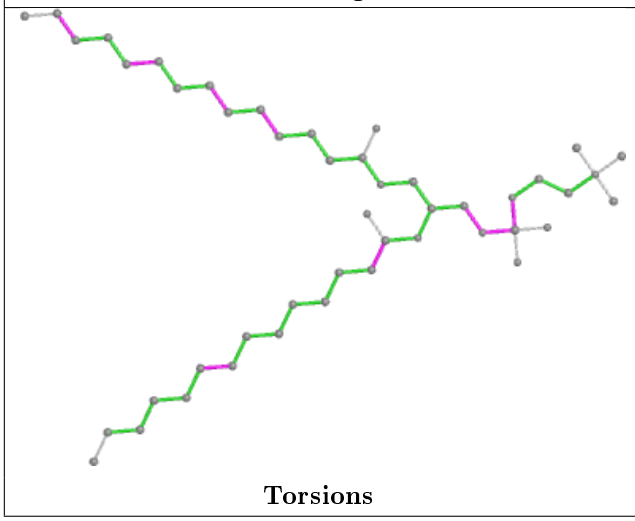
Ligand PX4 C 369



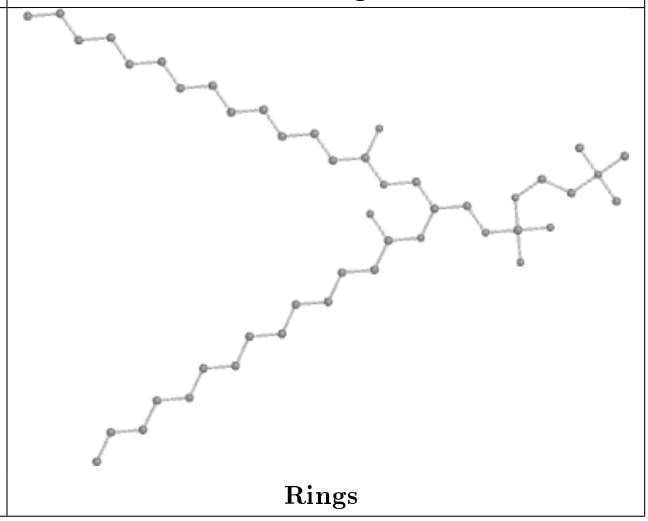
Bond lengths



Bond angles

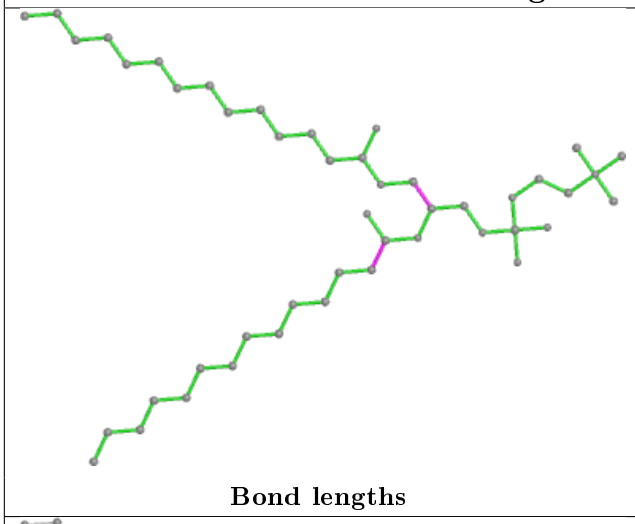


Torsions

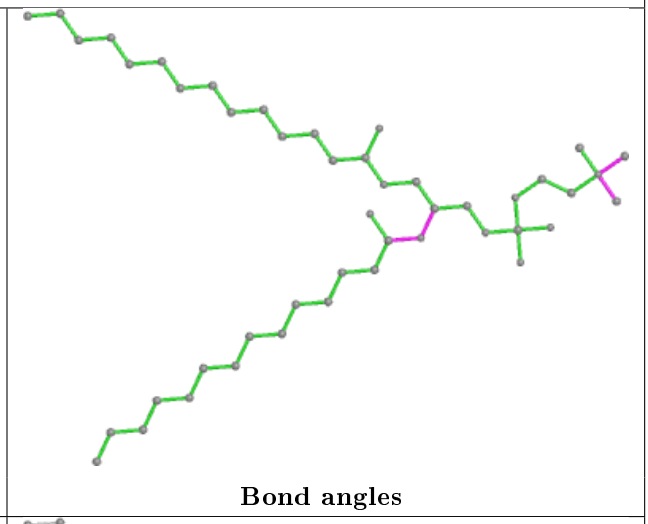


Rings

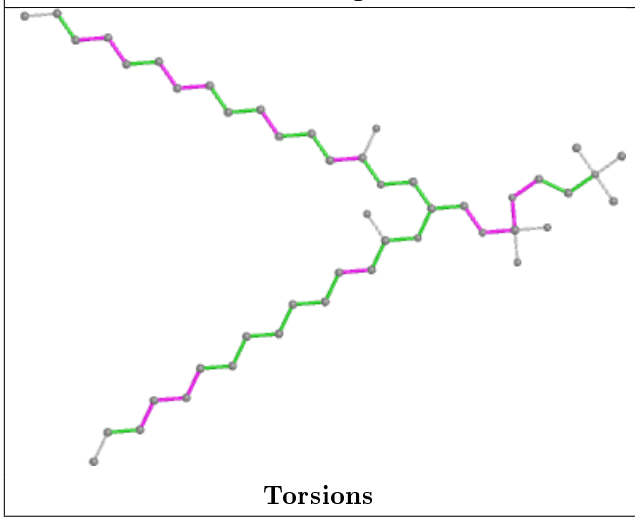
Ligand PX4 C 330



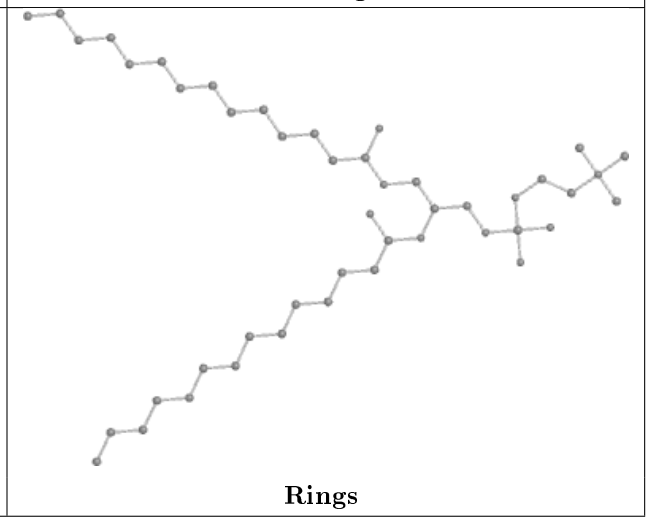
Bond lengths



Bond angles

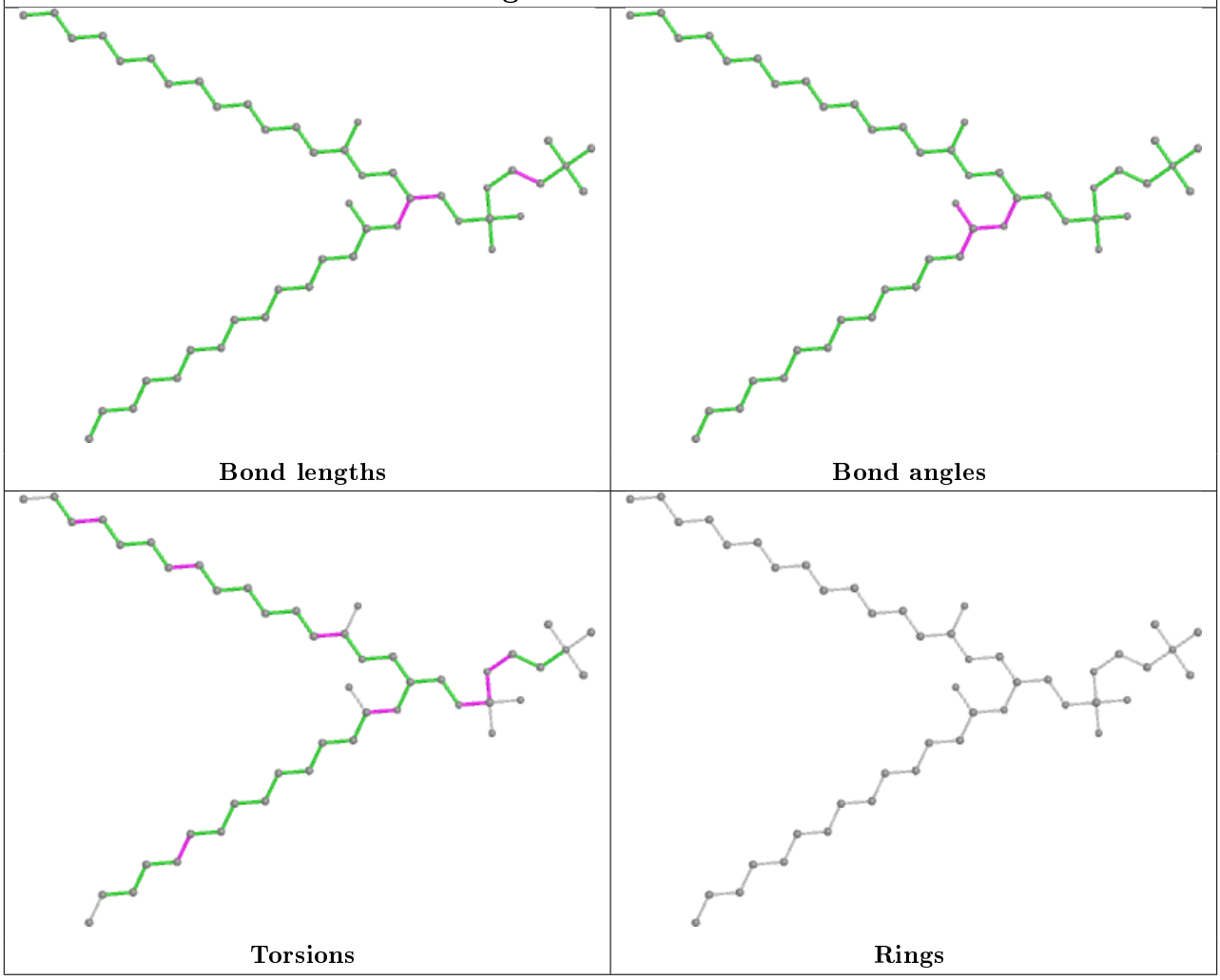


Torsions

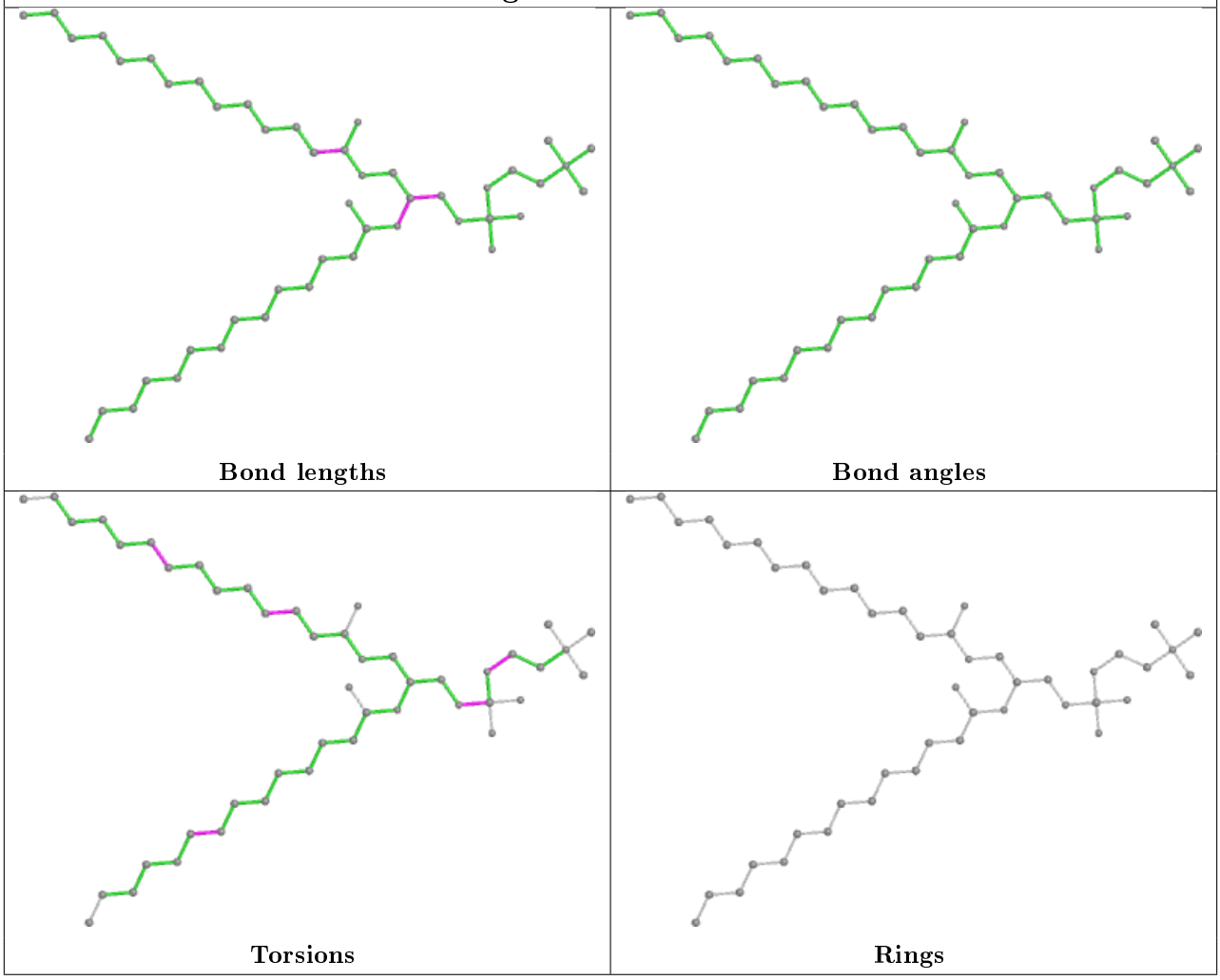


Rings

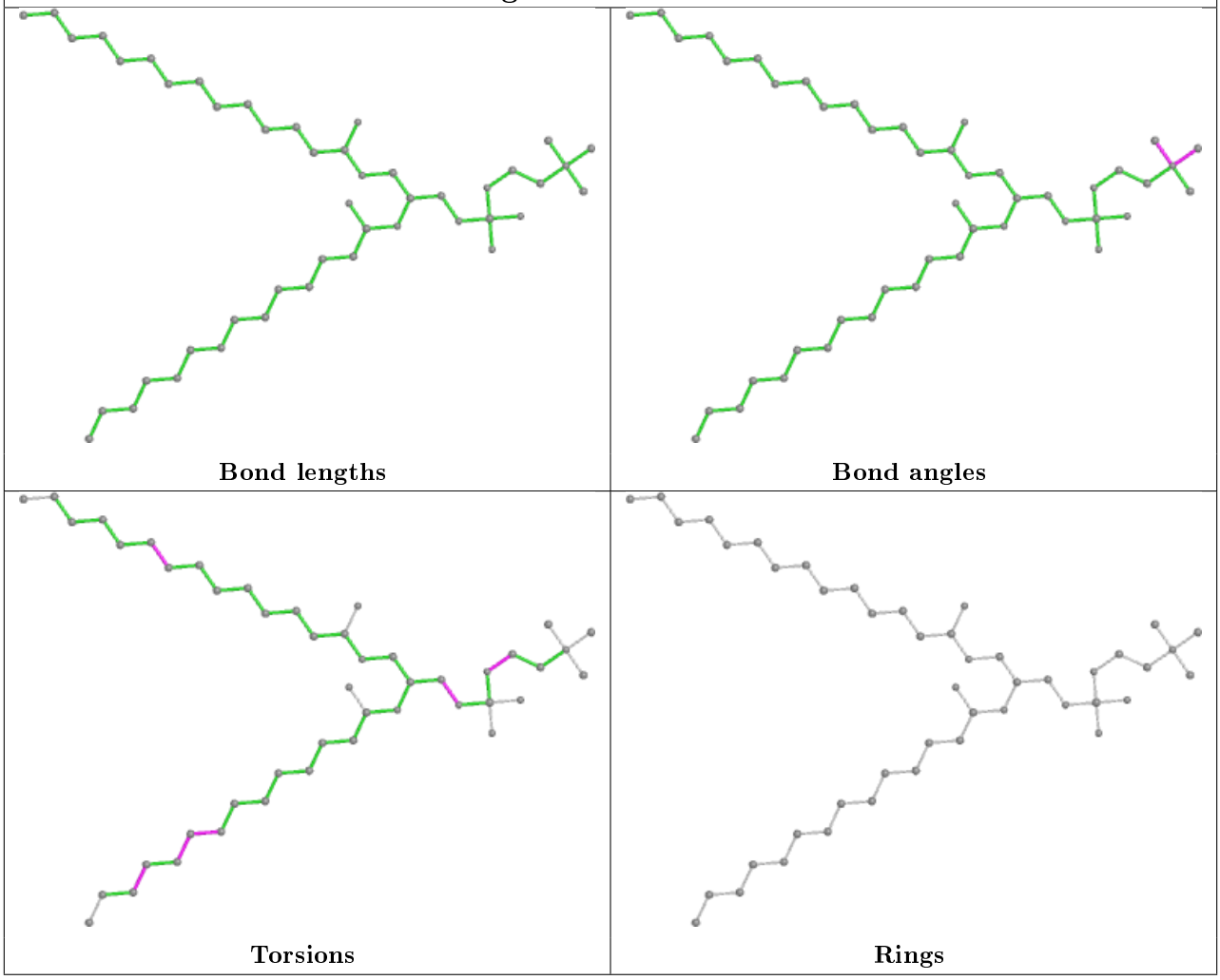
Ligand PX4 B 358



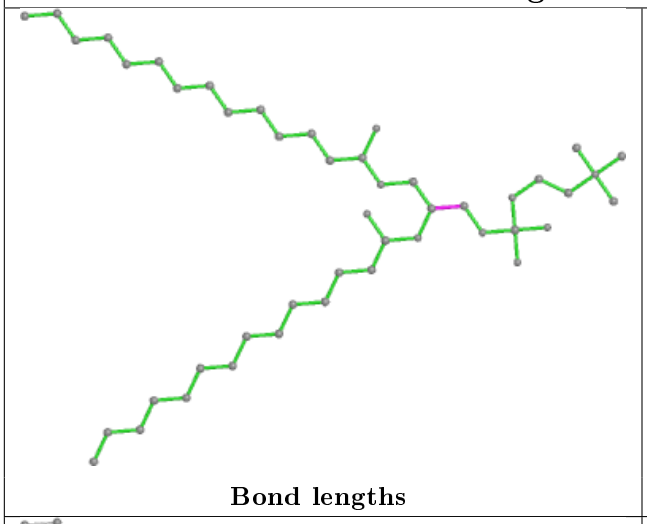
Ligand PX4 B 323



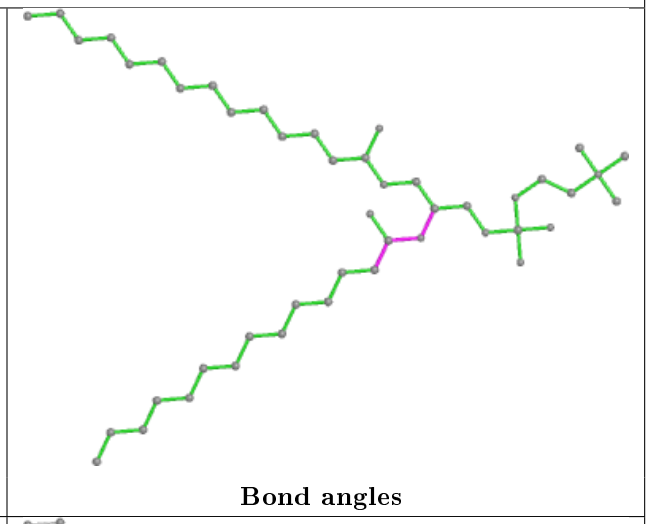
Ligand PX4 A 601



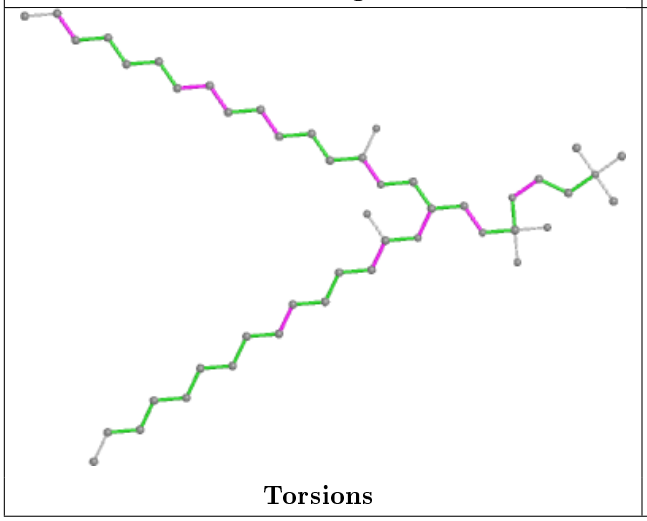
Ligand PX4 A 608



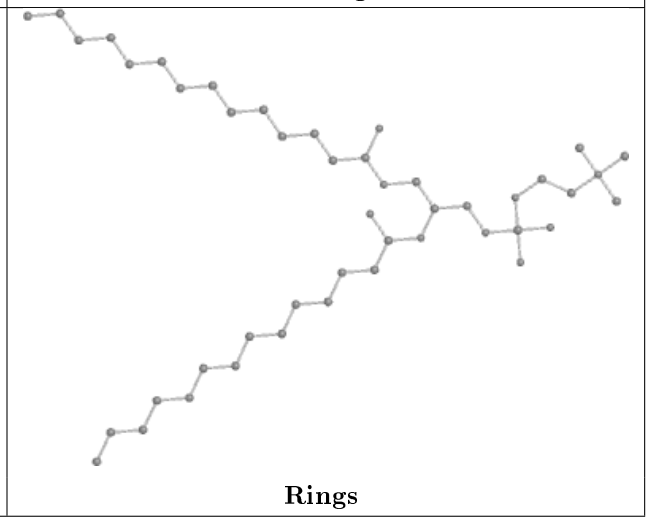
Bond lengths



Bond angles

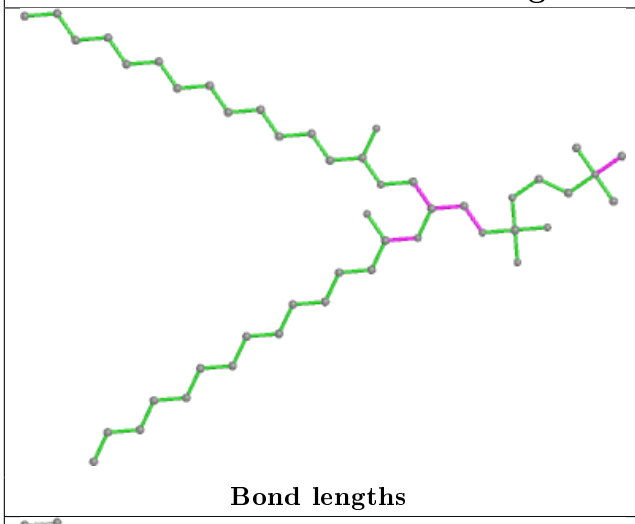


Torsions

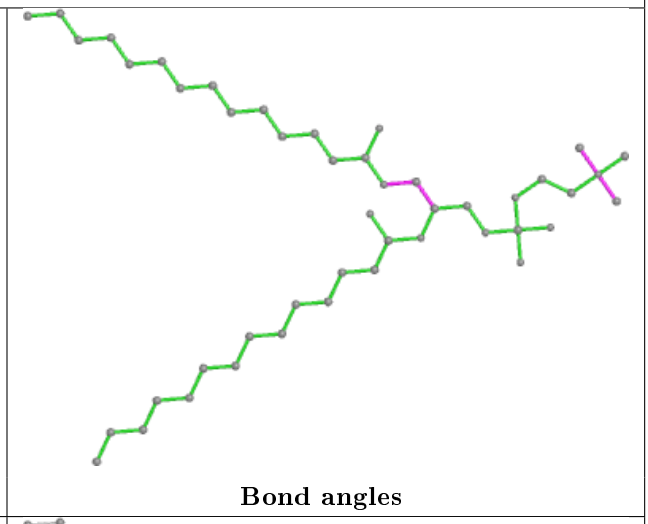


Rings

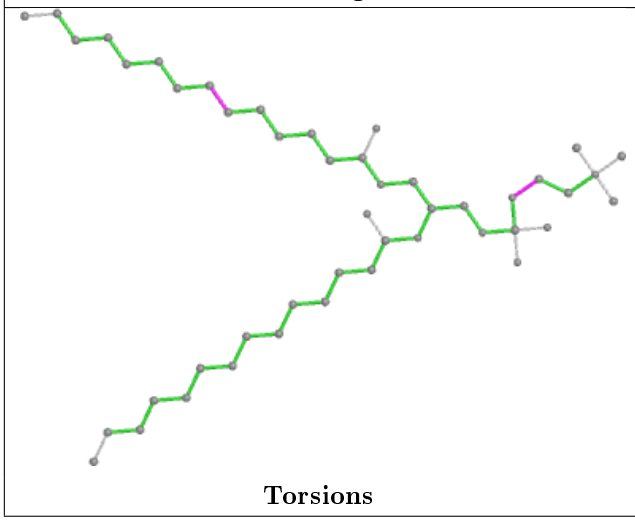
Ligand PX4 C 311



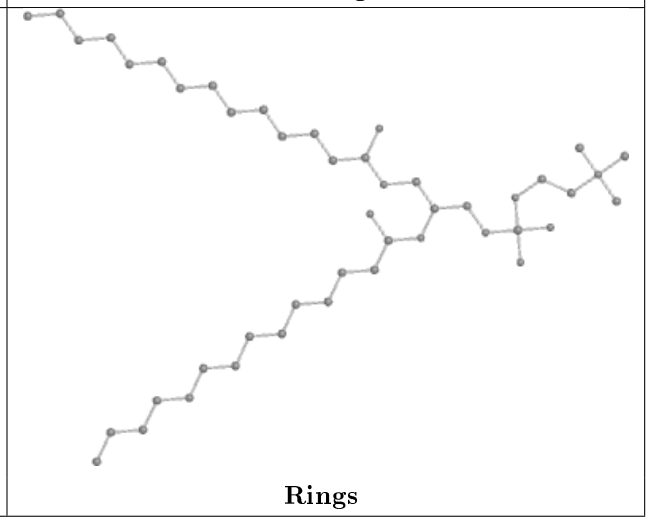
Bond lengths



Bond angles

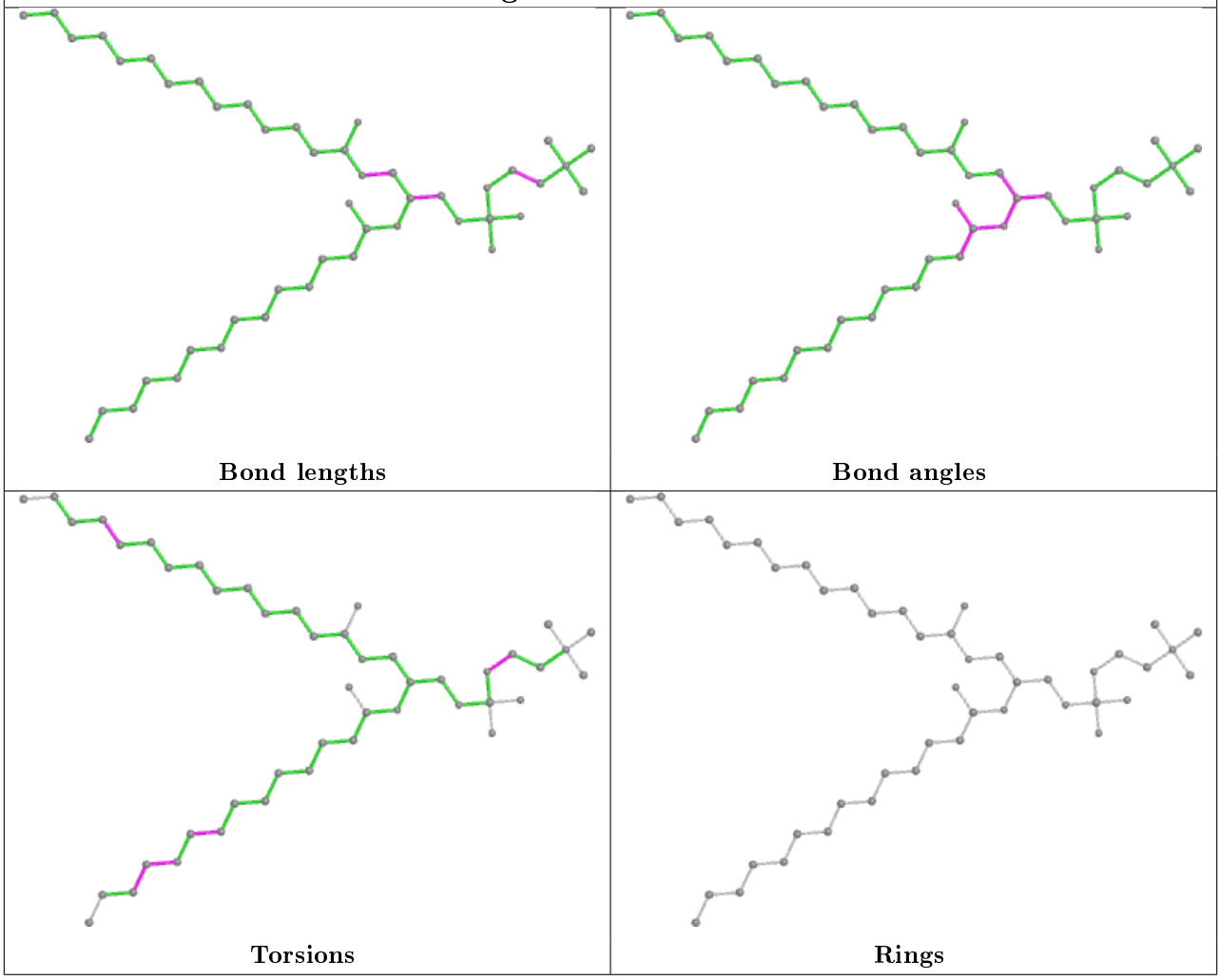


Torsions

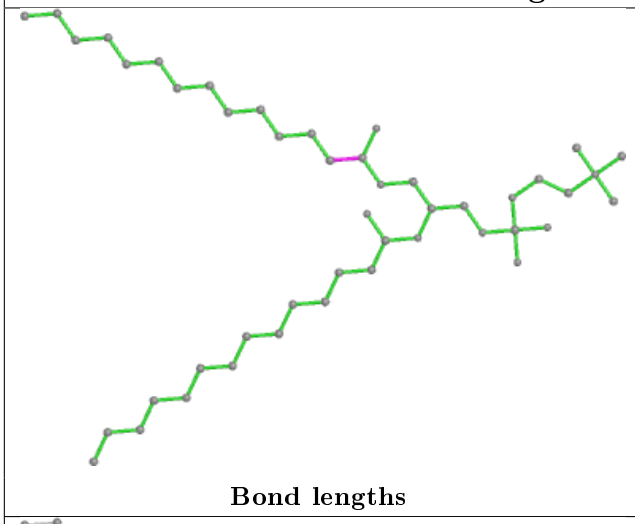


Rings

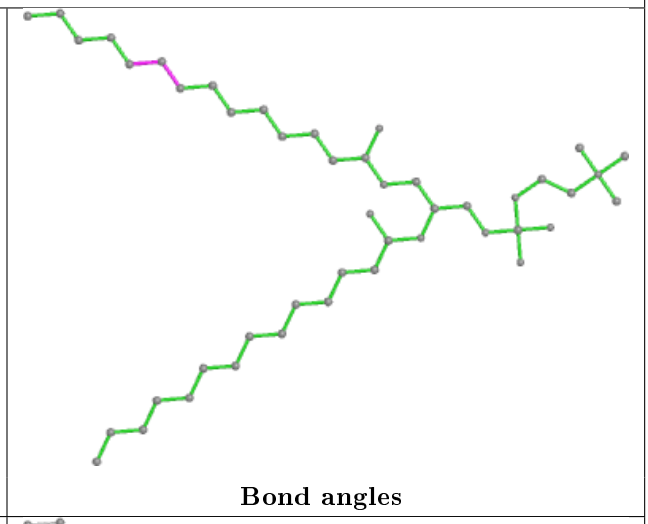
Ligand PX4 A 613



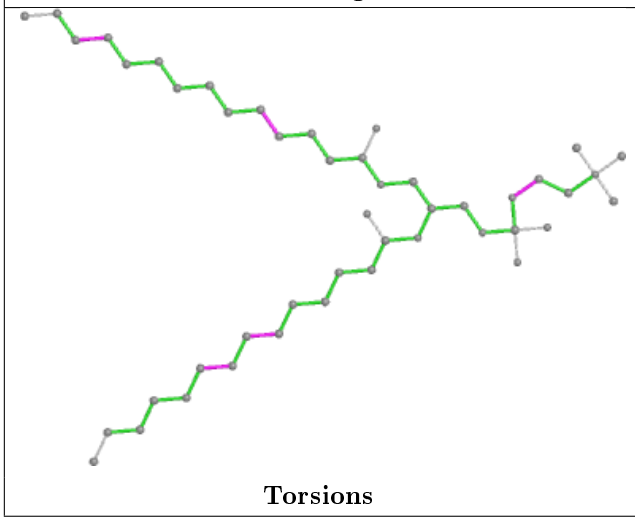
Ligand PX4 C 366



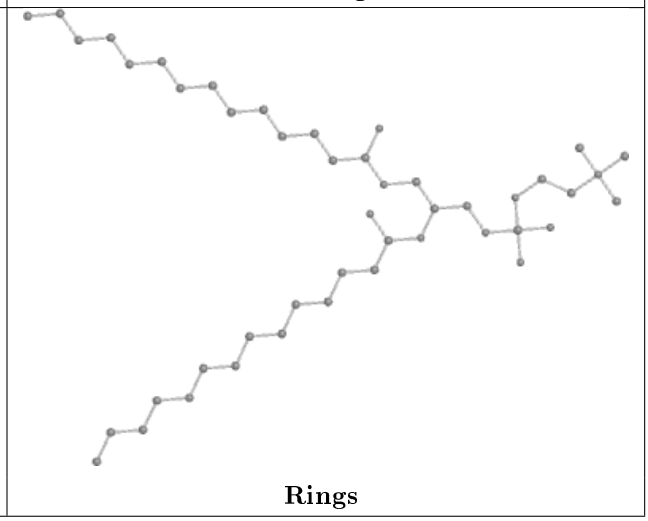
Bond lengths



Bond angles

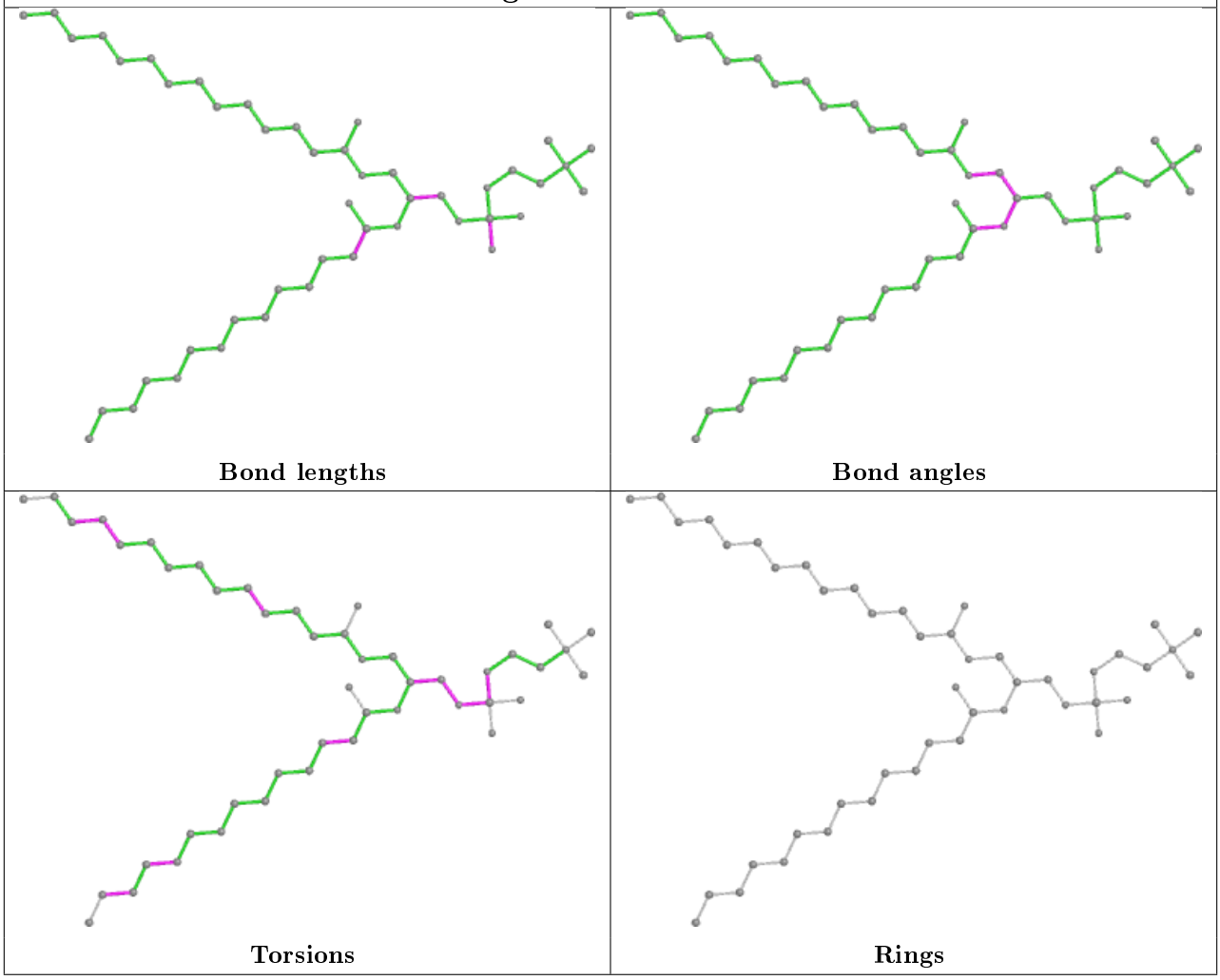


Torsions

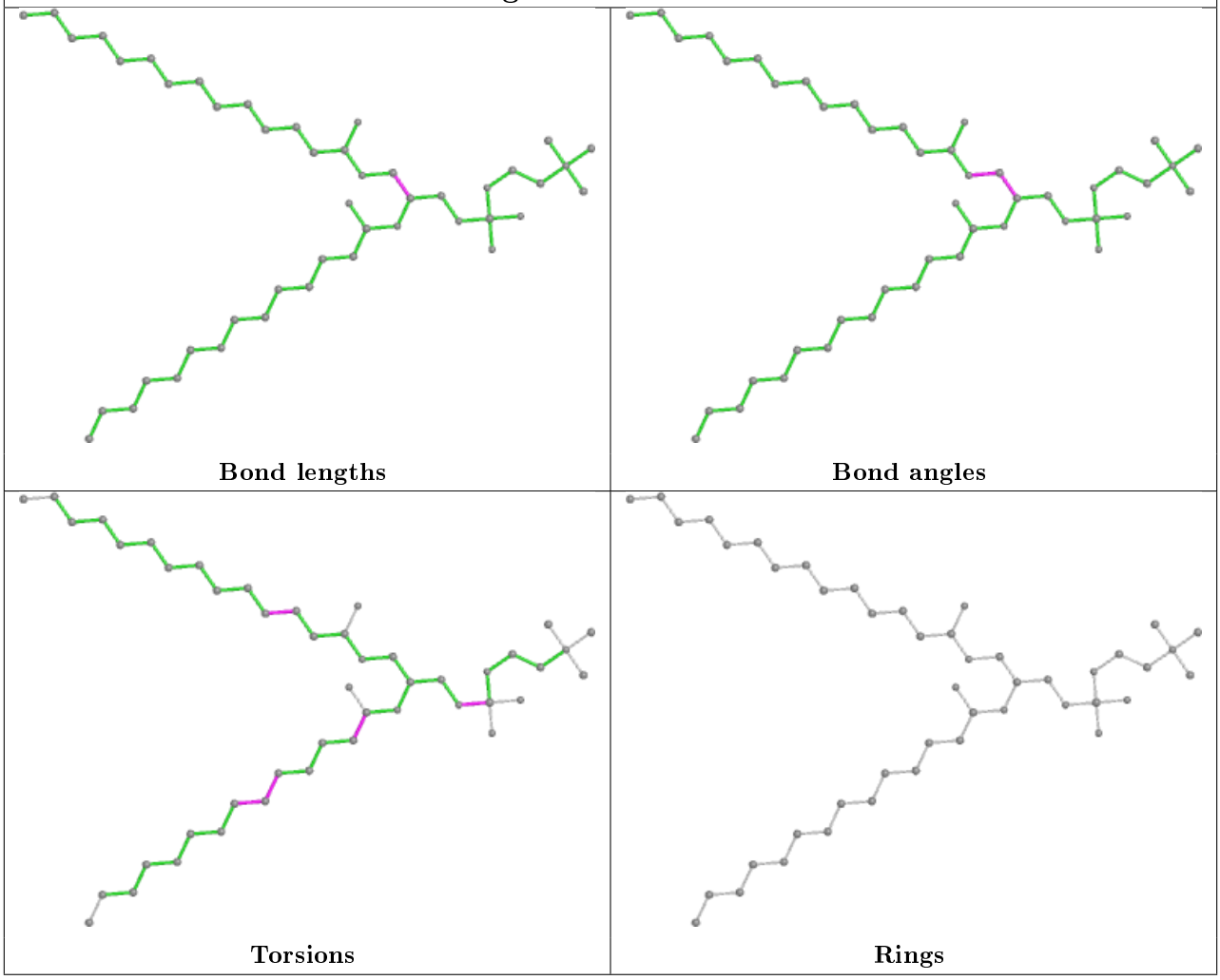


Rings

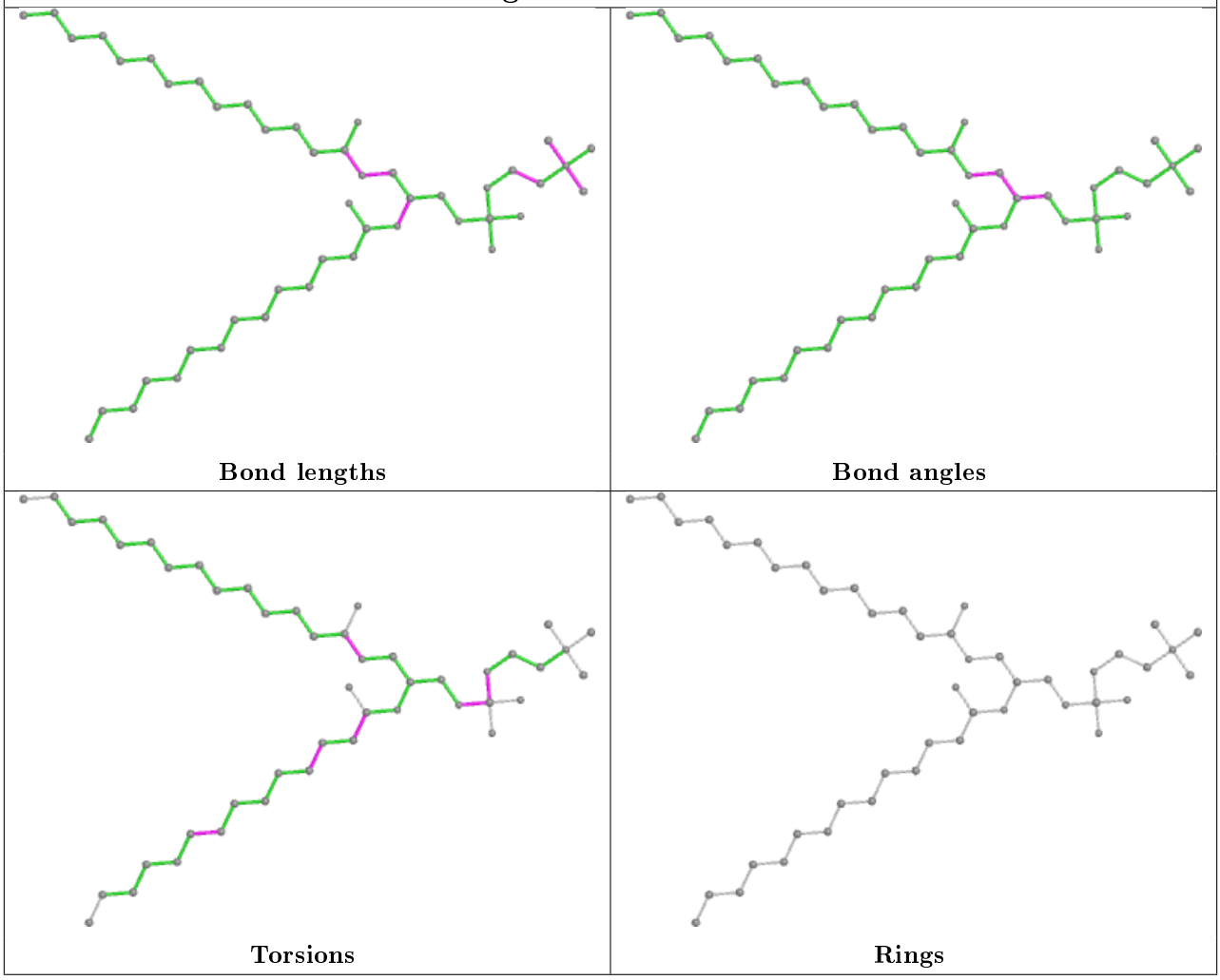
Ligand PX4 B 336



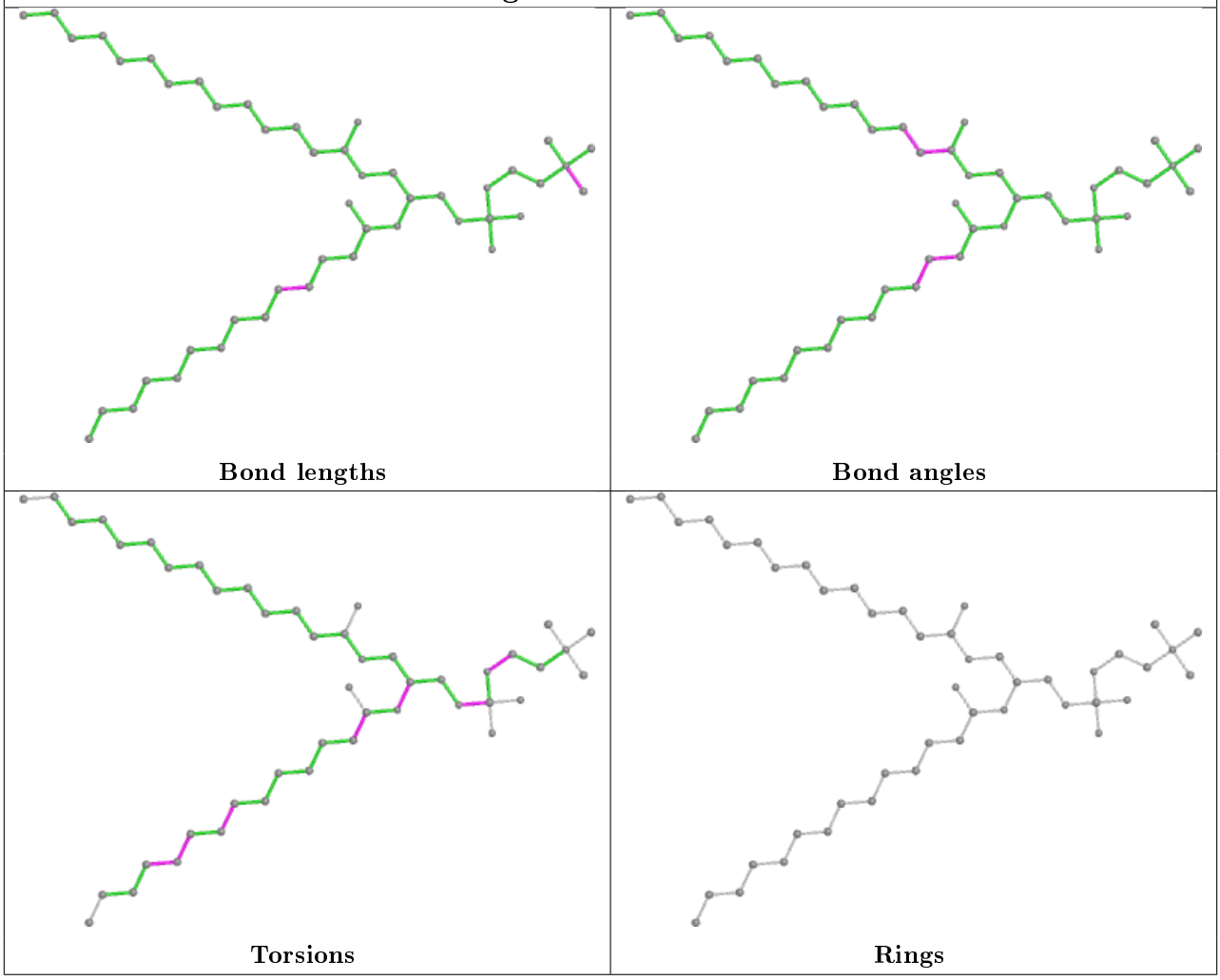
Ligand PX4 B 357



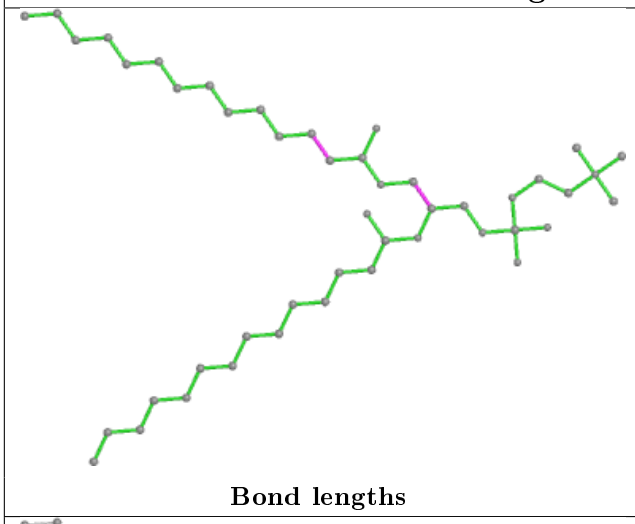
Ligand PX4 B 380



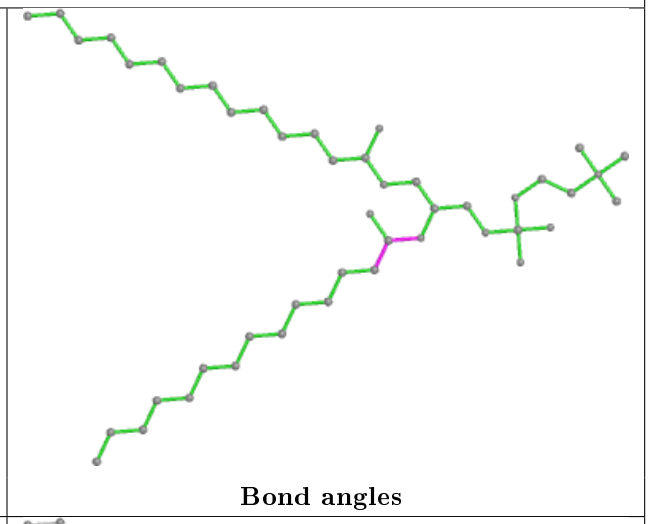
Ligand PX4 B 342



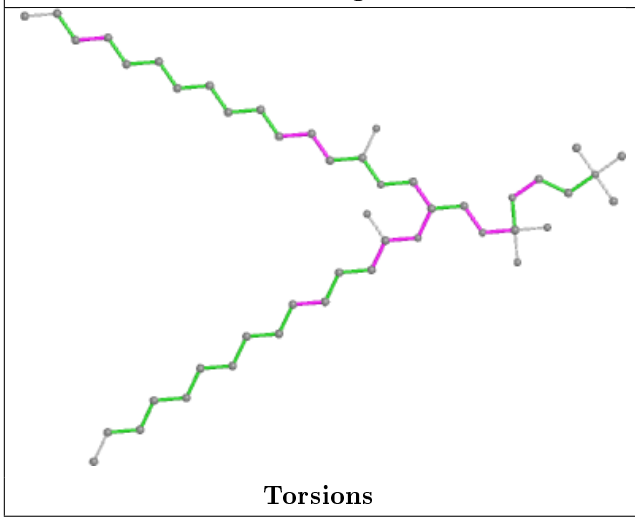
Ligand PX4 B 364



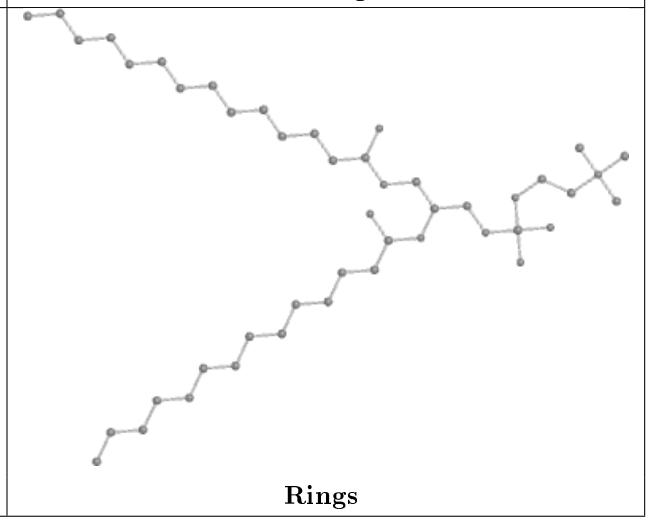
Bond lengths



Bond angles

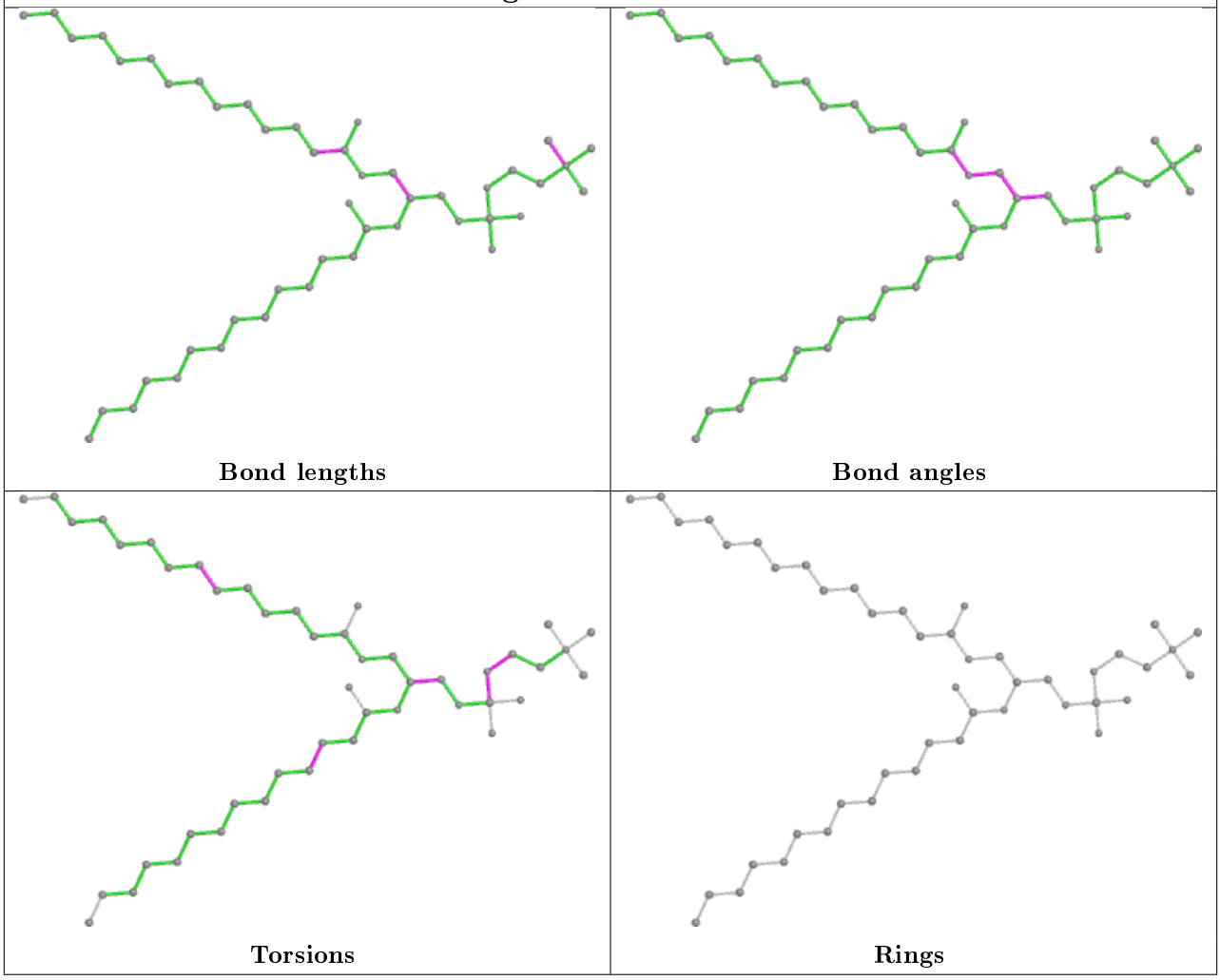


Torsions

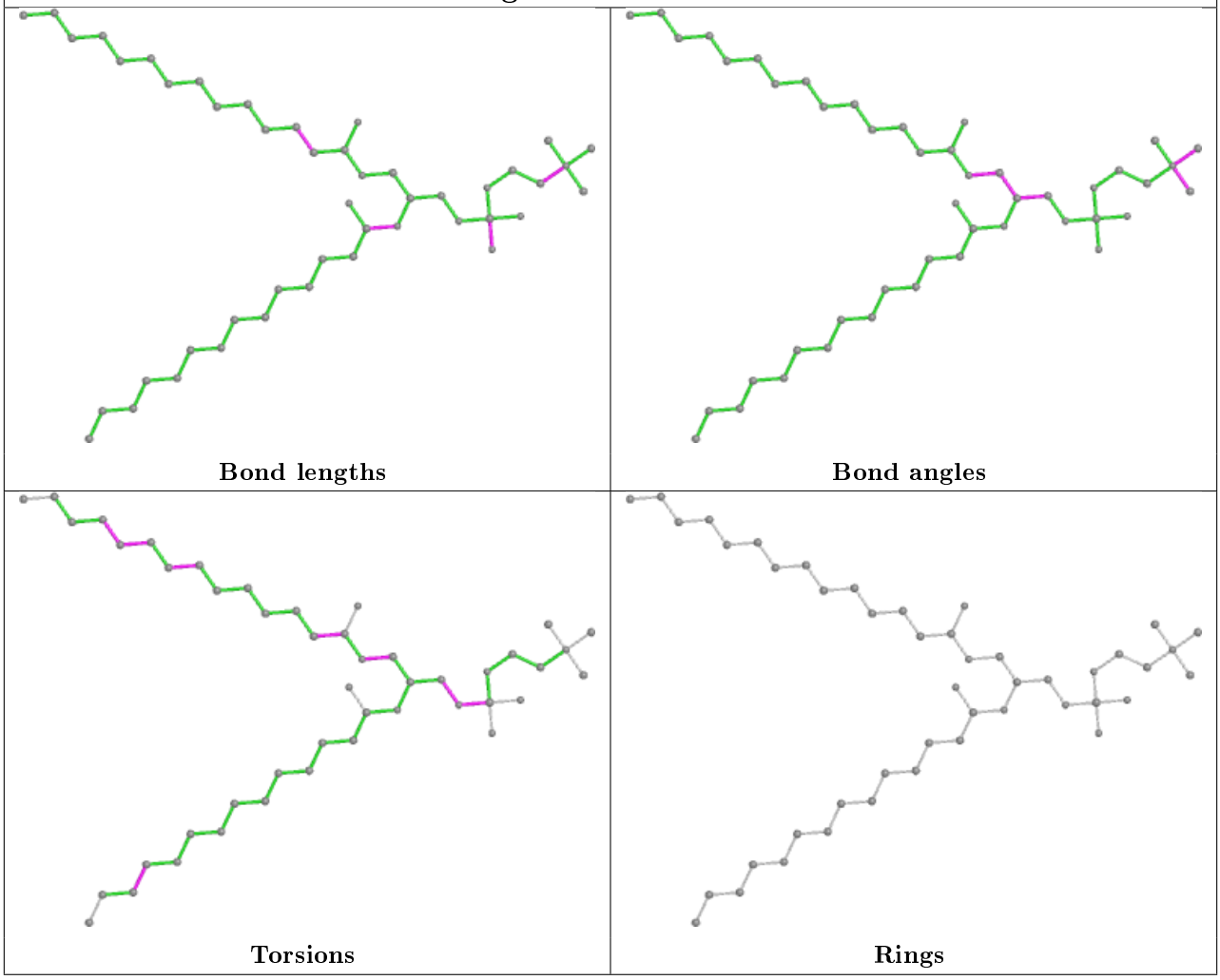


Rings

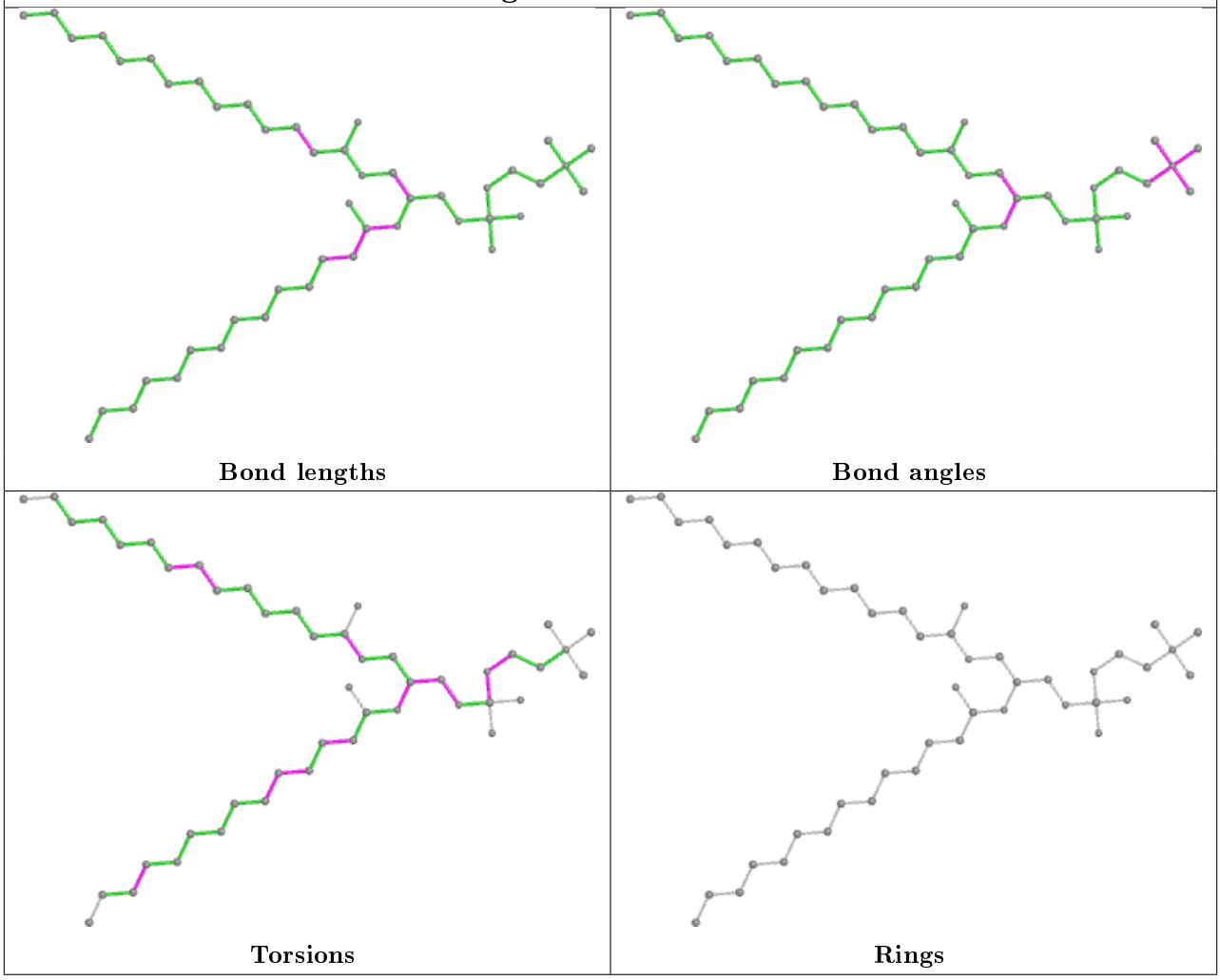
Ligand PX4 B 363



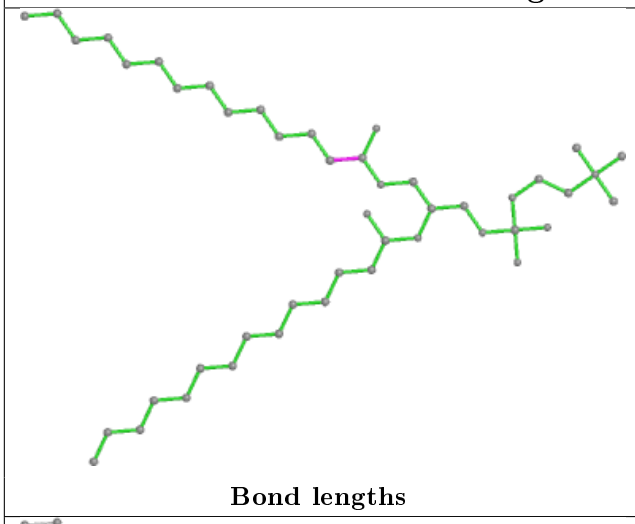
Ligand PX4 A 636



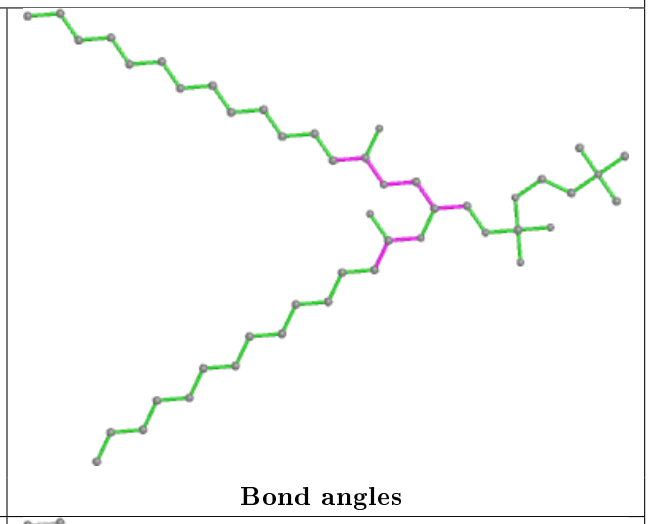
Ligand PX4 A 644



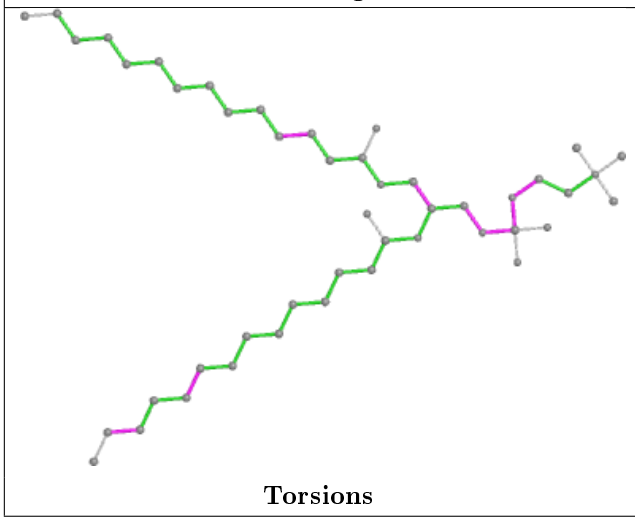
Ligand PX4 A 618



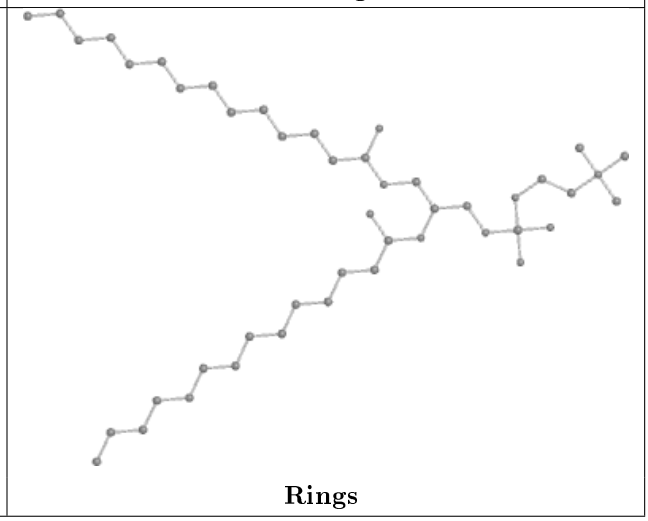
Bond lengths



Bond angles

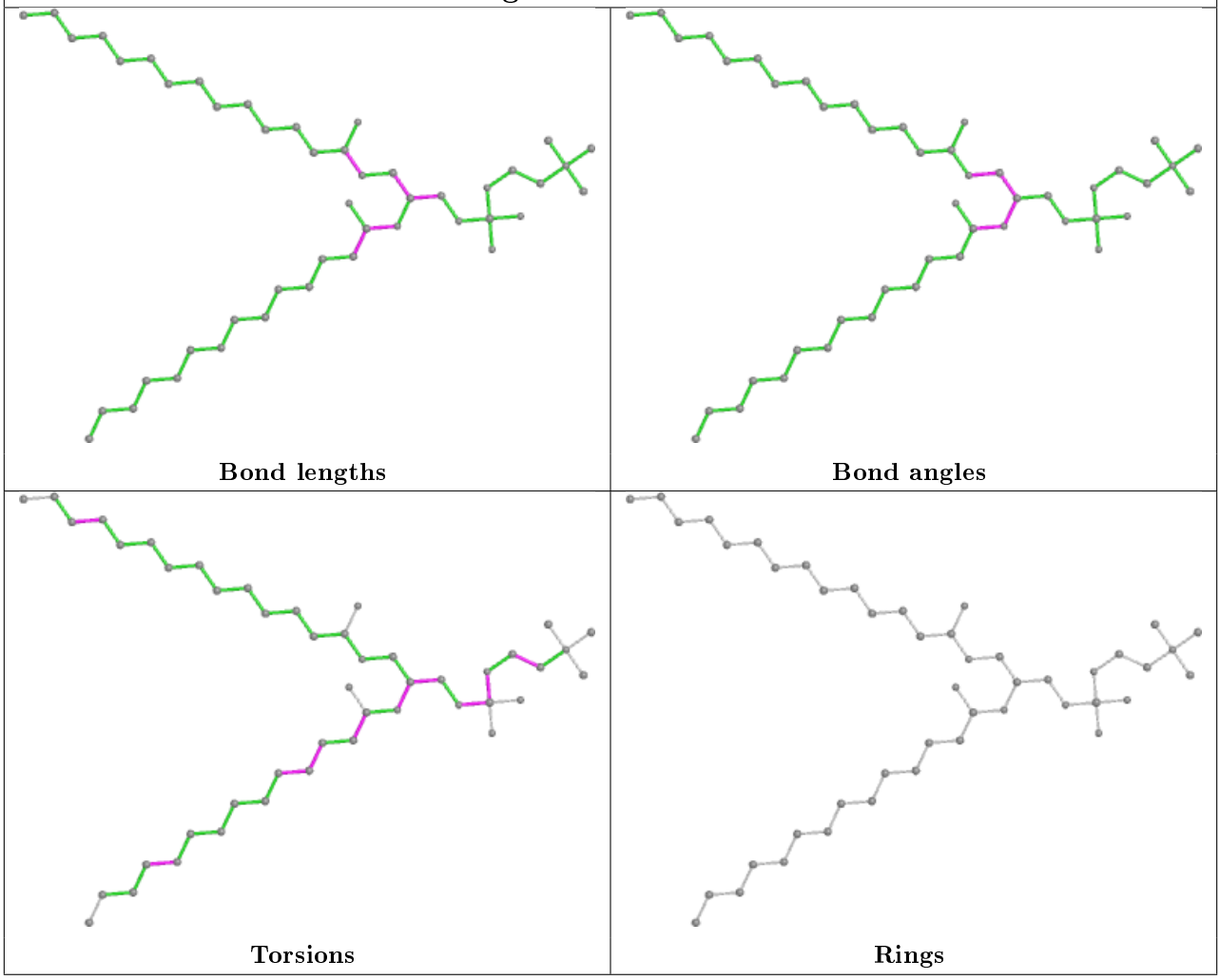


Torsions

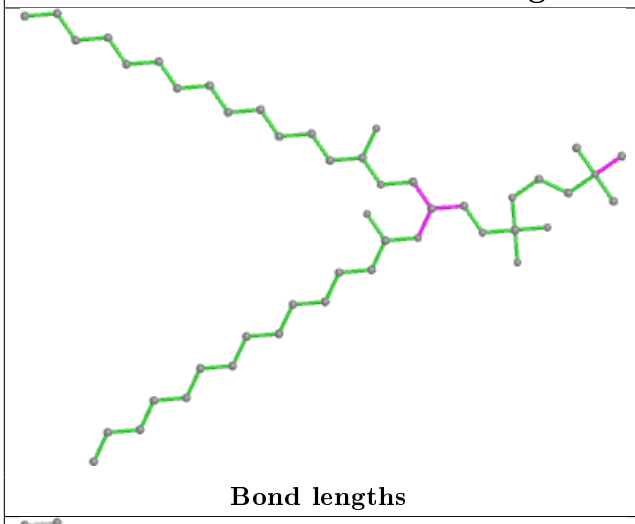


Rings

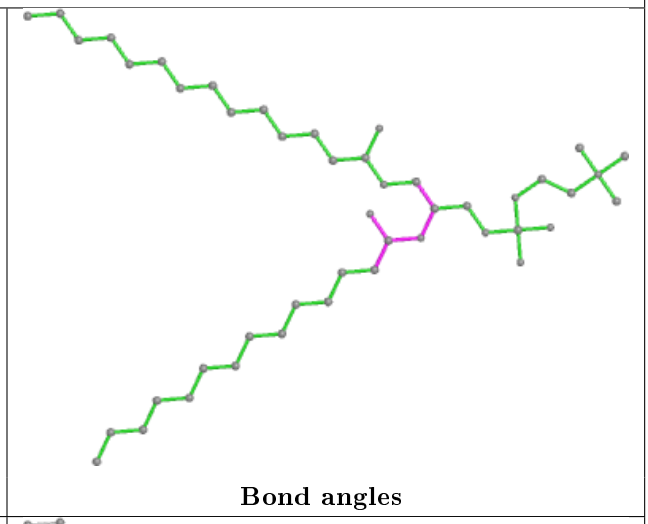
Ligand PX4 C 350



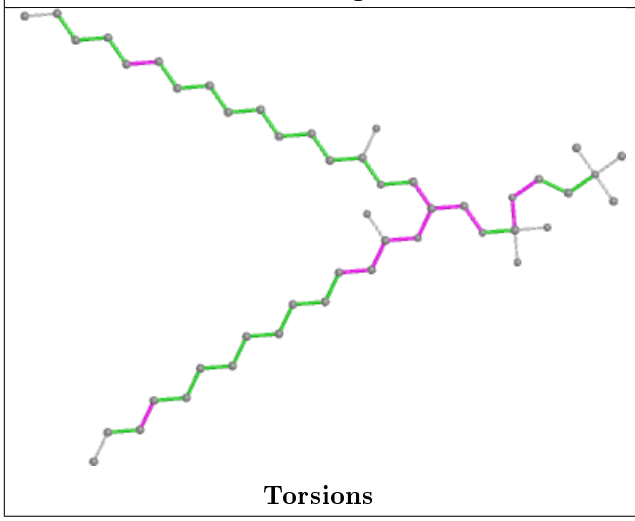
Ligand PX4 C 309



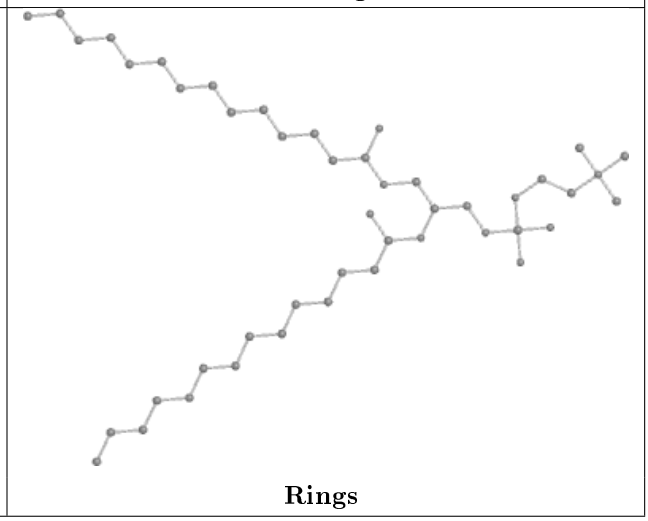
Bond lengths



Bond angles

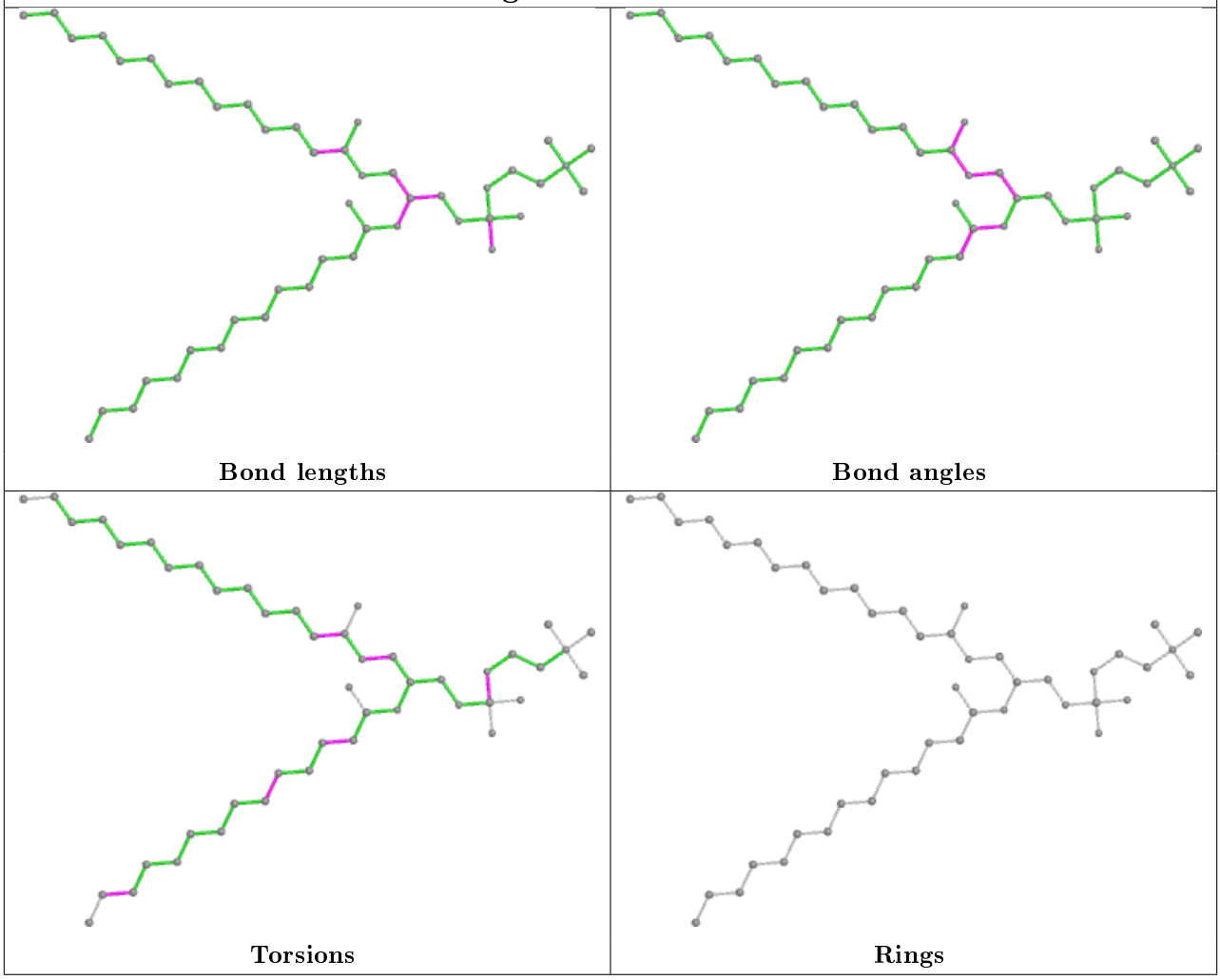


Torsions

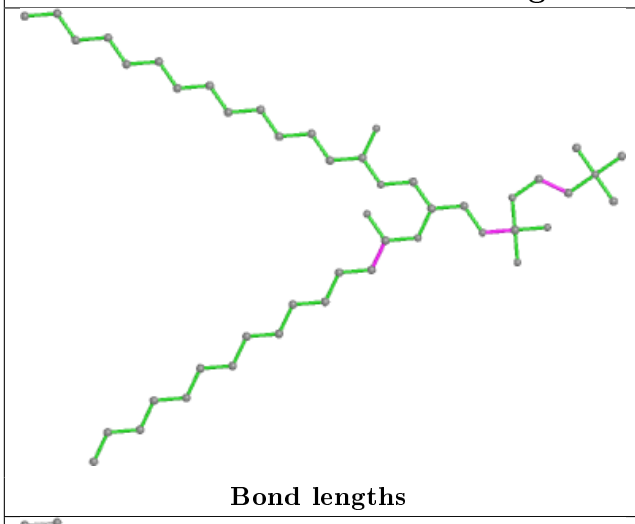


Rings

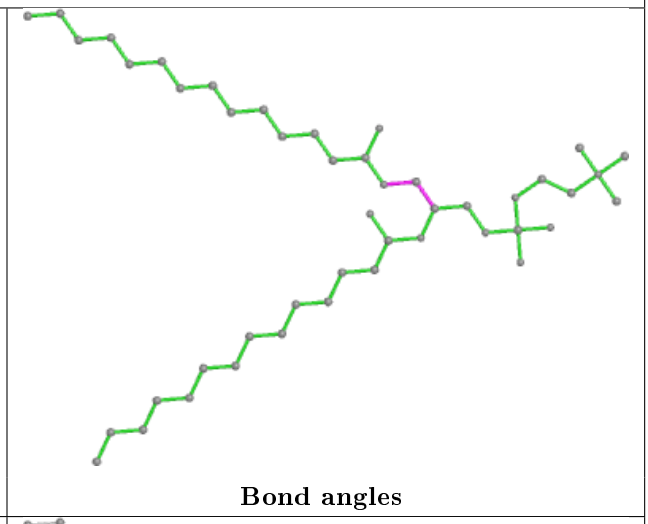
Ligand PX4 B 387



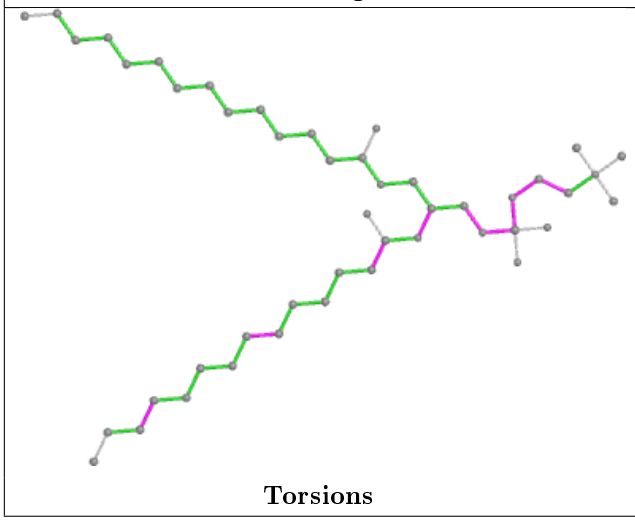
Ligand PX4 C 305



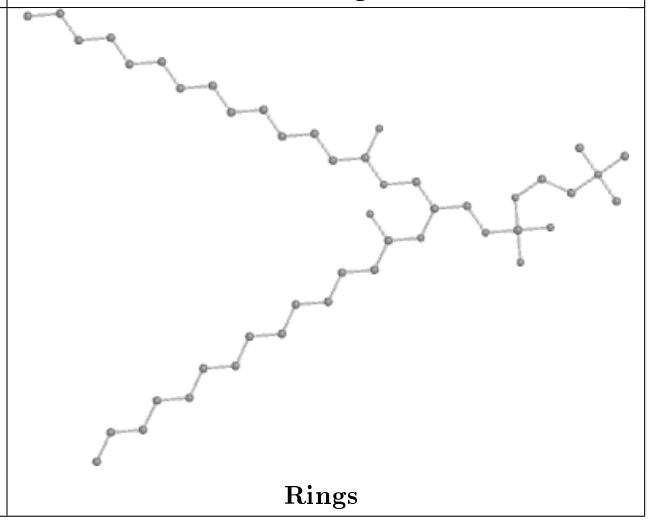
Bond lengths



Bond angles

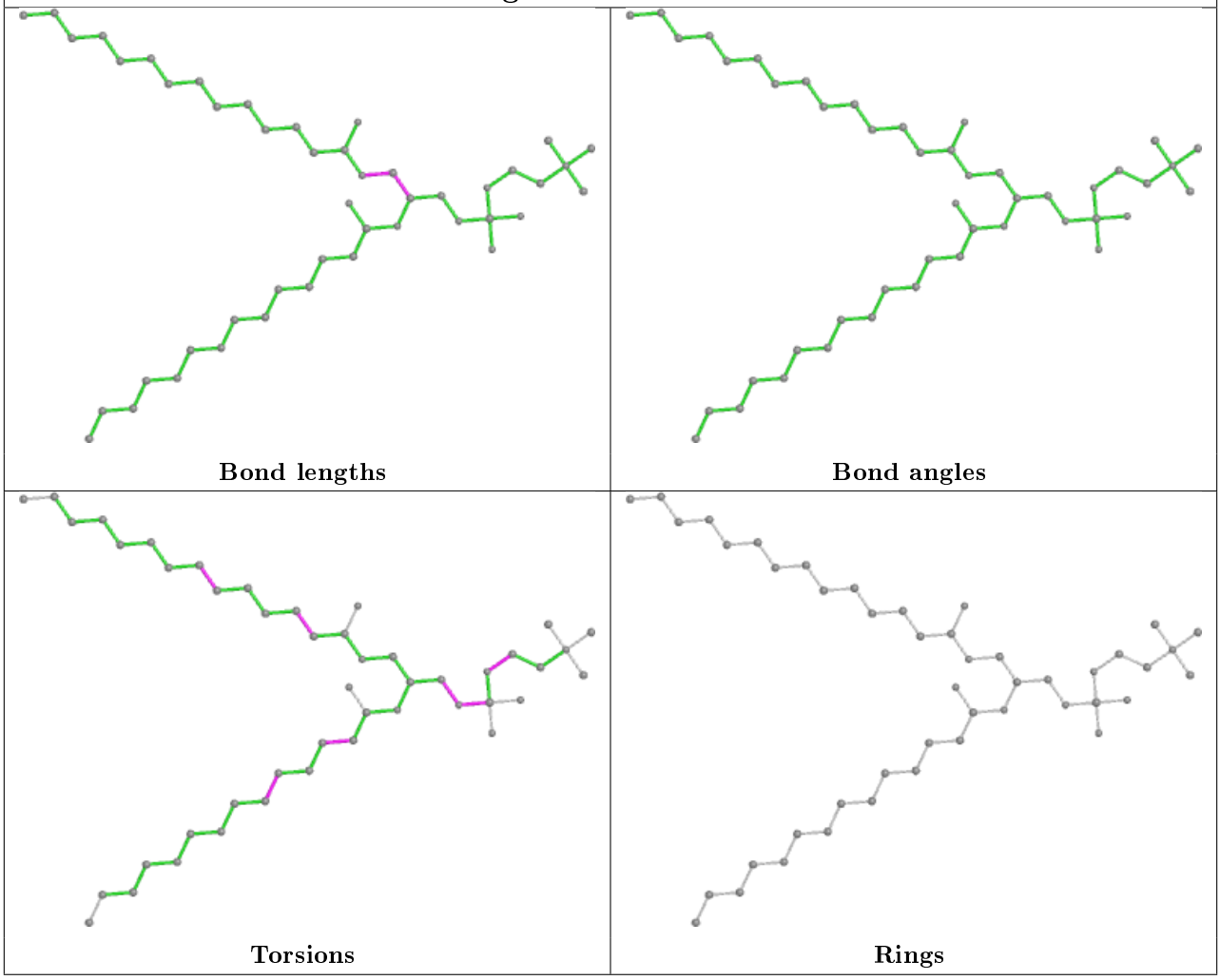


Torsions

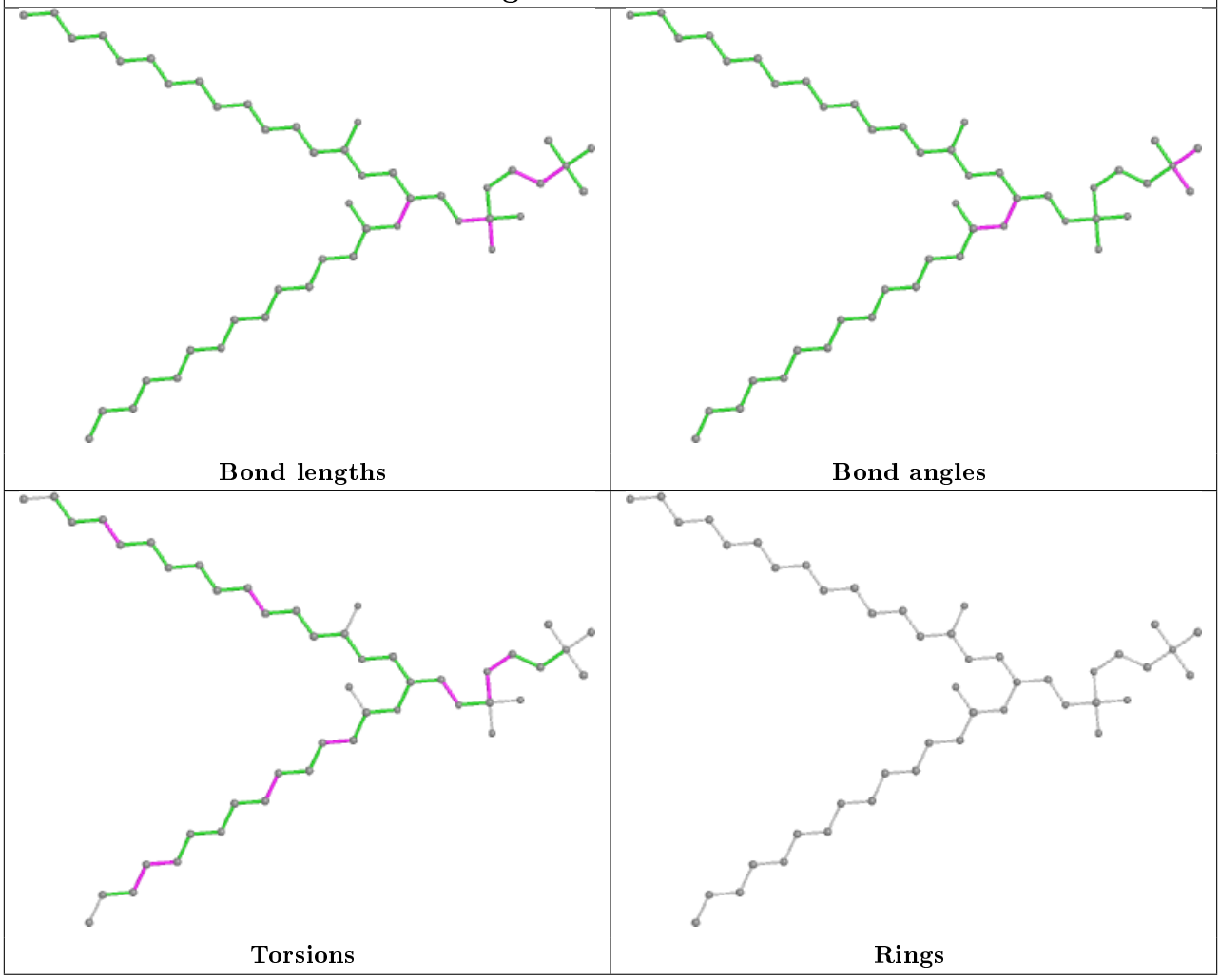


Rings

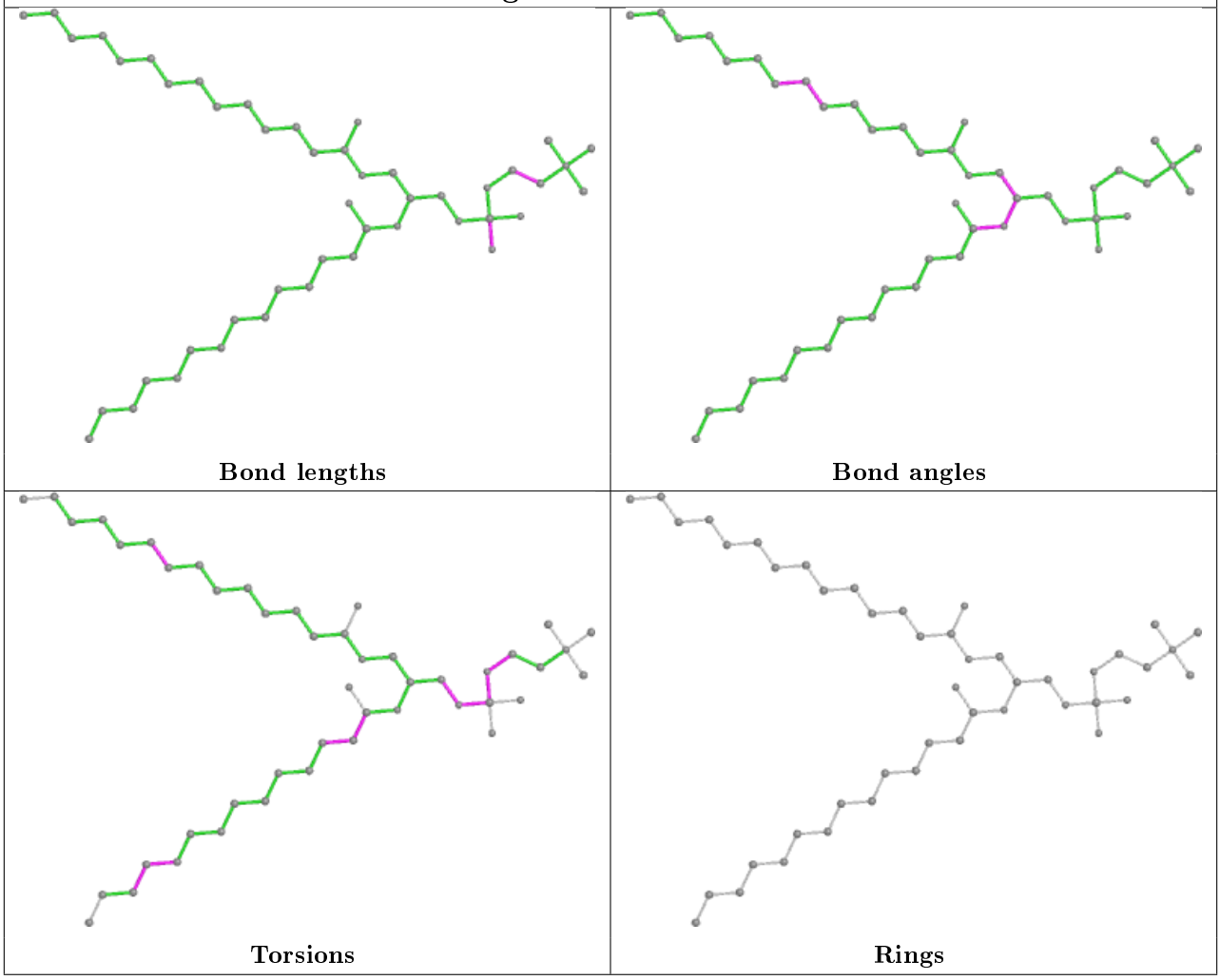
Ligand PX4 B 394



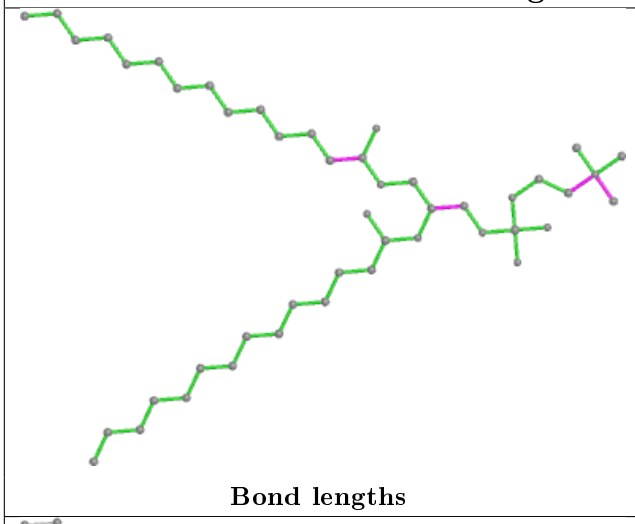
Ligand PX4 B 372



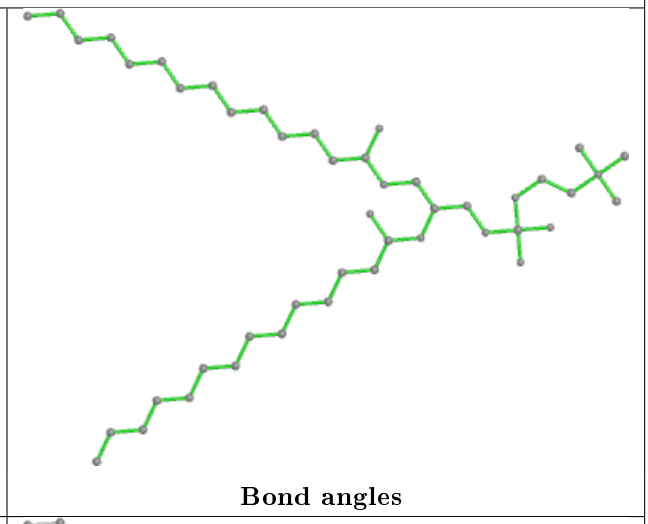
Ligand PX4 B 384



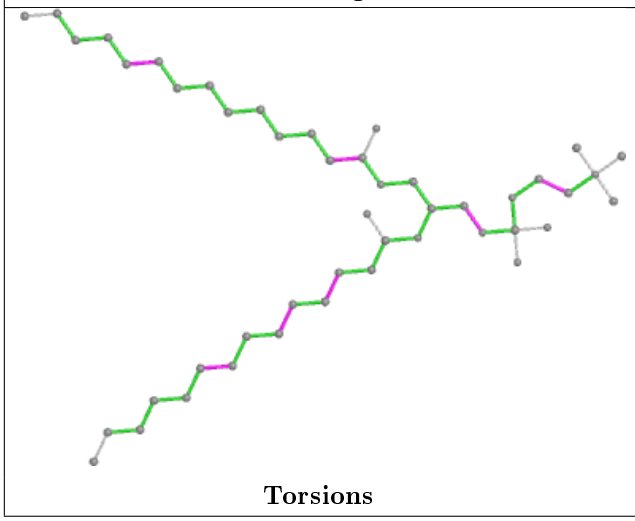
Ligand PX4 A 629



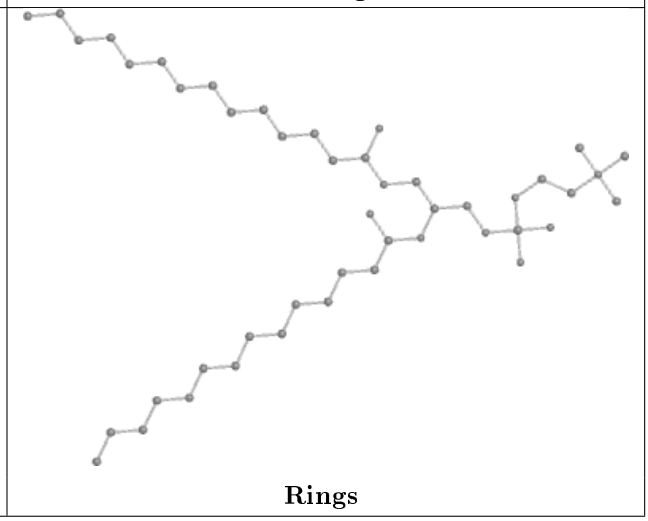
Bond lengths



Bond angles

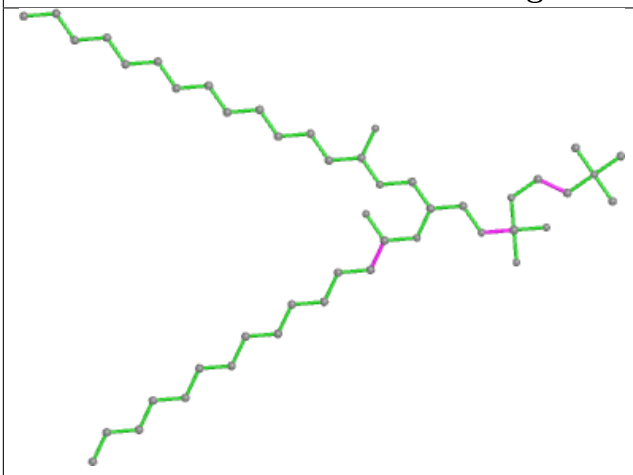


Torsions

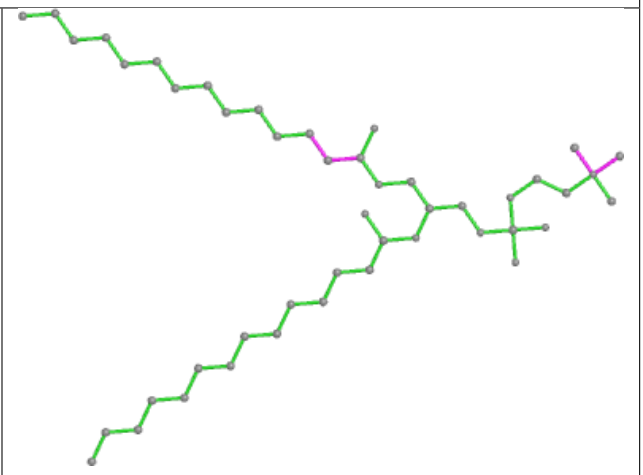


Rings

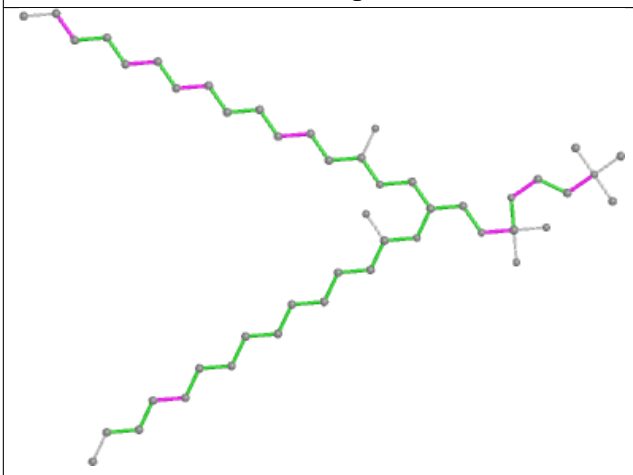
Ligand PX4 A 619



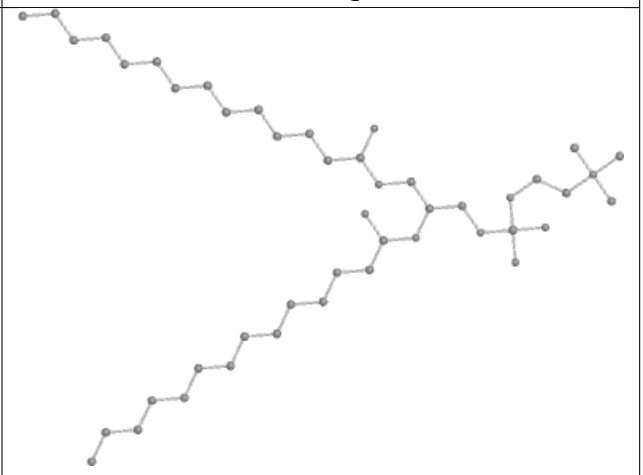
Bond lengths



Bond angles

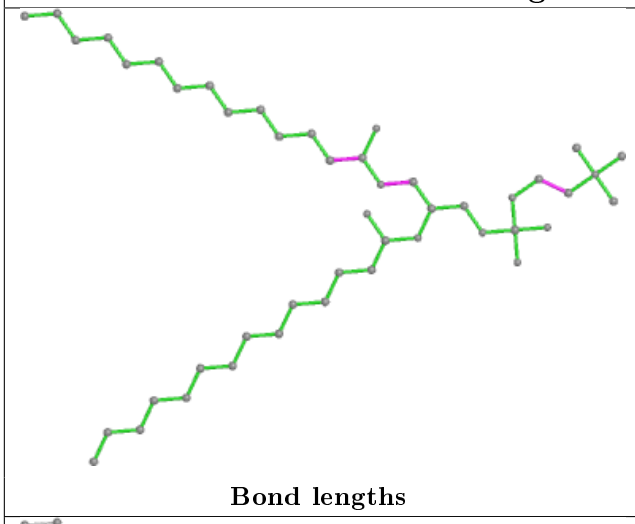


Torsions

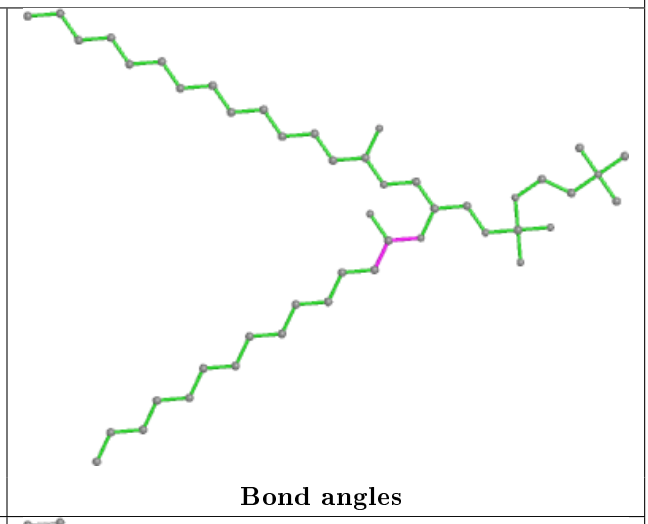


Rings

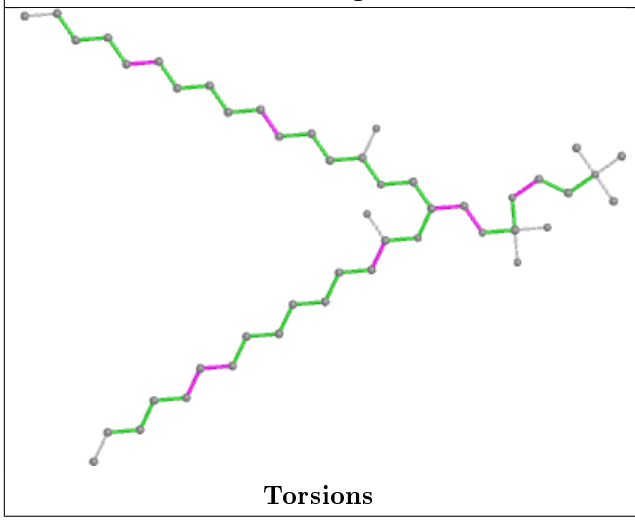
Ligand PX4 C 306



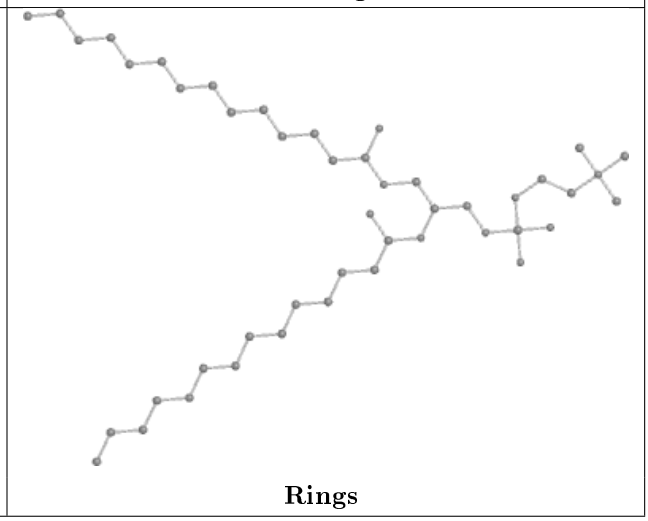
Bond lengths



Bond angles

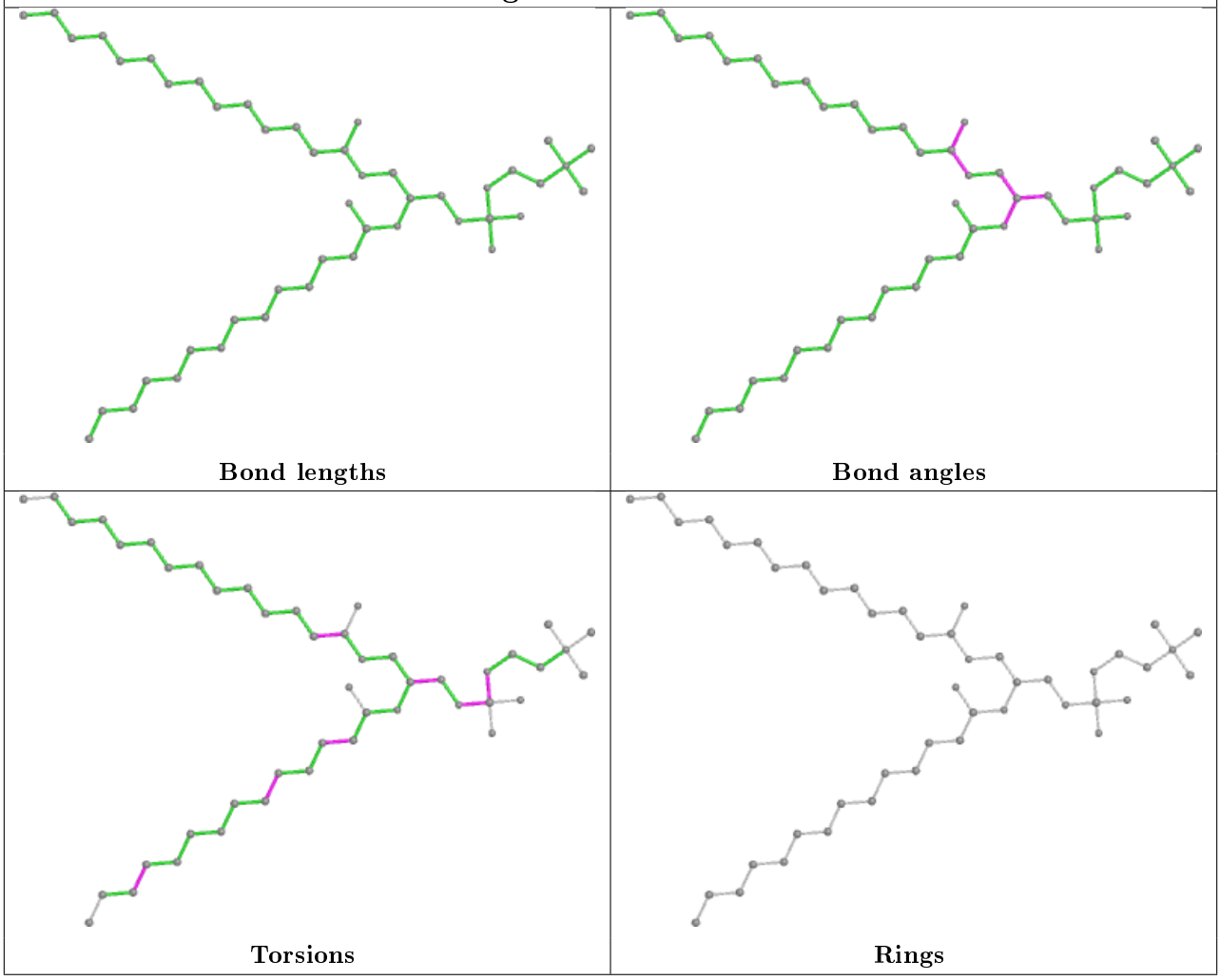


Torsions

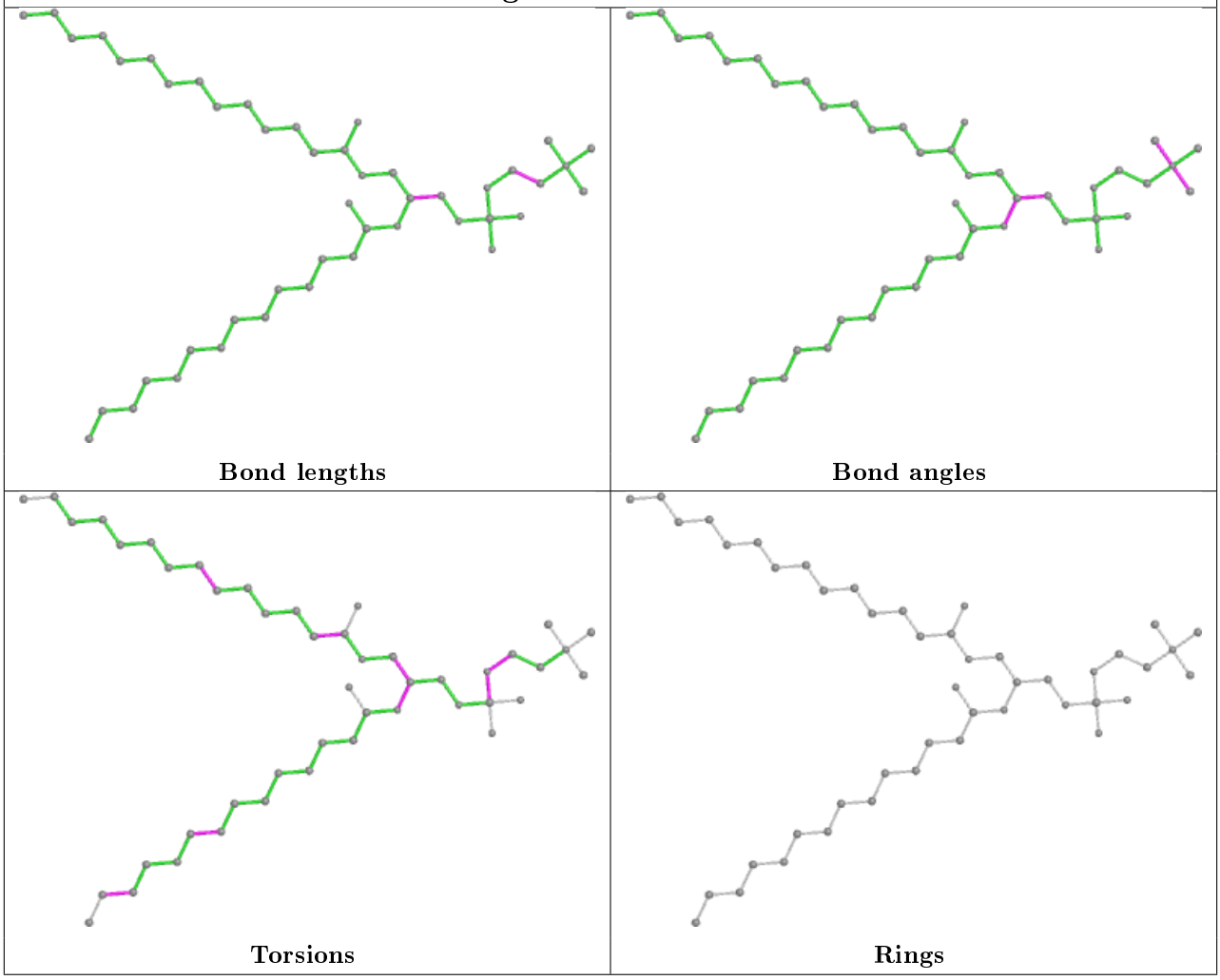


Rings

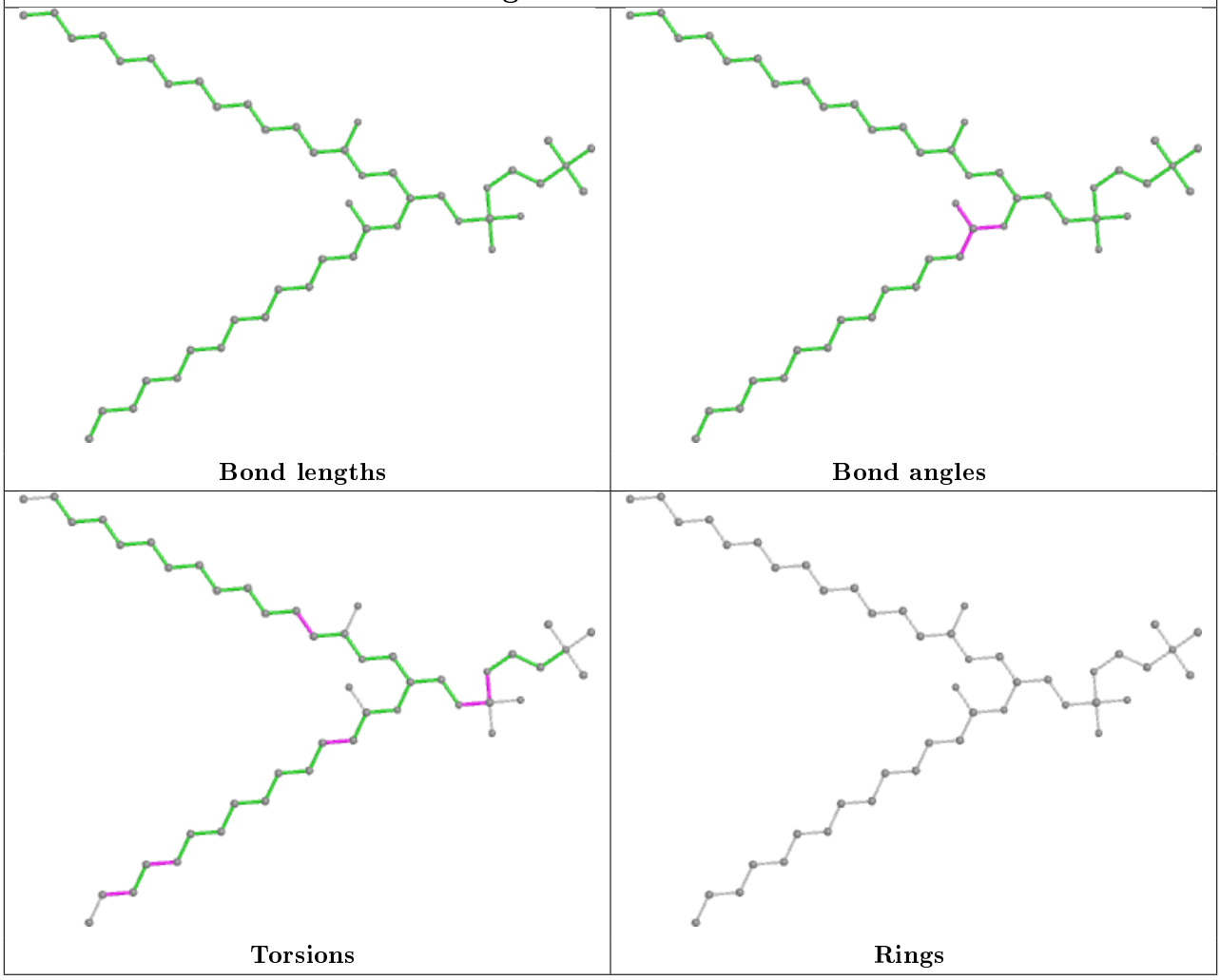
Ligand PX4 B 365



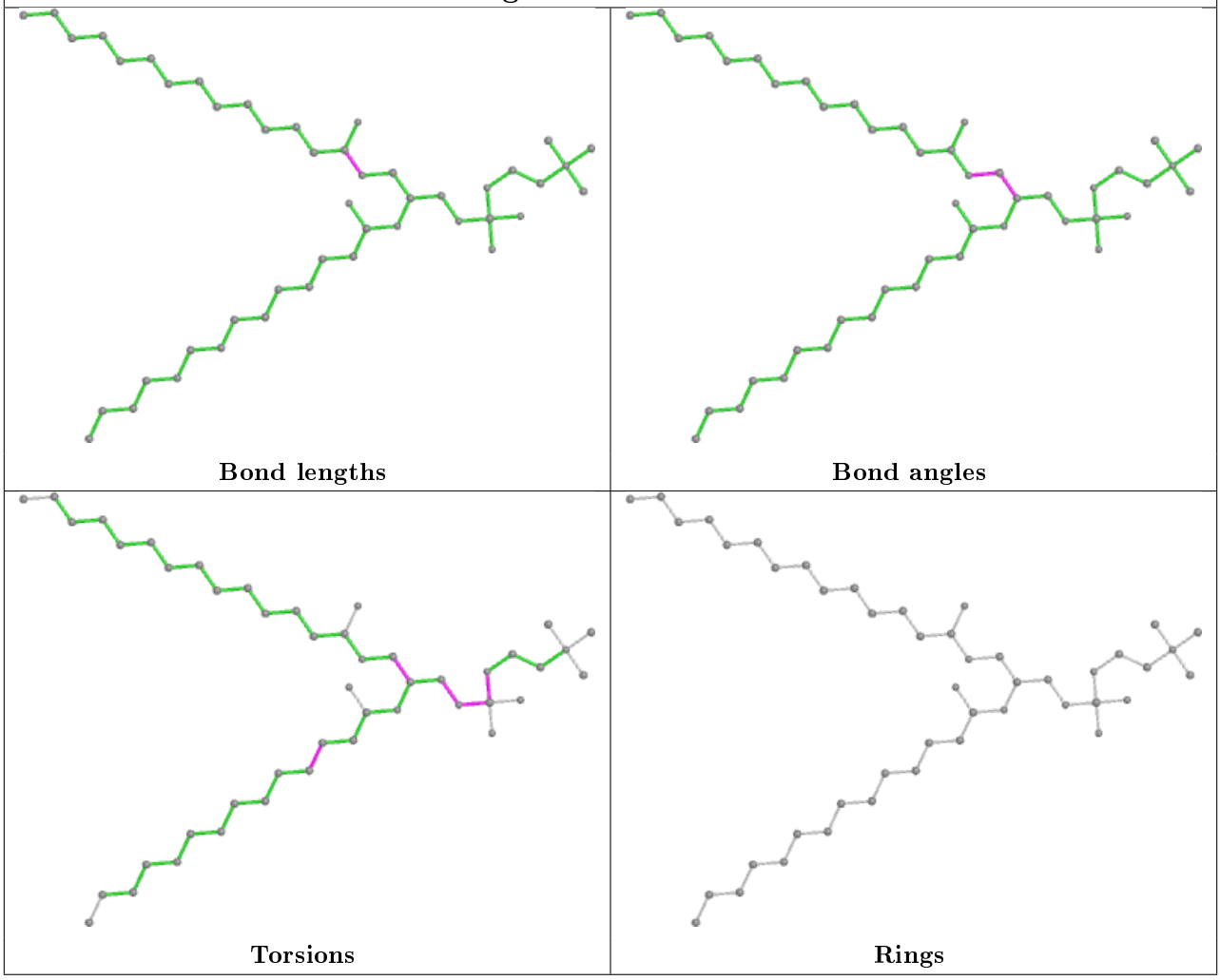
Ligand PX4 C 320



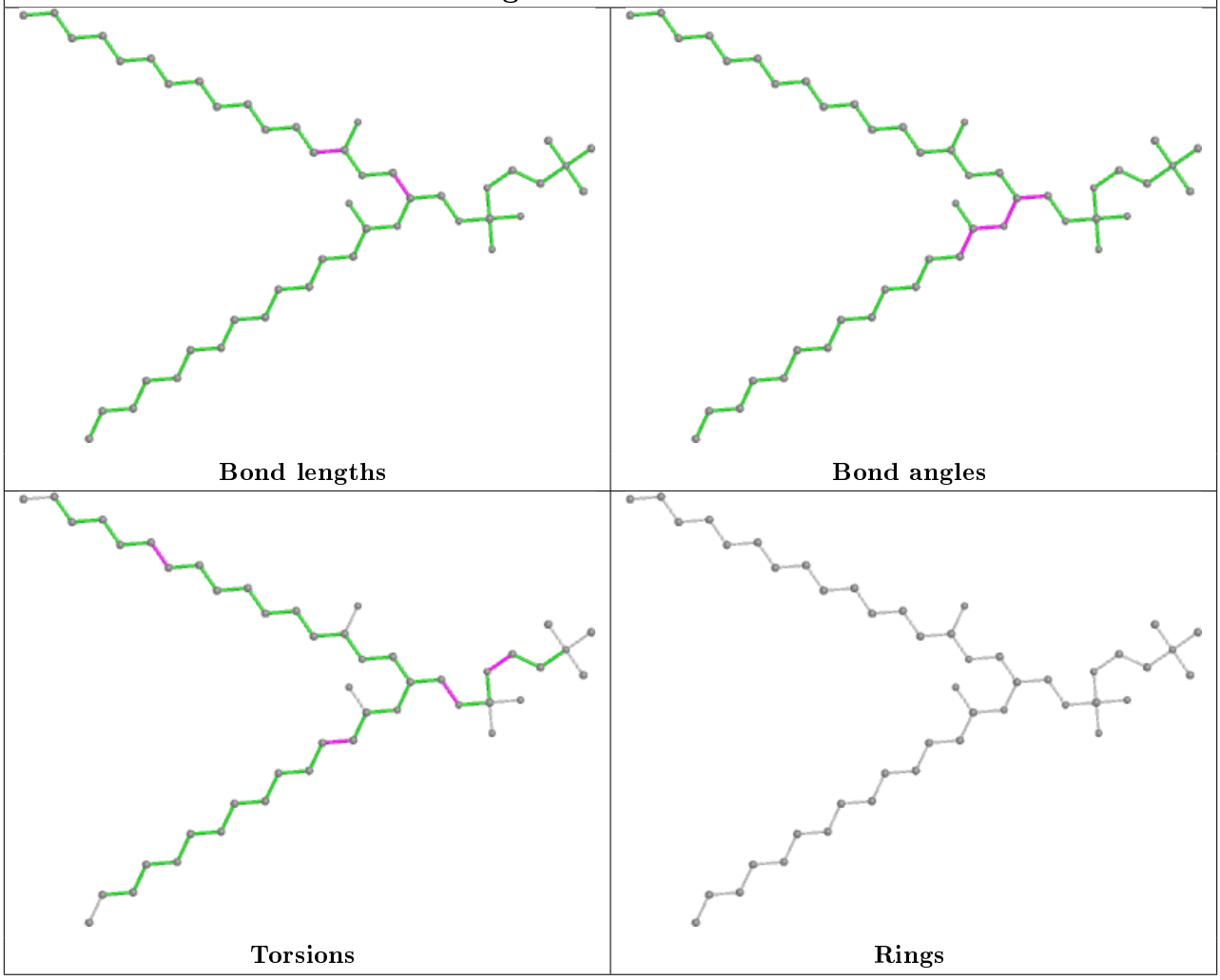
Ligand PX4 B 338



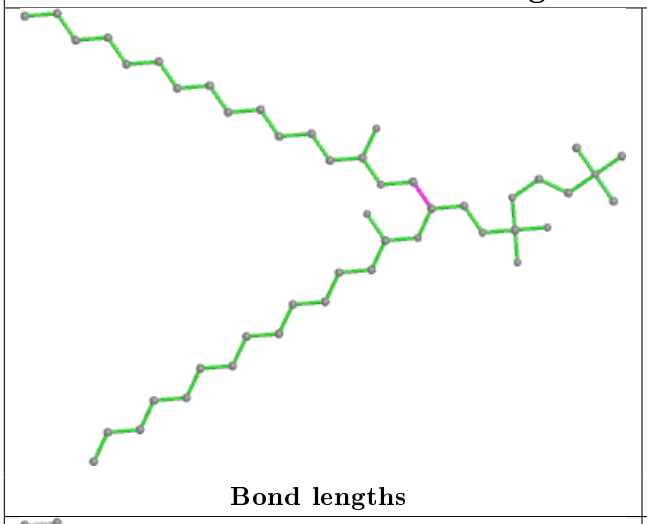
Ligand PX4 B 395



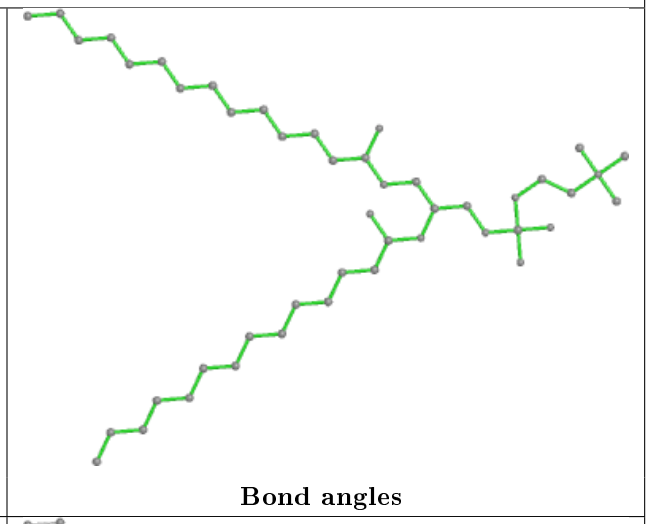
Ligand PX4 B 347



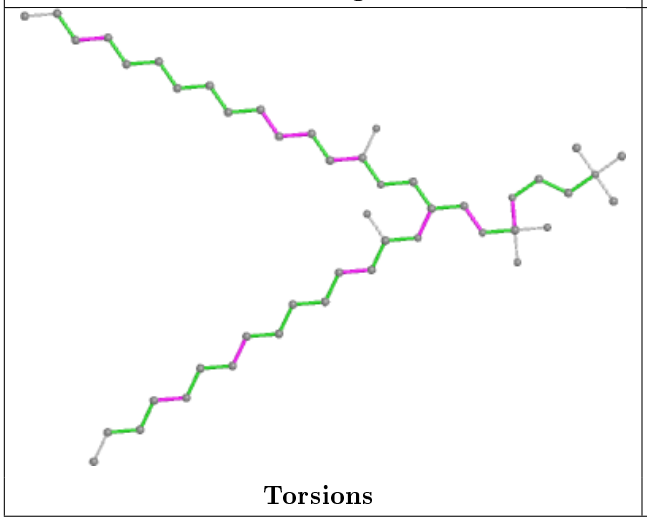
Ligand PX4 B 334



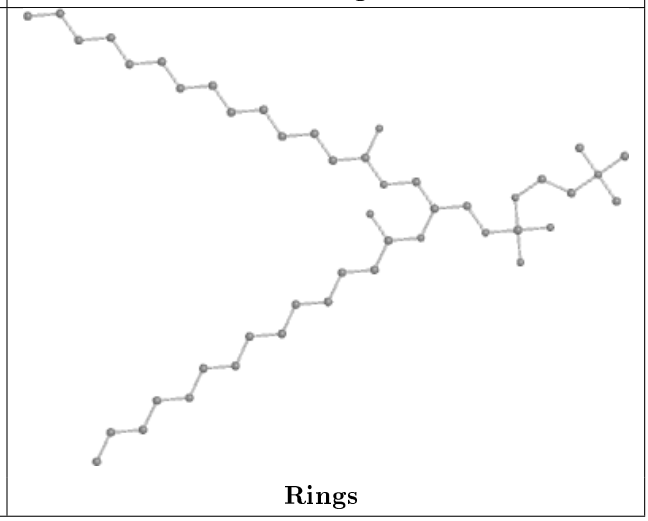
Bond lengths



Bond angles

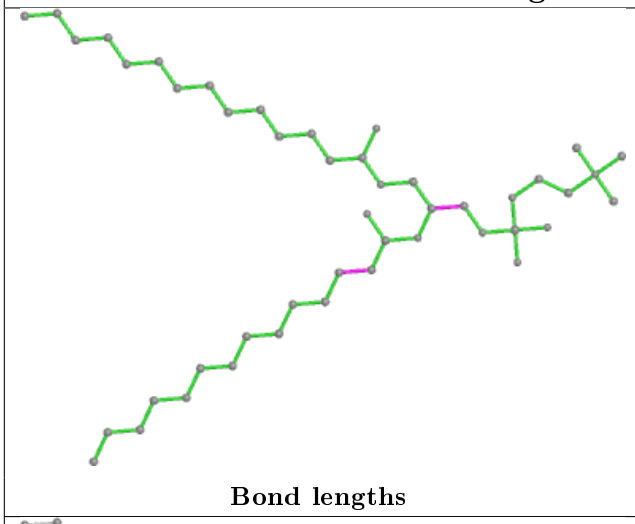


Torsions

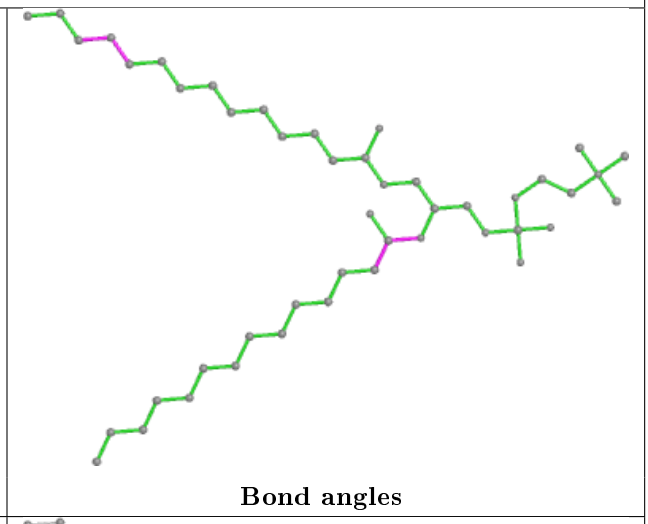


Rings

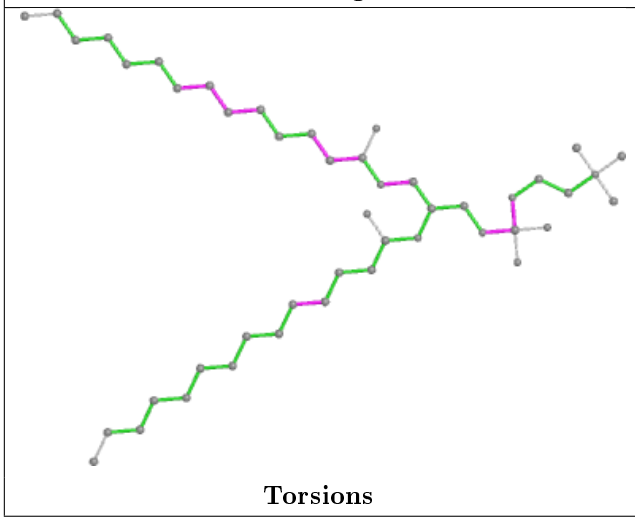
Ligand PX4 C 367



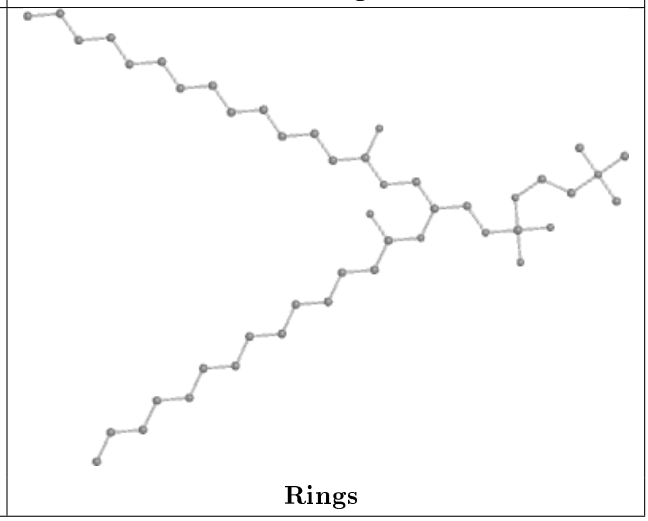
Bond lengths



Bond angles

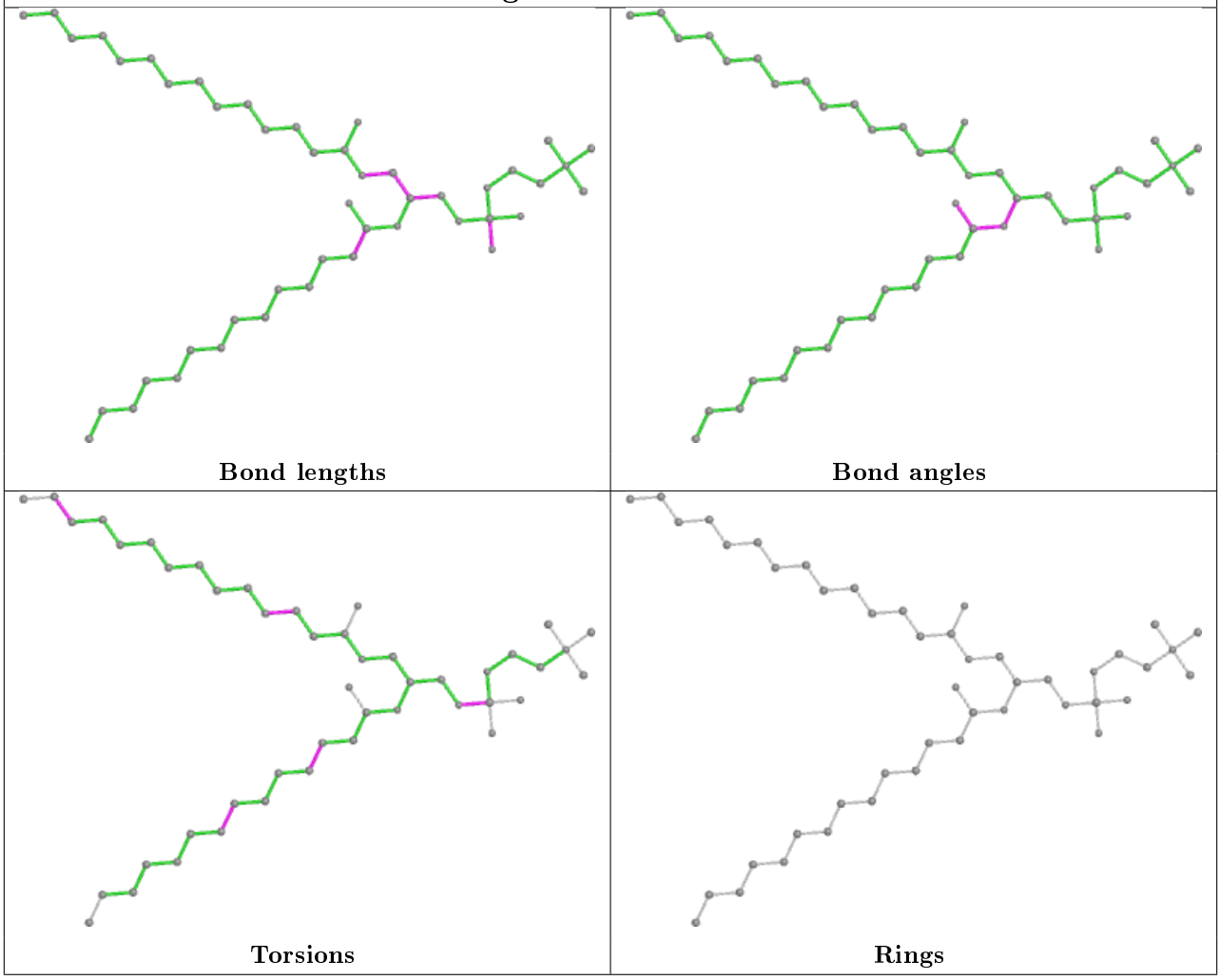


Torsions

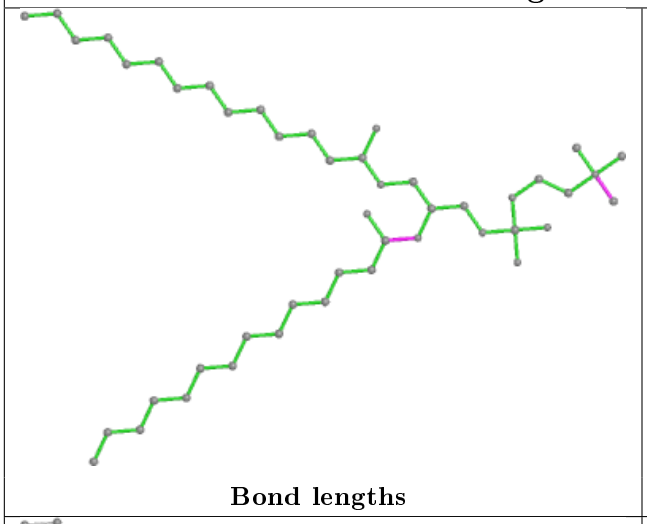


Rings

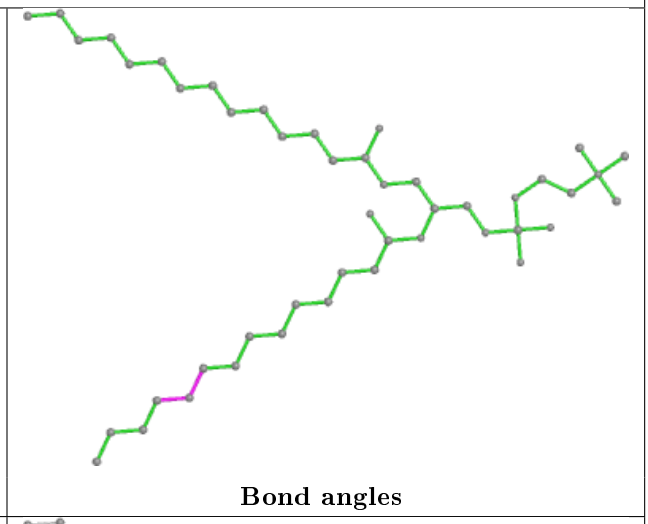
Ligand PX4 B 316



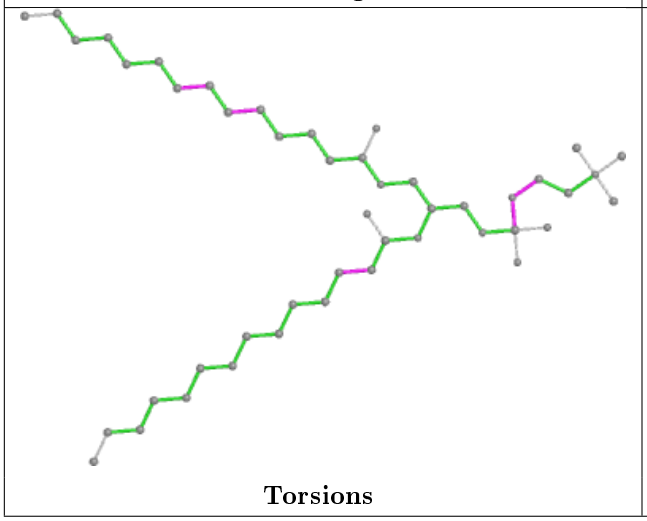
Ligand PX4 A 635



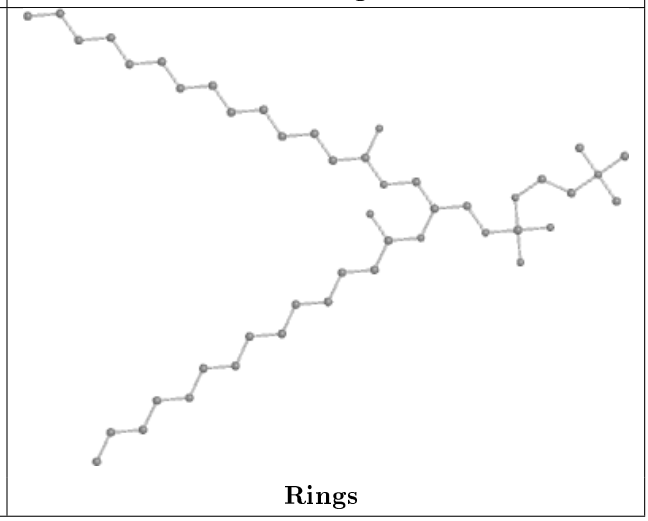
Bond lengths



Bond angles

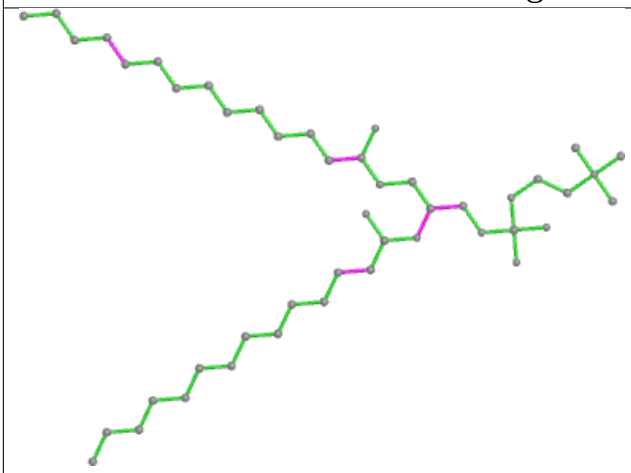


Torsions

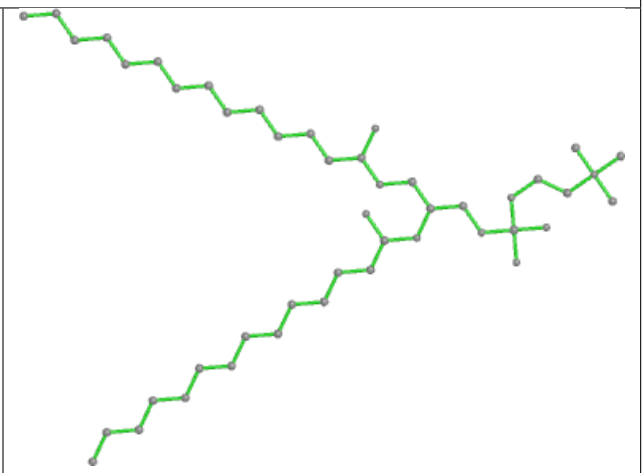


Rings

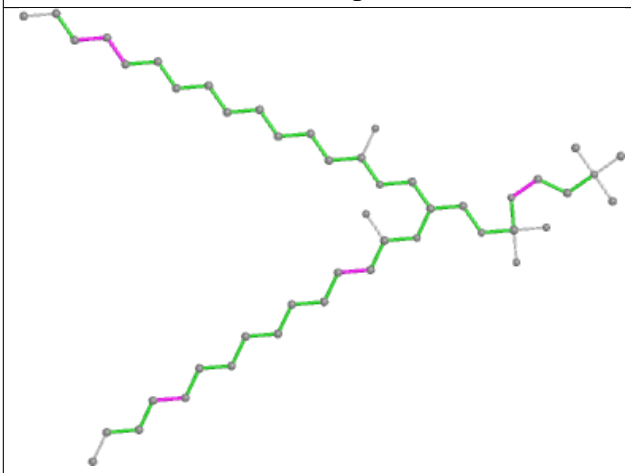
Ligand PX4 A 642



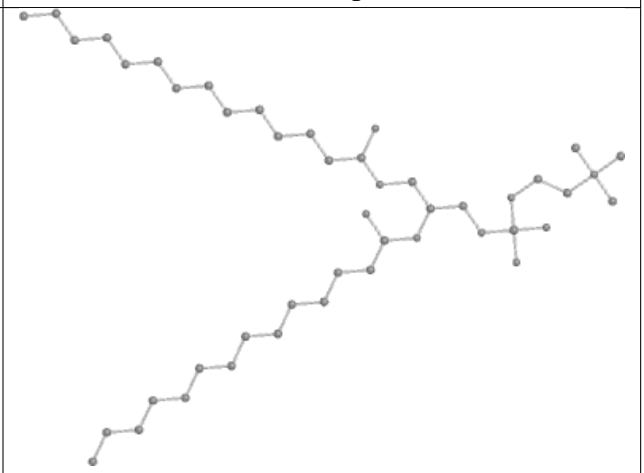
Bond lengths



Bond angles

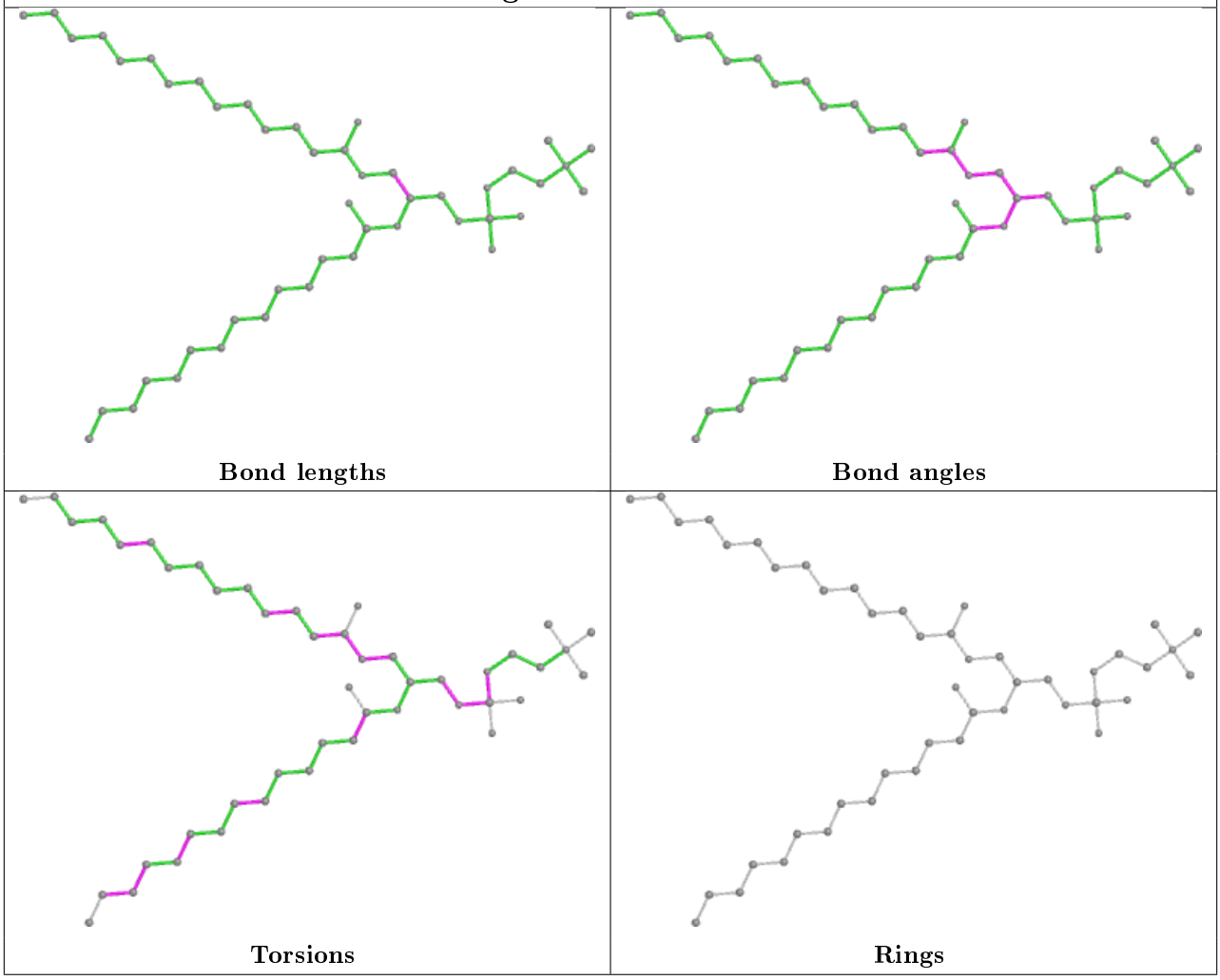


Torsions

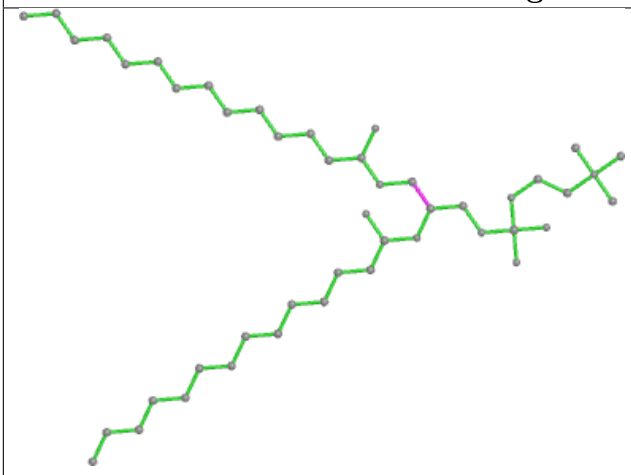


Rings

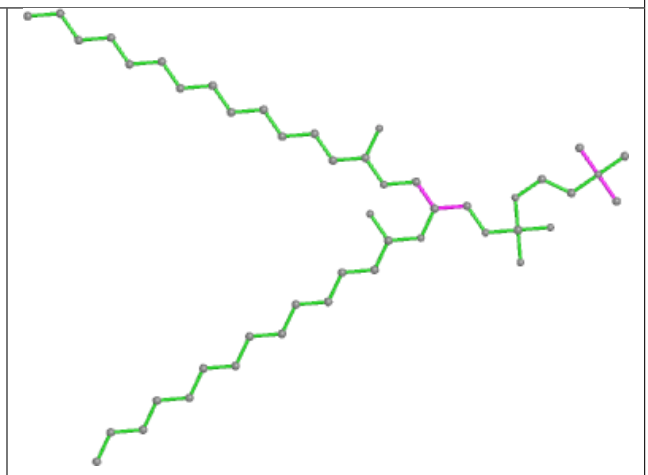
Ligand PX4 C 333



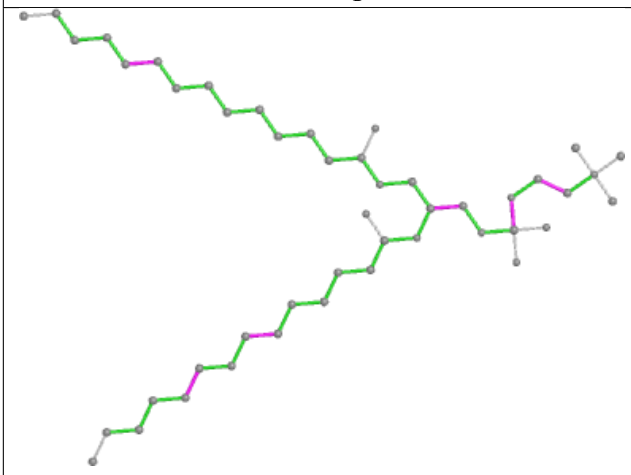
Ligand PX4 A 605



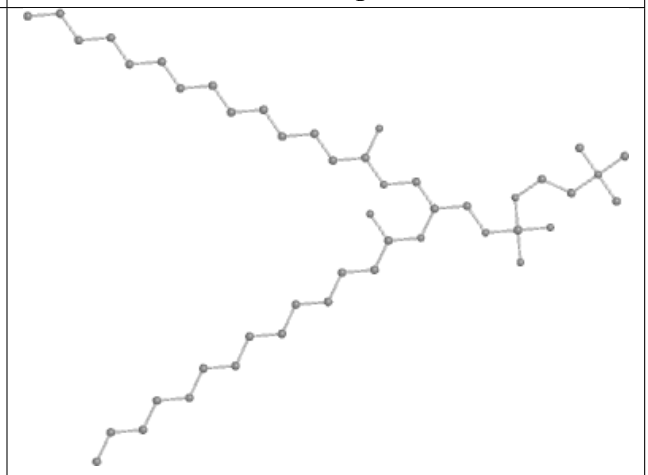
Bond lengths



Bond angles

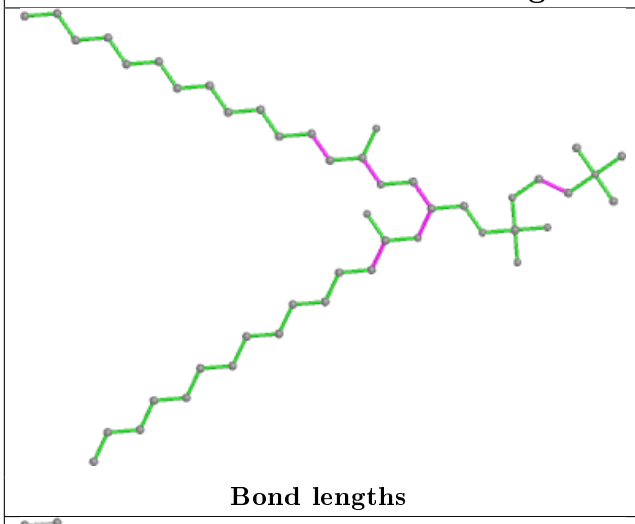


Torsions

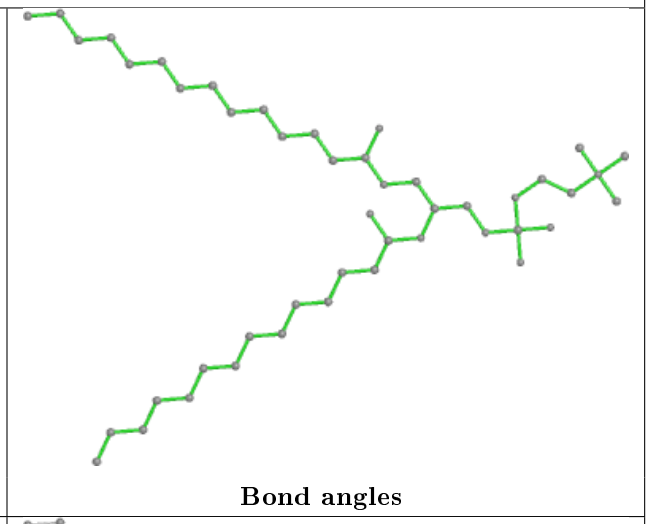


Rings

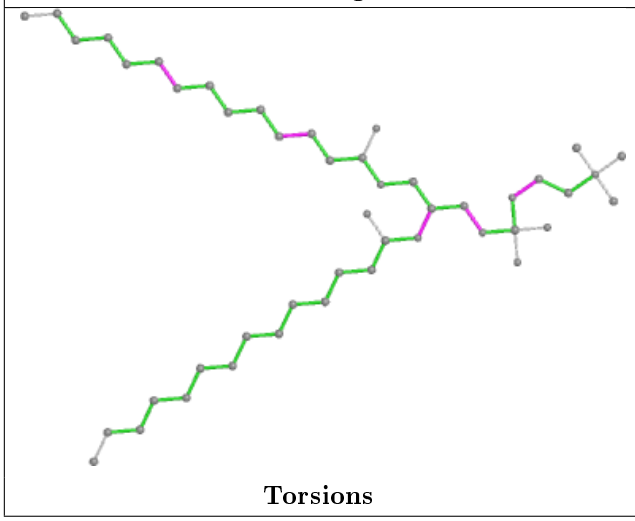
Ligand PX4 C 336



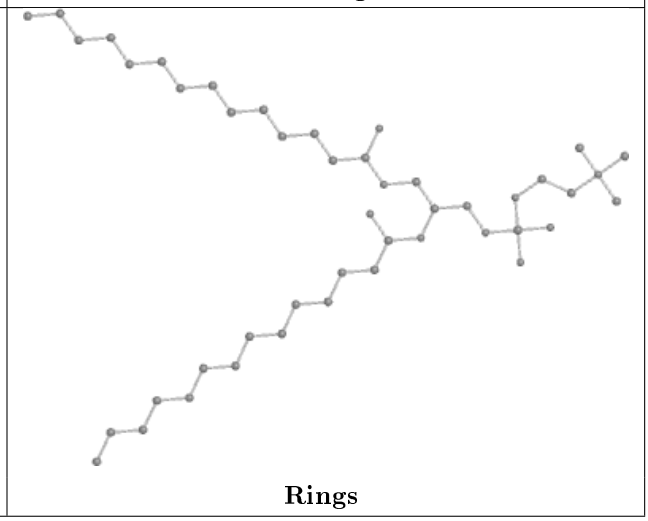
Bond lengths



Bond angles

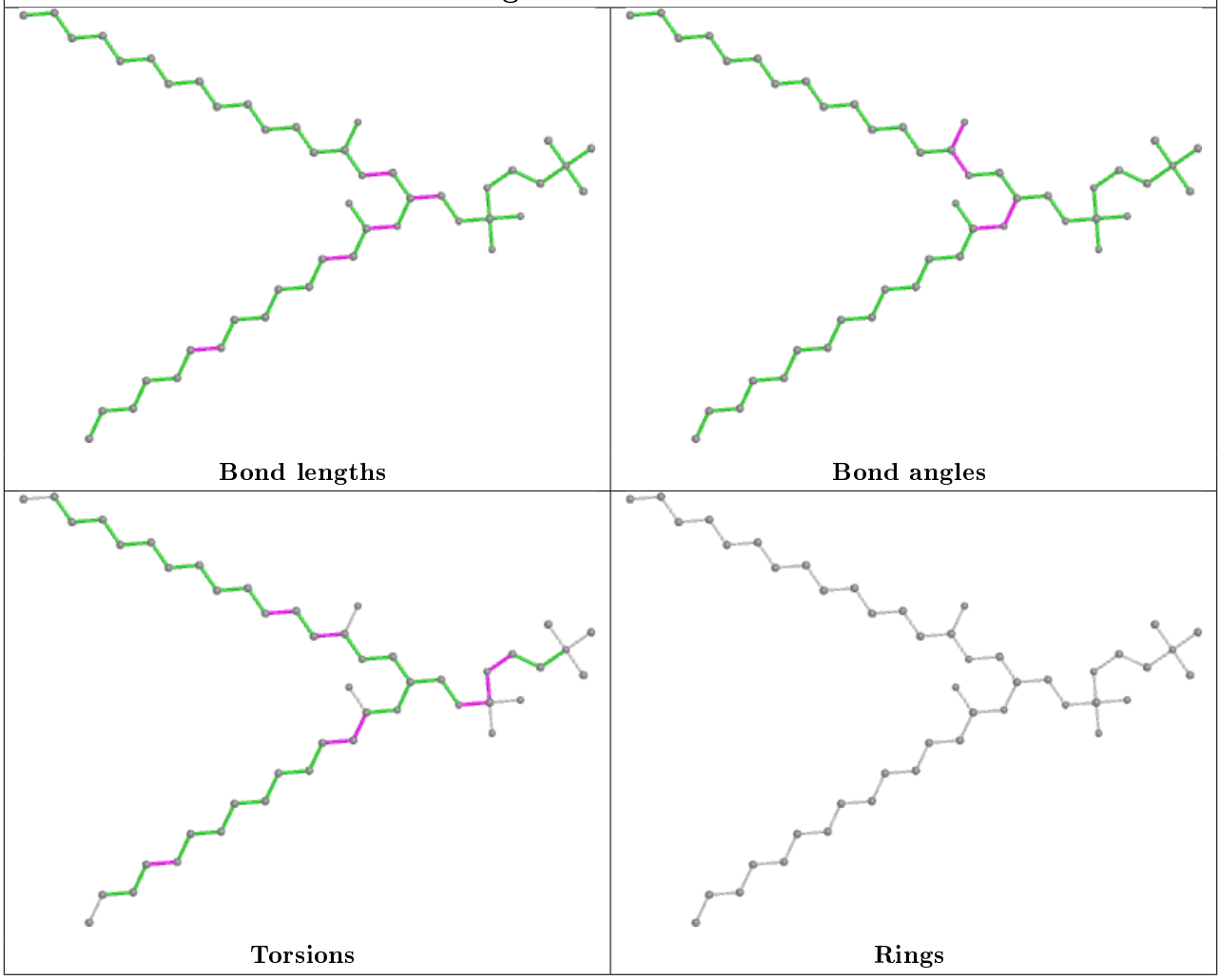


Torsions

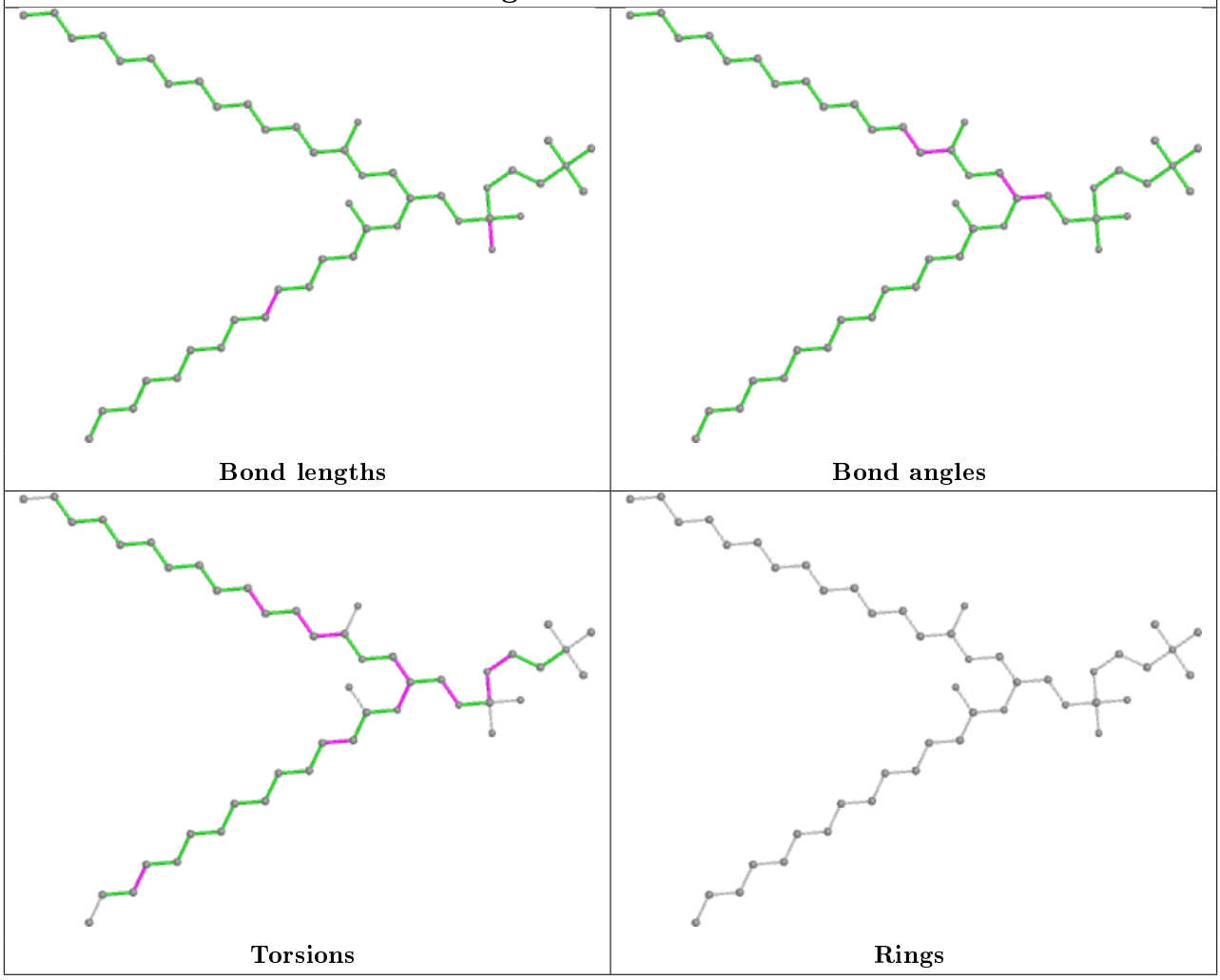


Rings

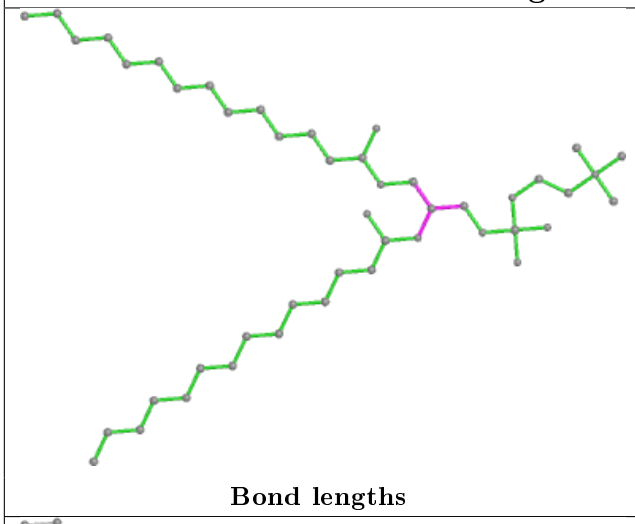
Ligand PX4 C 368



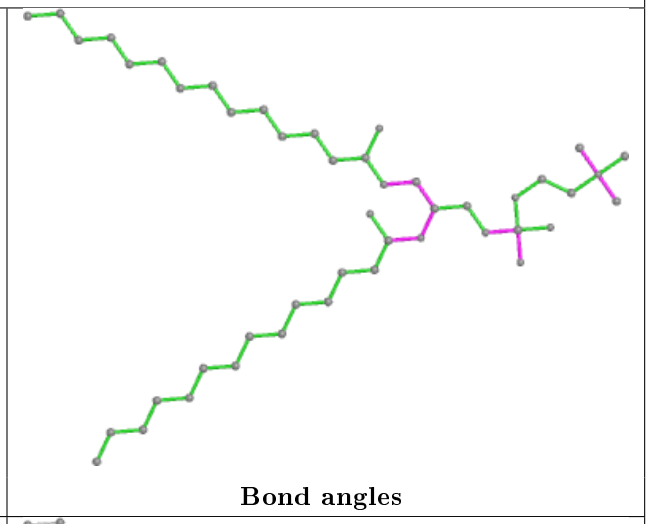
Ligand PX4 A 638



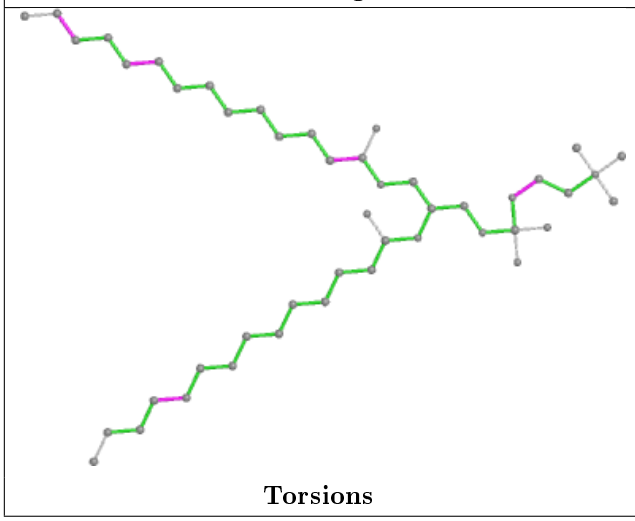
Ligand PX4 B 314



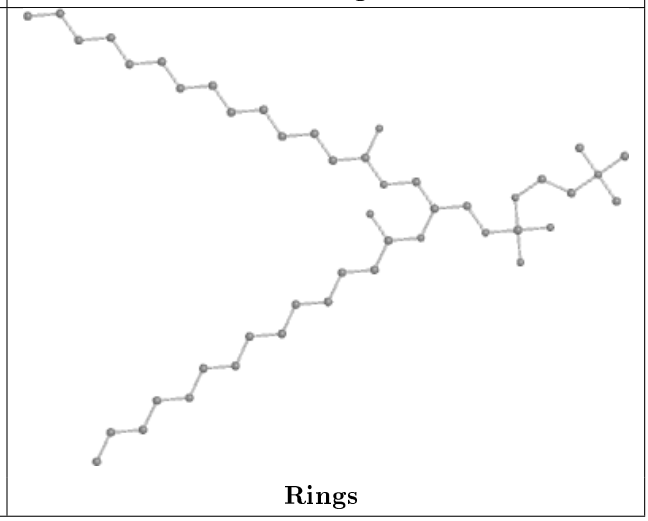
Bond lengths



Bond angles

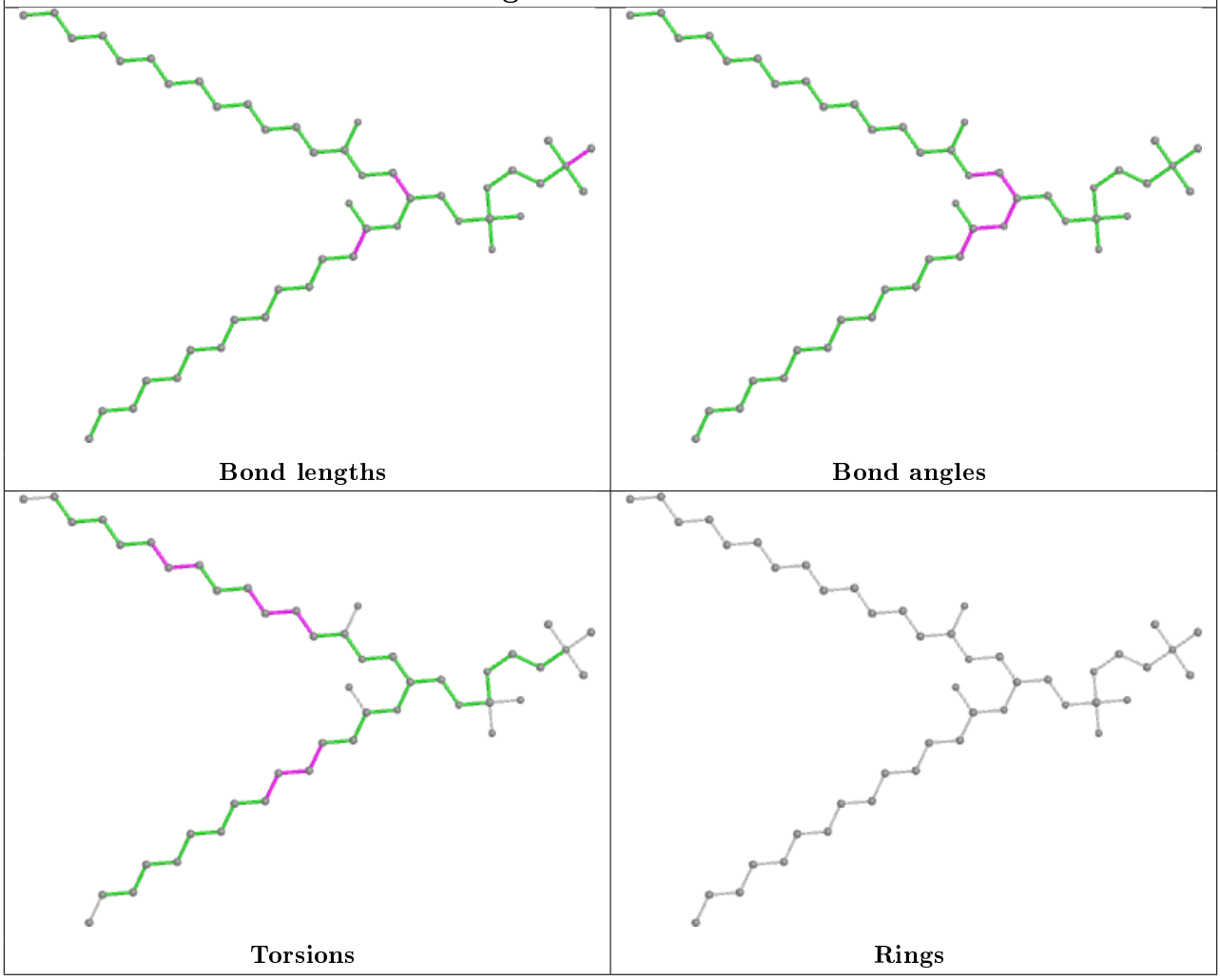


Torsions

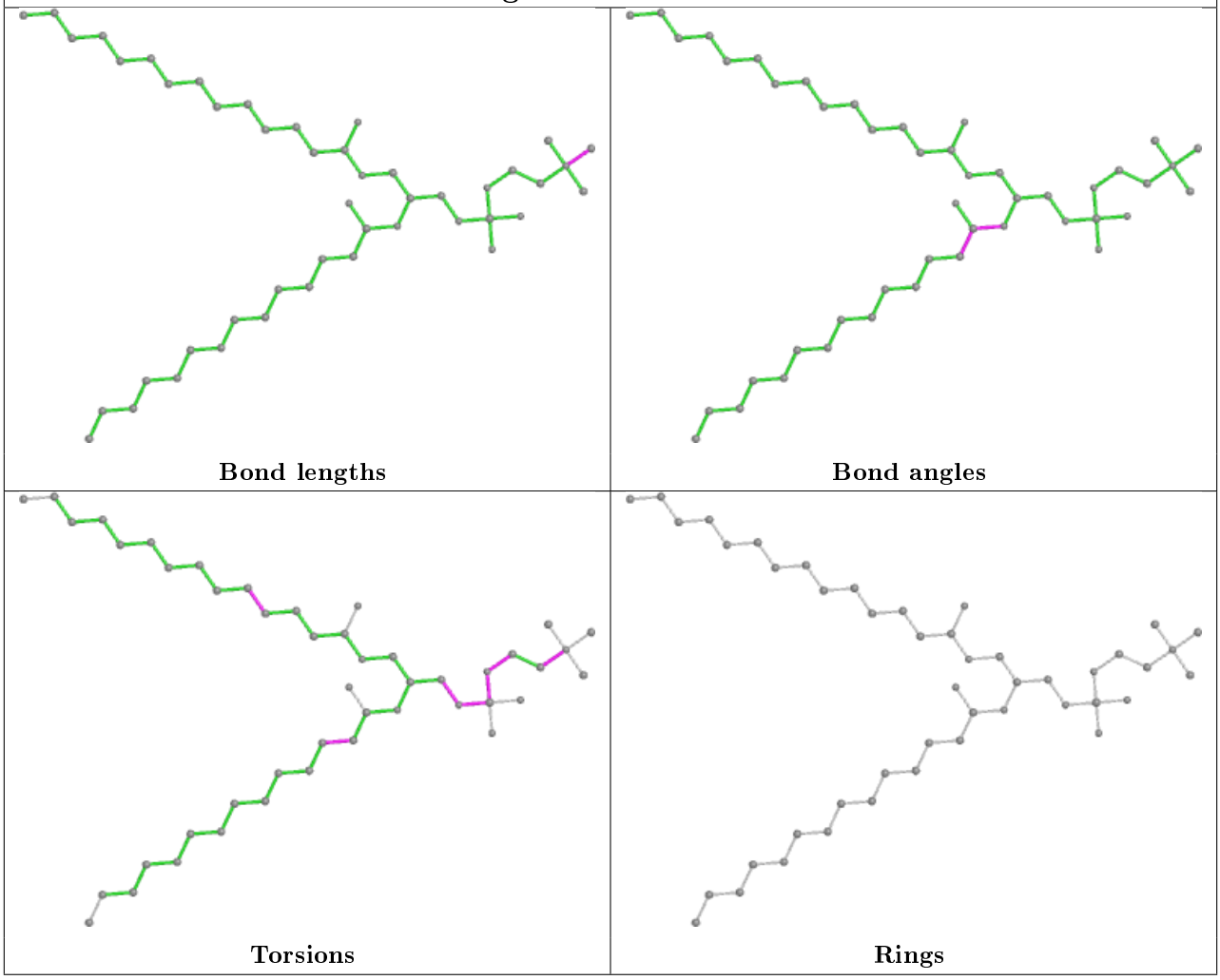


Rings

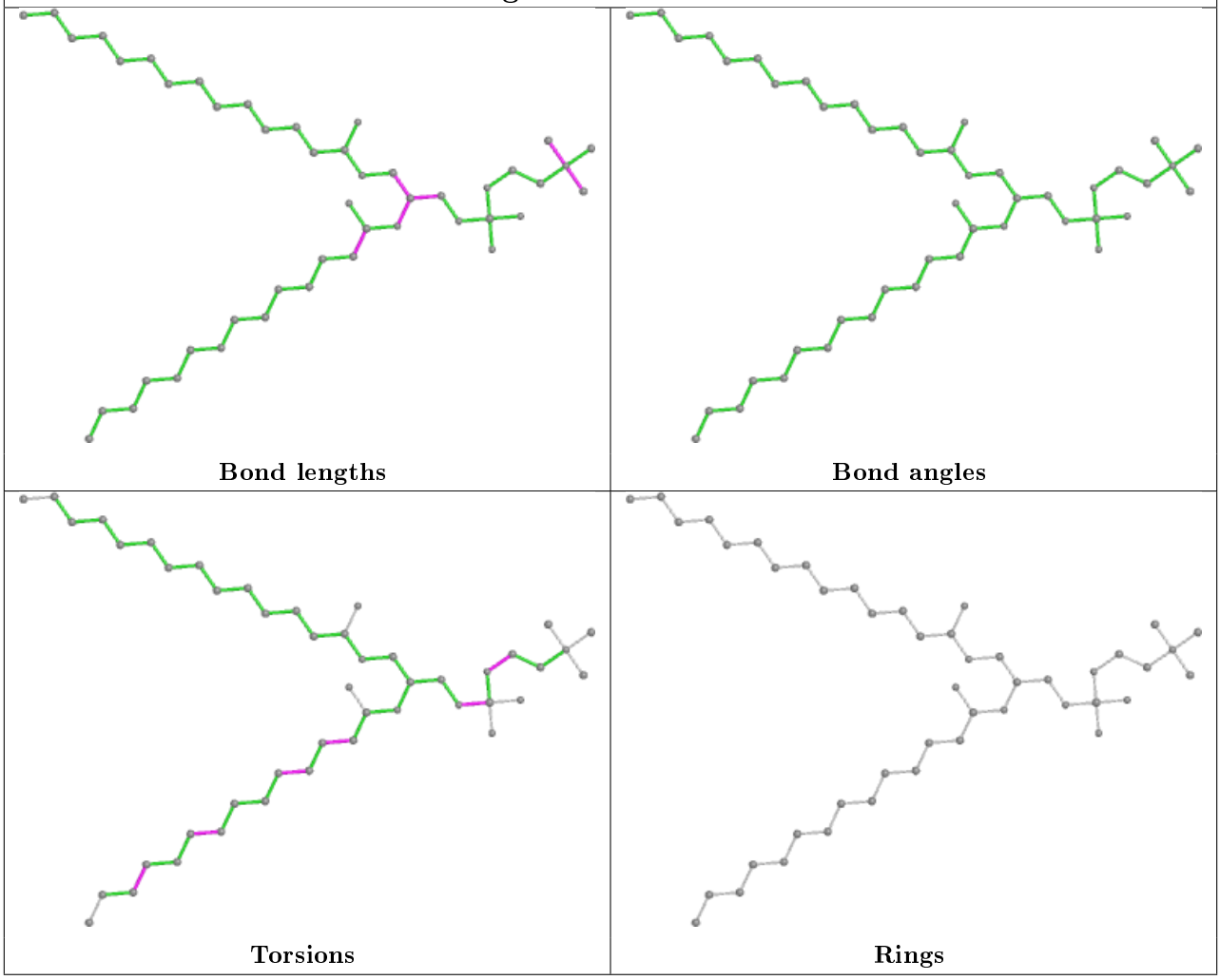
Ligand PX4 B 333



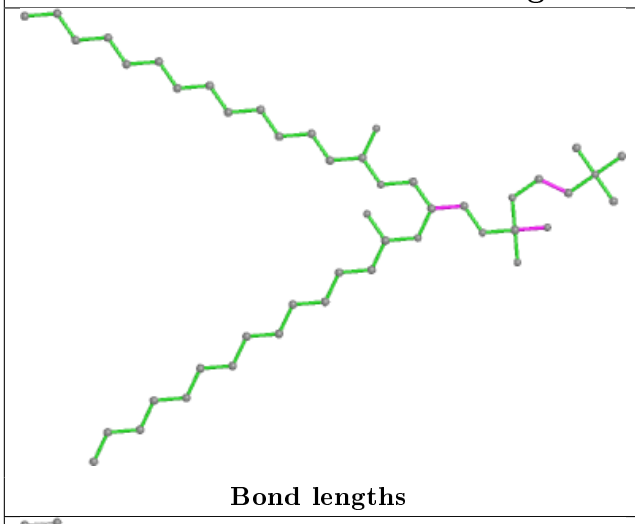
Ligand PX4 C 349



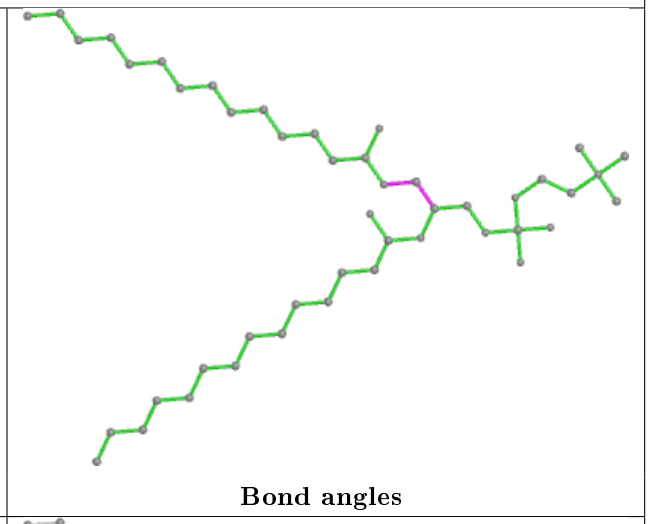
Ligand PX4 B 385



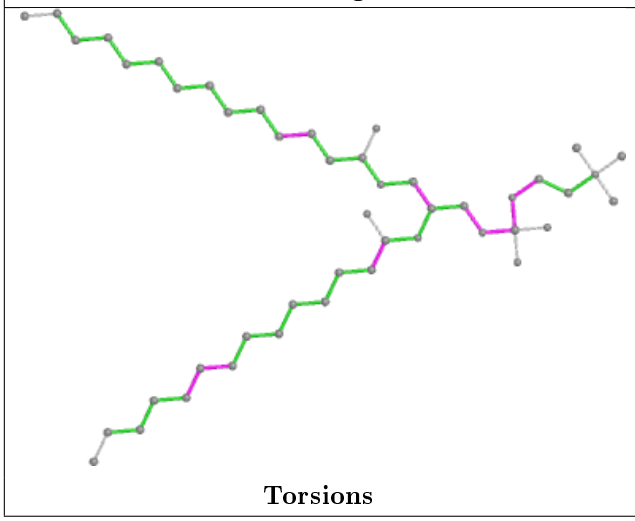
Ligand PX4 A 645



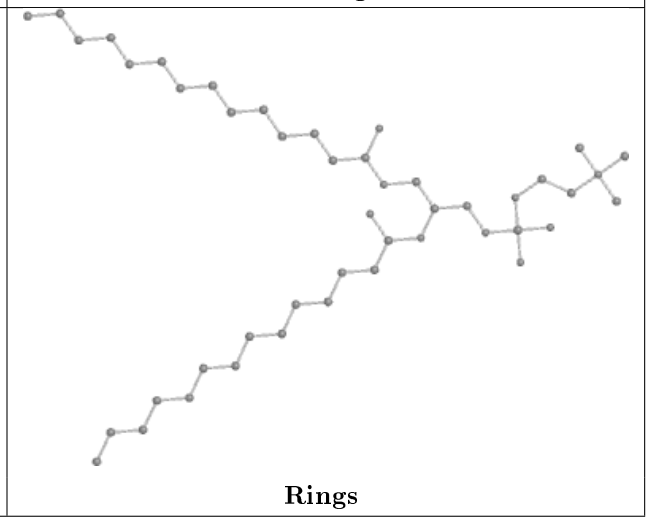
Bond lengths



Bond angles

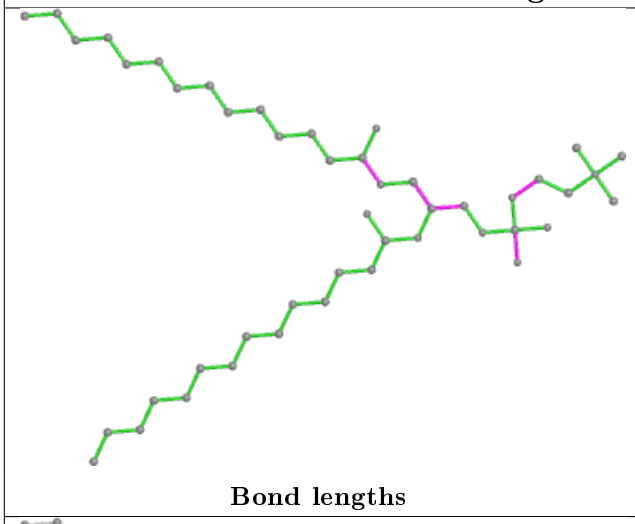


Torsions

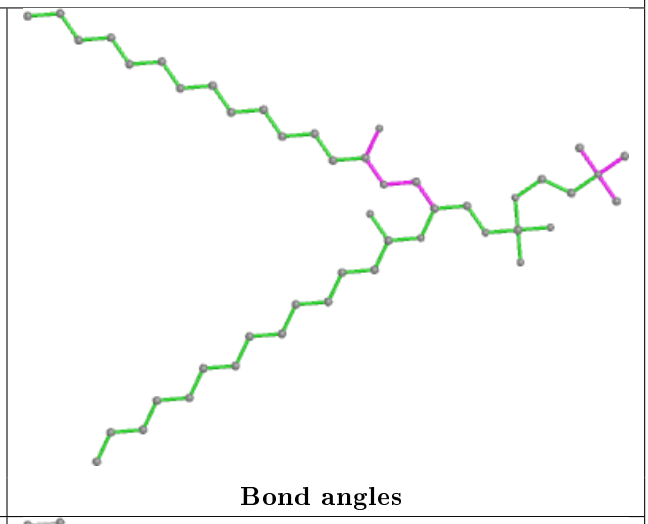


Rings

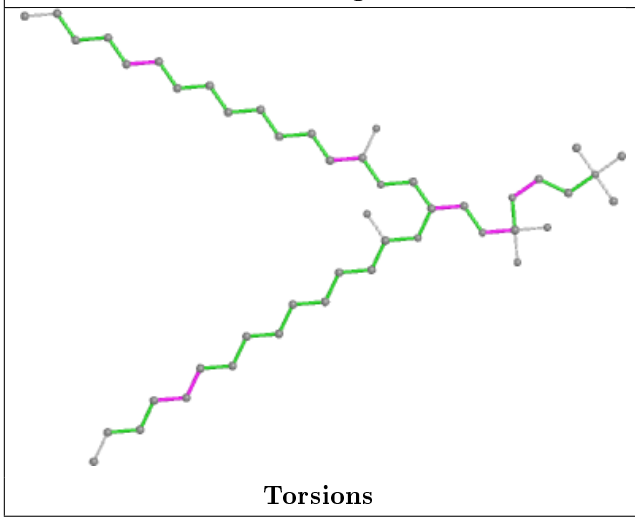
Ligand PX4 A 609



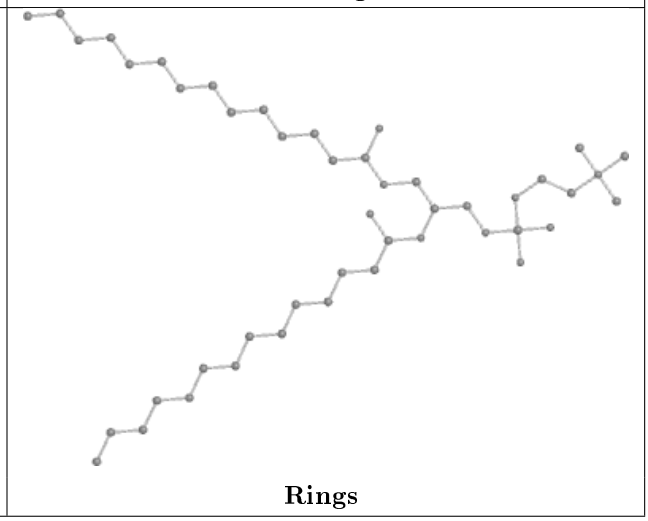
Bond lengths



Bond angles

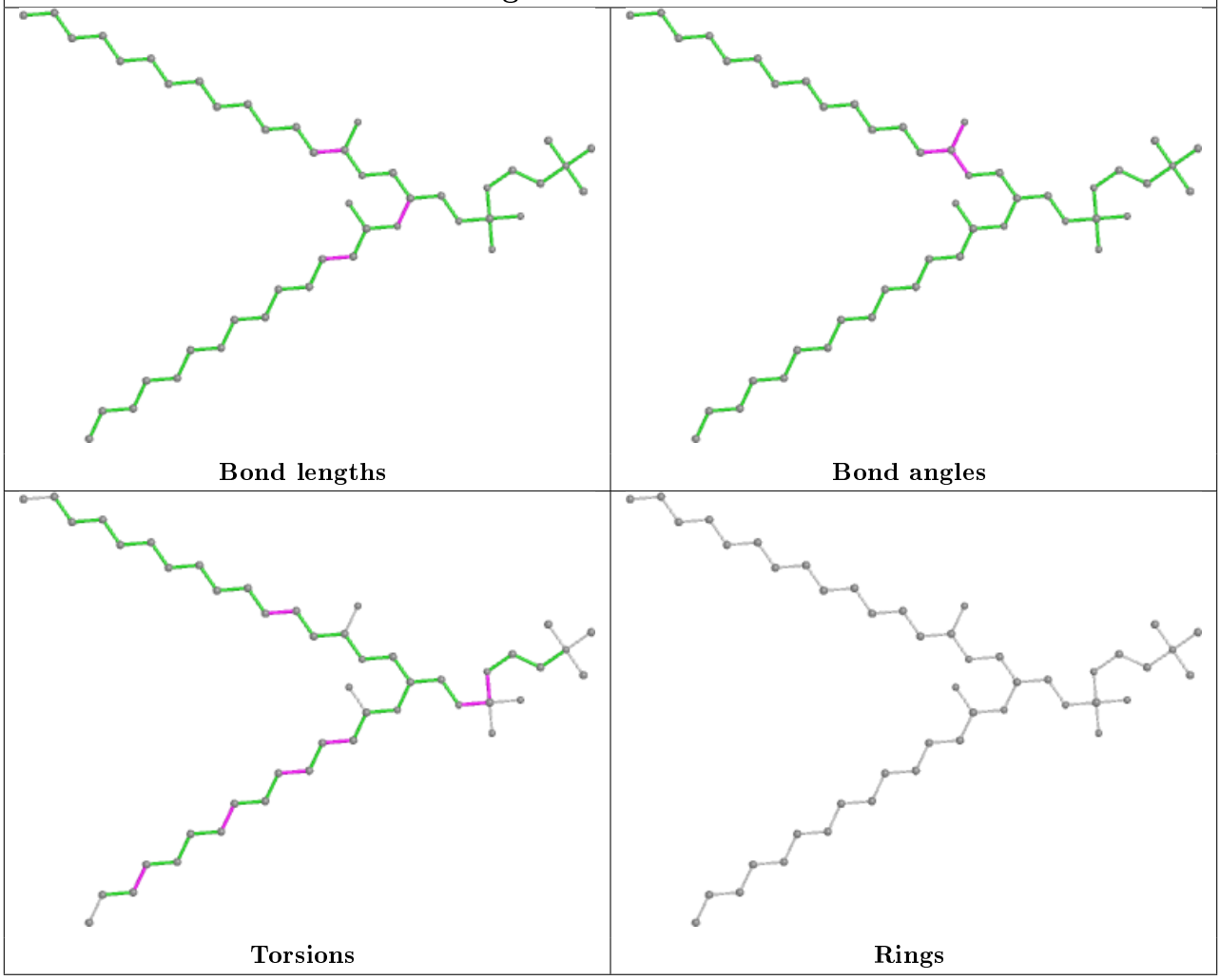


Torsions

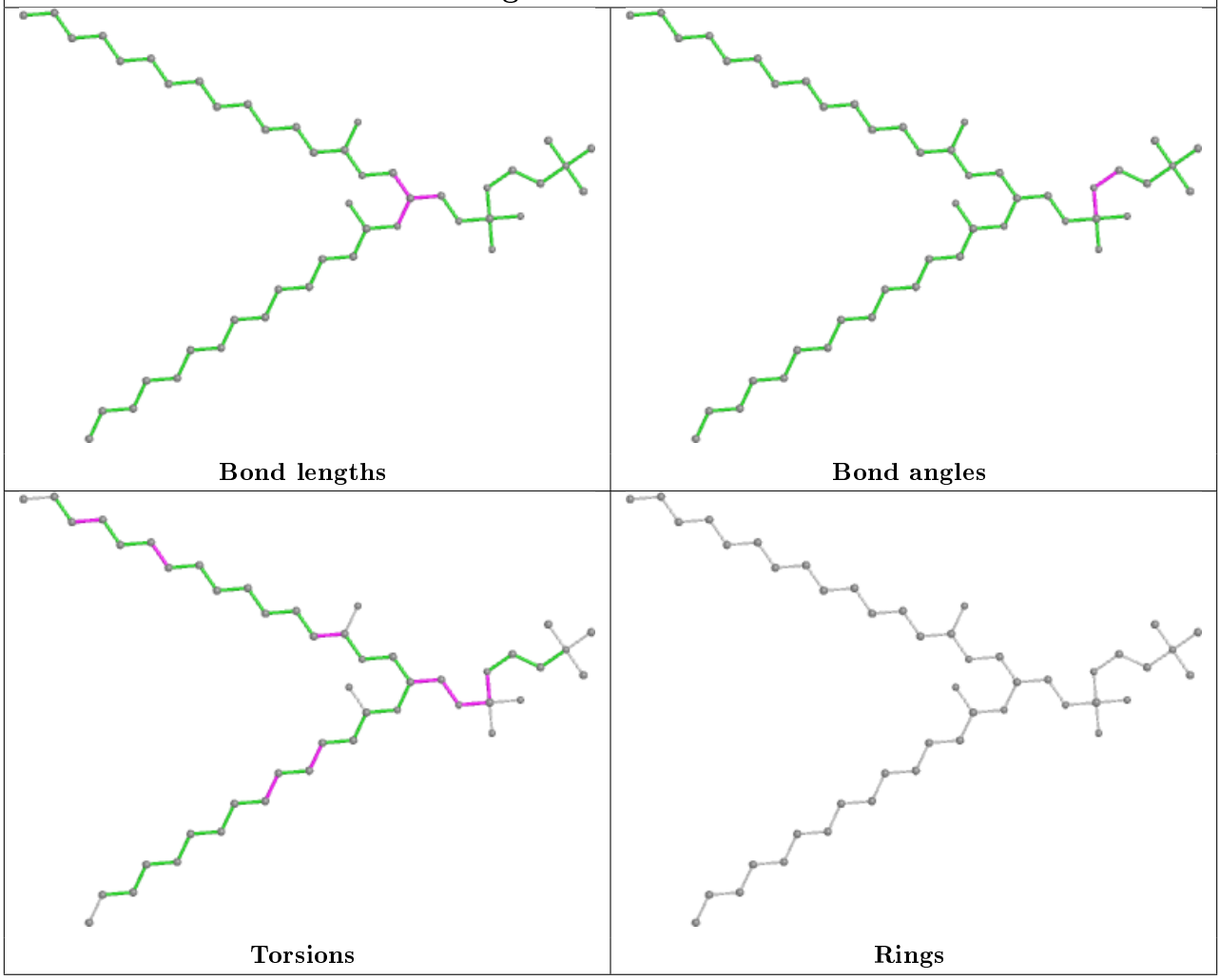


Rings

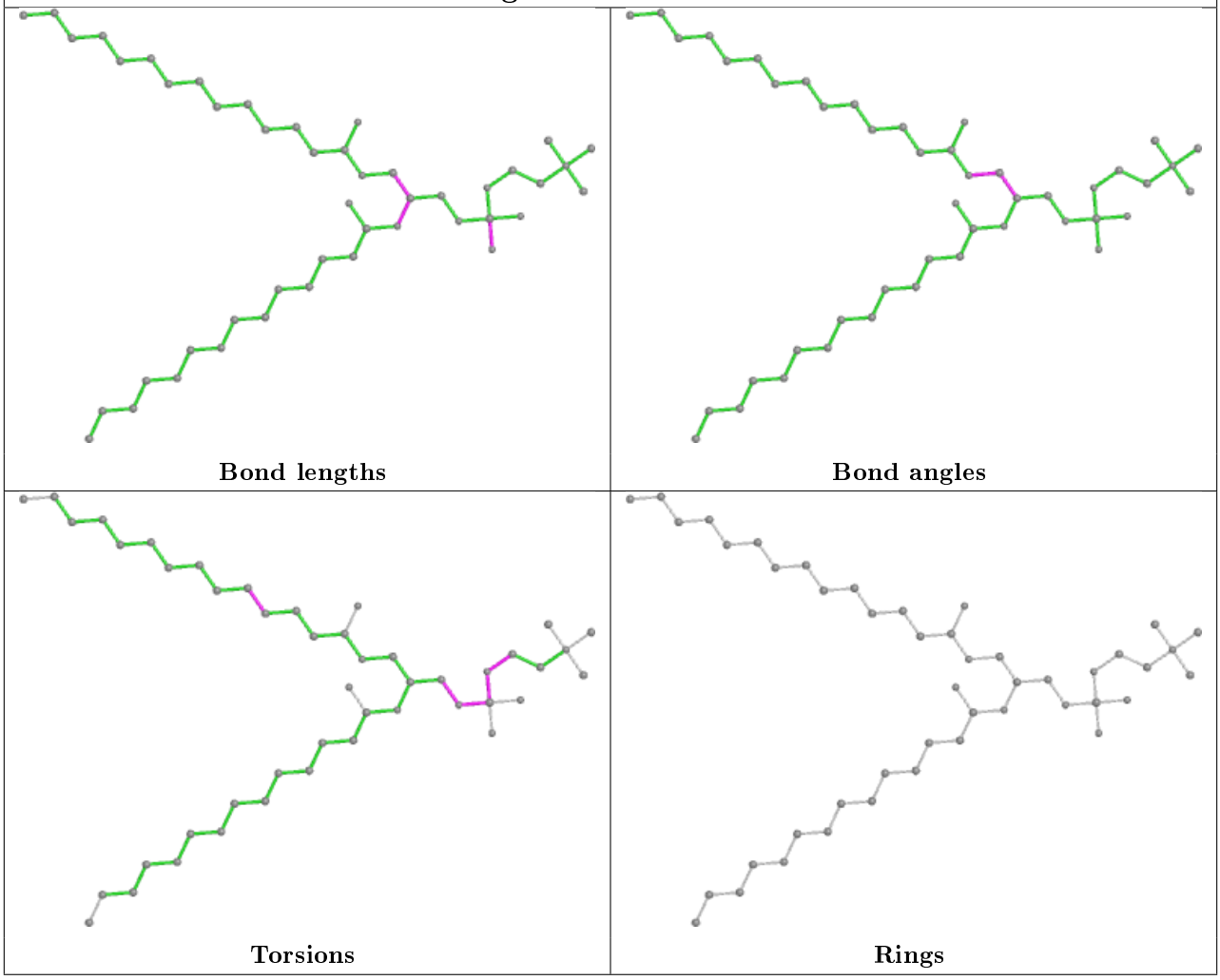
Ligand PX4 B 345



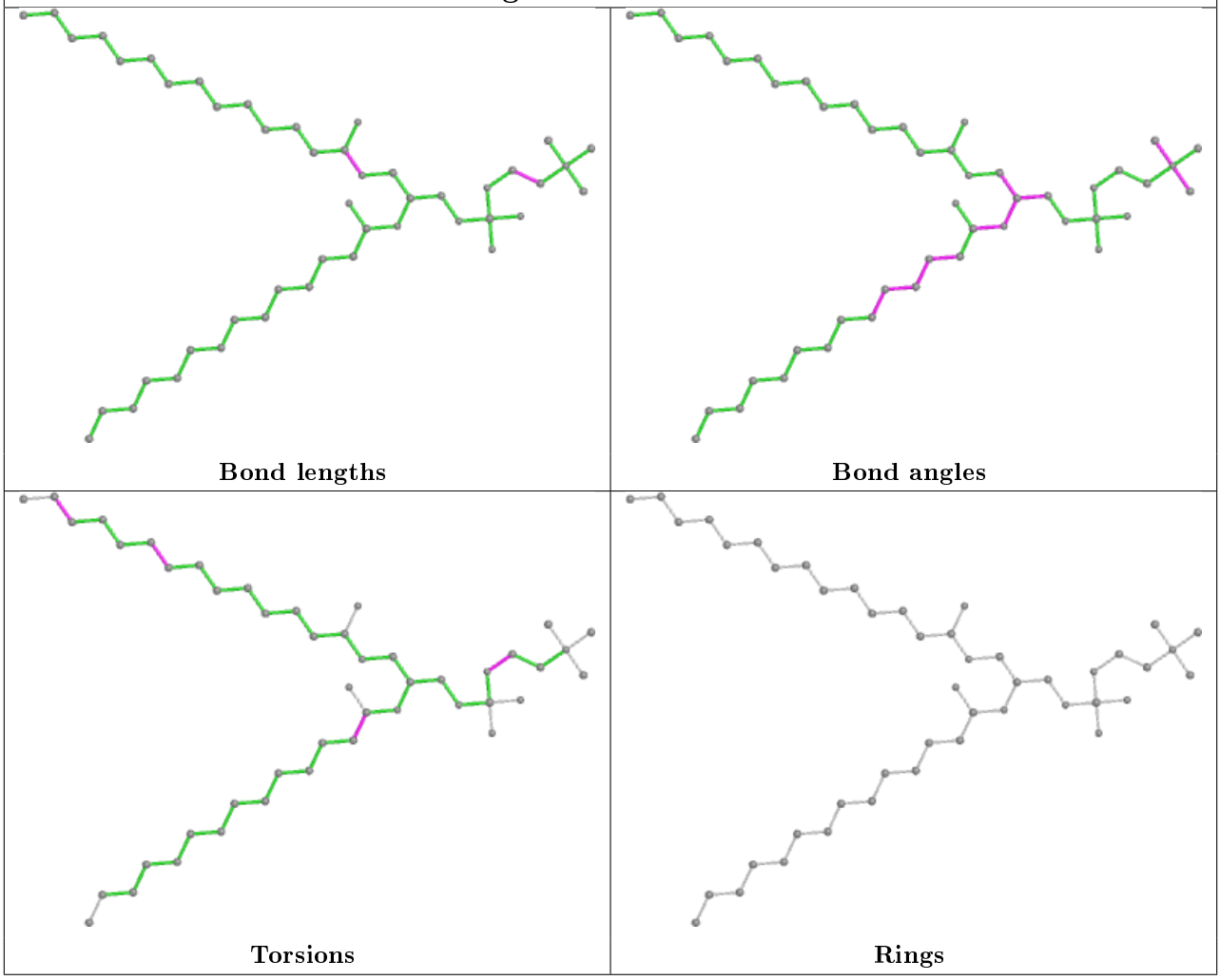
Ligand PX4 B 354



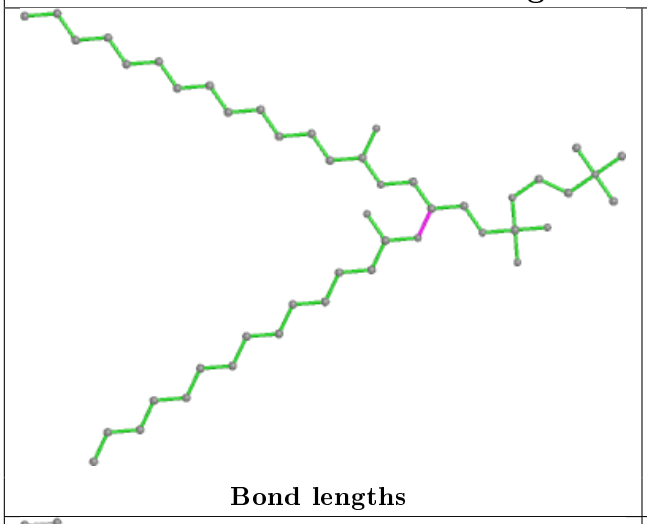
Ligand PX4 A 620



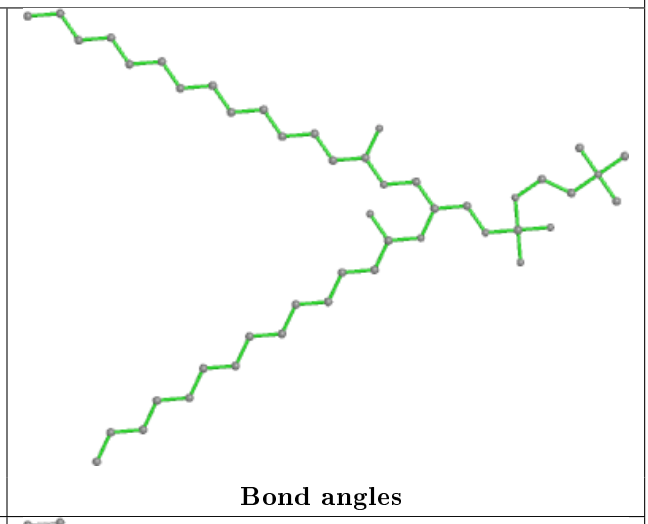
Ligand PX4 B 374



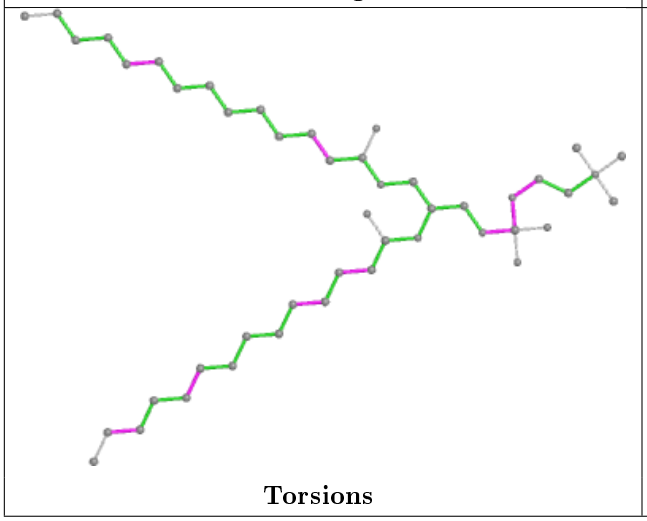
Ligand PX4 A 640



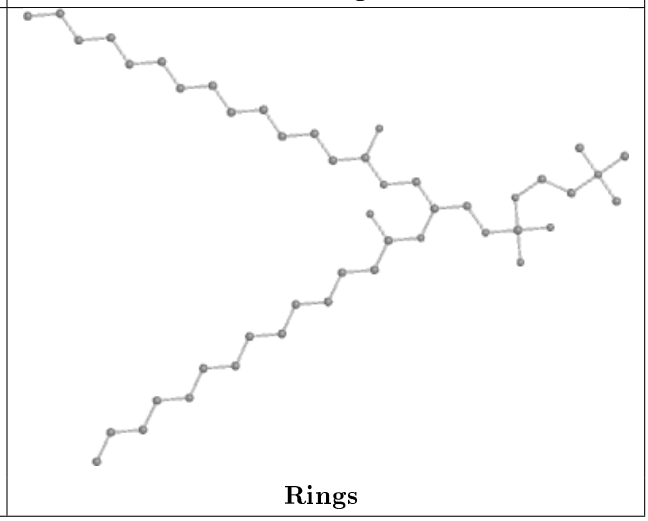
Bond lengths



Bond angles

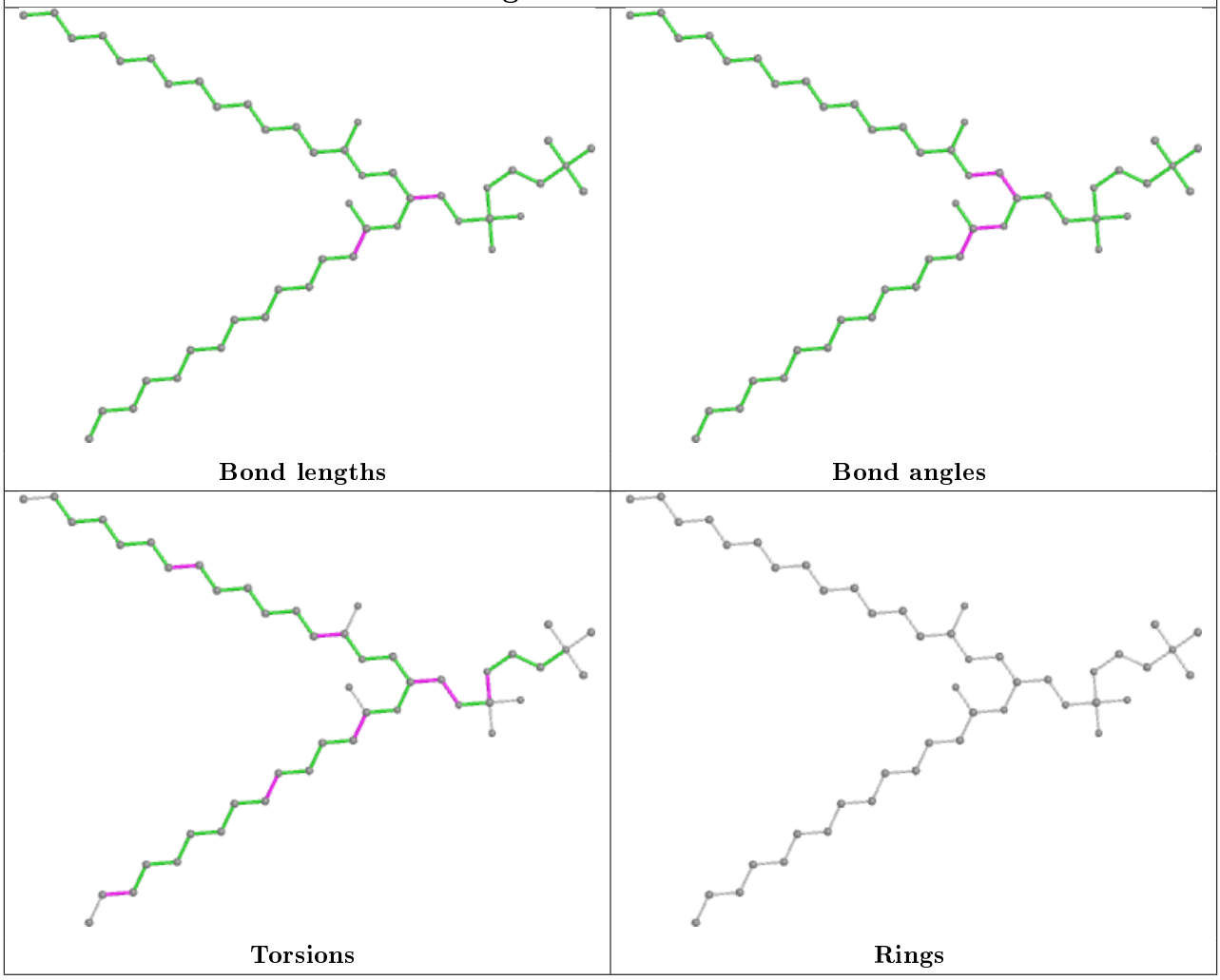


Torsions

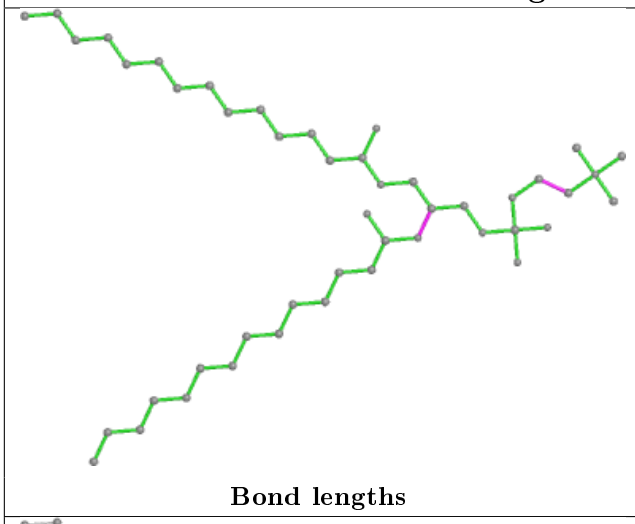


Rings

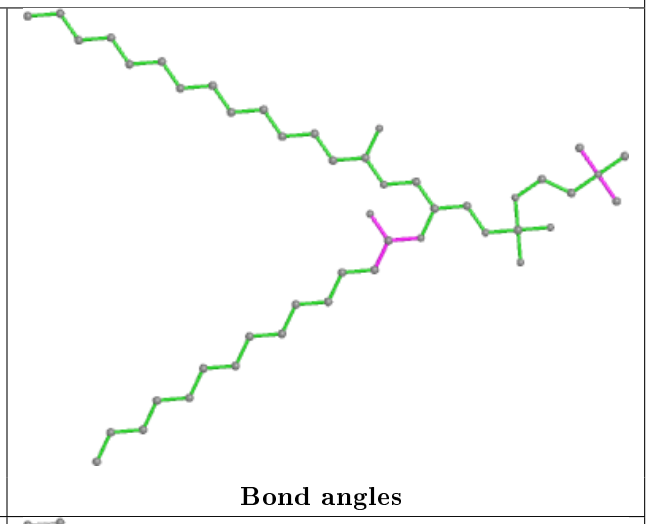
Ligand PX4 B 352



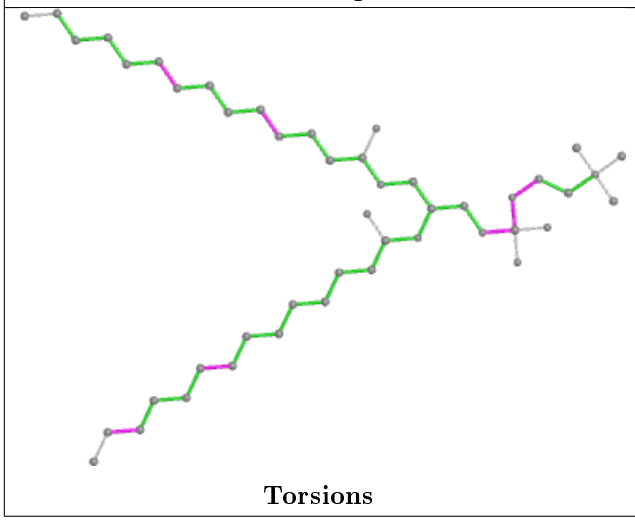
Ligand PX4 C 303



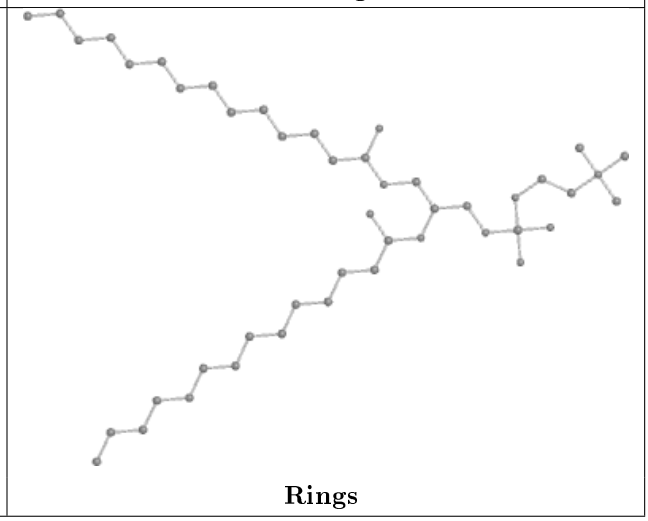
Bond lengths



Bond angles

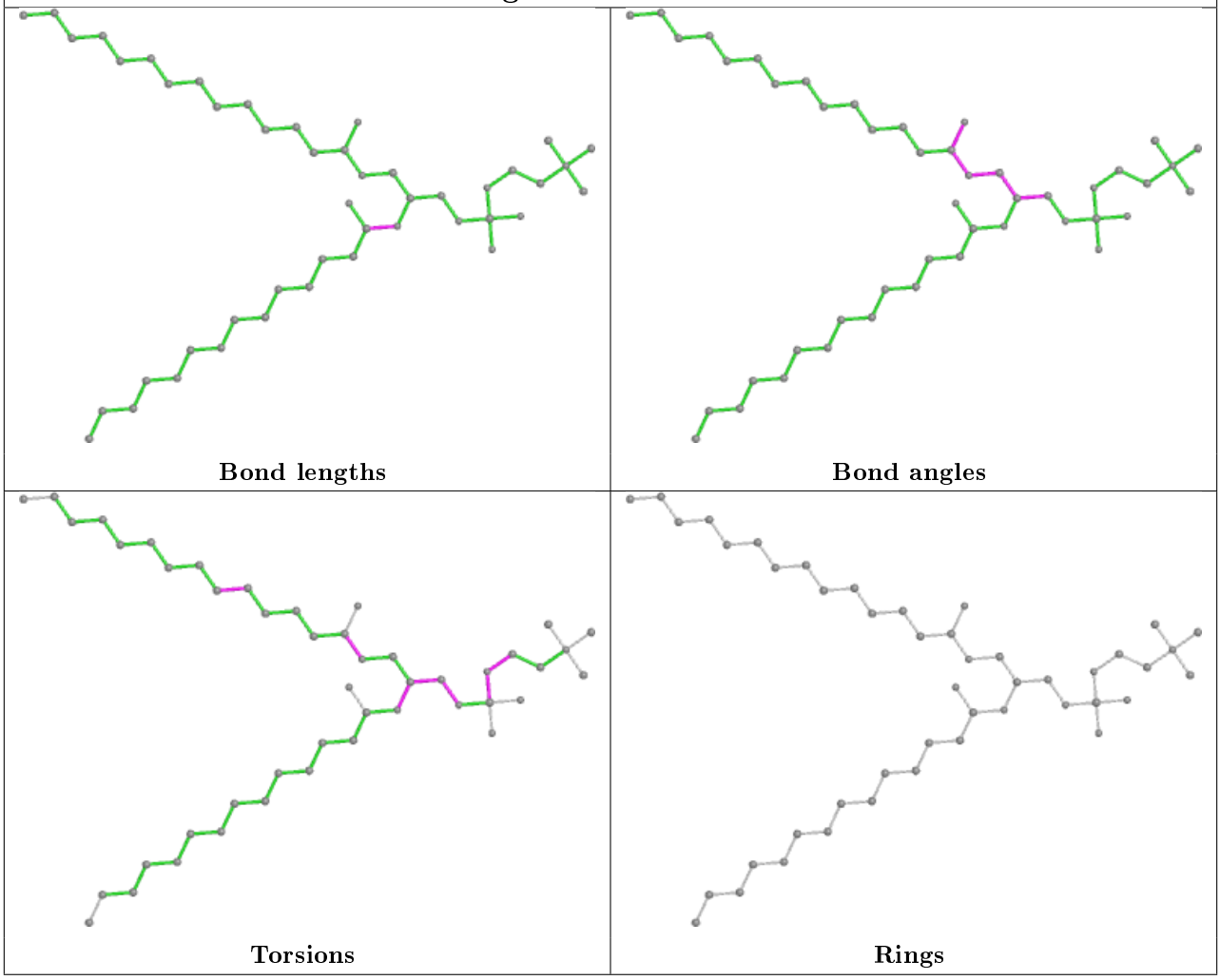


Torsions

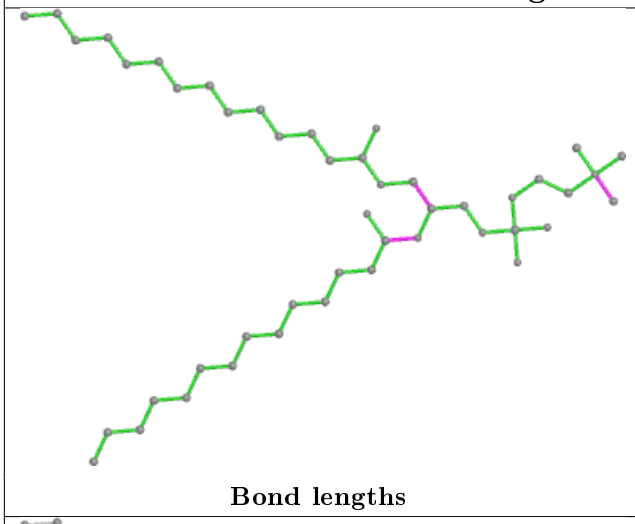


Rings

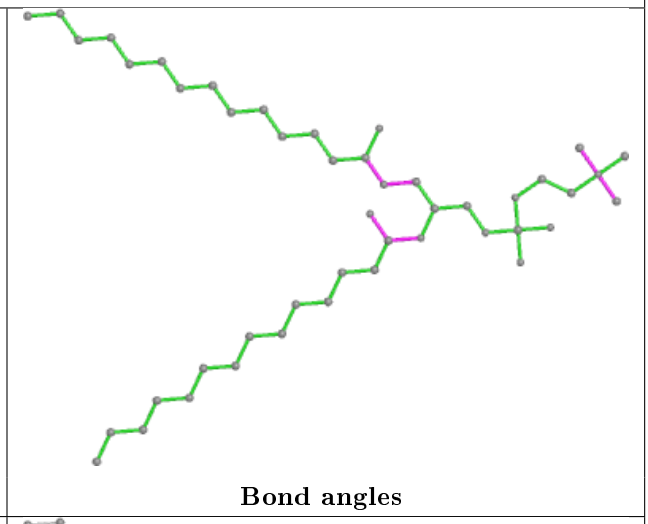
Ligand PX4 B 343



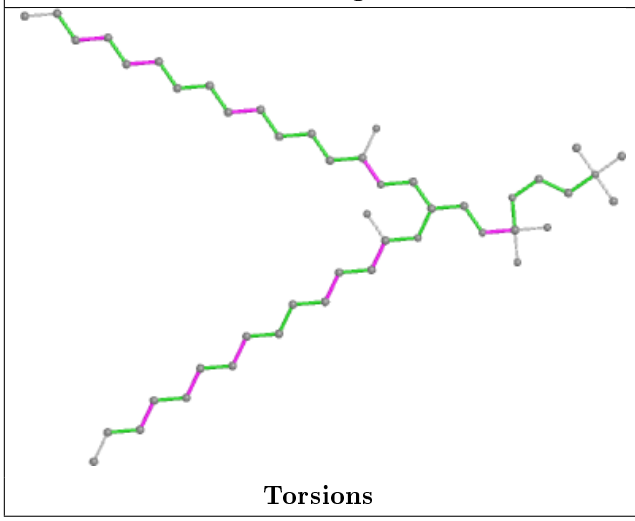
Ligand PX4 C 322



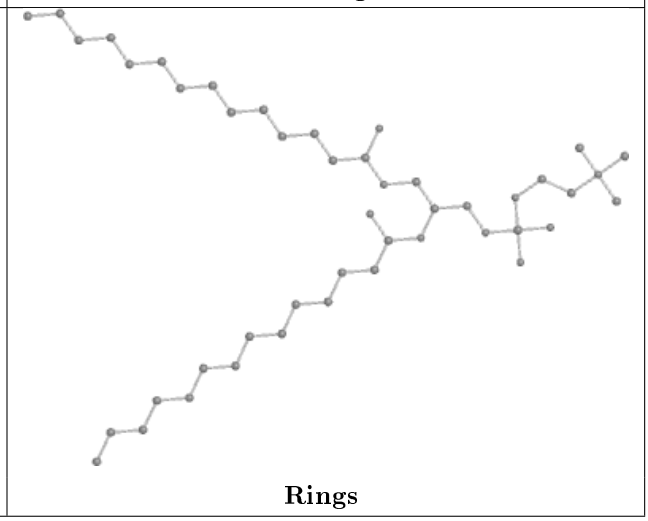
Bond lengths



Bond angles

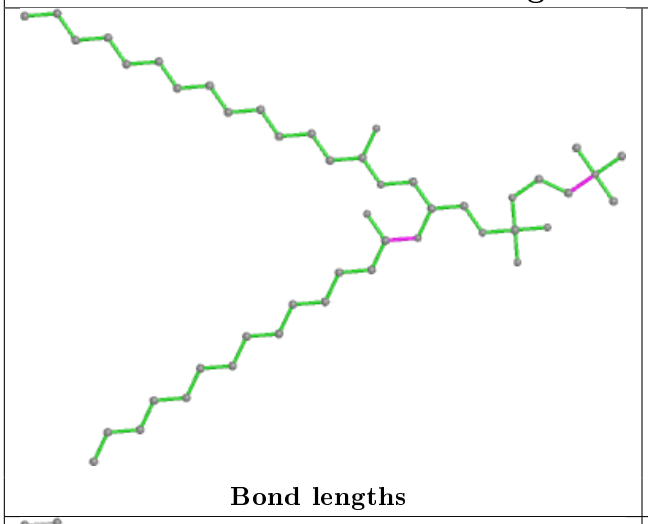


Torsions

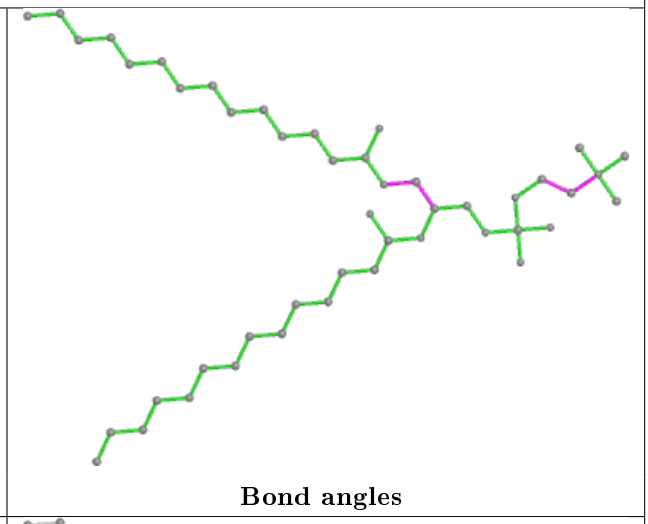


Rings

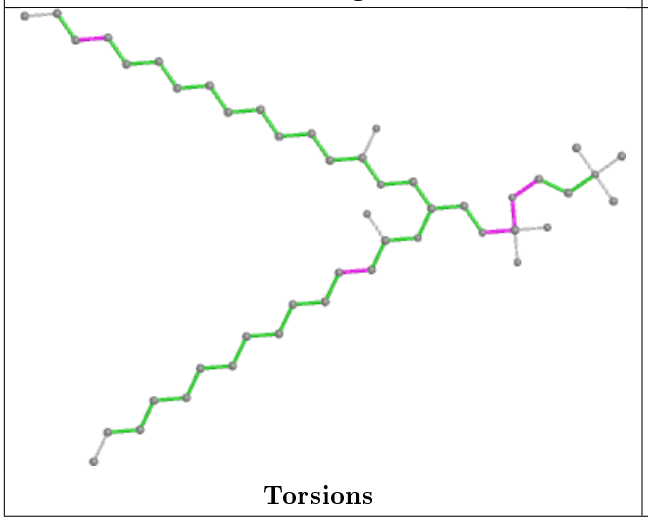
Ligand PX4 A 630



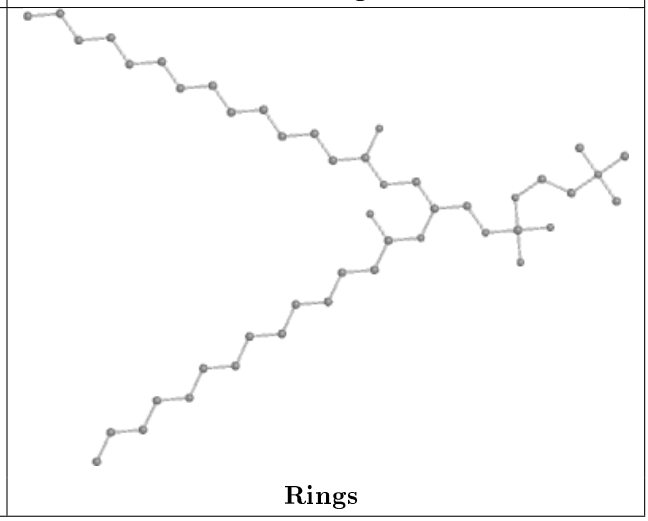
Bond lengths



Bond angles

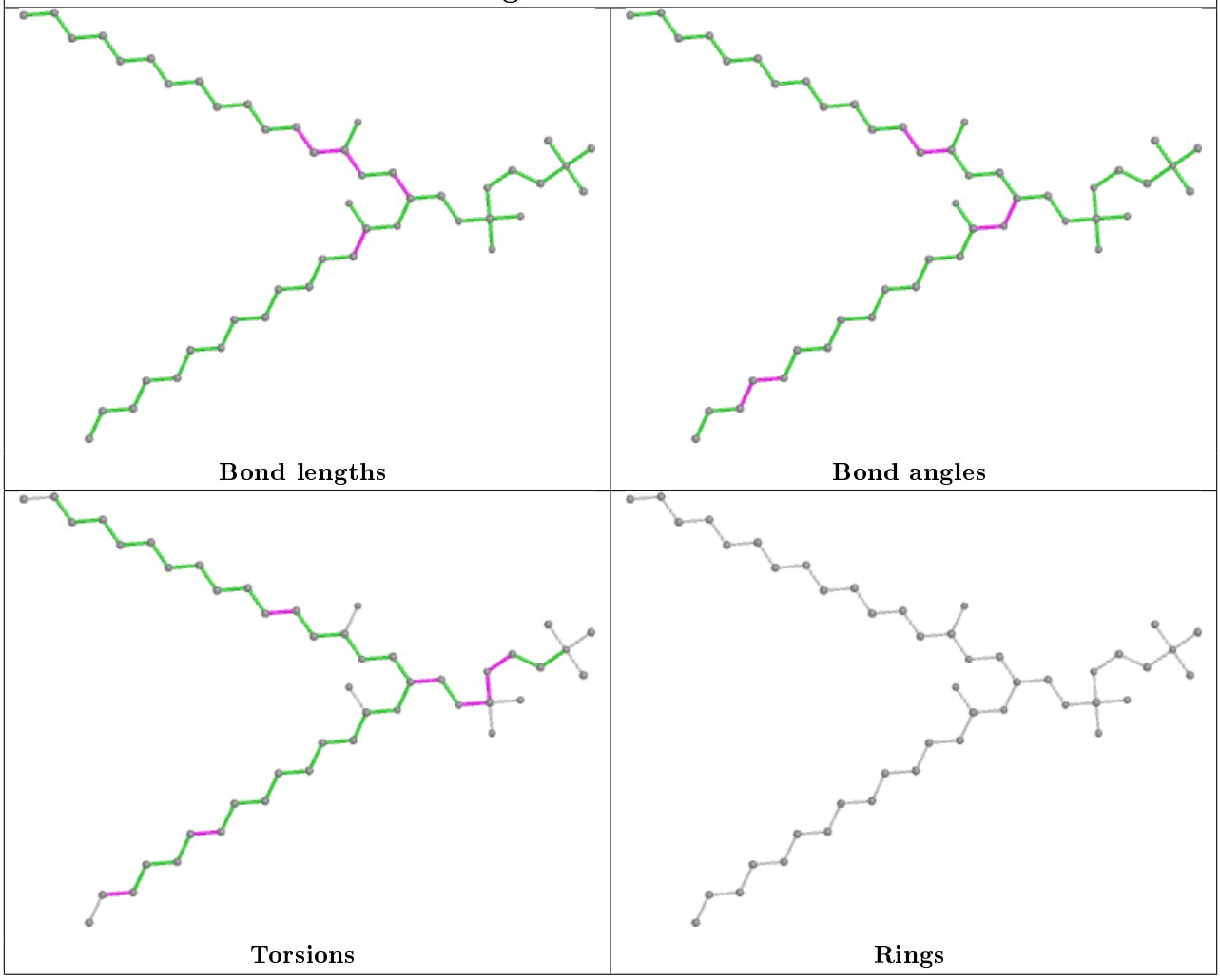


Torsions

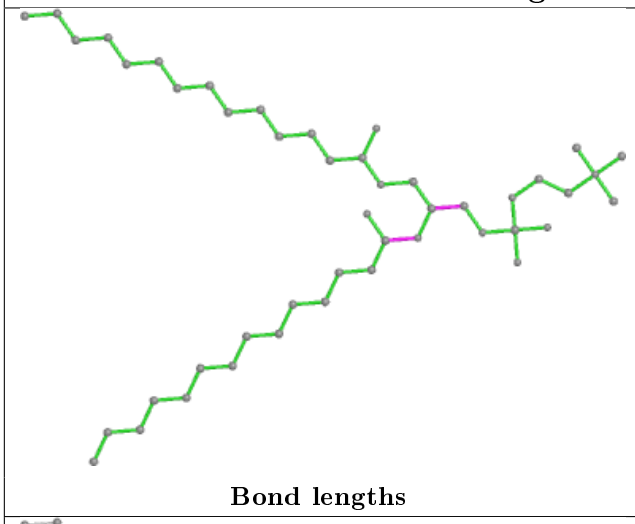


Rings

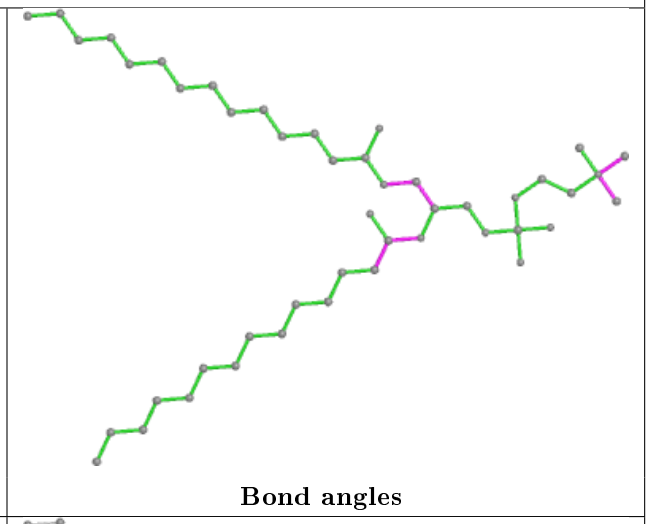
Ligand PX4 B 340



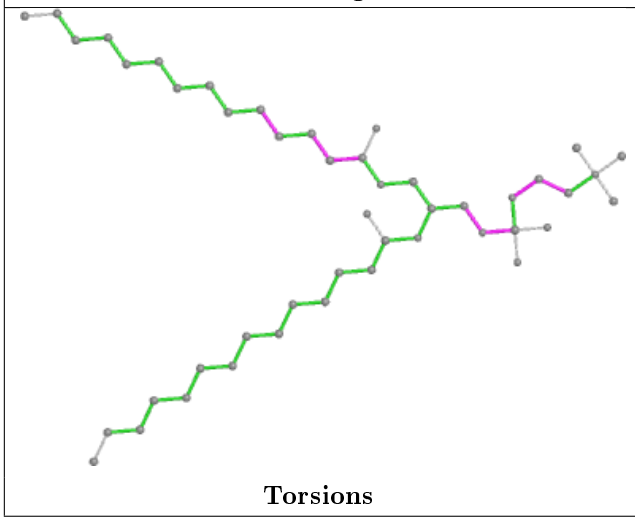
Ligand PX4 B 328



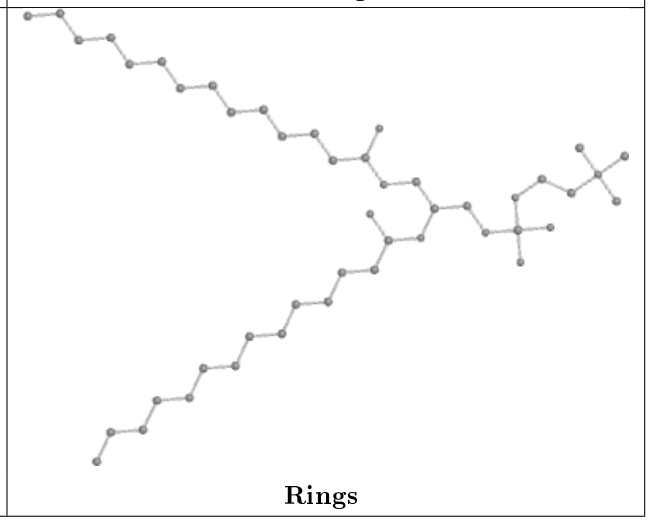
Bond lengths



Bond angles

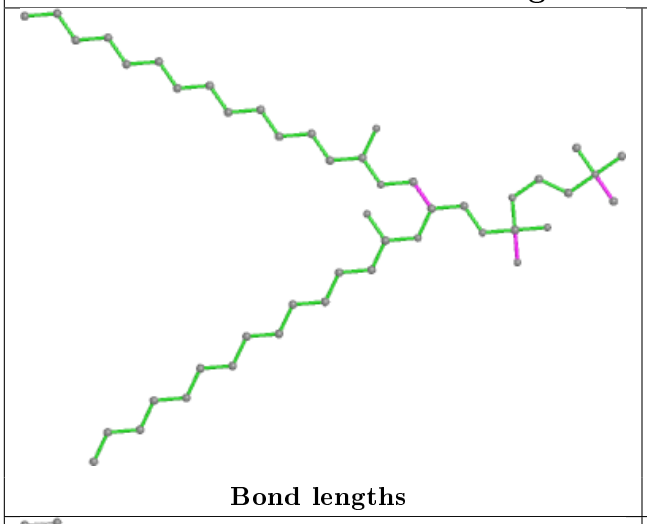


Torsions

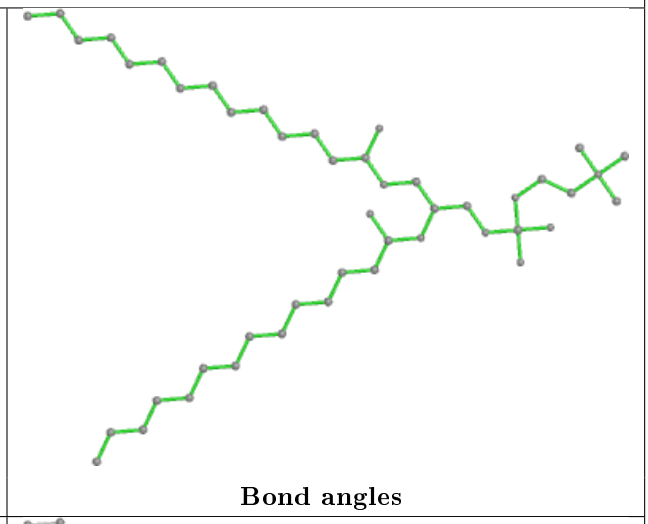


Rings

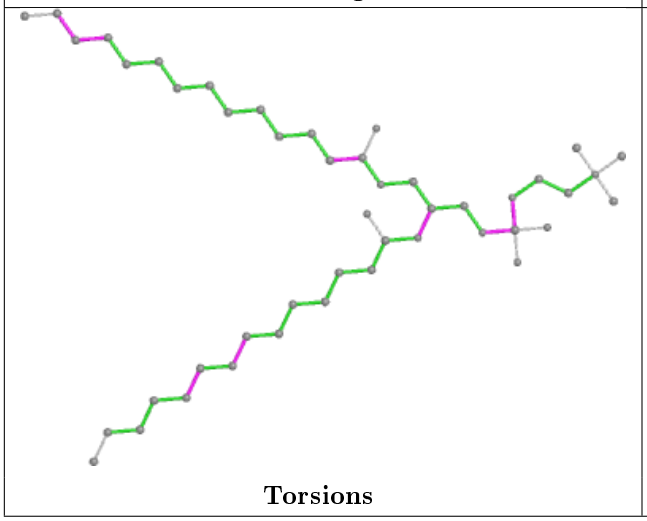
Ligand PX4 B 308



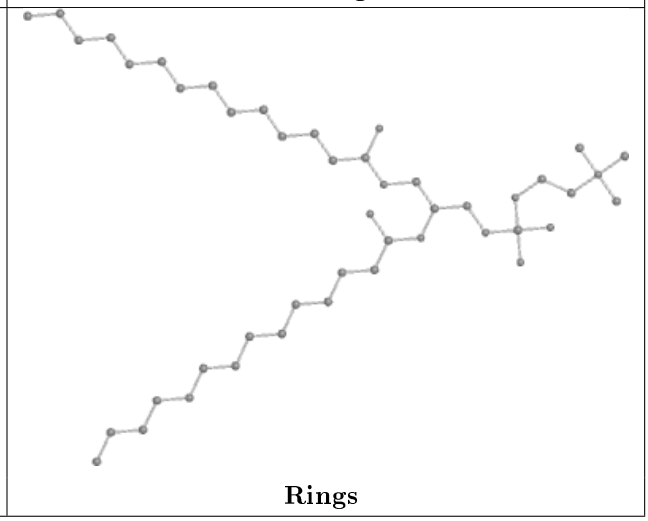
Bond lengths



Bond angles

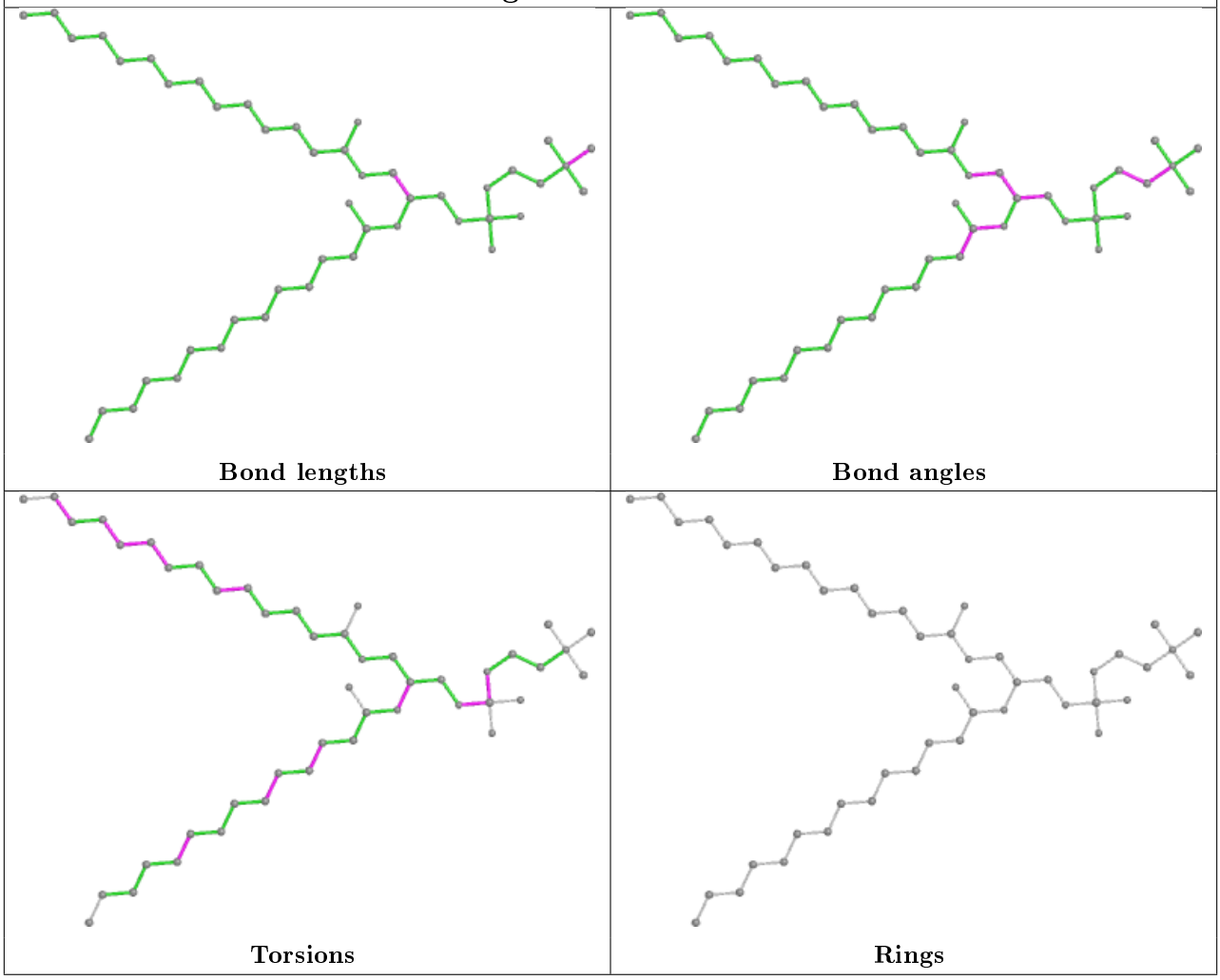


Torsions

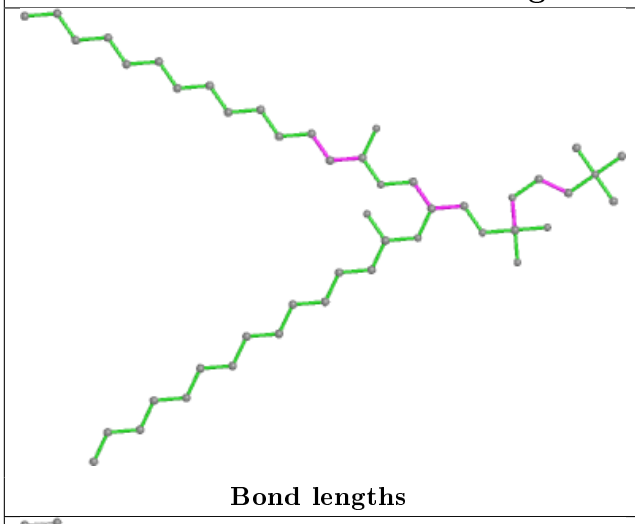


Rings

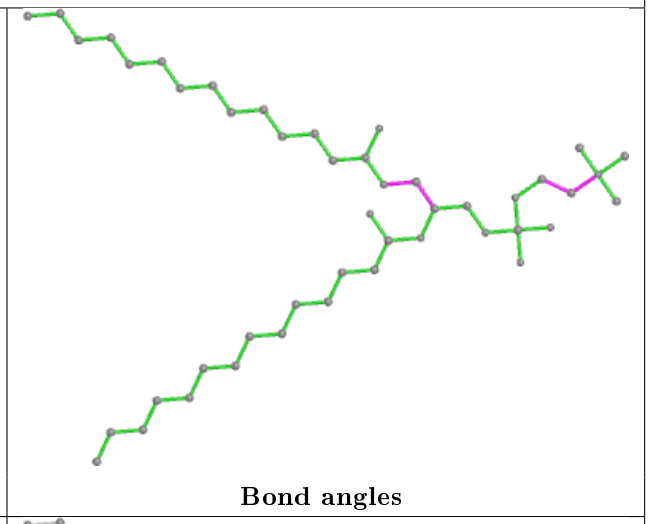
Ligand PX4 B 325



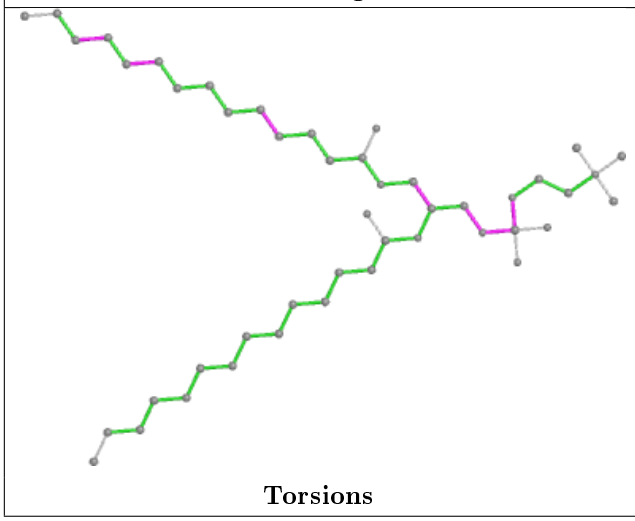
Ligand PX4 C 323



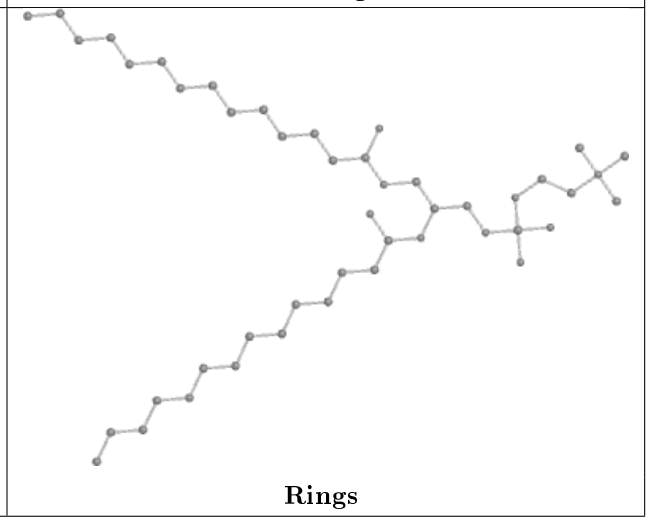
Bond lengths



Bond angles

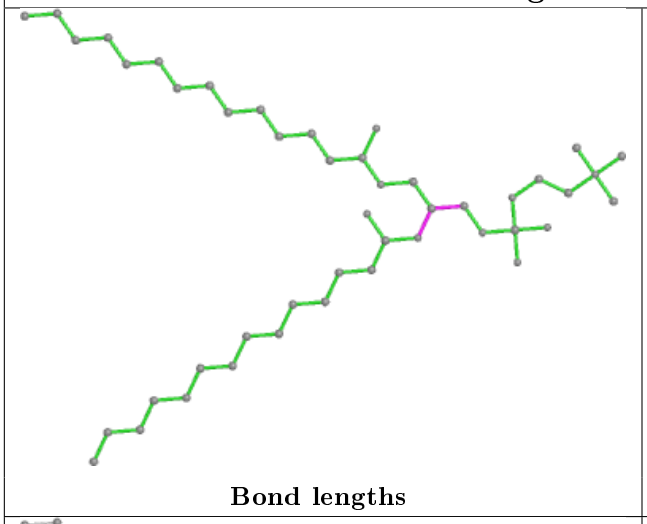


Torsions

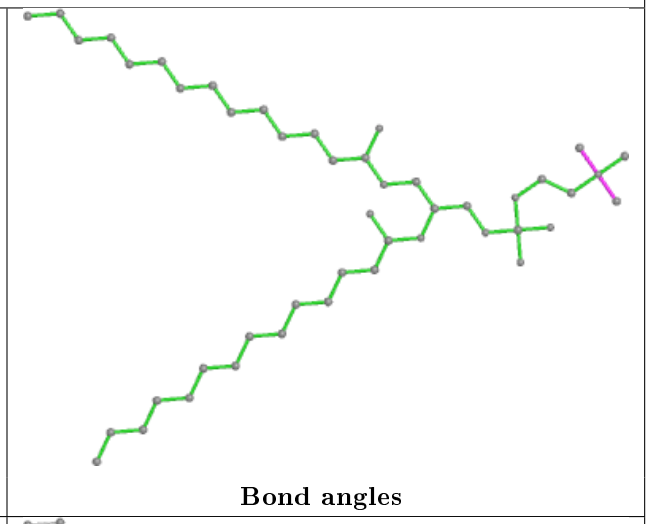


Rings

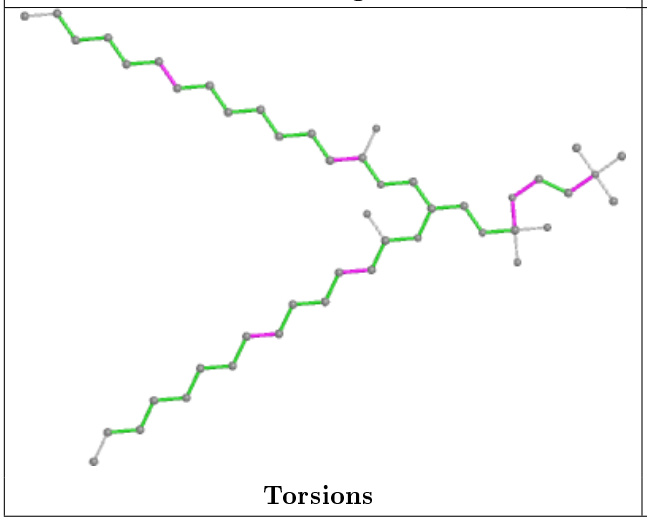
Ligand PX4 A 626



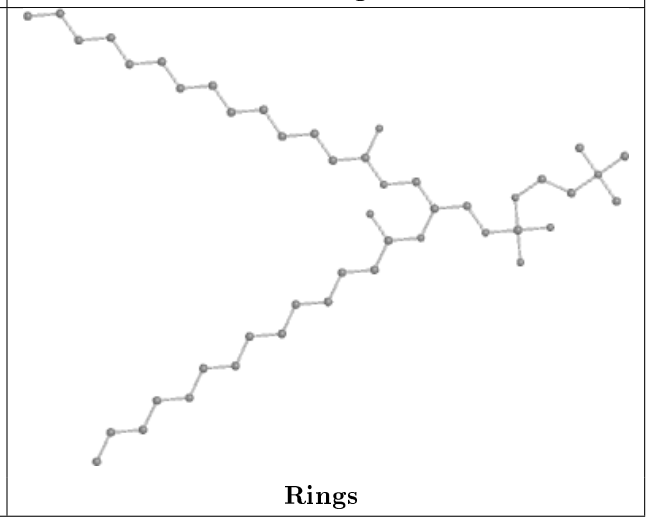
Bond lengths



Bond angles

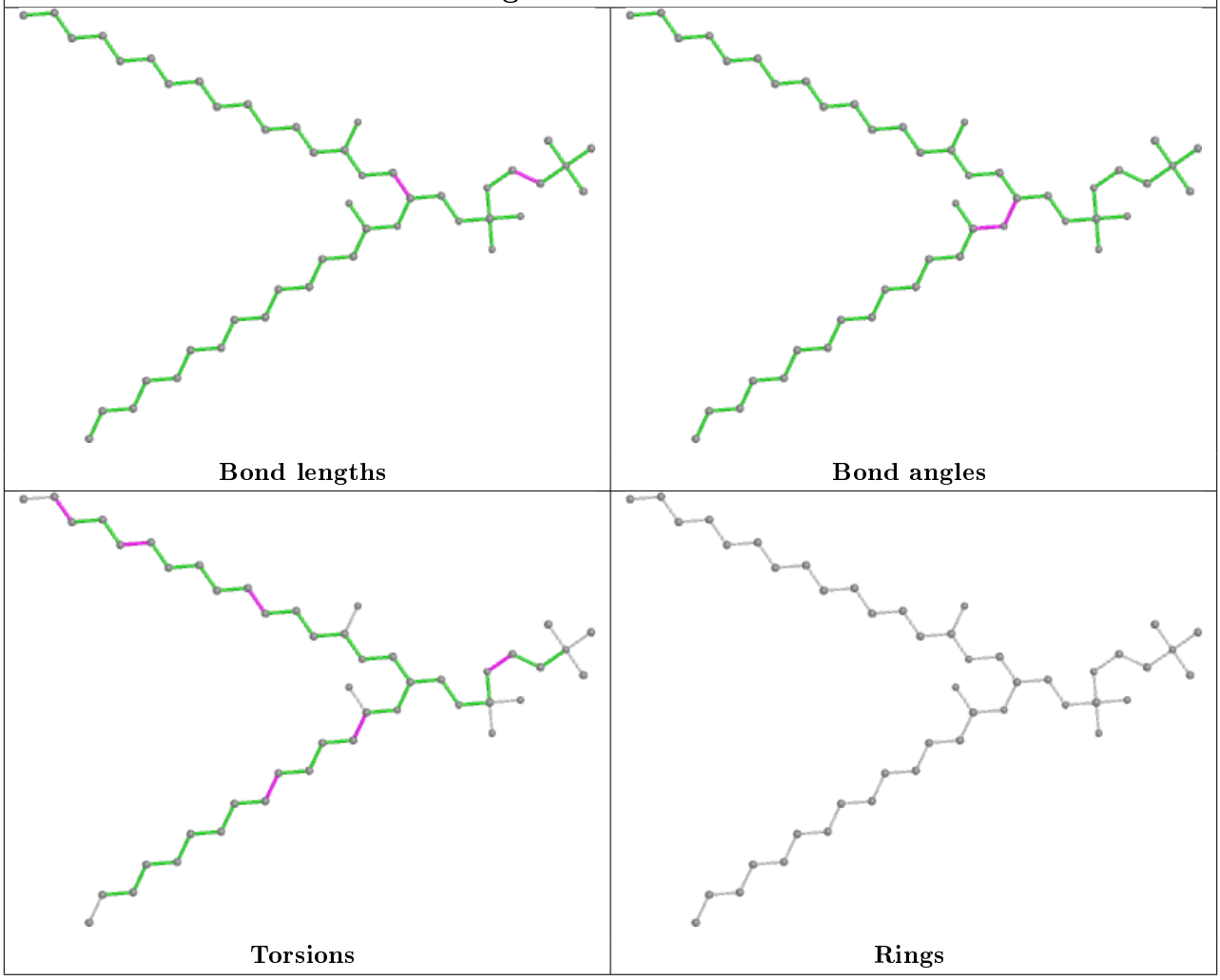


Torsions

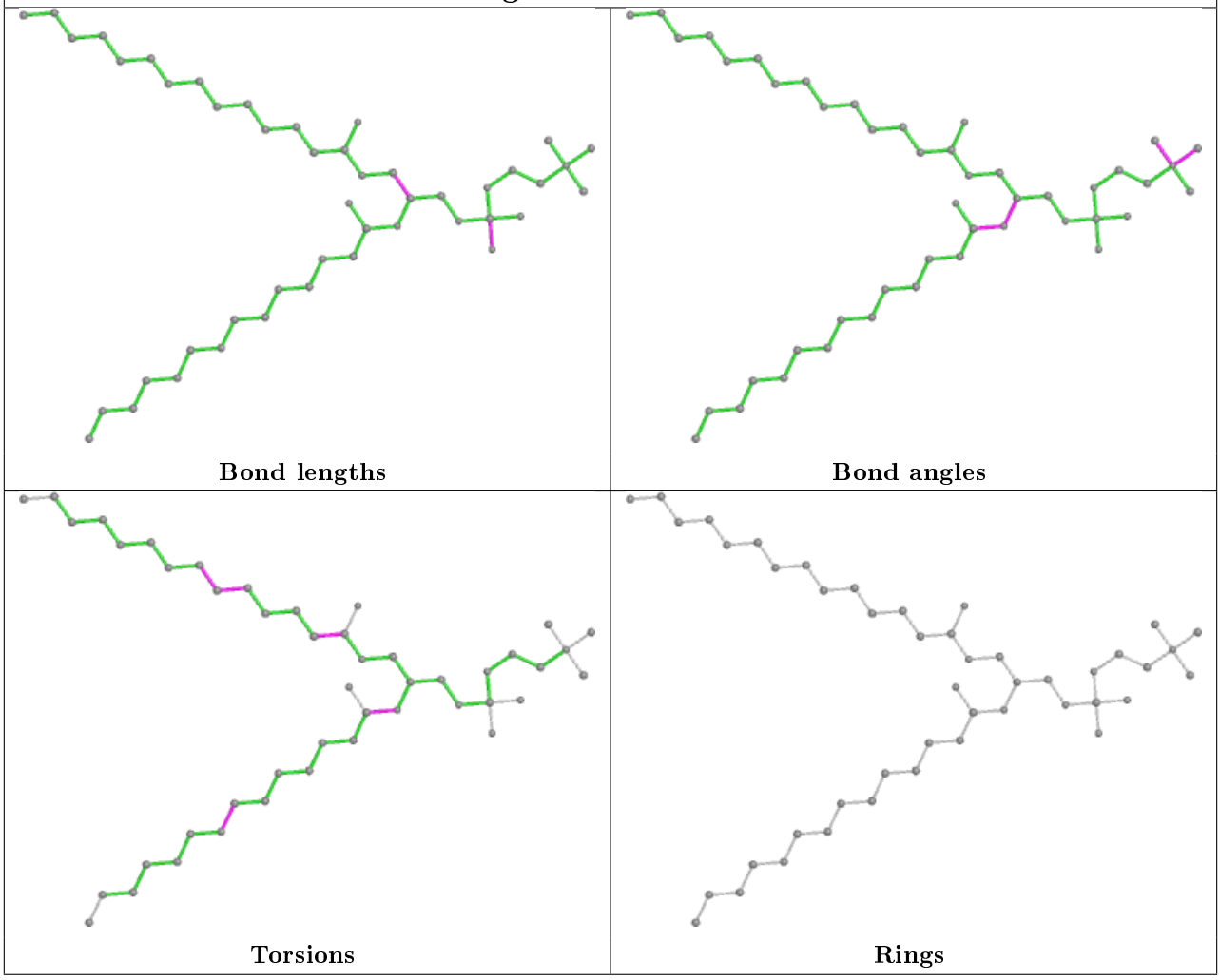


Rings

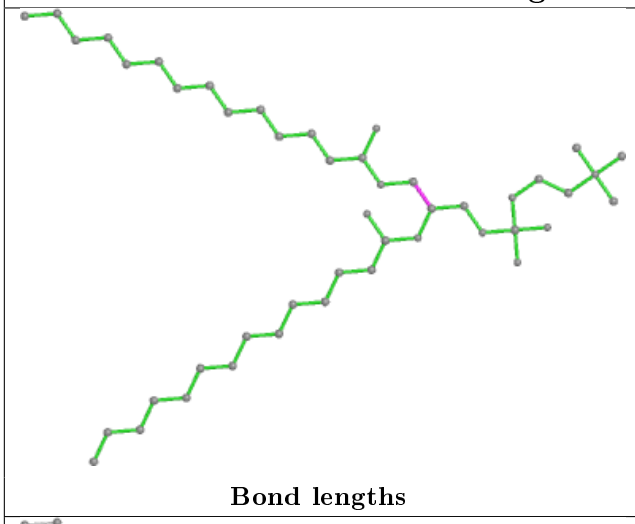
Ligand PX4 C 341



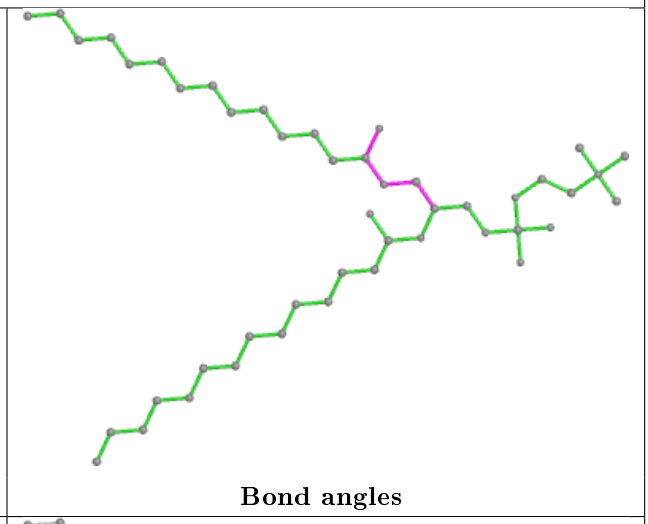
Ligand PX4 C 363



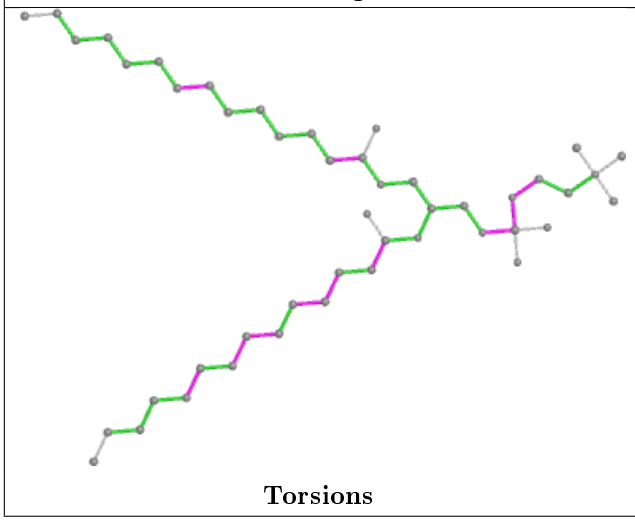
Ligand PX4 C 301



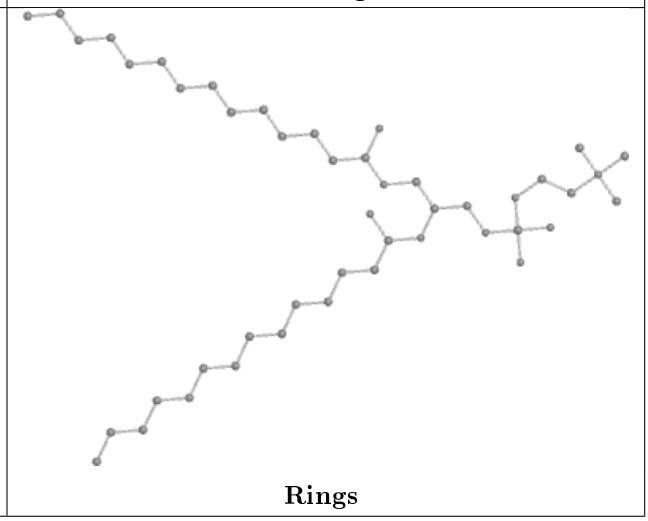
Bond lengths



Bond angles

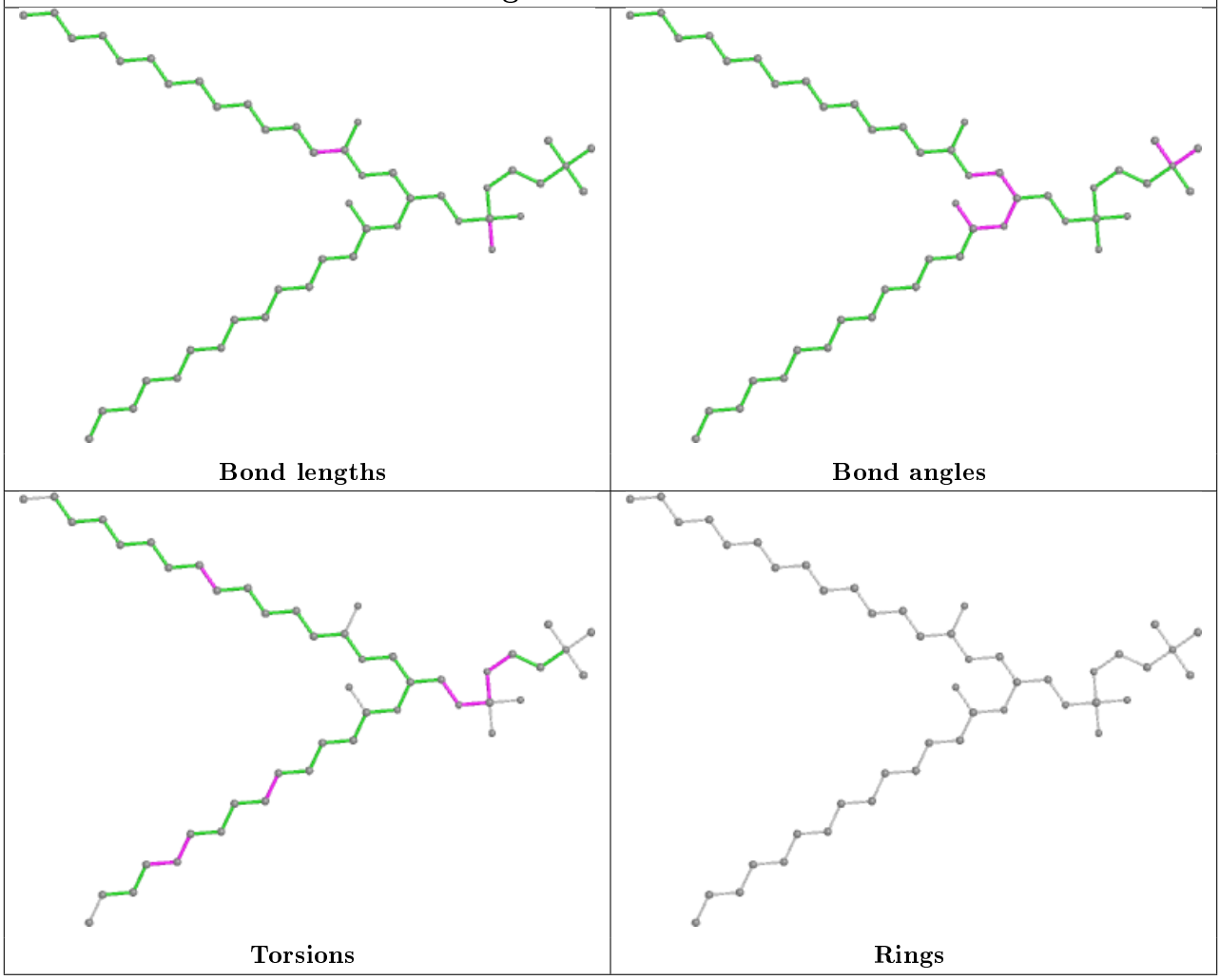


Torsions

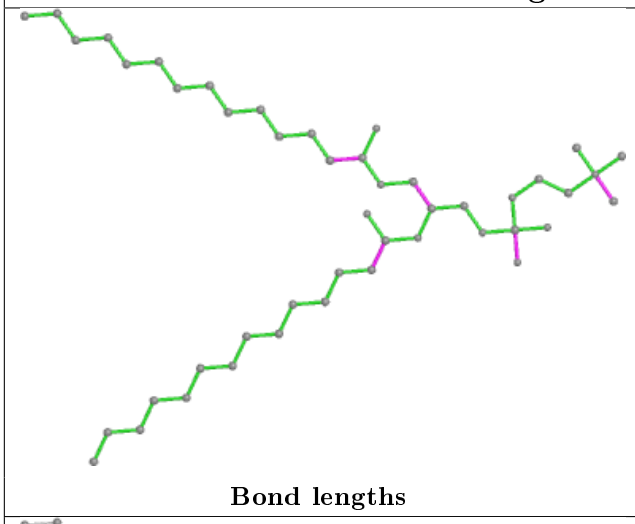


Rings

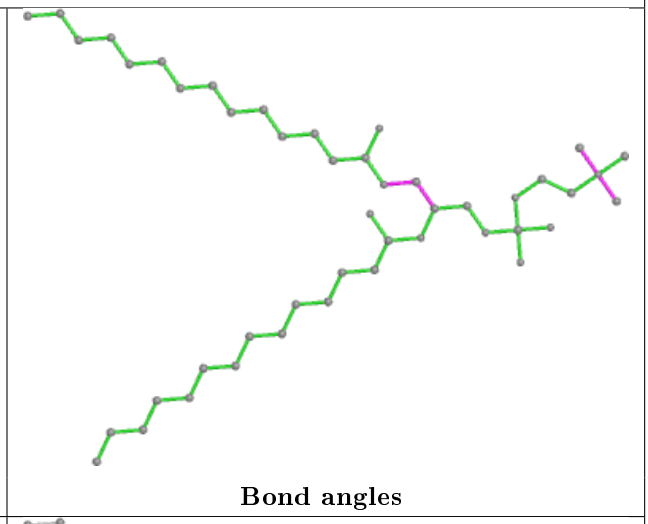
Ligand PX4 C 351



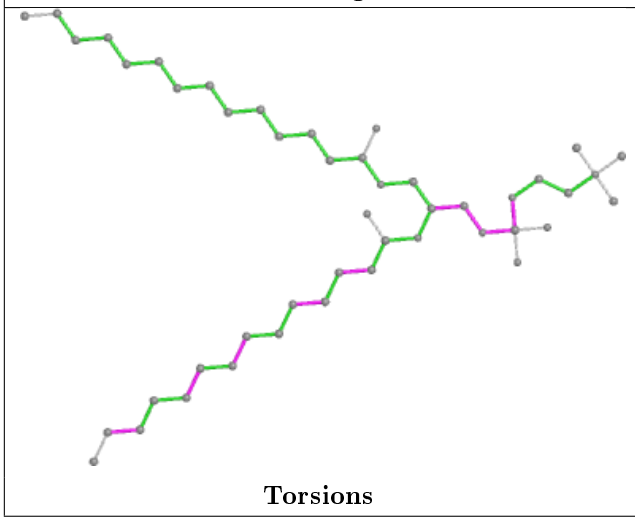
Ligand PX4 C 364



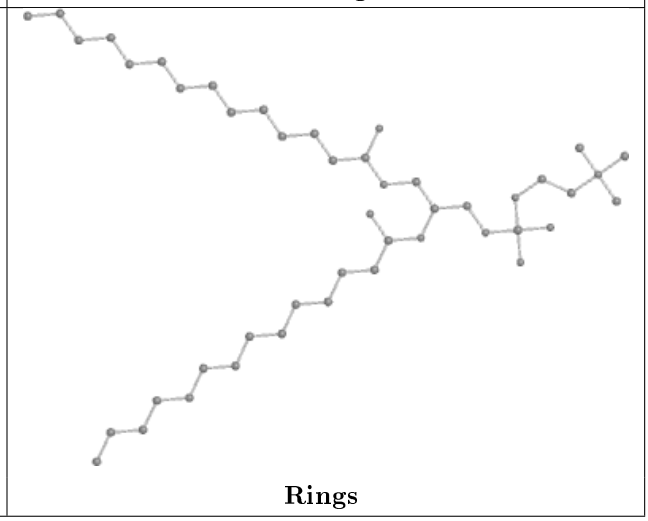
Bond lengths



Bond angles

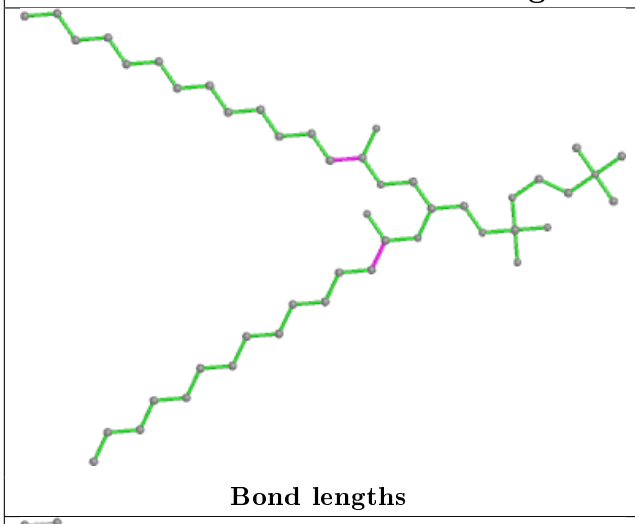


Torsions

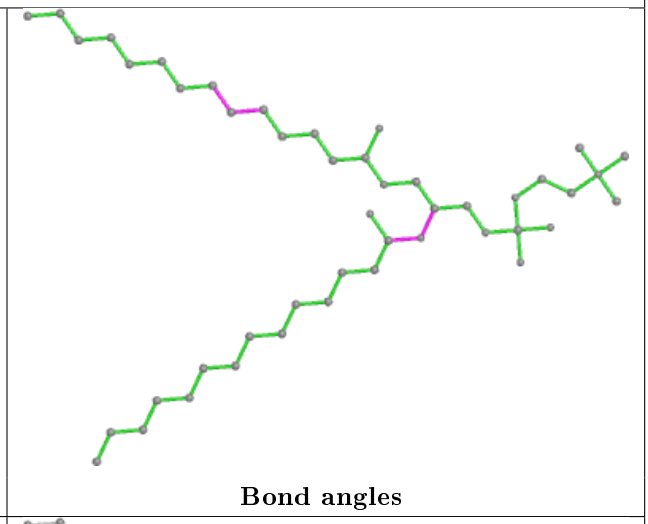


Rings

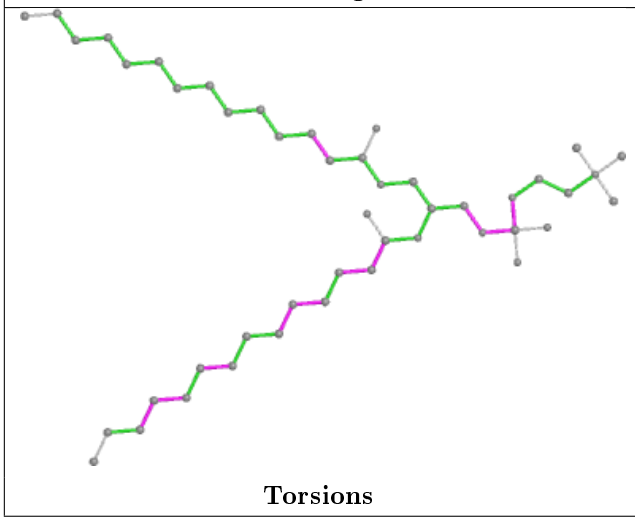
Ligand PX4 C 302



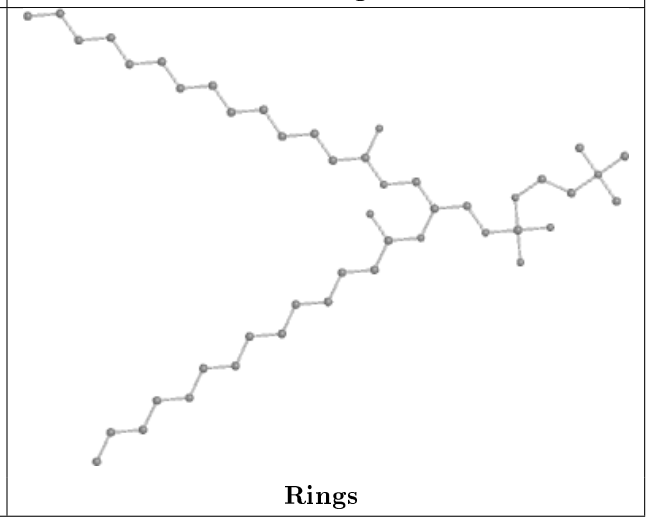
Bond lengths



Bond angles

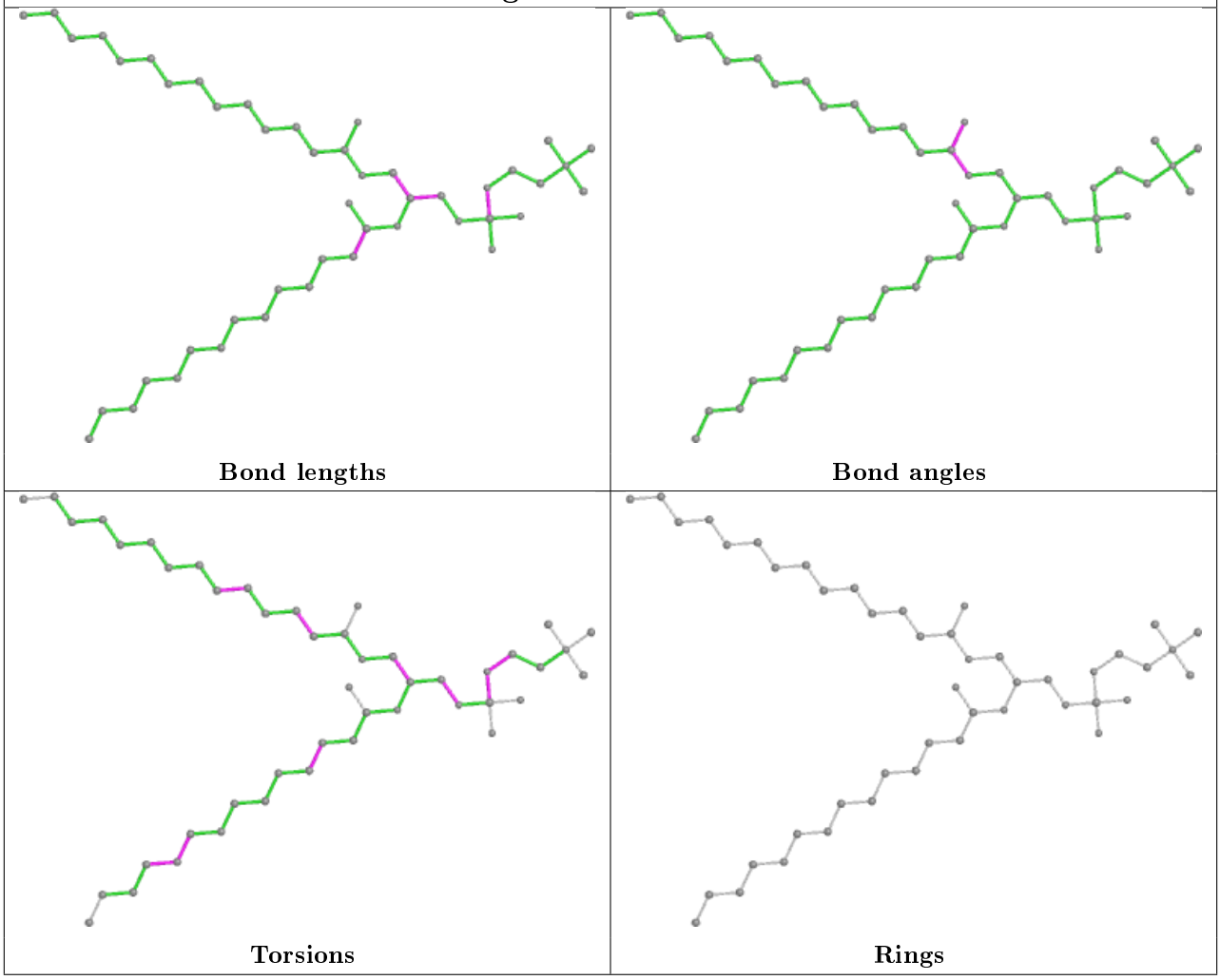


Torsions

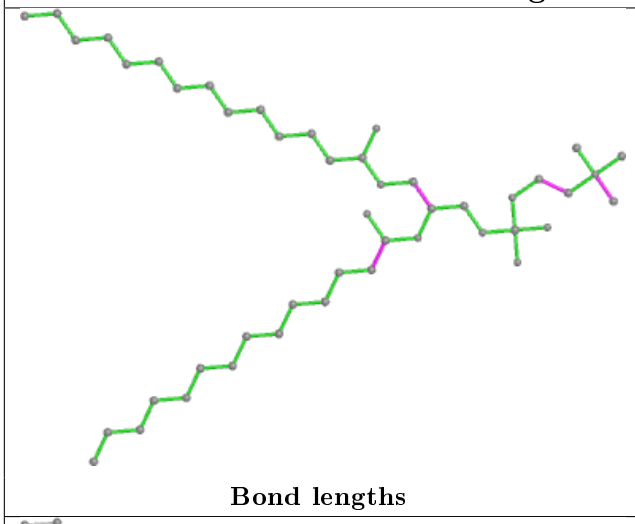


Rings

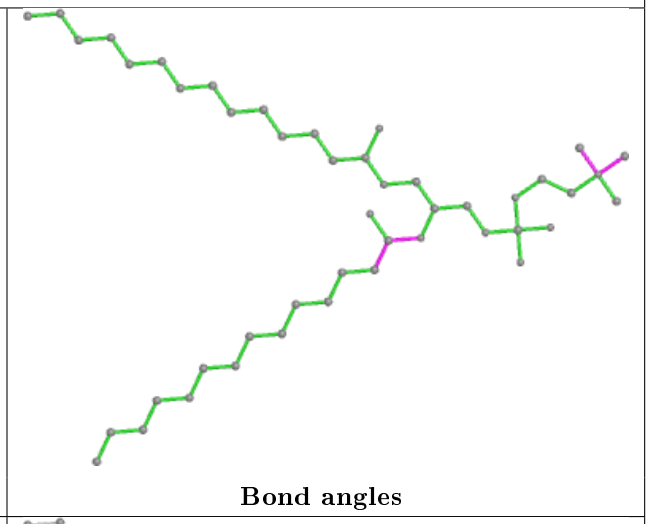
Ligand PX4 B 335



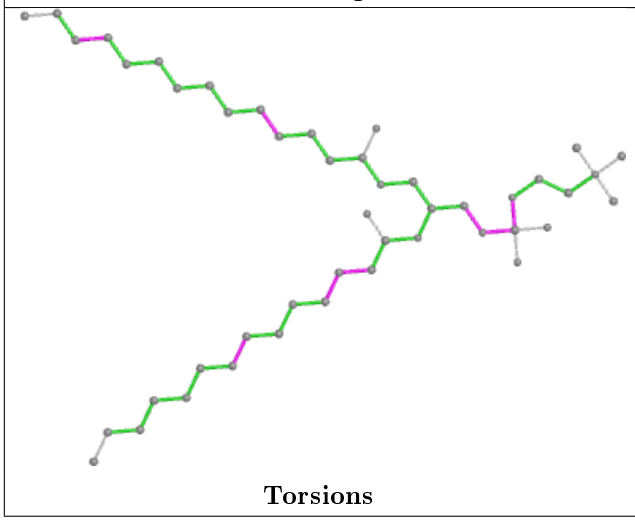
Ligand PX4 C 355



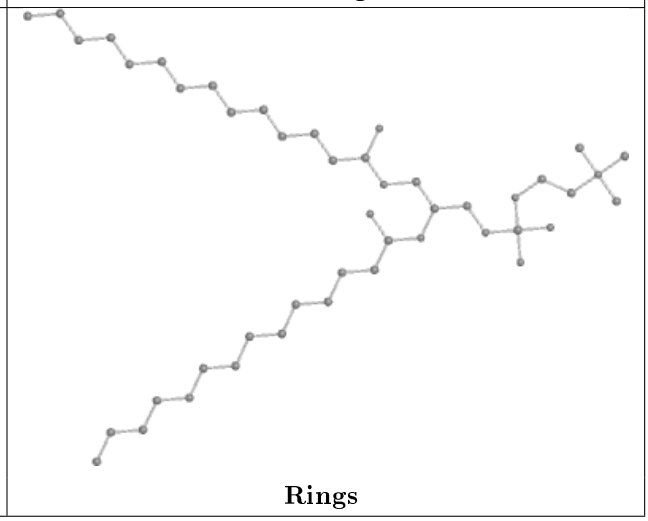
Bond lengths



Bond angles

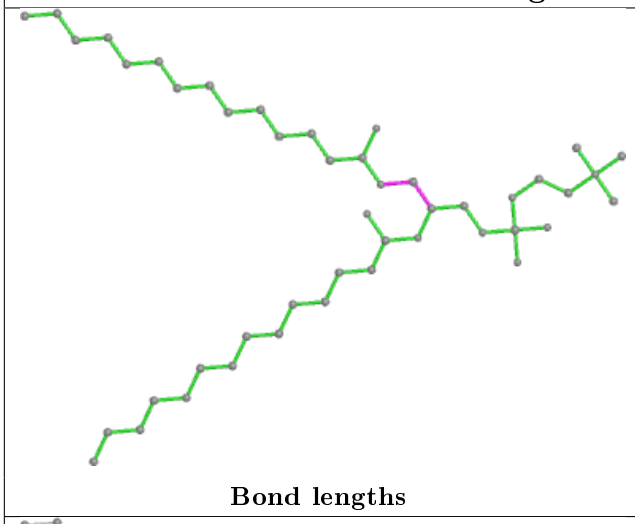


Torsions

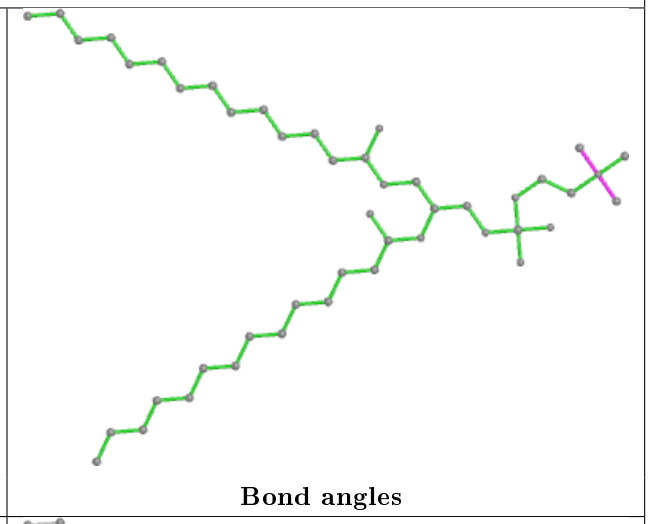


Rings

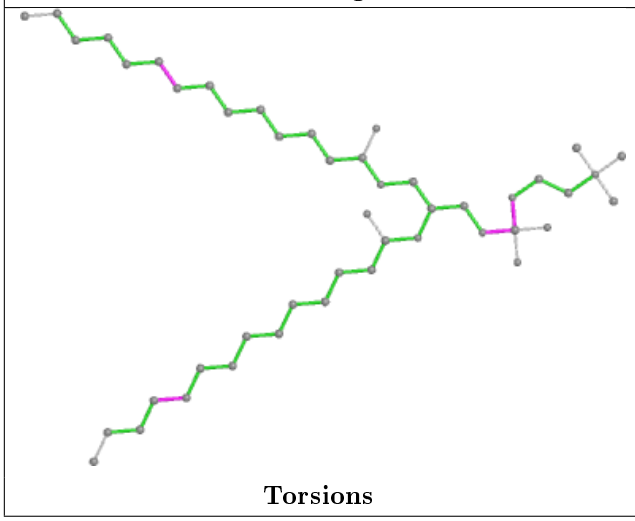
Ligand PX4 C 321



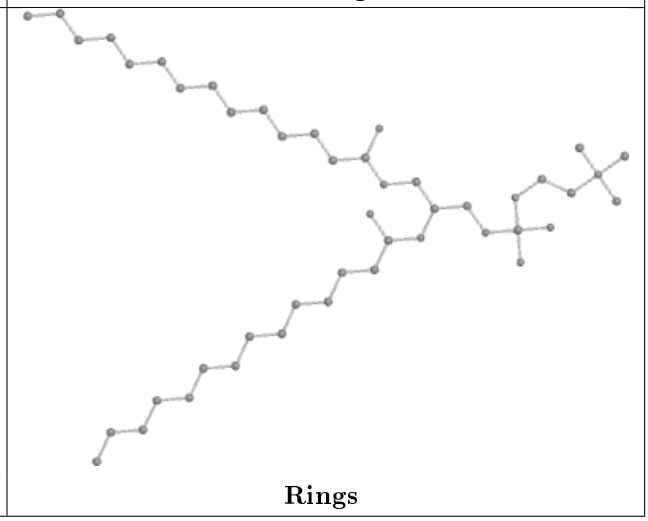
Bond lengths



Bond angles

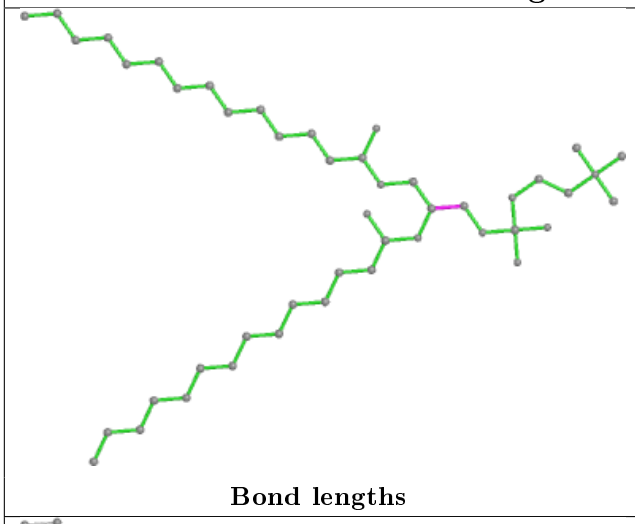


Torsions

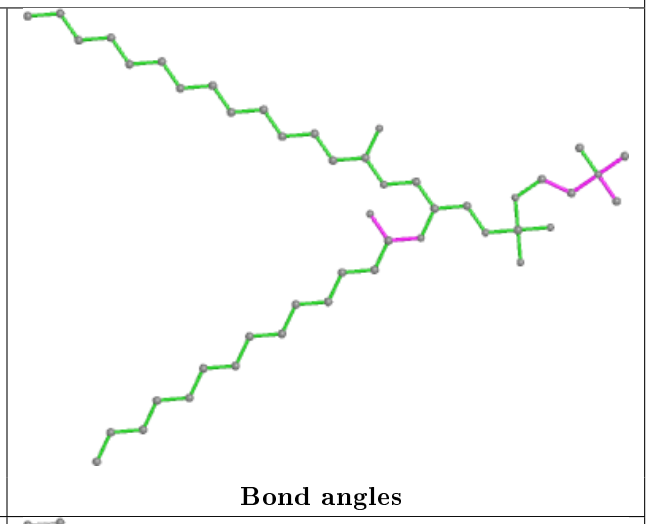


Rings

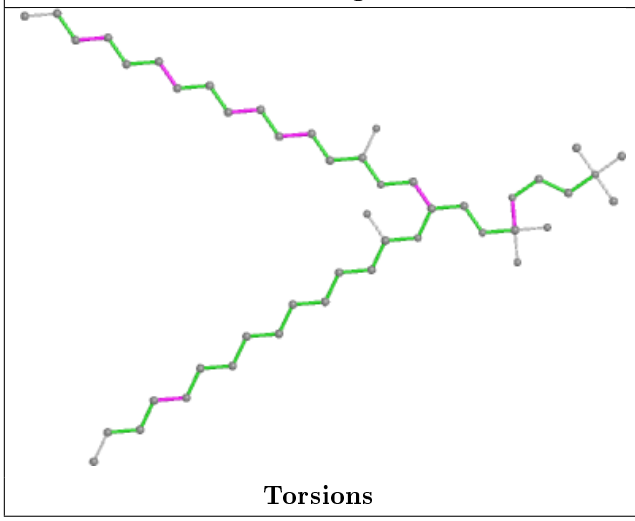
Ligand PX4 C 362



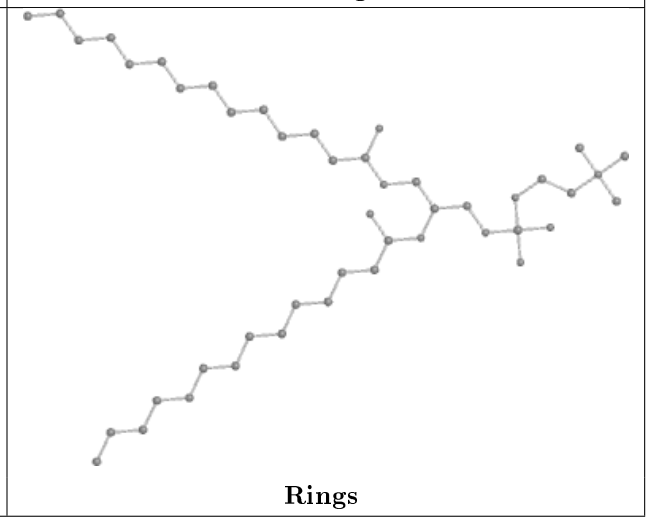
Bond lengths



Bond angles

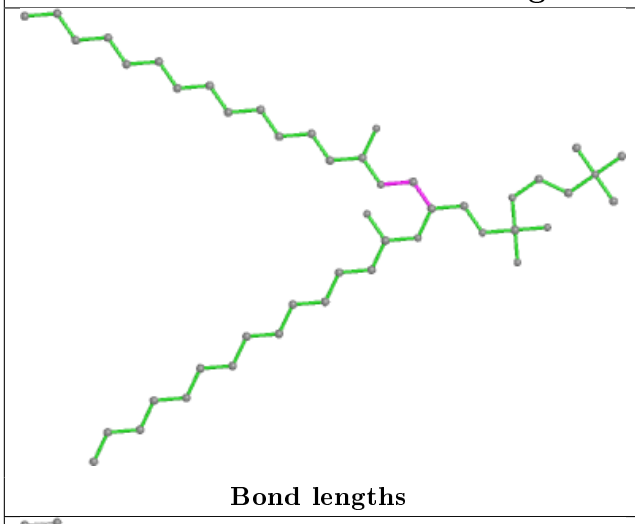


Torsions

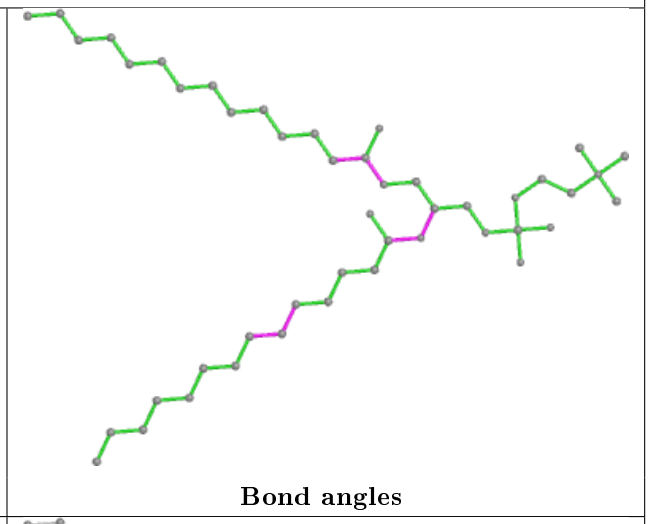


Rings

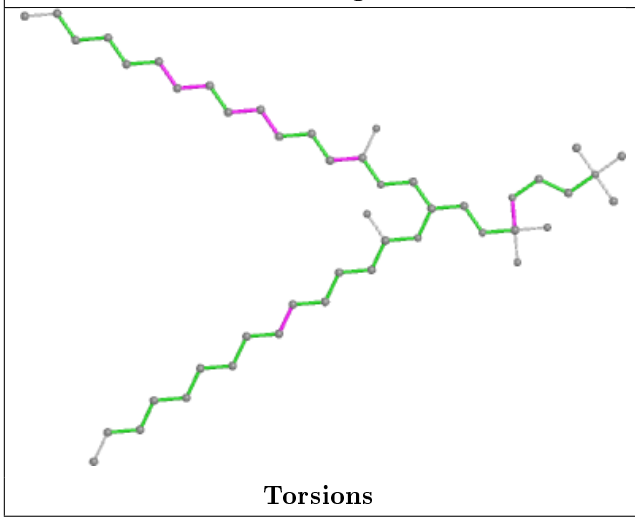
Ligand PX4 B 389



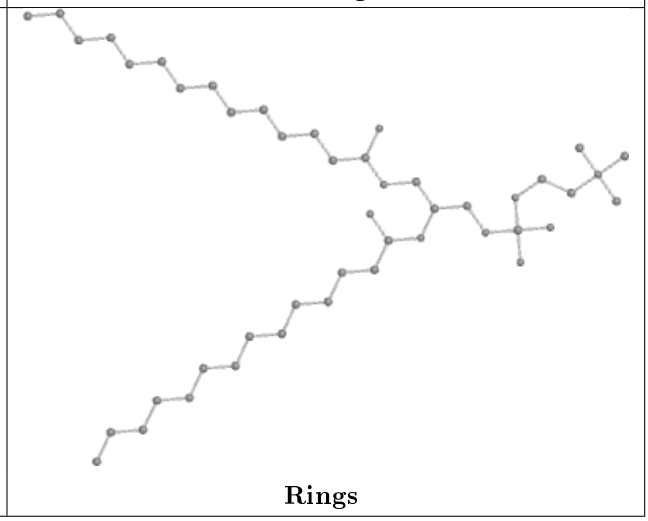
Bond lengths



Bond angles

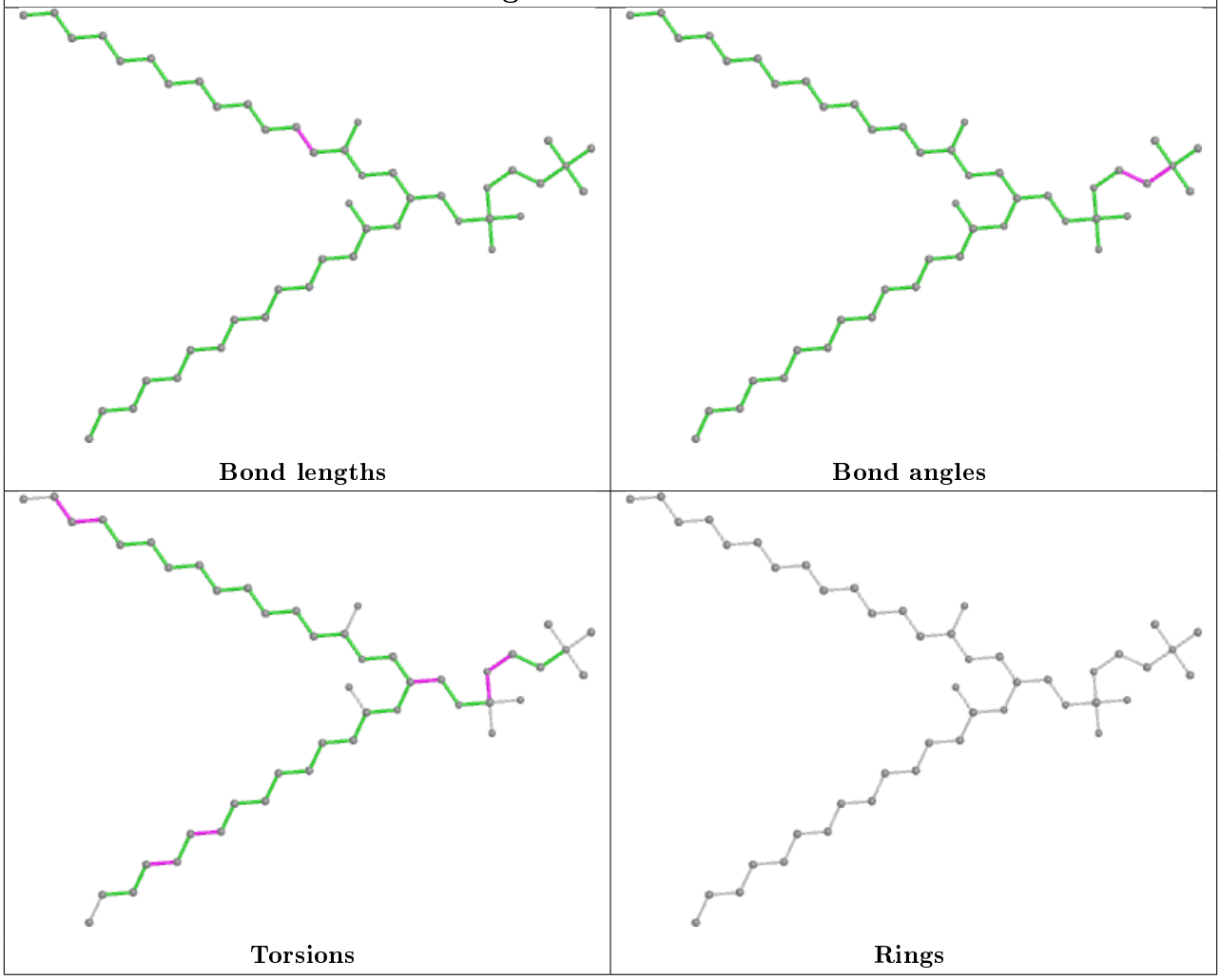


Torsions

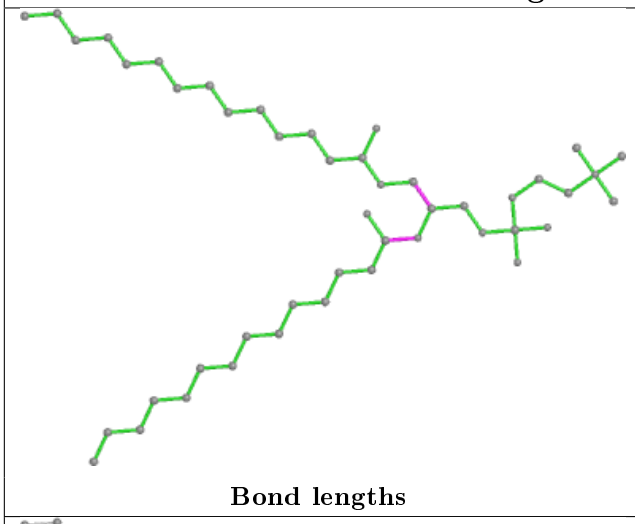


Rings

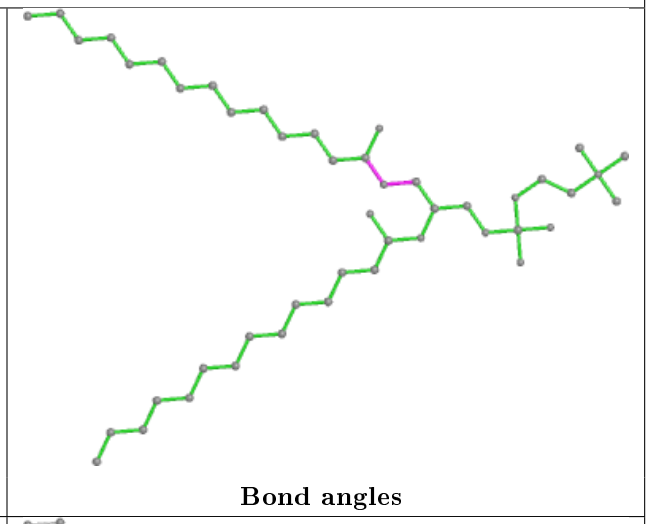
Ligand PX4 B 349



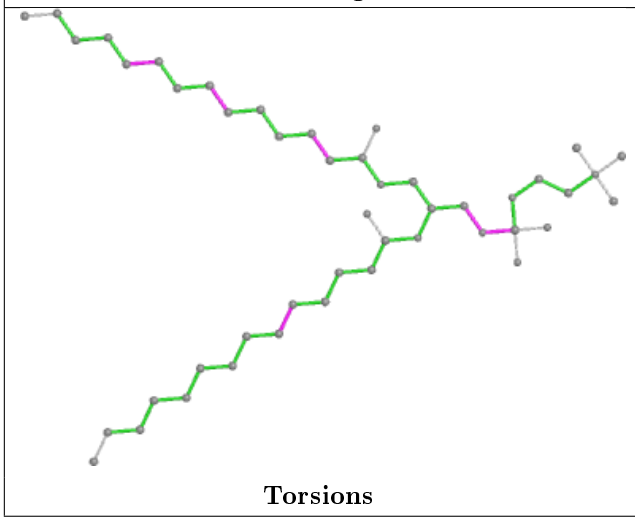
Ligand PX4 A 612



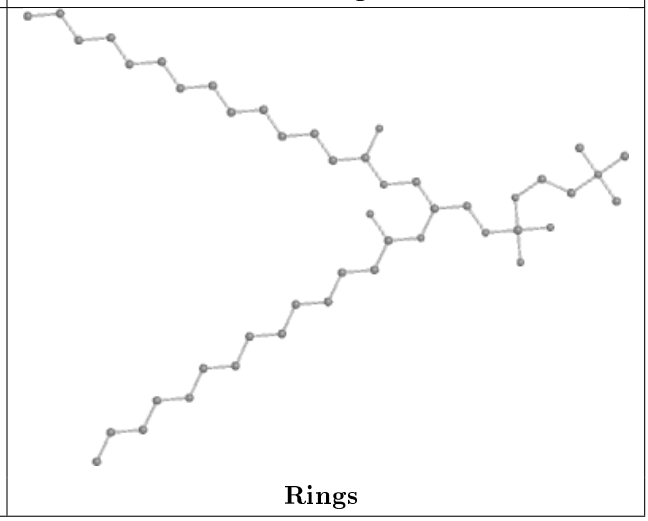
Bond lengths



Bond angles

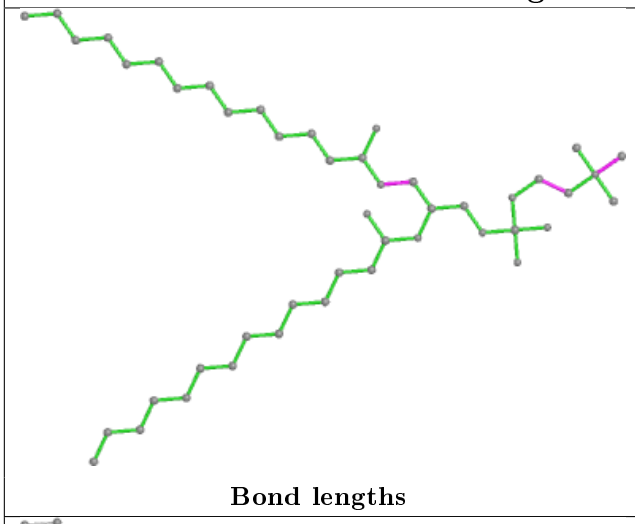


Torsions

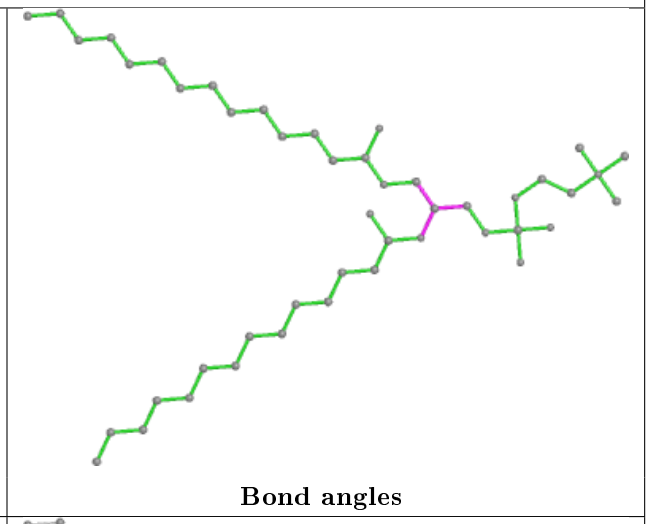


Rings

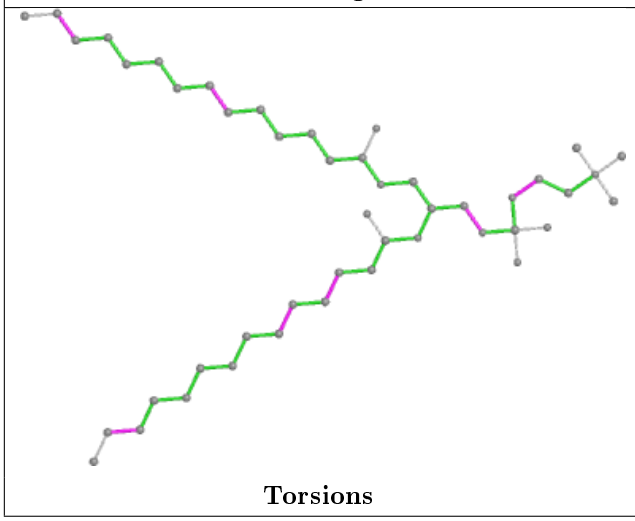
Ligand PX4 A 602



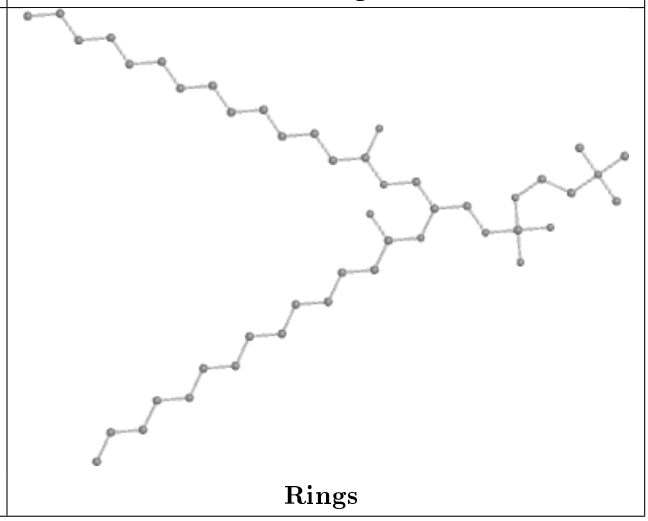
Bond lengths



Bond angles

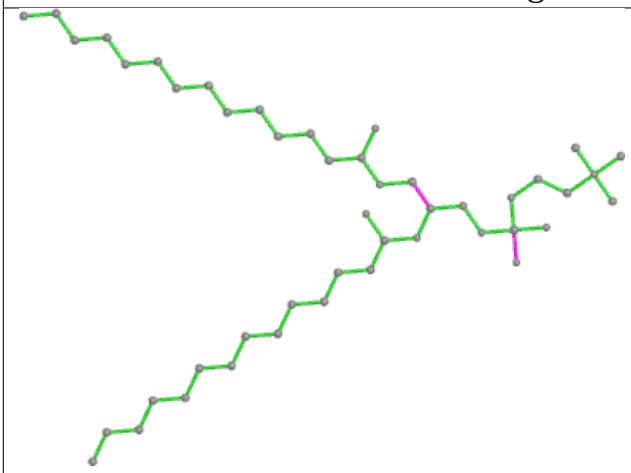


Torsions

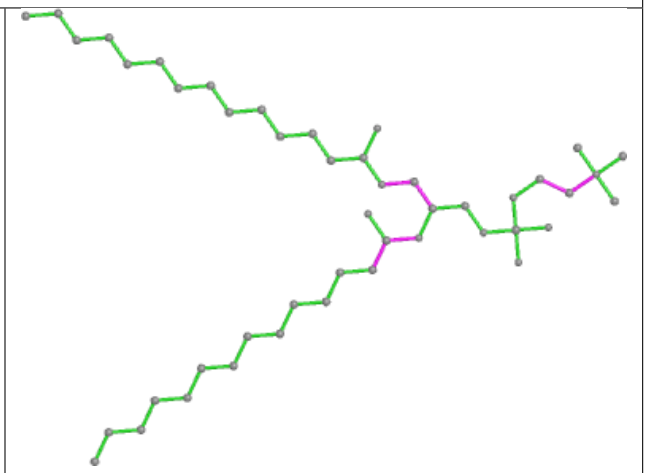


Rings

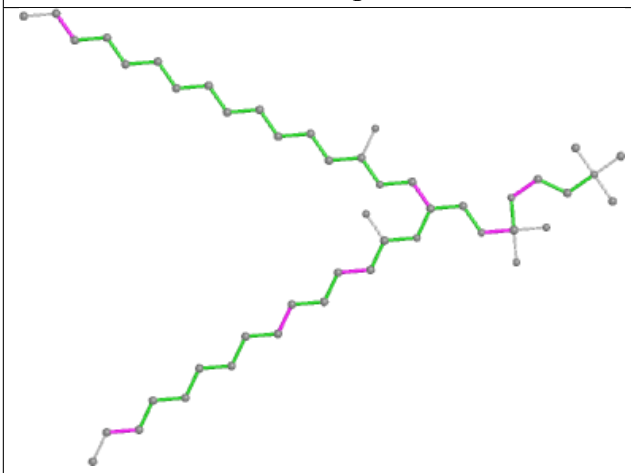
Ligand PX4 C 339



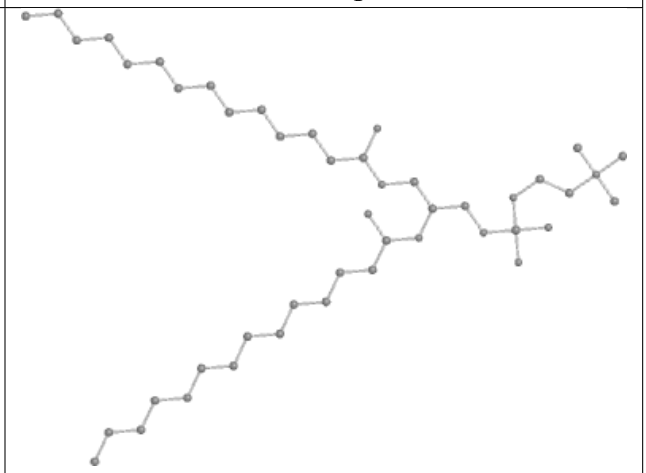
Bond lengths



Bond angles

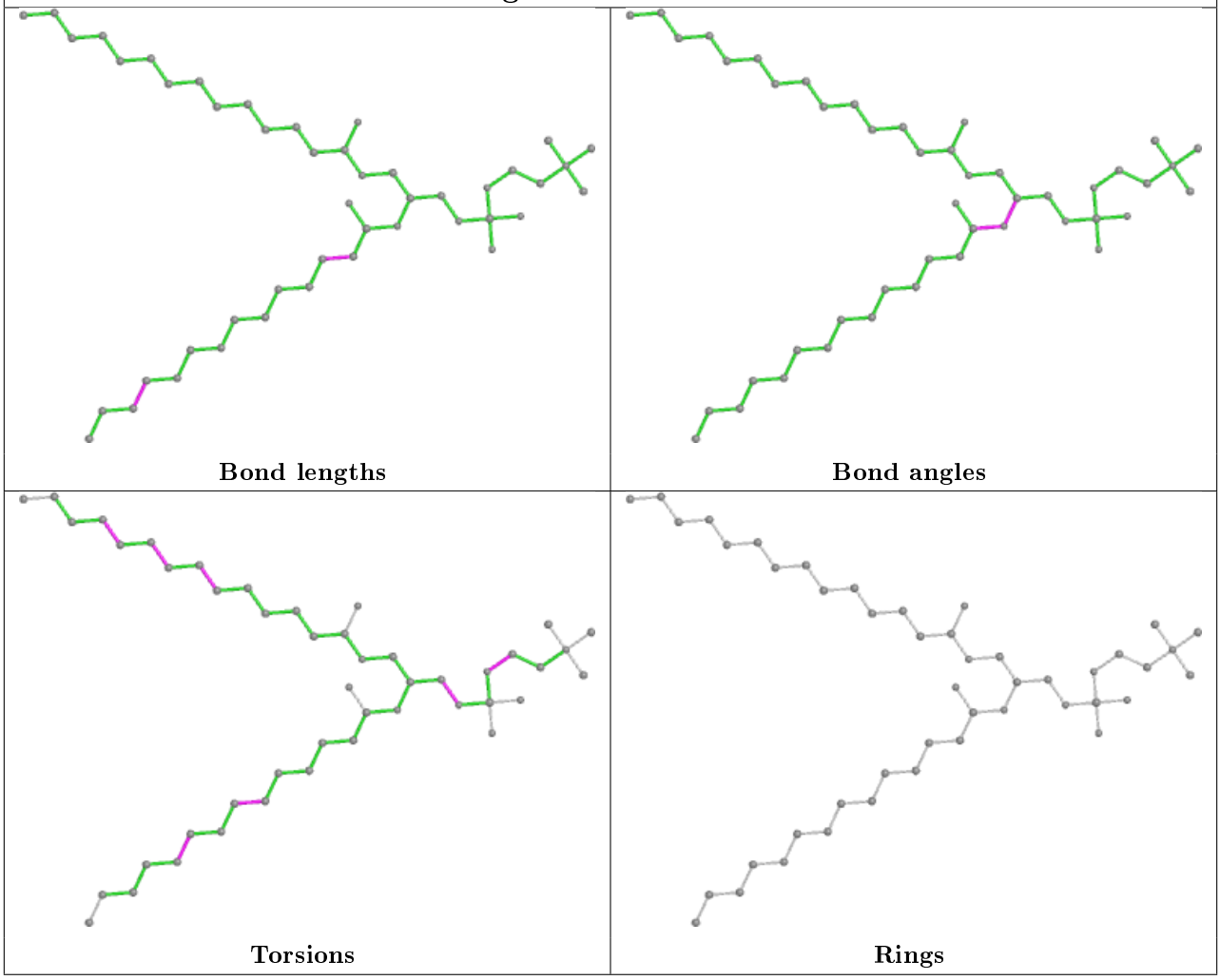


Torsions

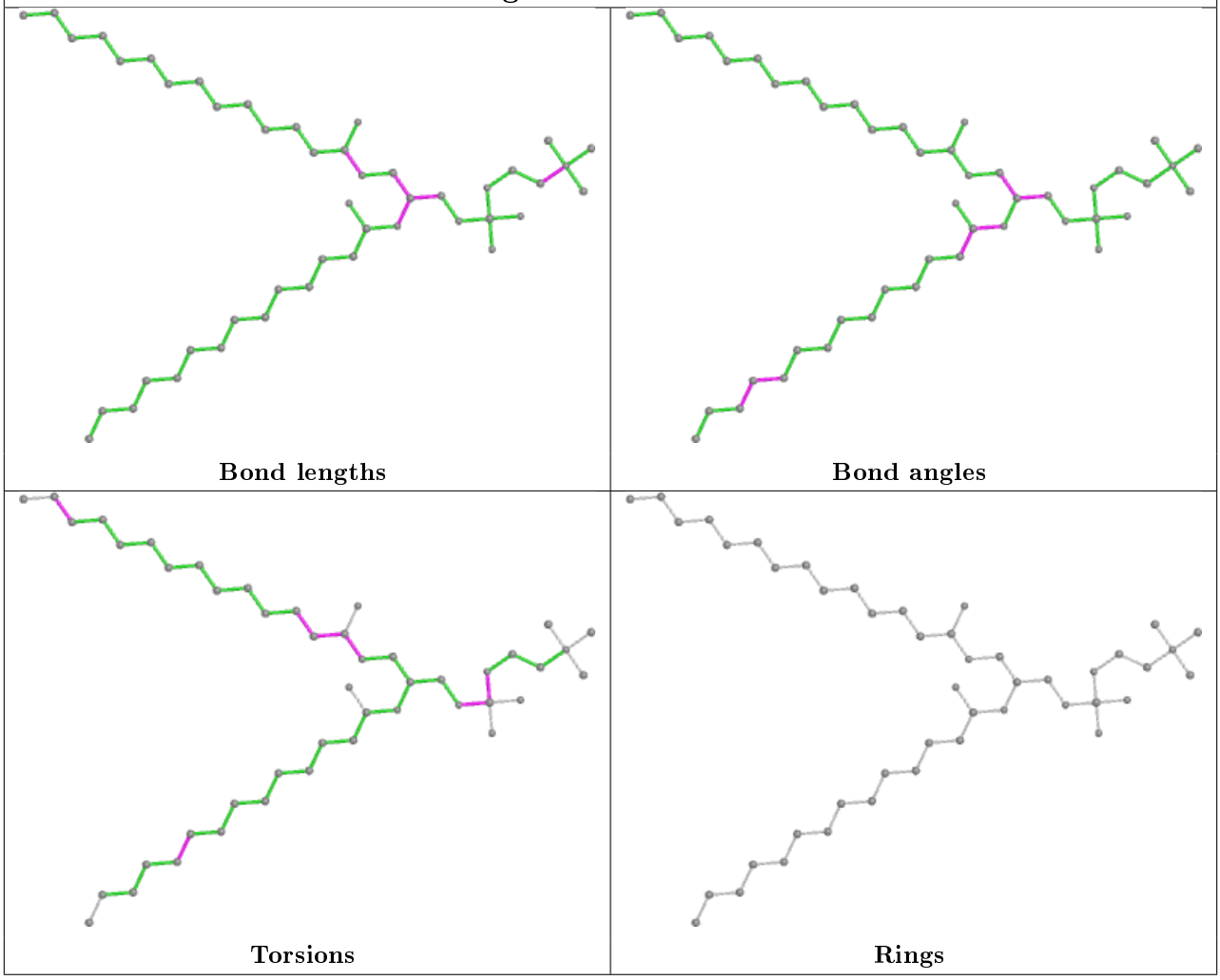


Rings

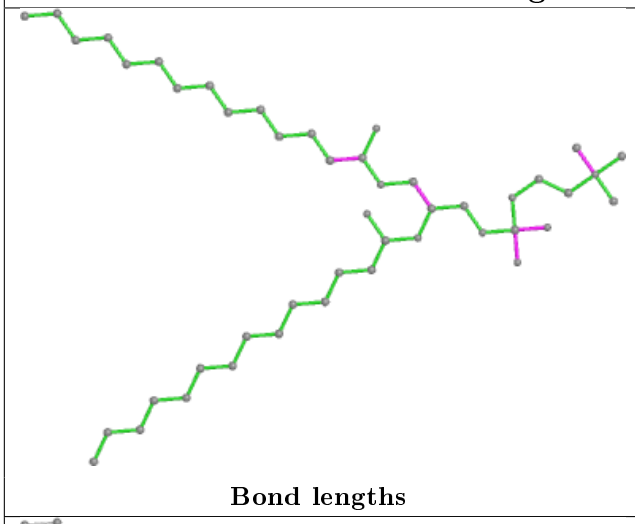
Ligand PX4 B 379



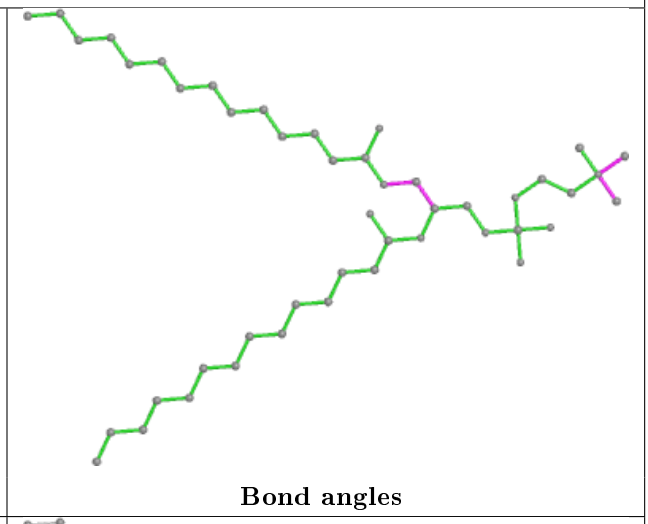
Ligand PX4 C 338



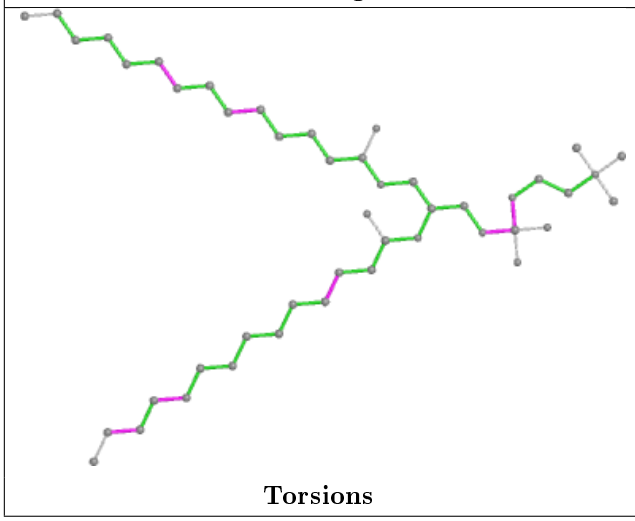
Ligand PX4 C 342



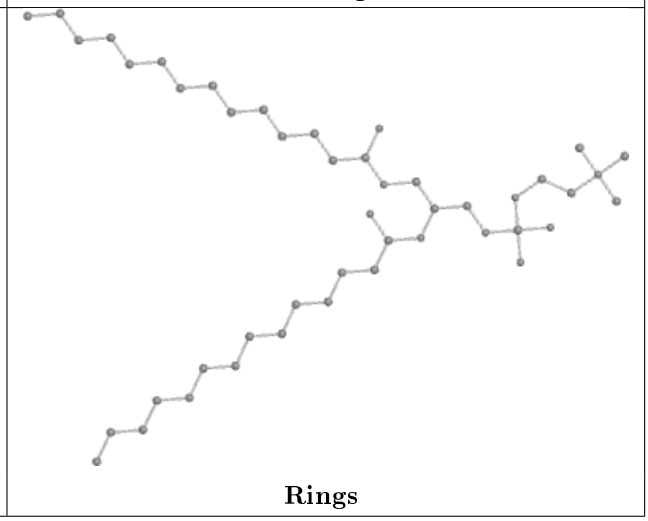
Bond lengths



Bond angles

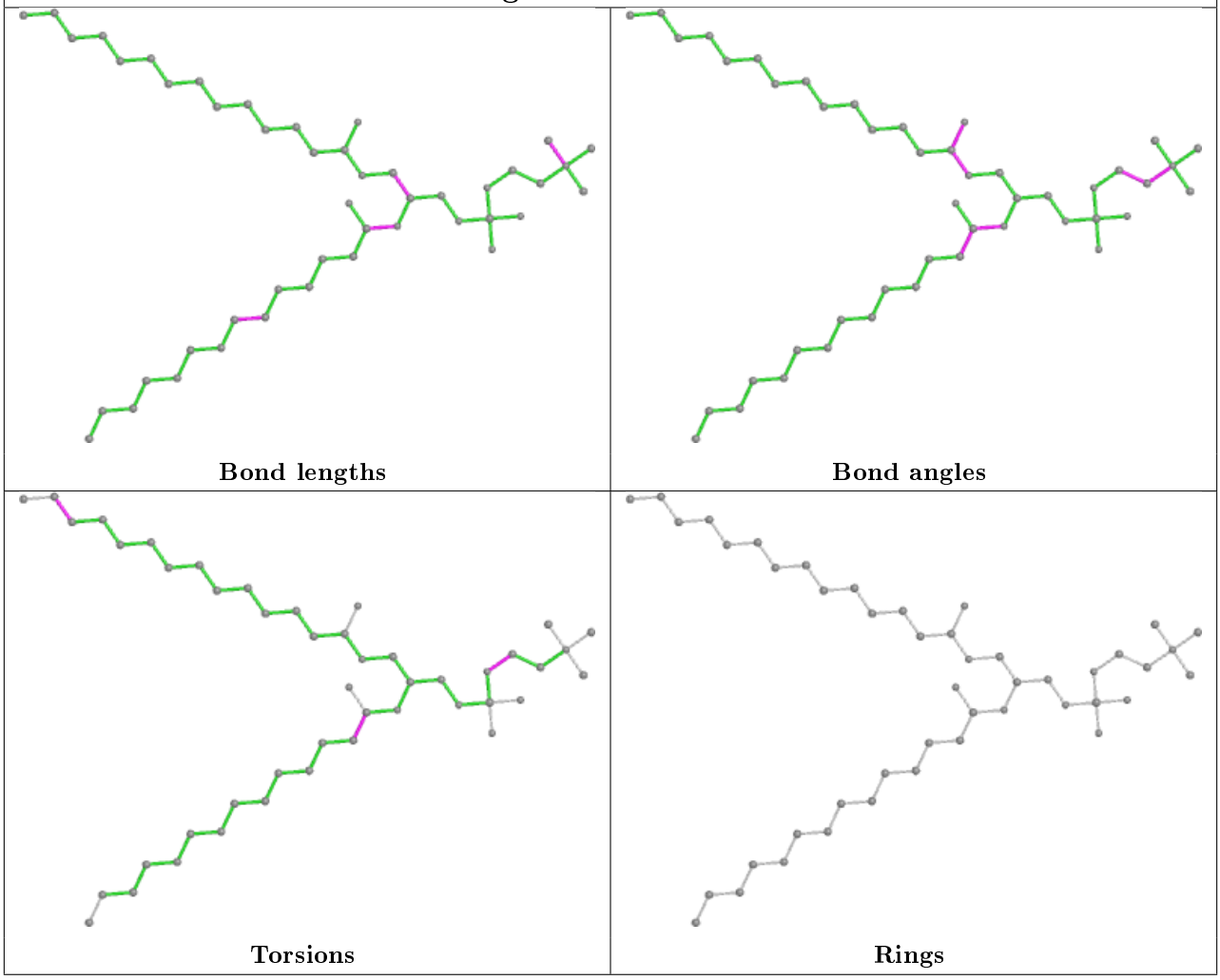


Torsions

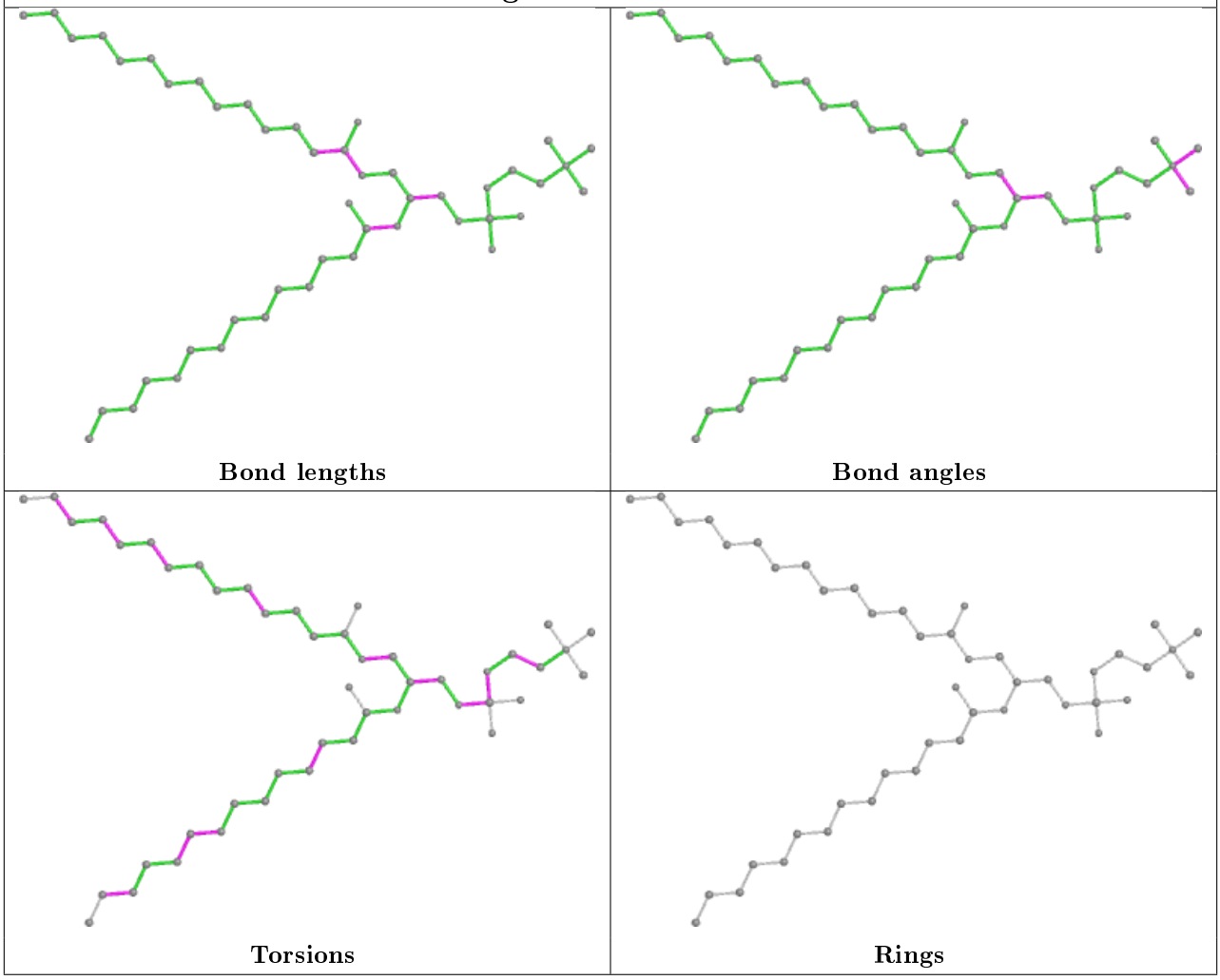


Rings

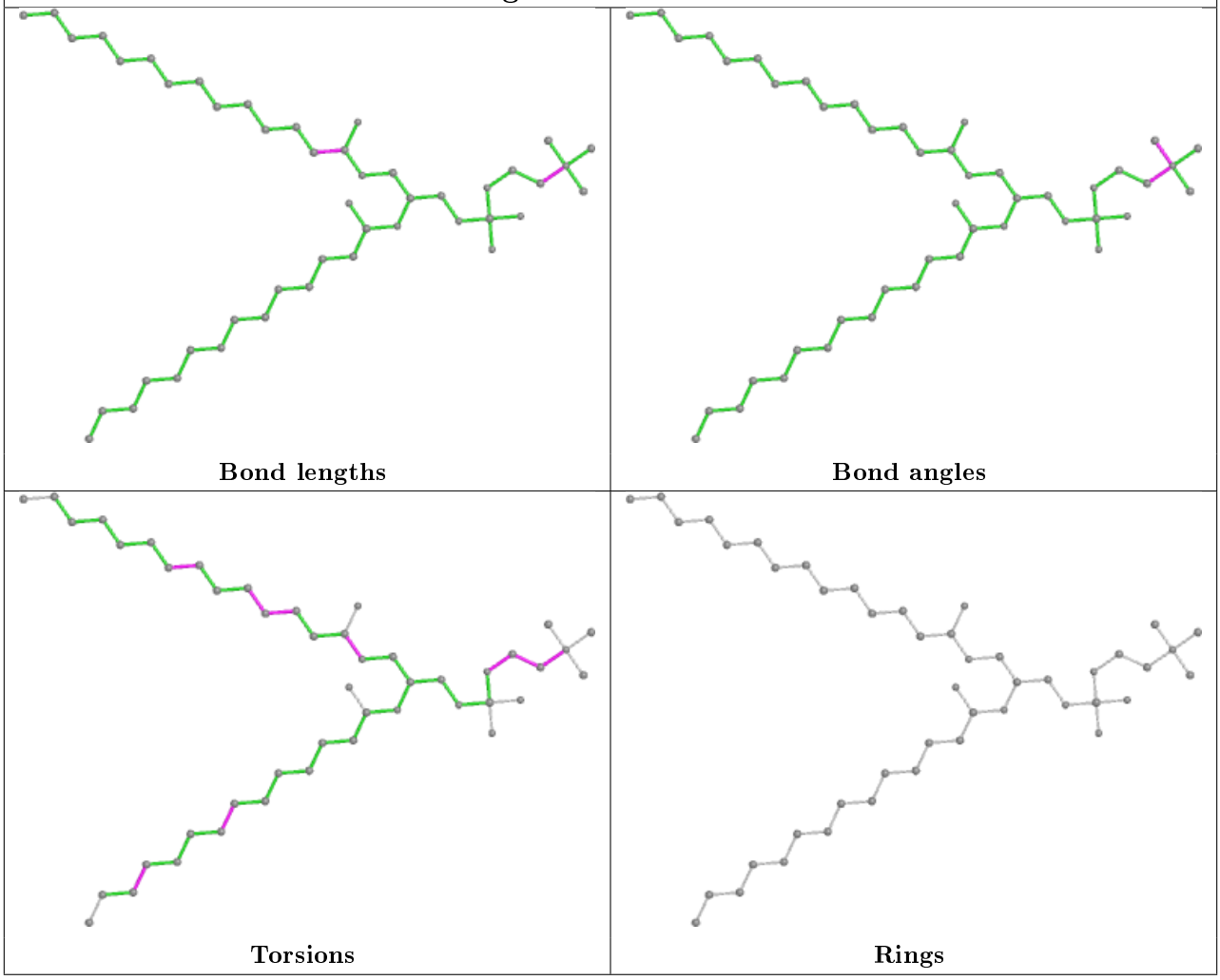
Ligand PX4 B 386



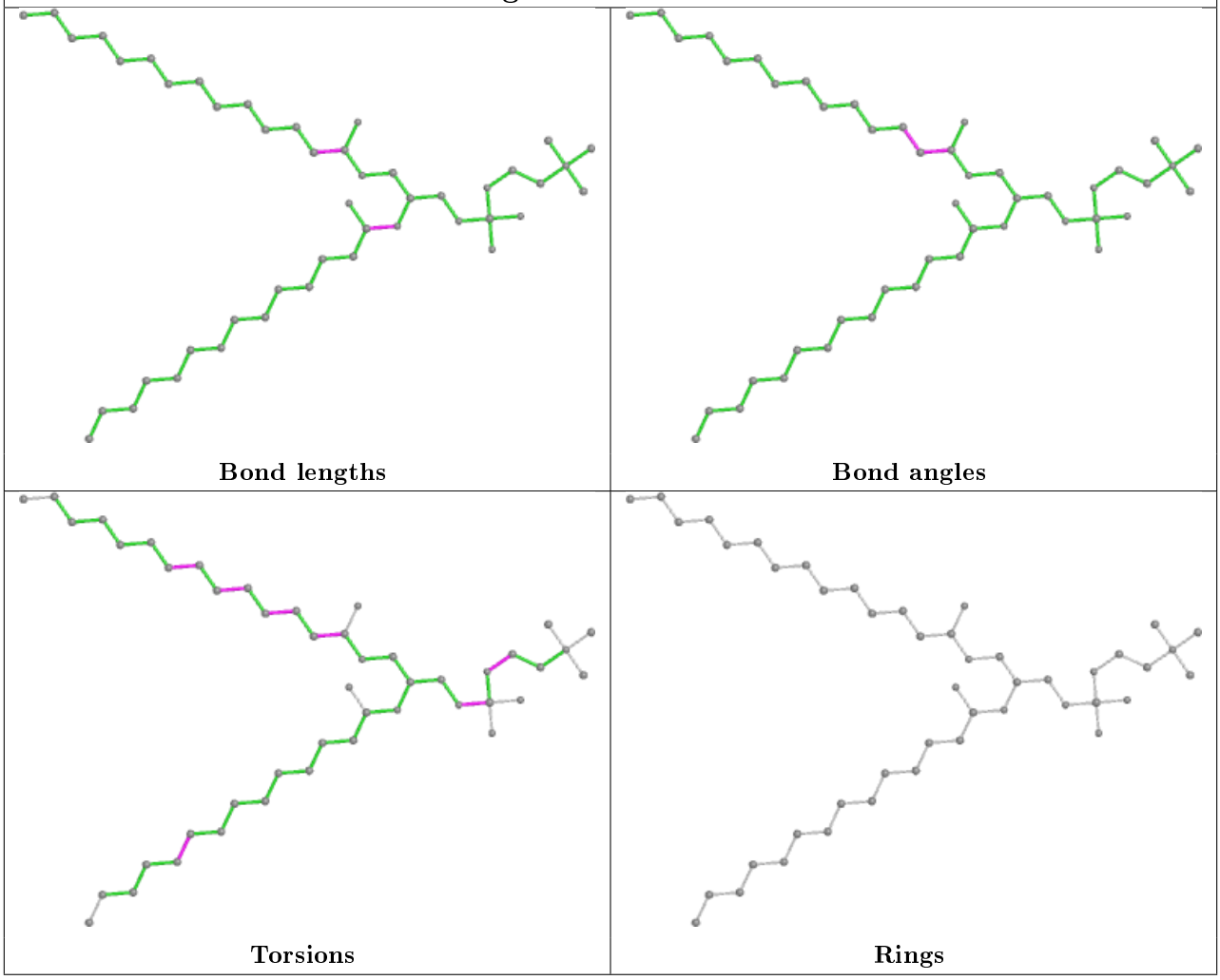
Ligand PX4 B 307



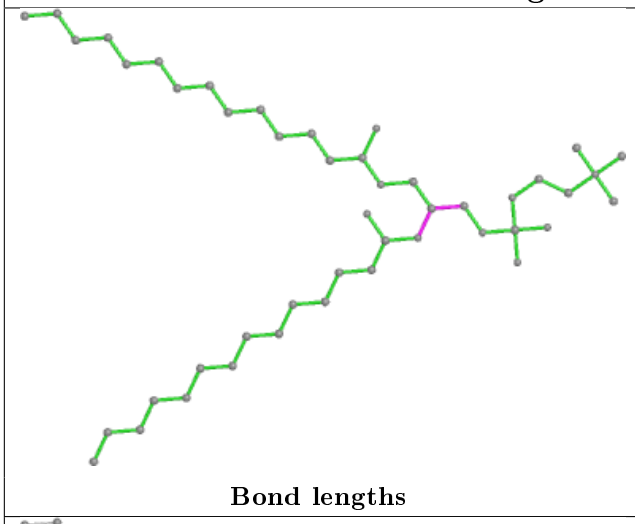
Ligand PX4 B 362



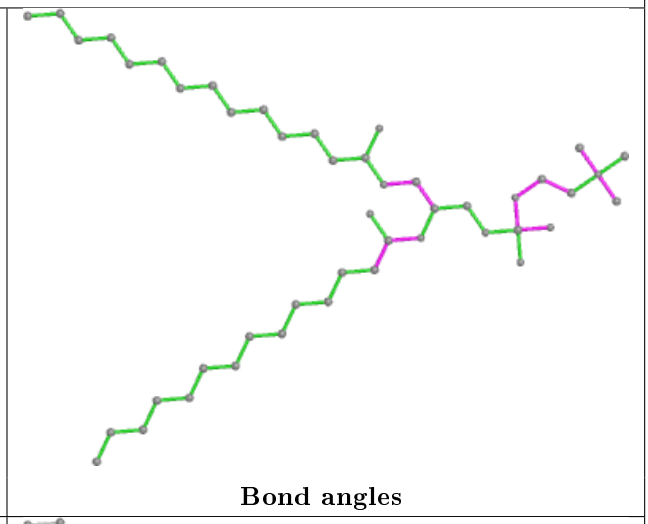
Ligand PX4 C 353



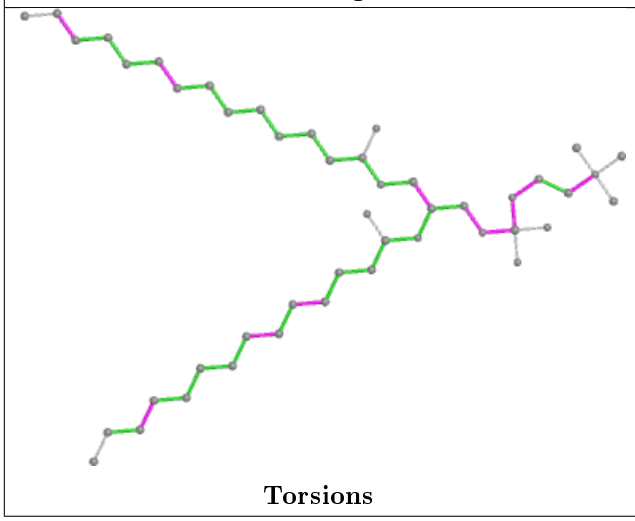
Ligand PX4 A 627



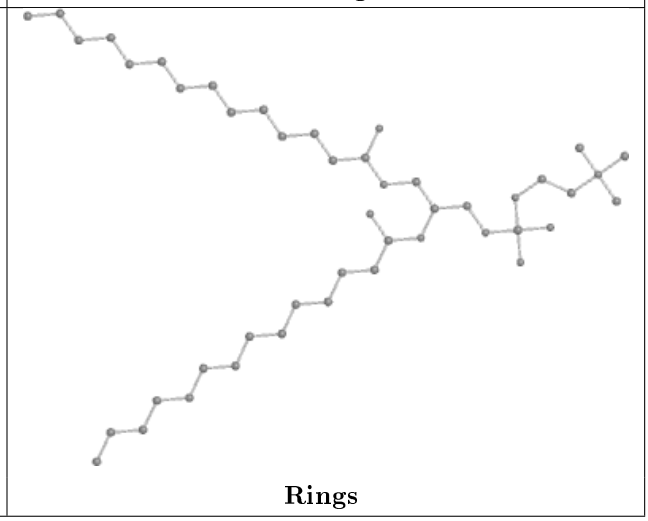
Bond lengths



Bond angles

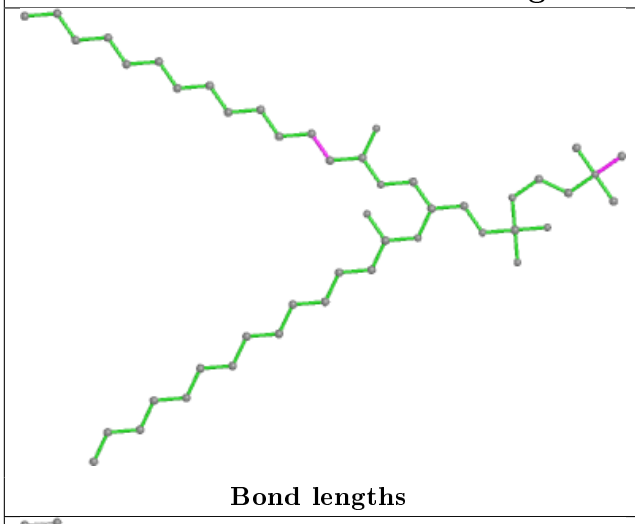


Torsions

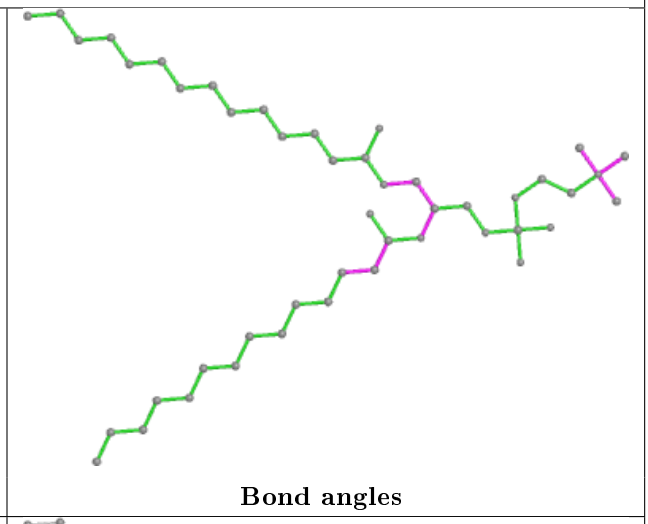


Rings

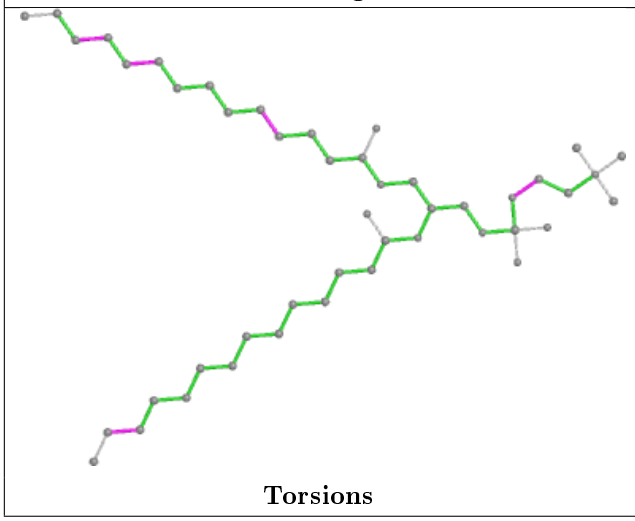
Ligand PX4 C 332



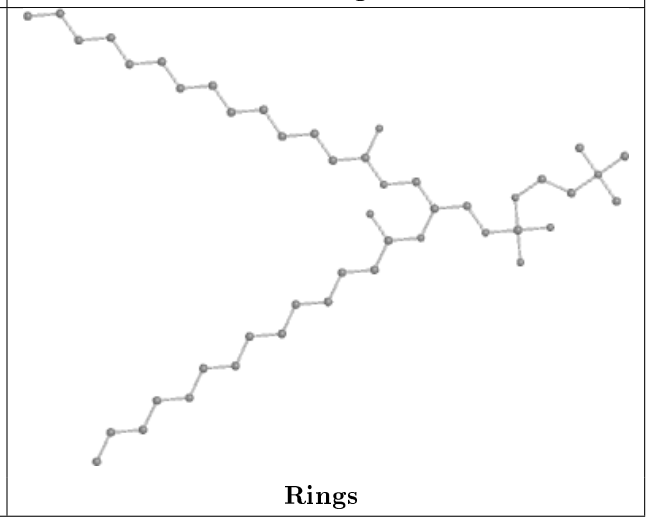
Bond lengths



Bond angles

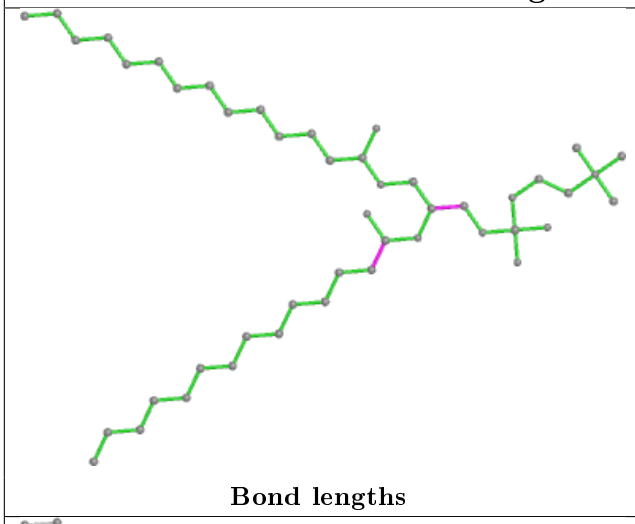


Torsions

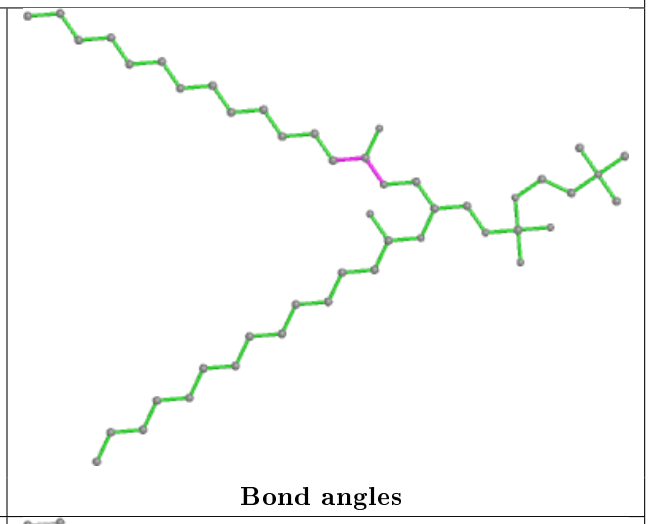


Rings

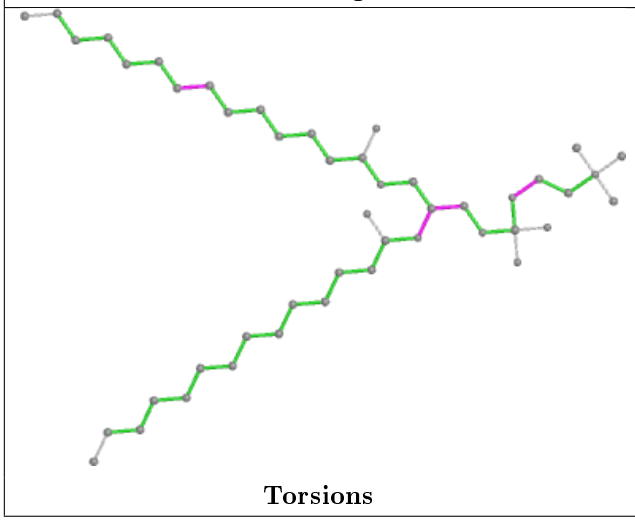
Ligand PX4 C 325



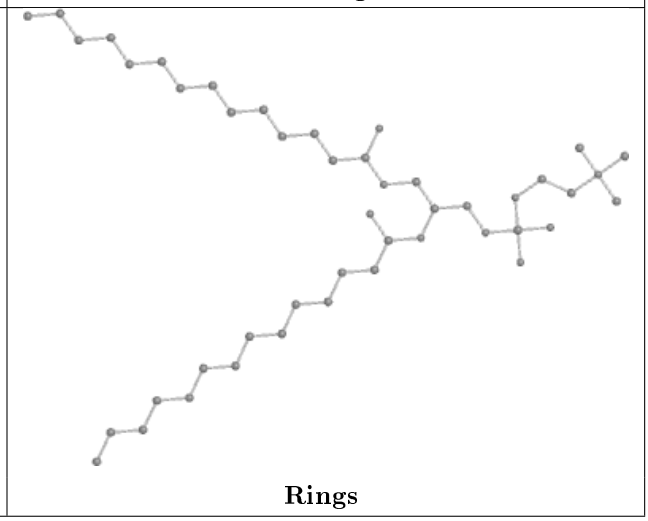
Bond lengths



Bond angles

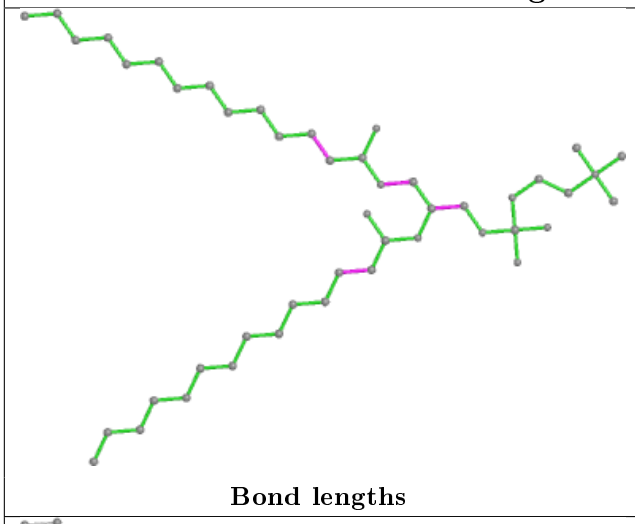


Torsions

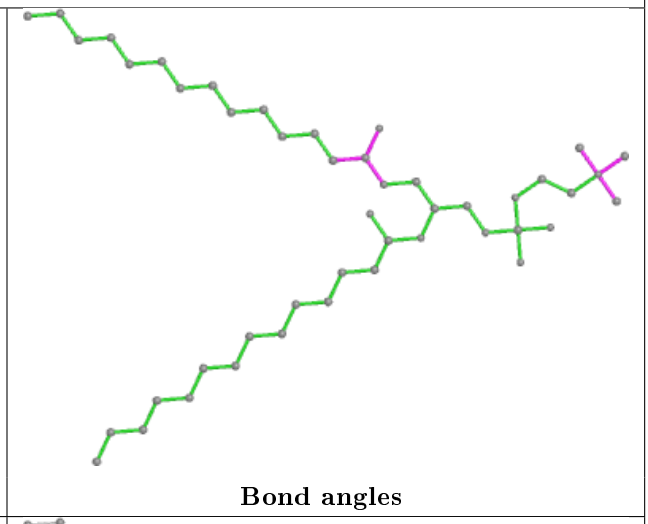


Rings

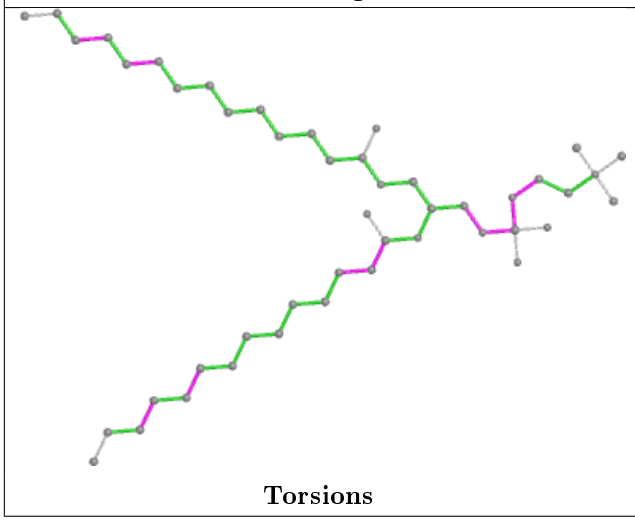
Ligand PX4 B 377



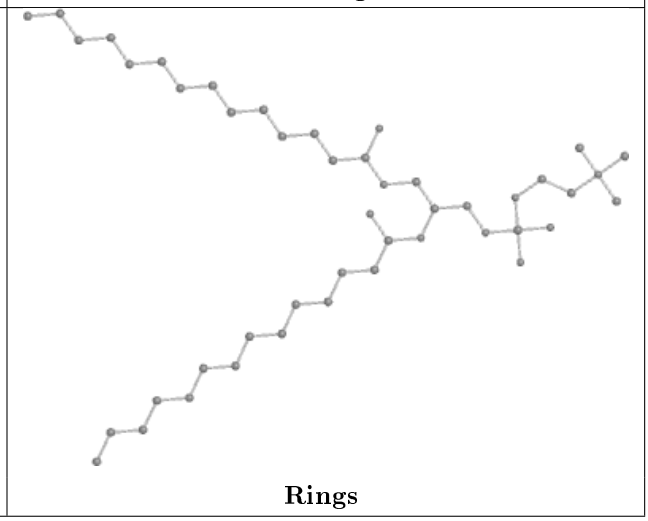
Bond lengths



Bond angles

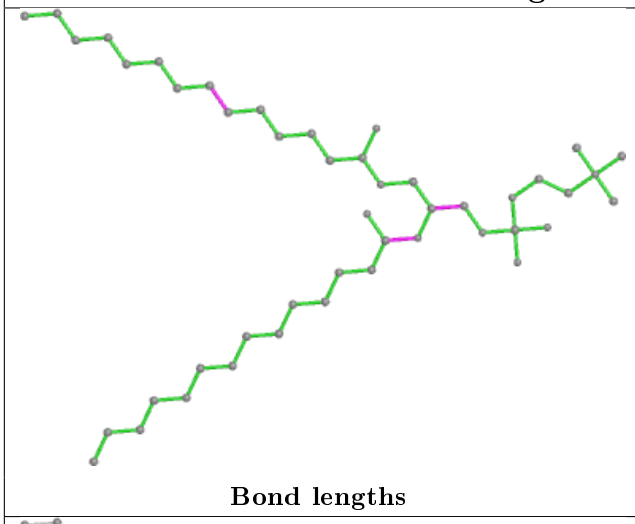


Torsions

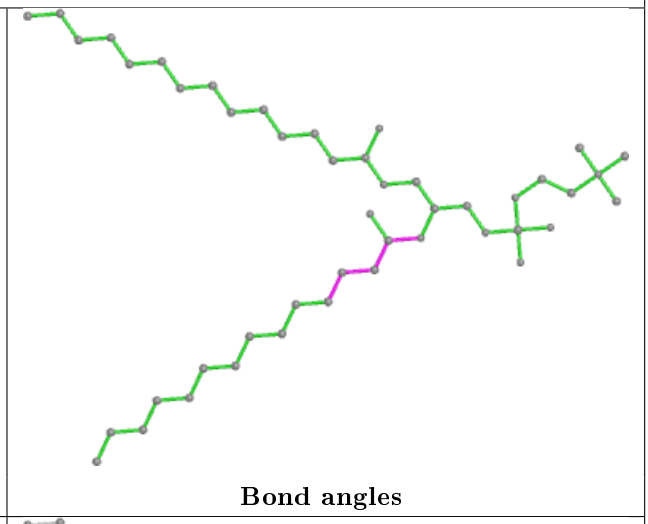


Rings

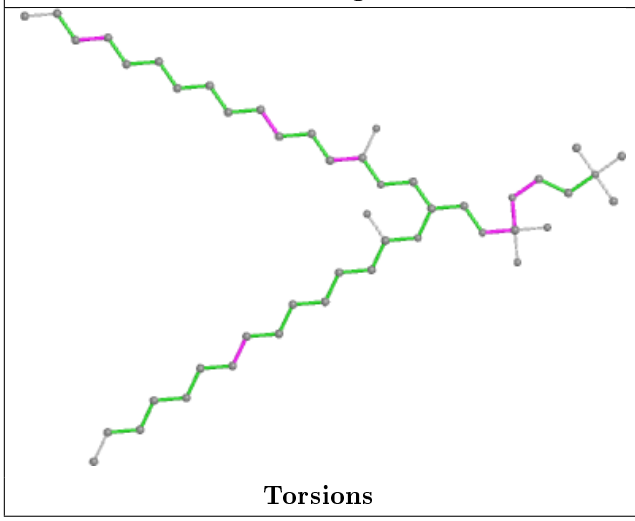
Ligand PX4 B 398



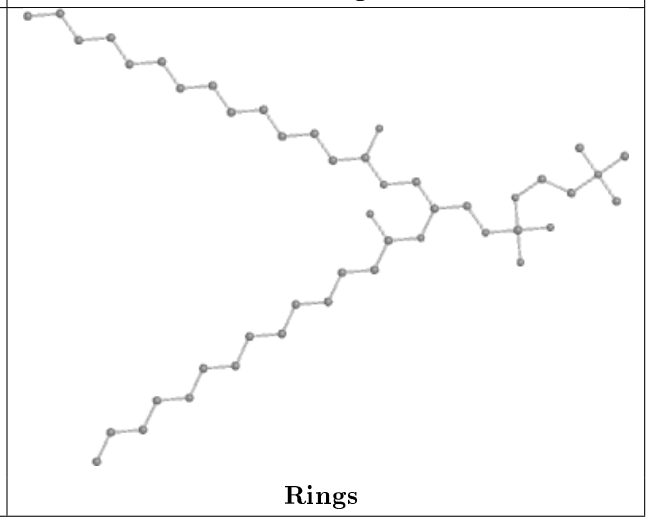
Bond lengths



Bond angles

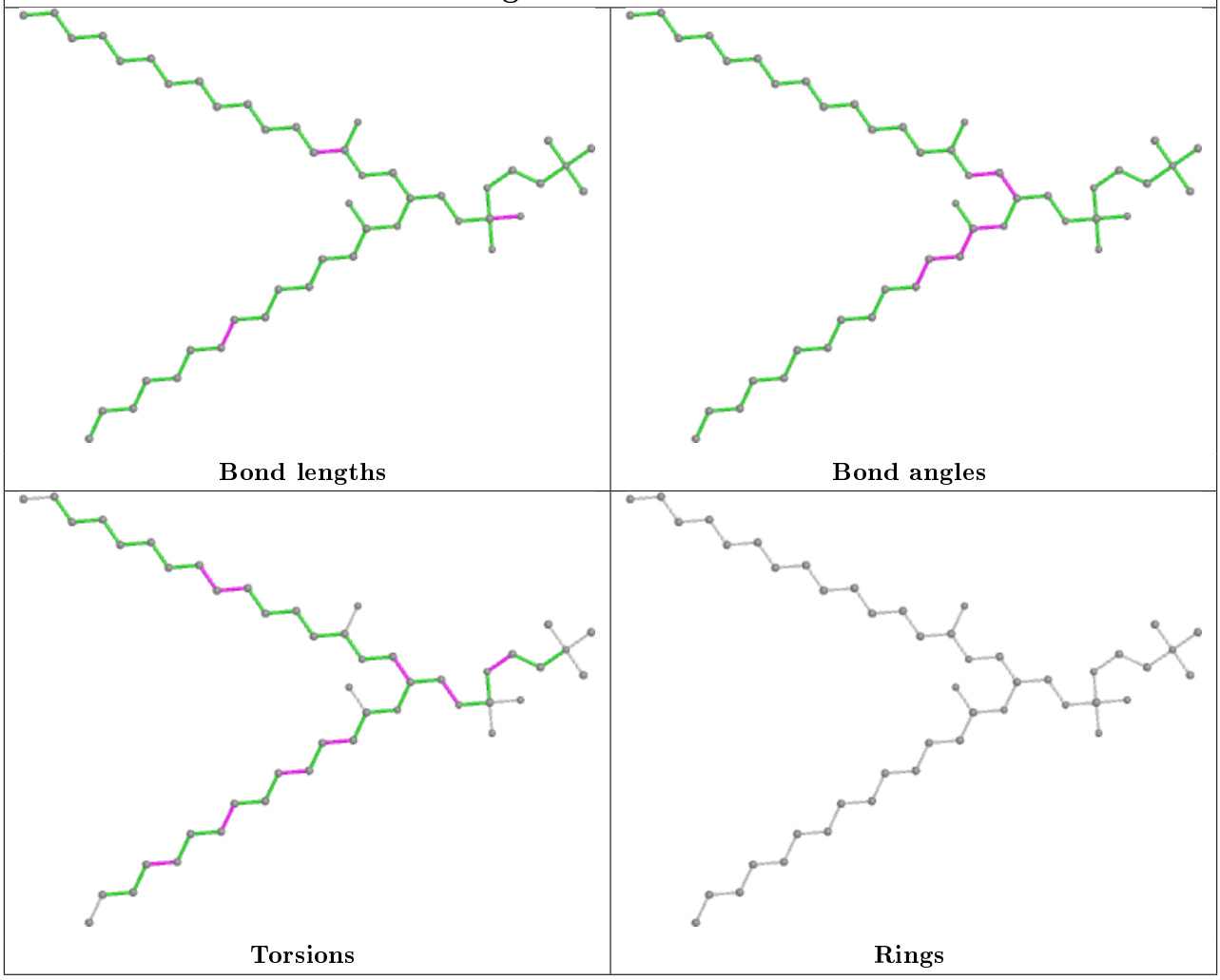


Torsions

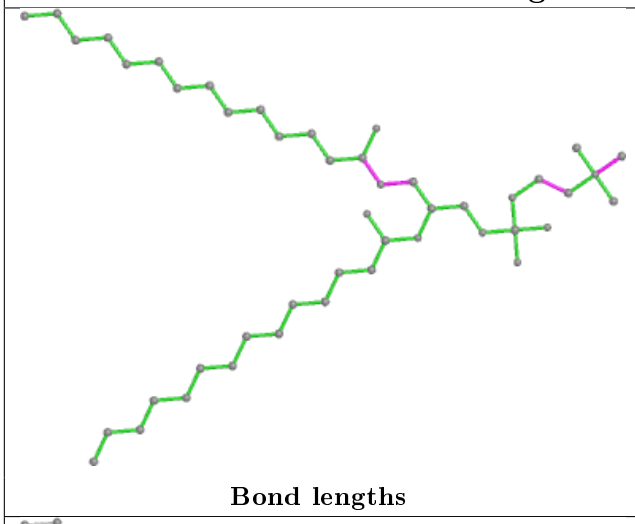


Rings

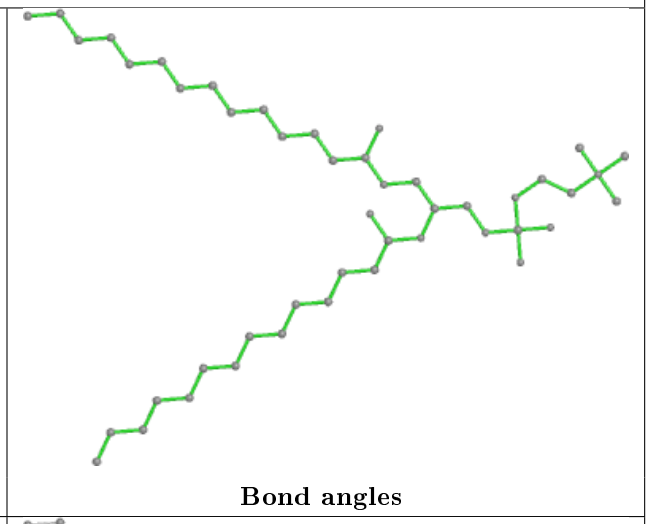
Ligand PX4 B 391



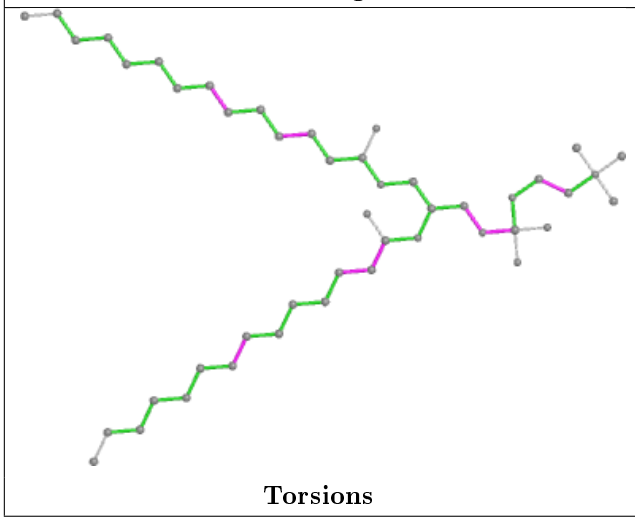
Ligand PX4 B 311



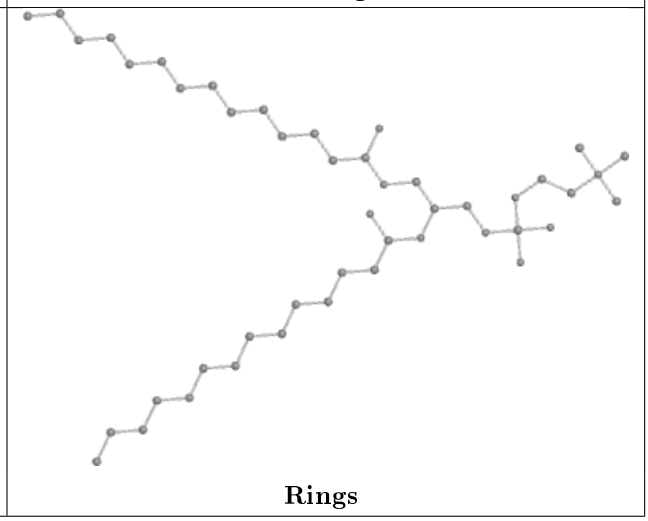
Bond lengths



Bond angles

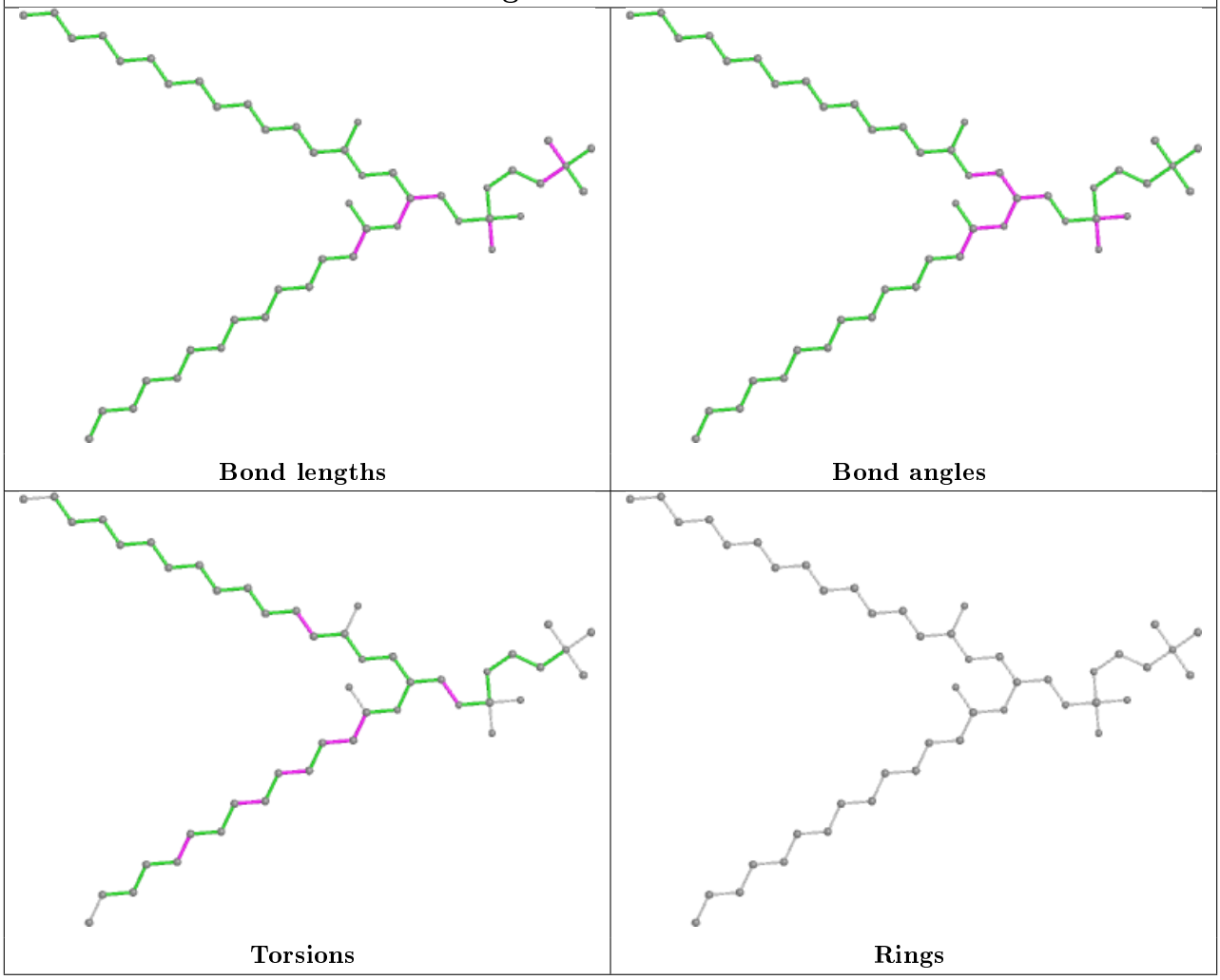


Torsions

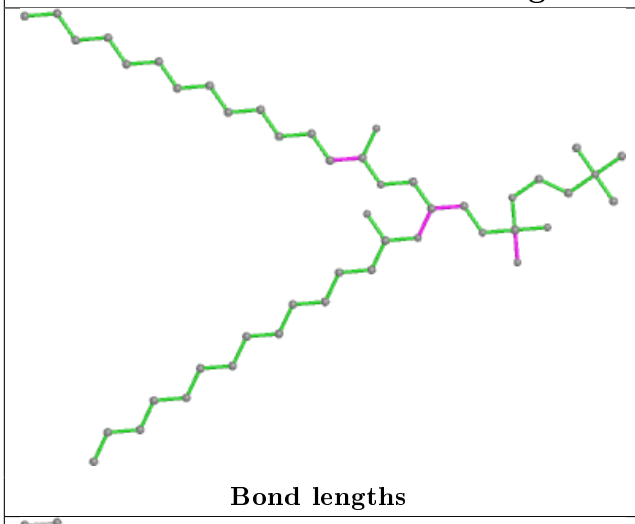


Rings

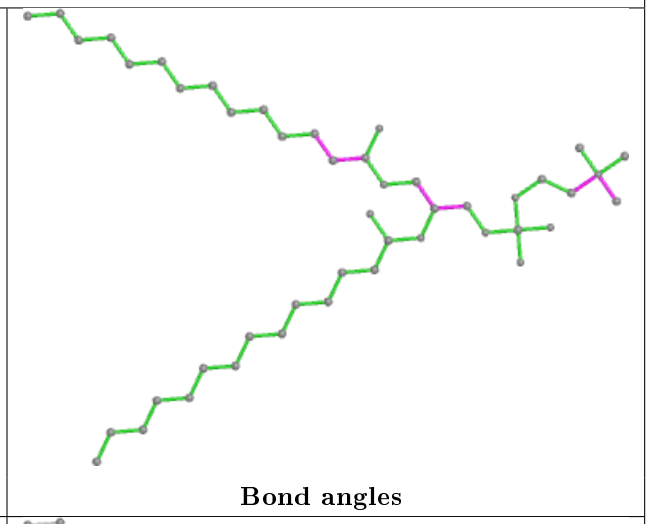
Ligand PX4 B 390



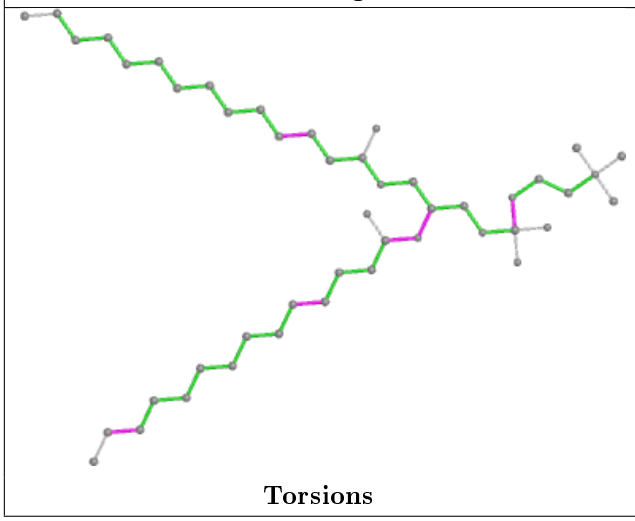
Ligand PX4 C 370



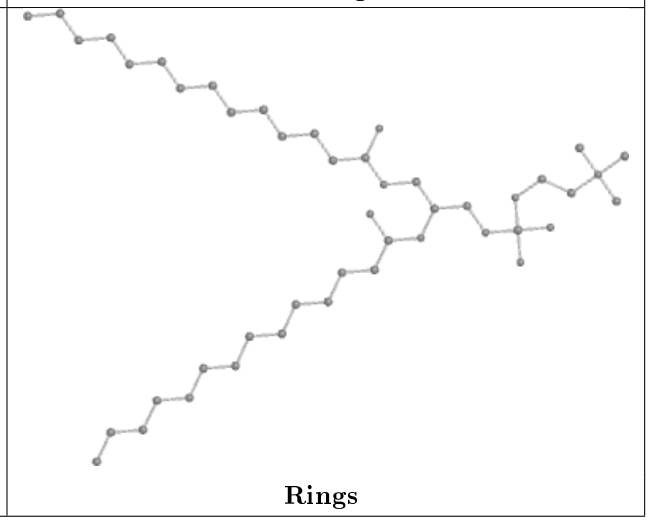
Bond lengths



Bond angles

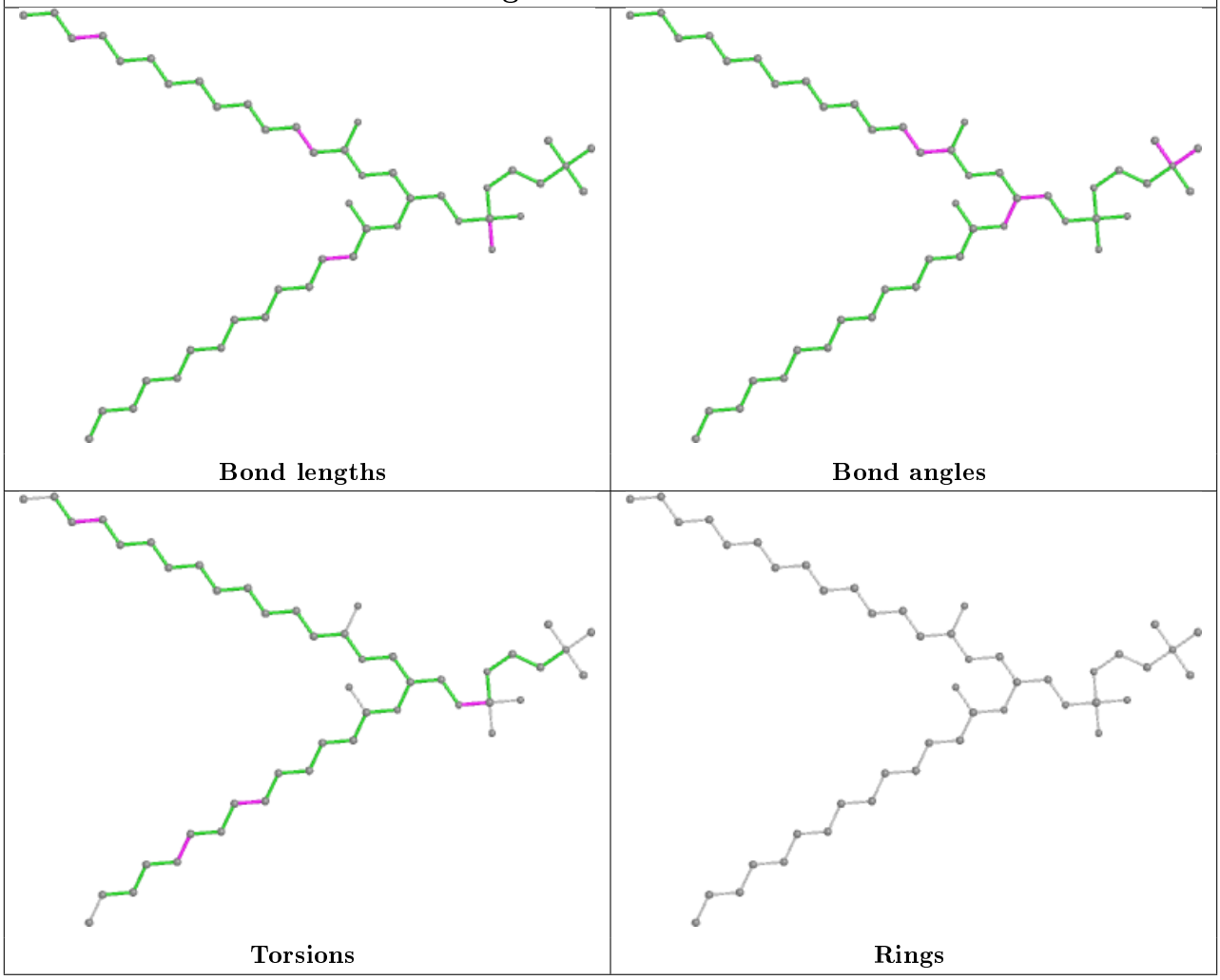


Torsions

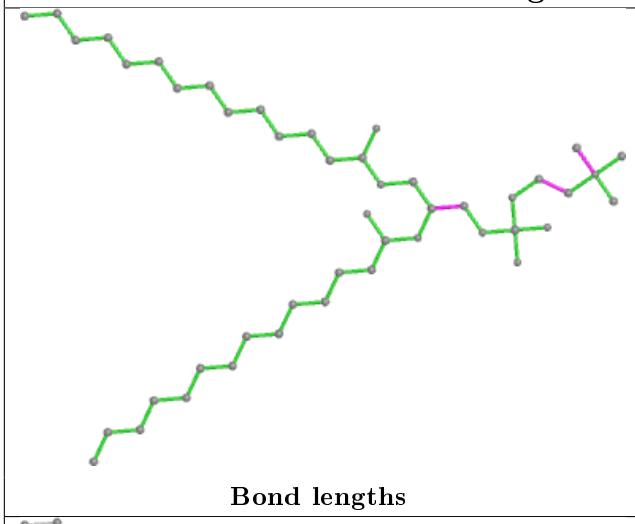


Rings

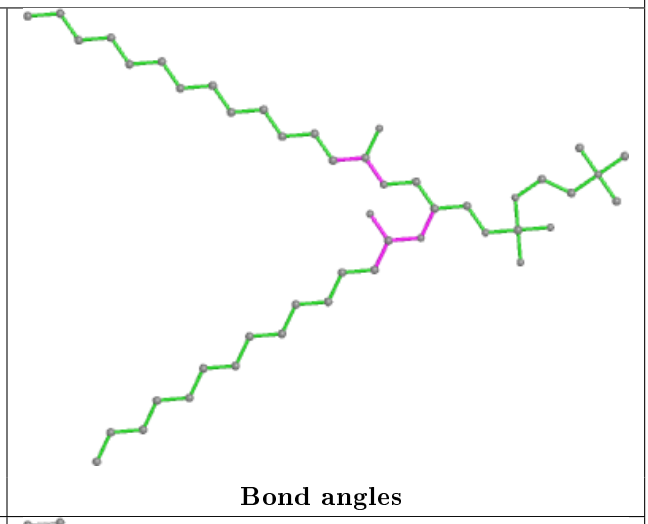
Ligand PX4 B 319



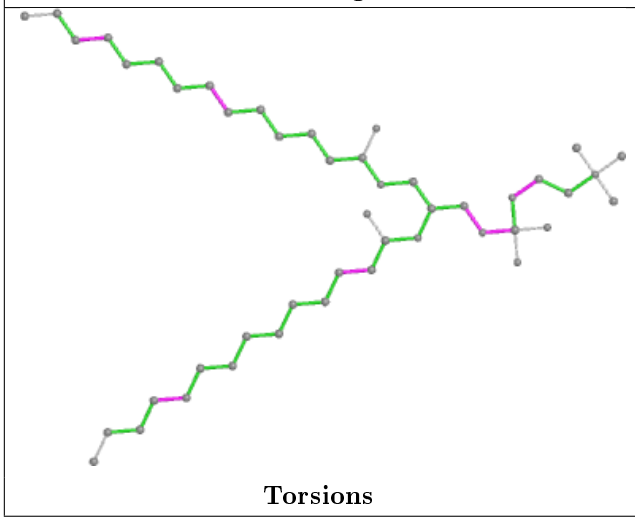
Ligand PX4 A 641



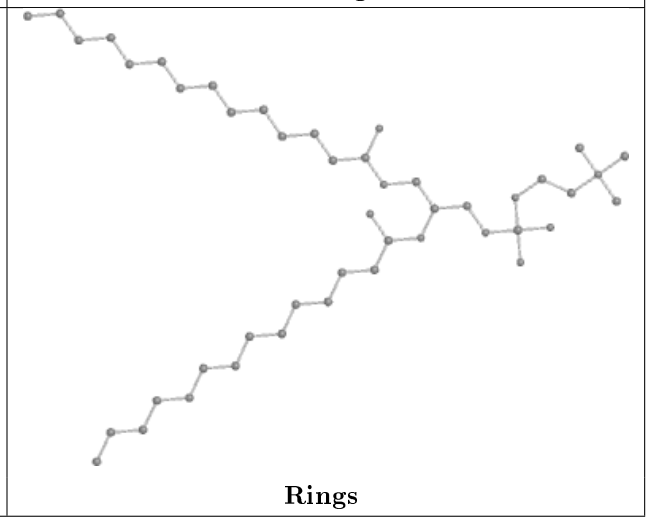
Bond lengths



Bond angles

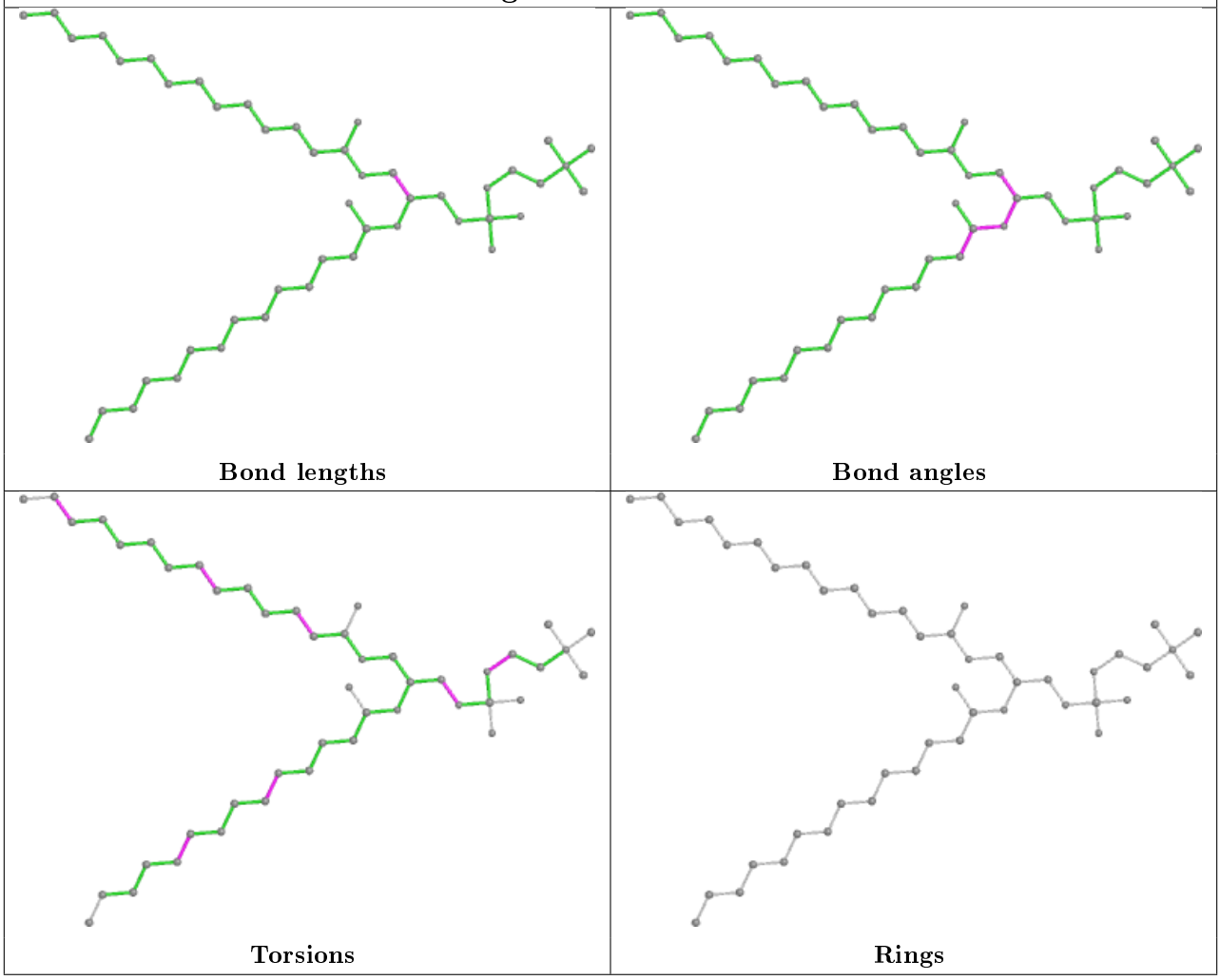


Torsions

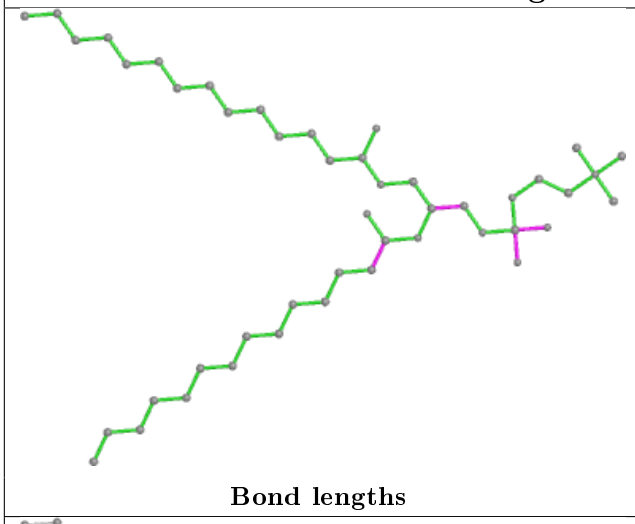


Rings

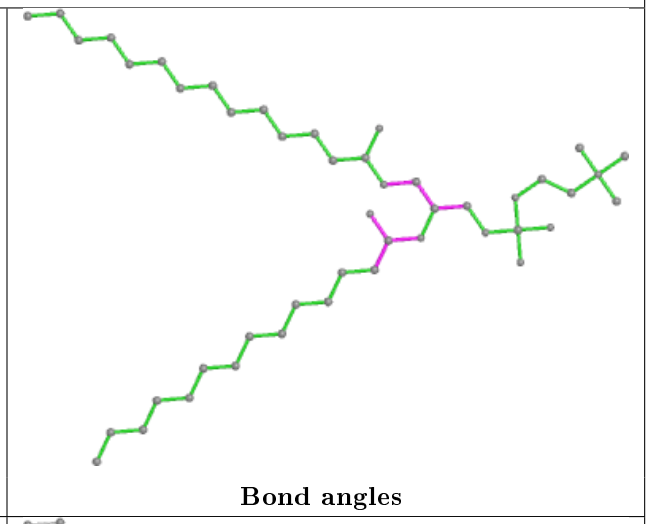
Ligand PX4 A 628



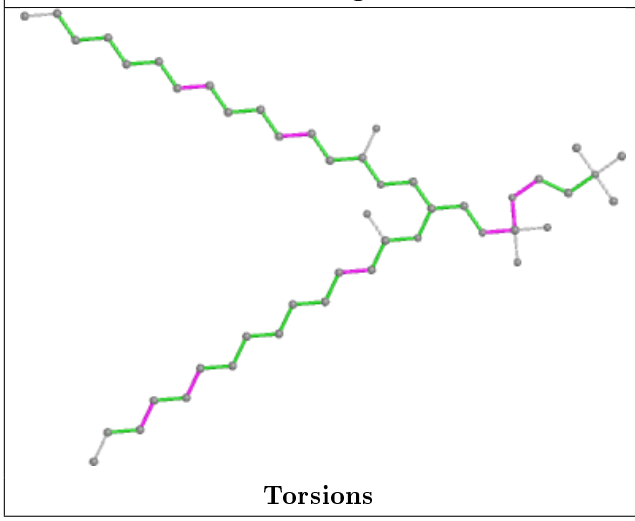
Ligand PX4 C 337



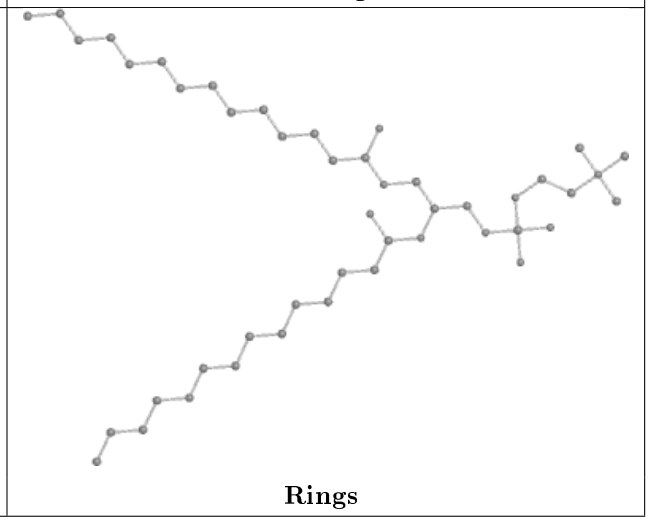
Bond lengths



Bond angles

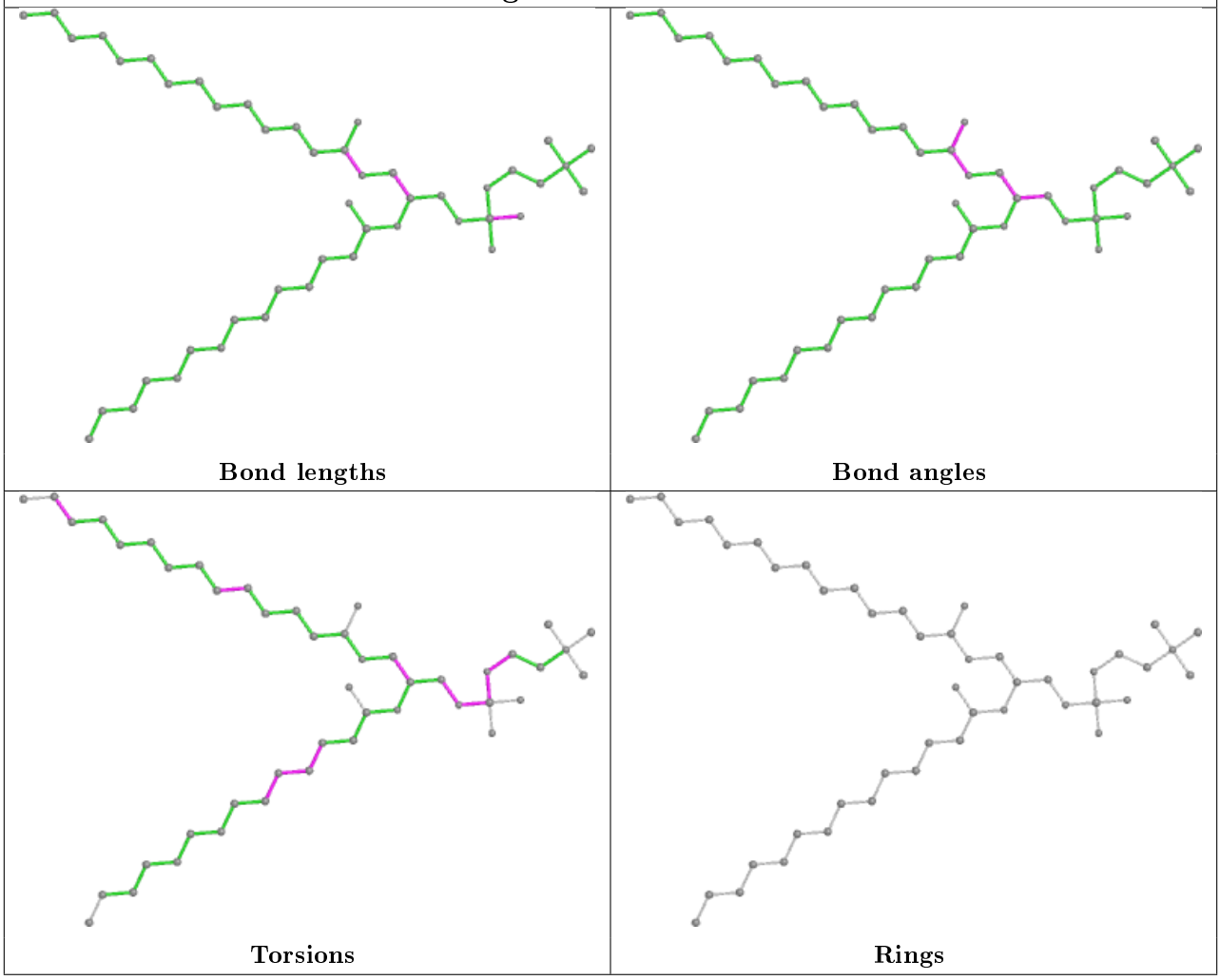


Torsions

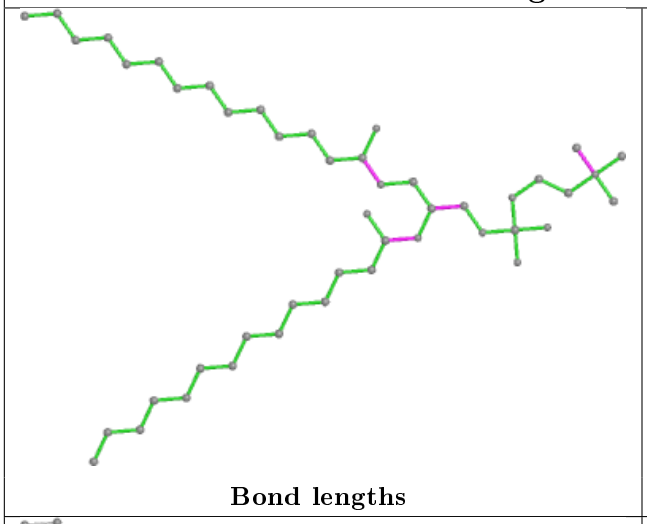


Rings

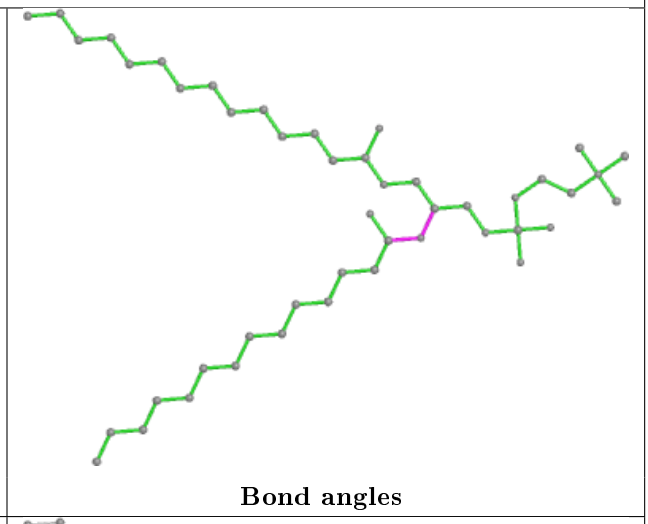
Ligand PX4 B 331



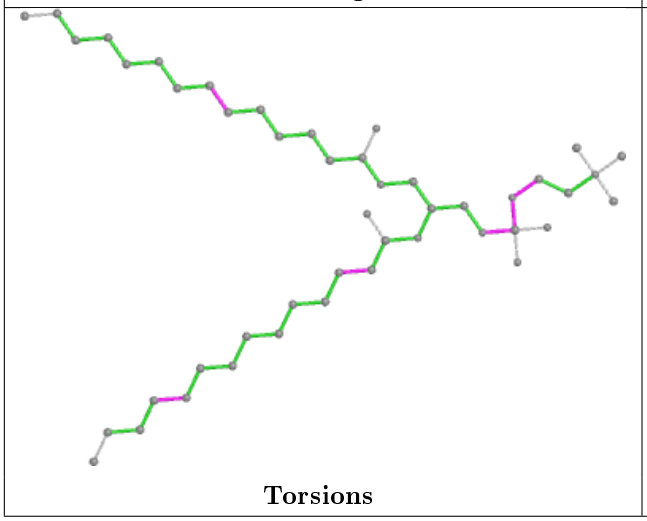
Ligand PX4 B 301



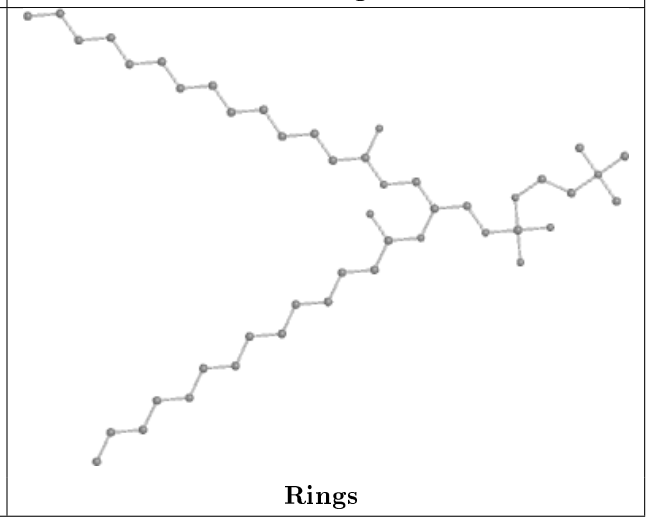
Bond lengths



Bond angles

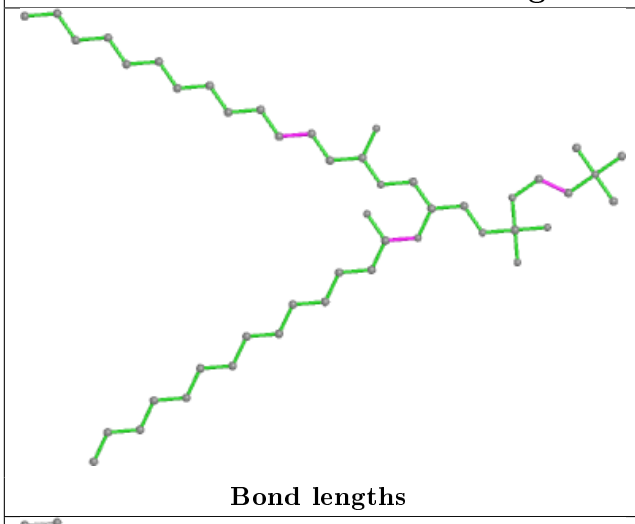


Torsions

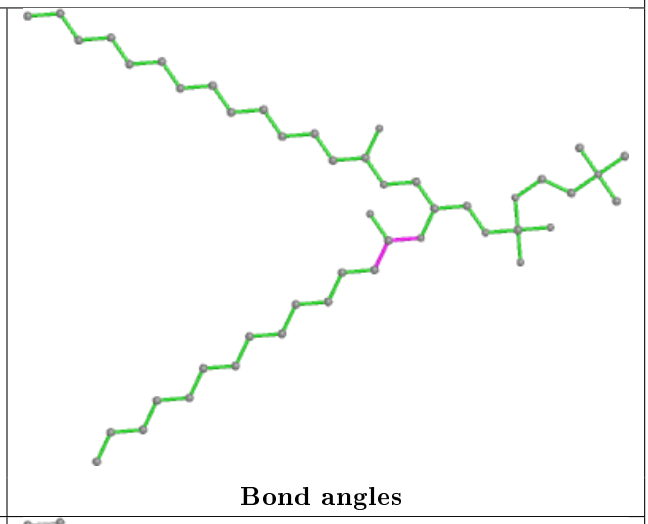


Rings

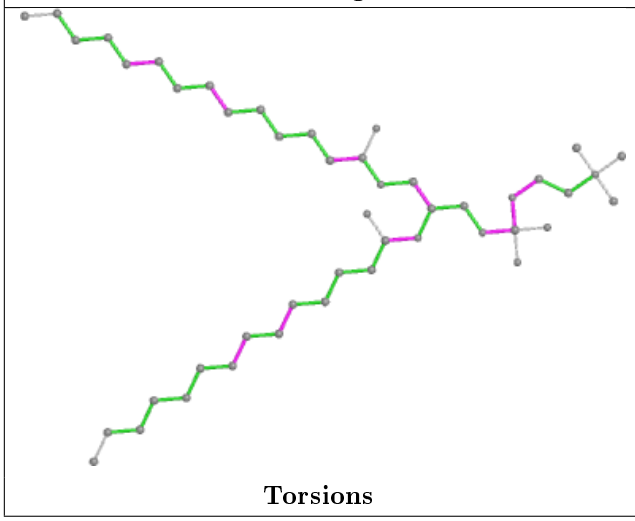
Ligand PX4 C 327



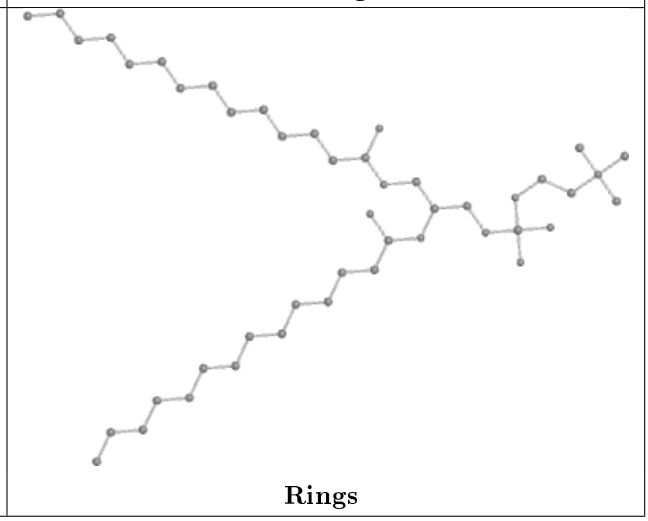
Bond lengths



Bond angles

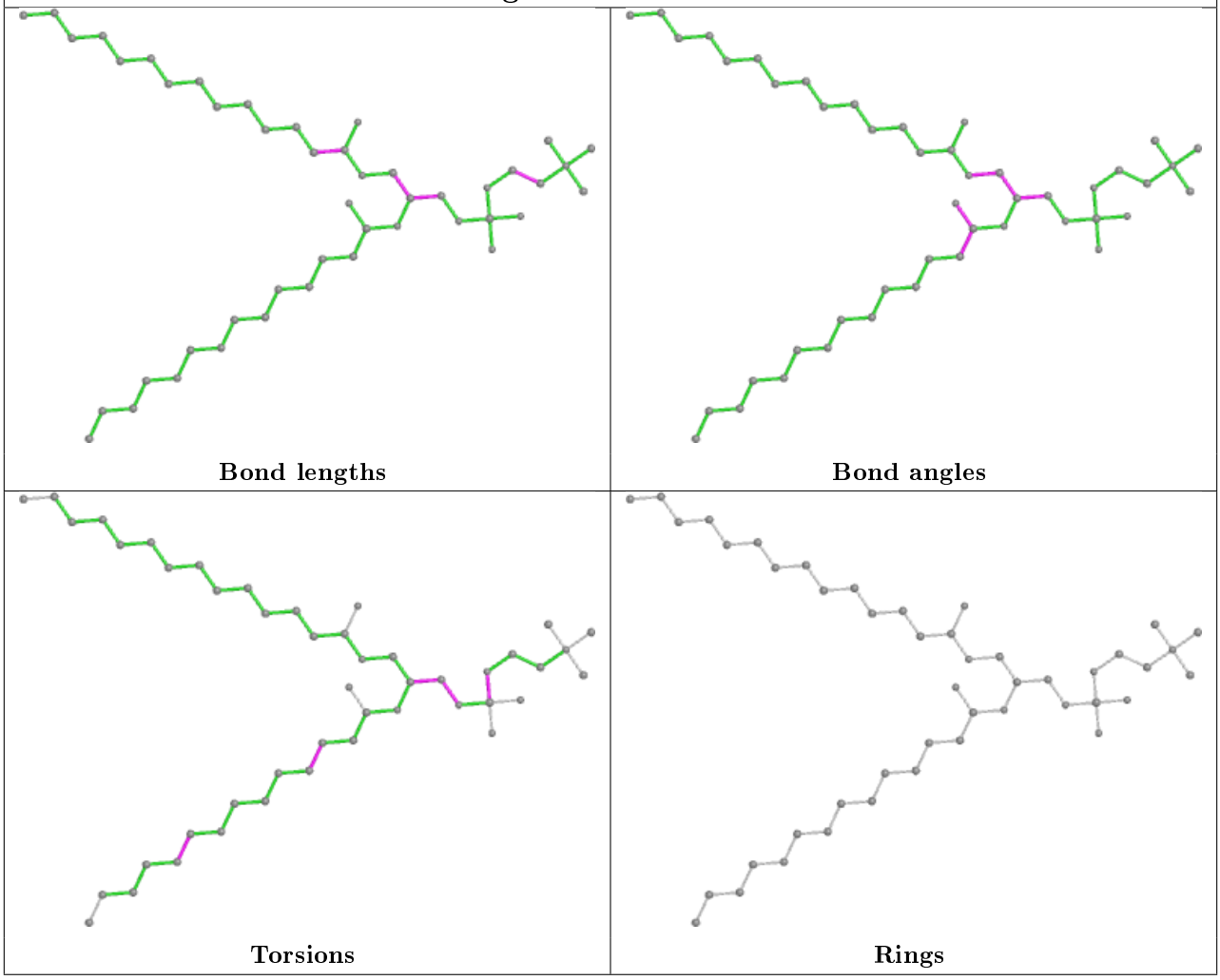


Torsions

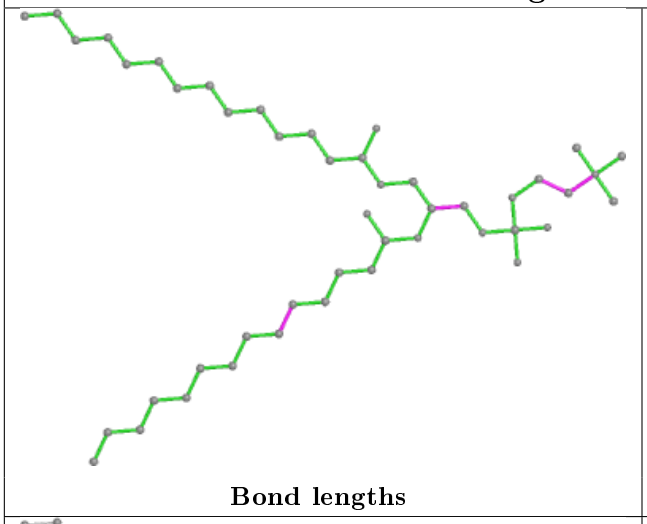


Rings

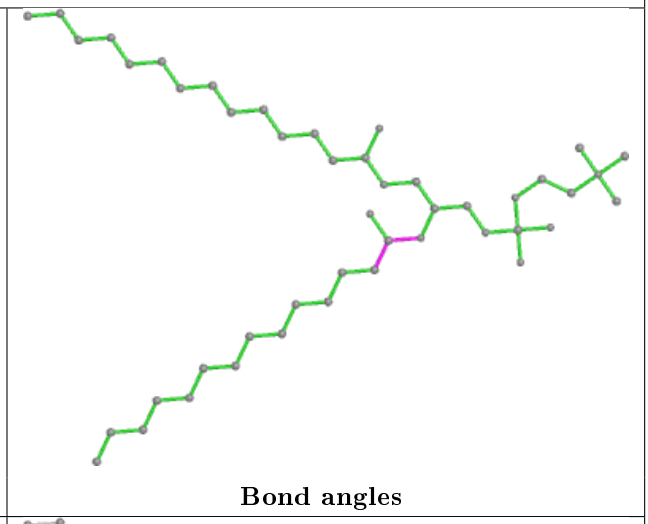
Ligand PX4 B 341



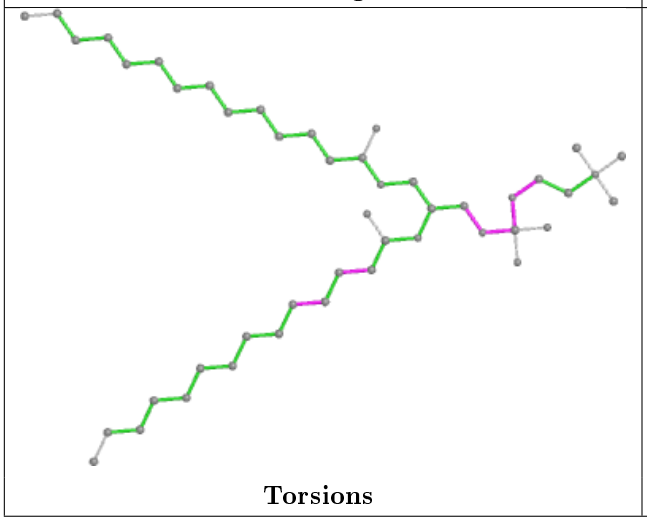
Ligand PX4 B 373



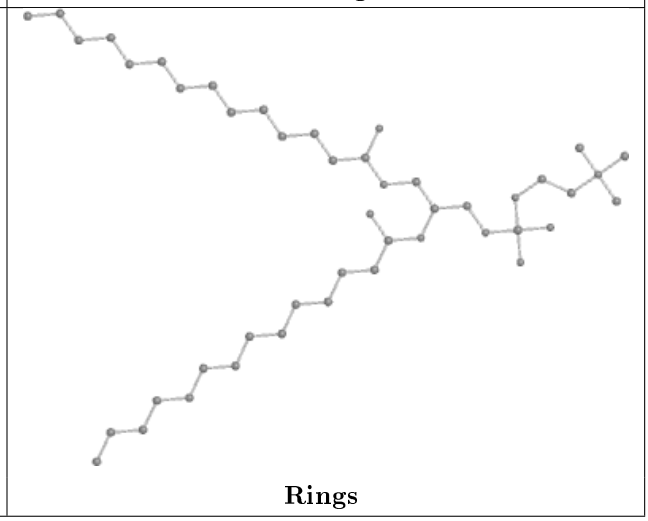
Bond lengths



Bond angles

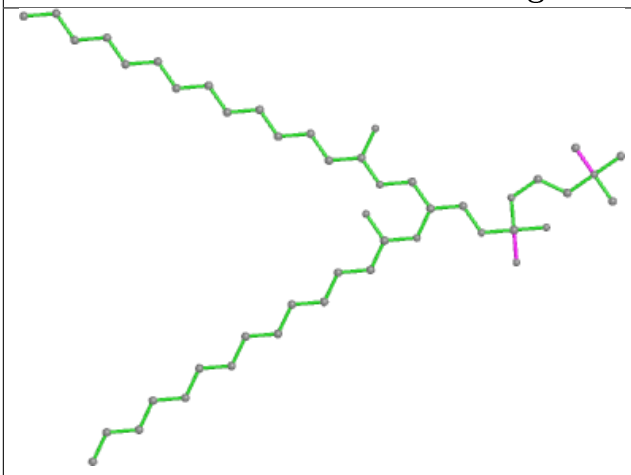


Torsions

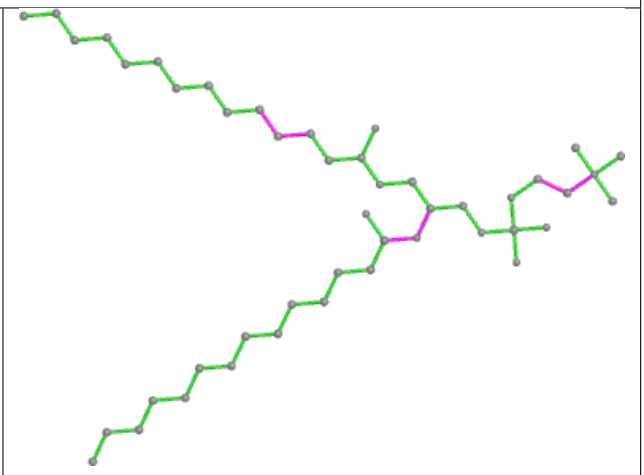


Rings

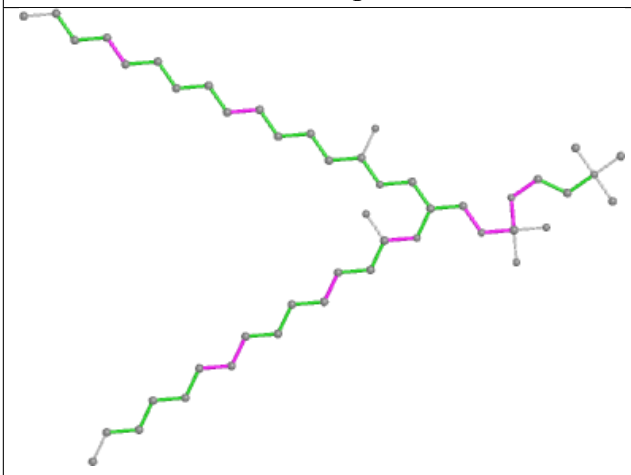
Ligand PX4 C 313



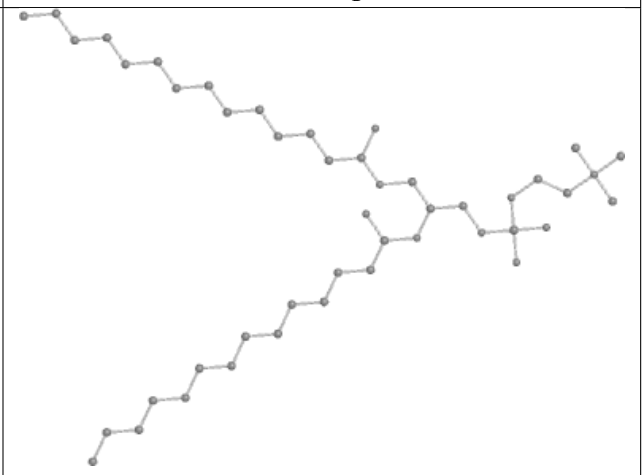
Bond lengths



Bond angles

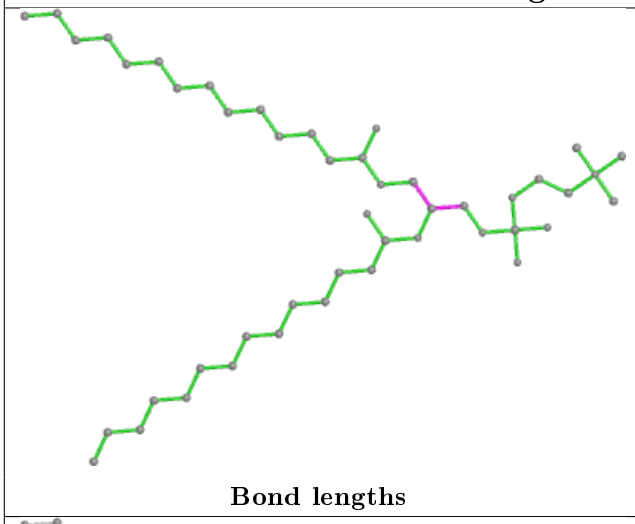


Torsions

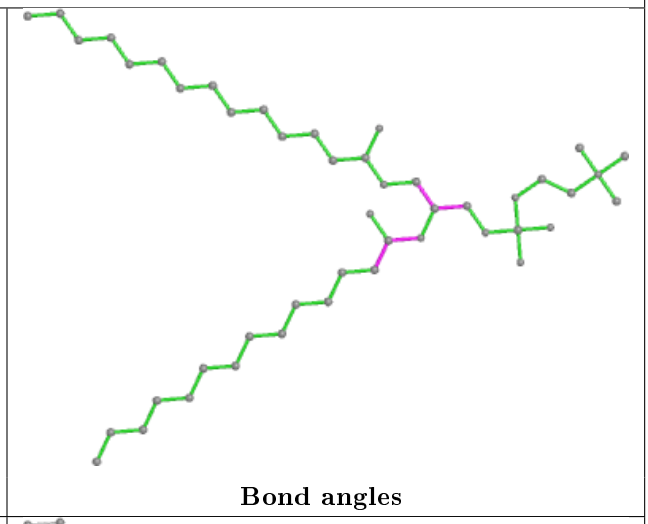


Rings

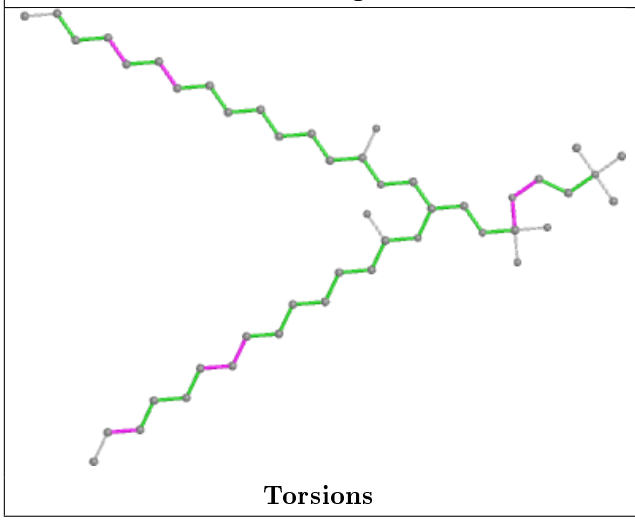
Ligand PX4 B 317



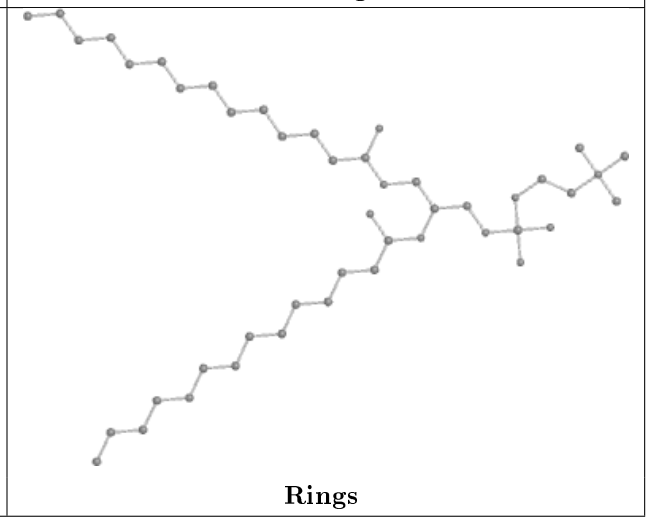
Bond lengths



Bond angles

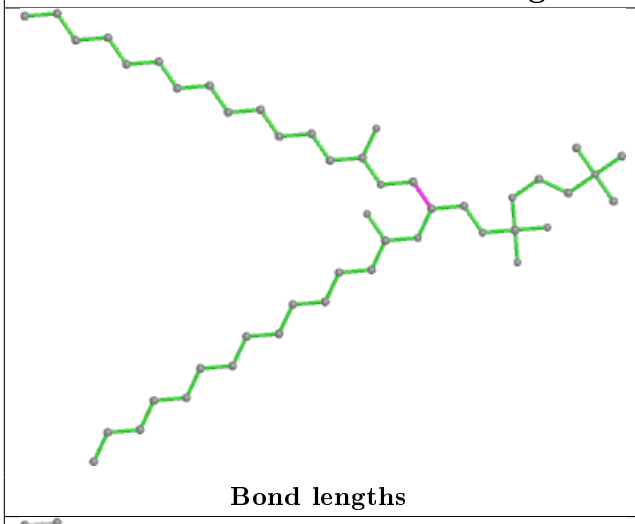


Torsions

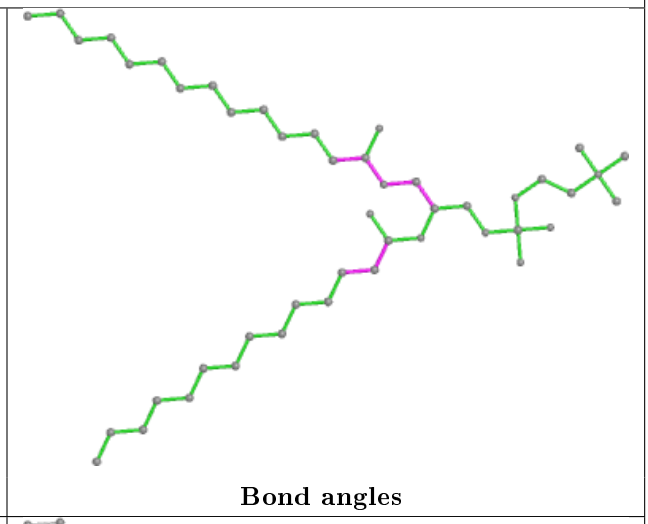


Rings

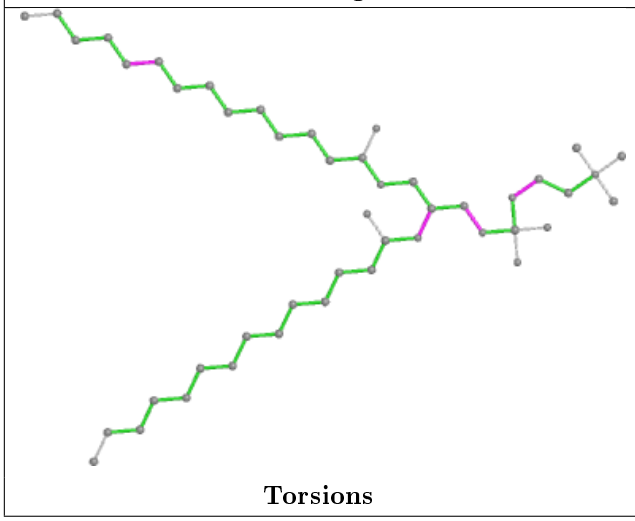
Ligand PX4 B 369



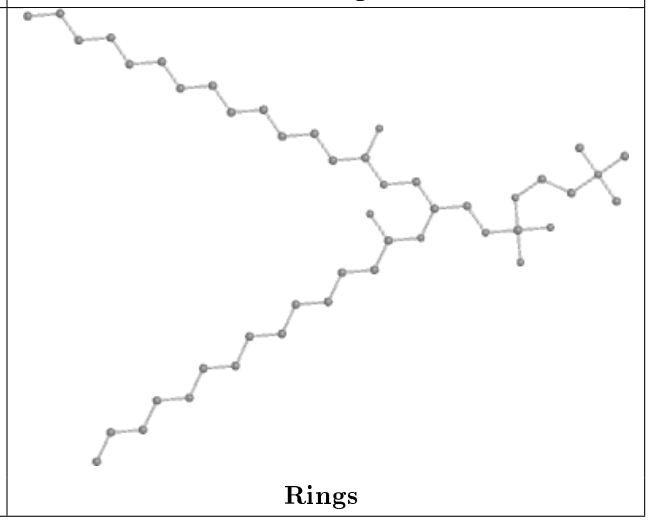
Bond lengths



Bond angles

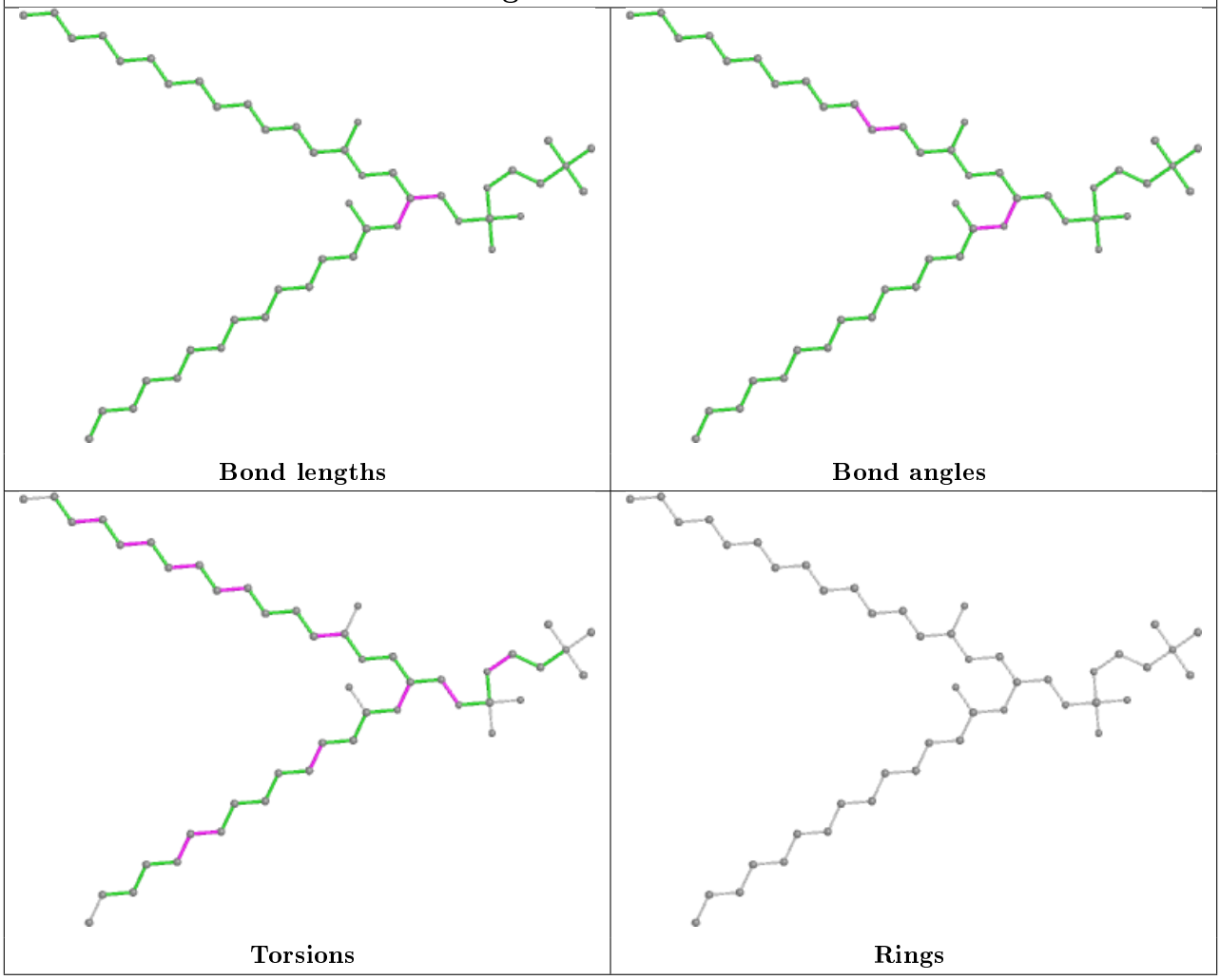


Torsions

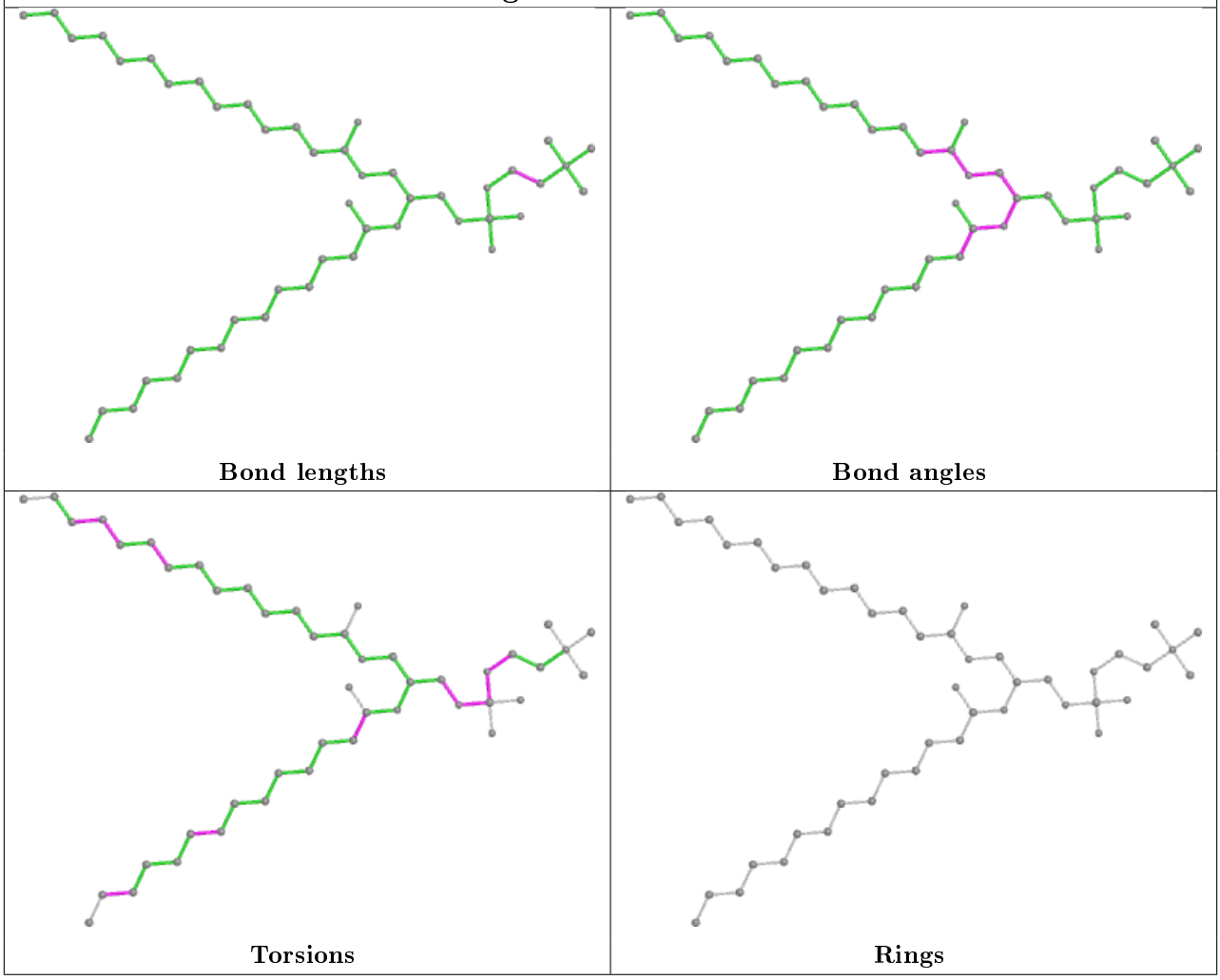


Rings

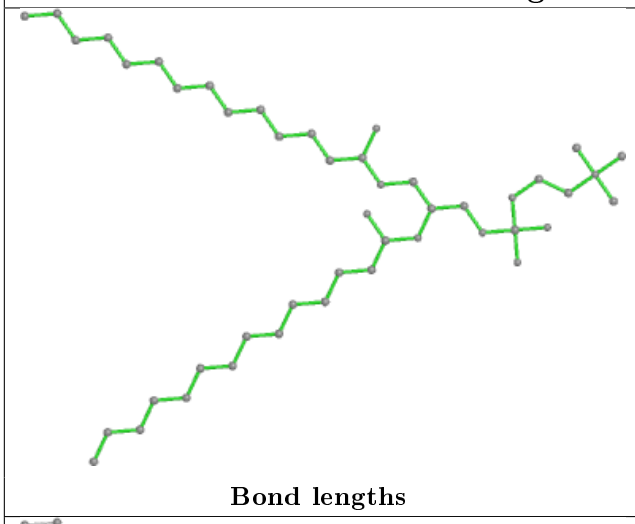
Ligand PX4 B 306



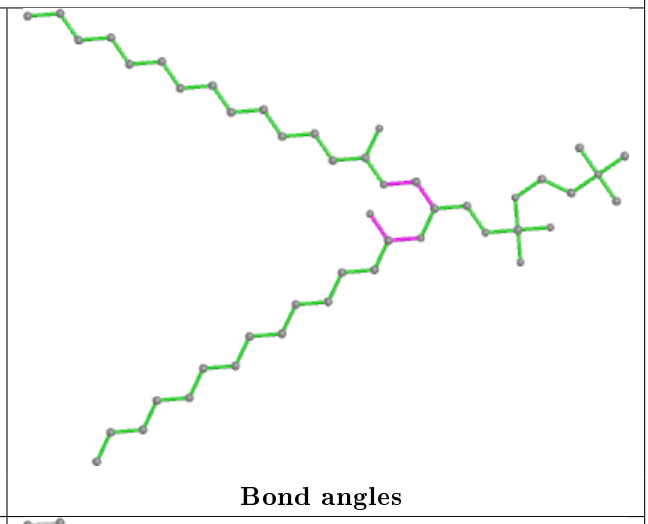
Ligand PX4 B 313



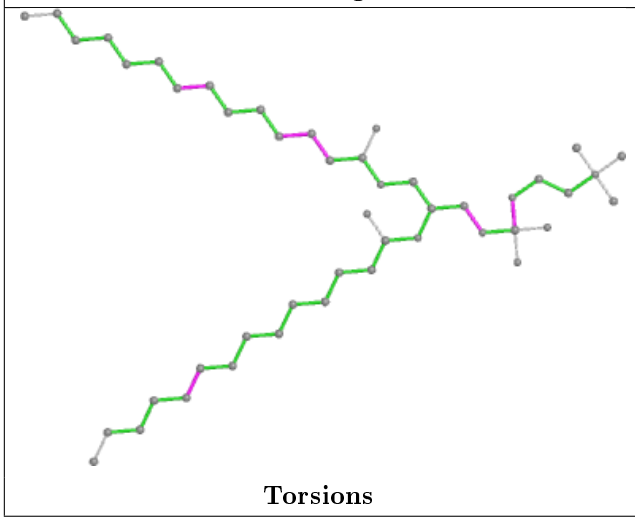
Ligand PX4 A 621



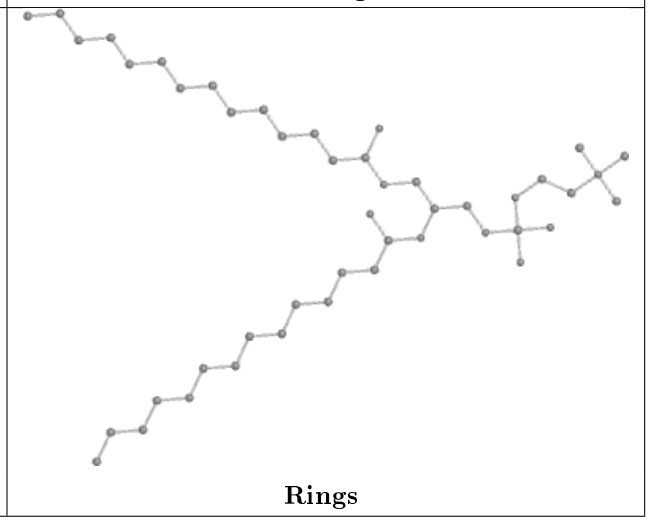
Bond lengths



Bond angles

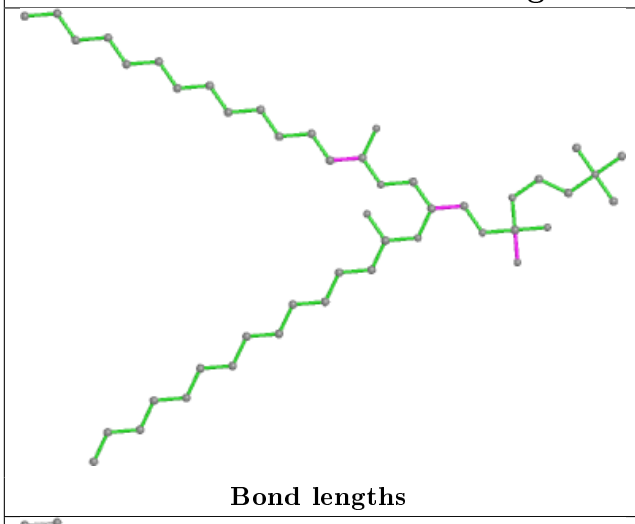


Torsions

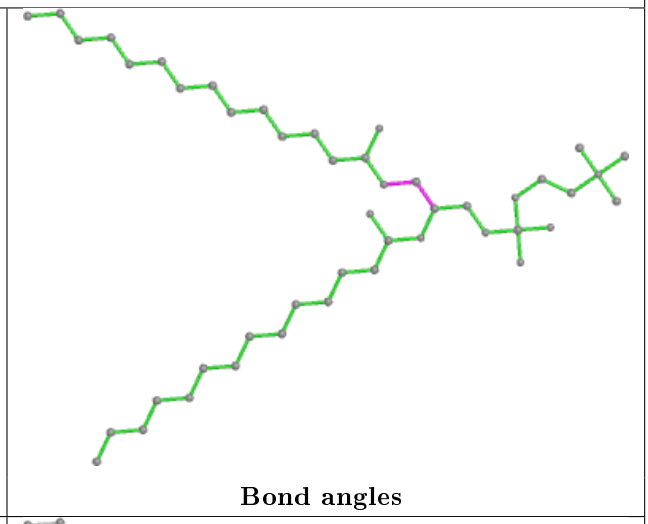


Rings

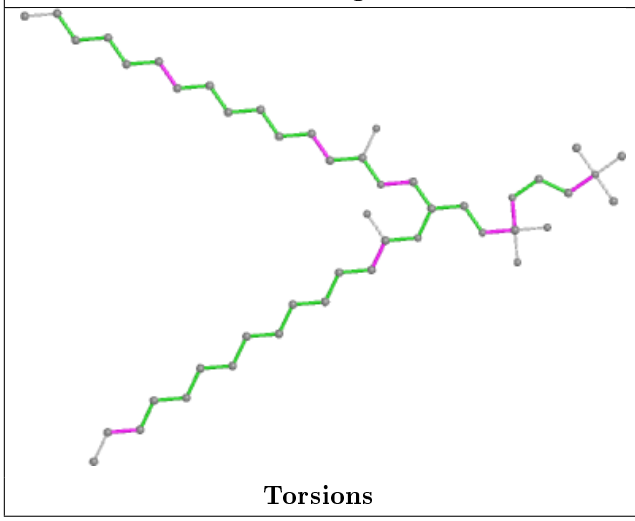
Ligand PX4 A 639



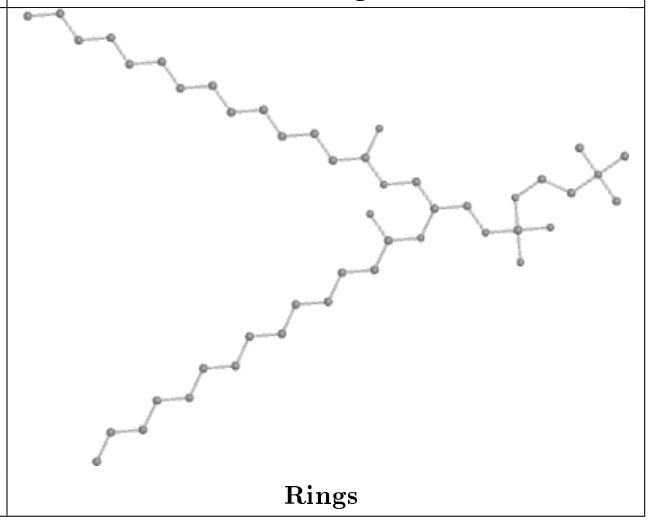
Bond lengths



Bond angles

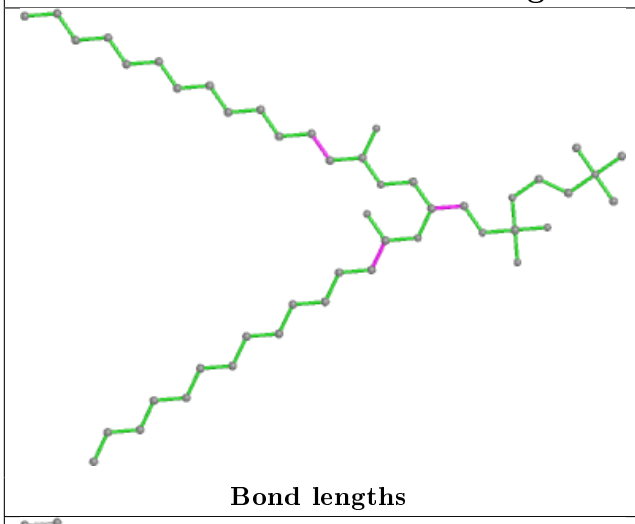


Torsions

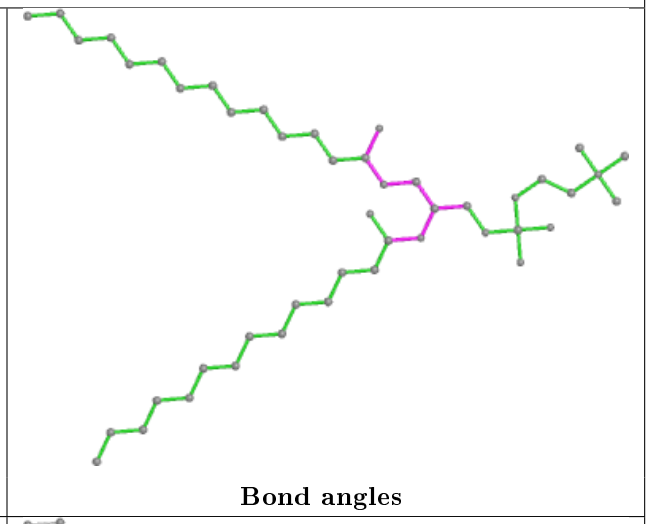


Rings

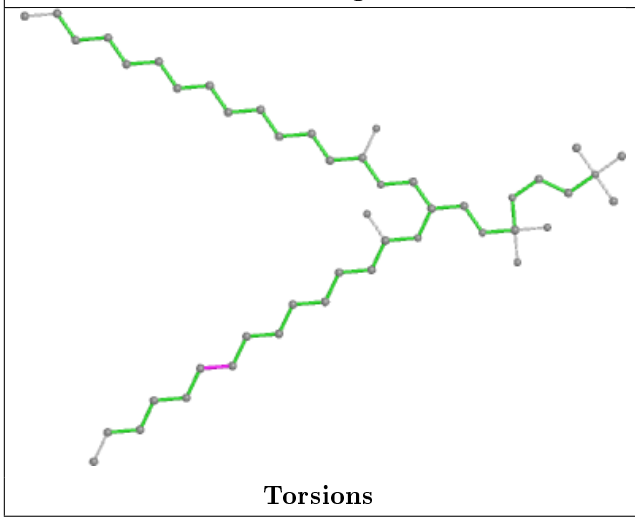
Ligand PX4 A 648



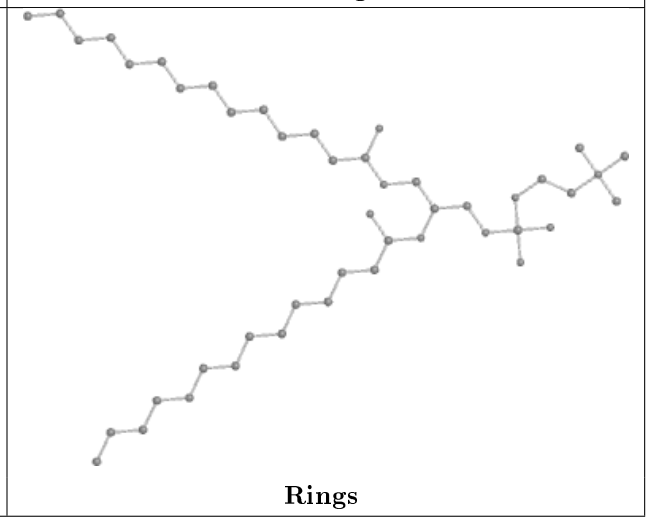
Bond lengths



Bond angles

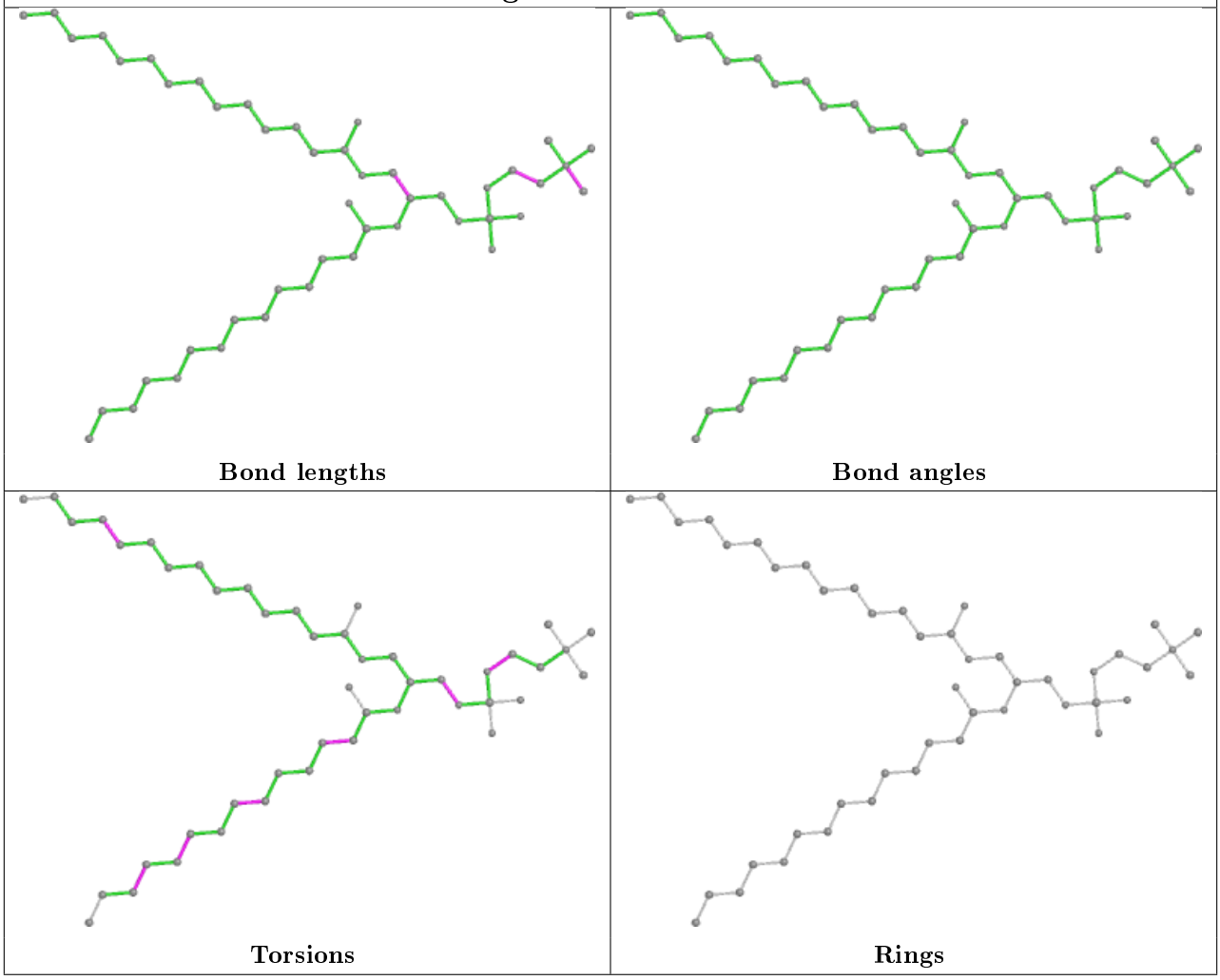


Torsions

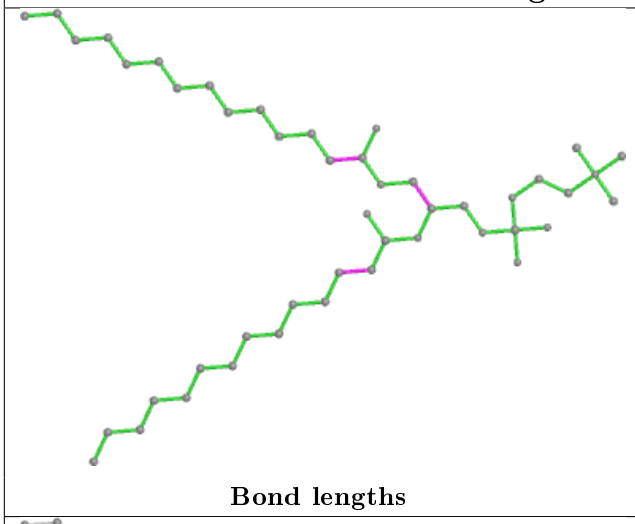


Rings

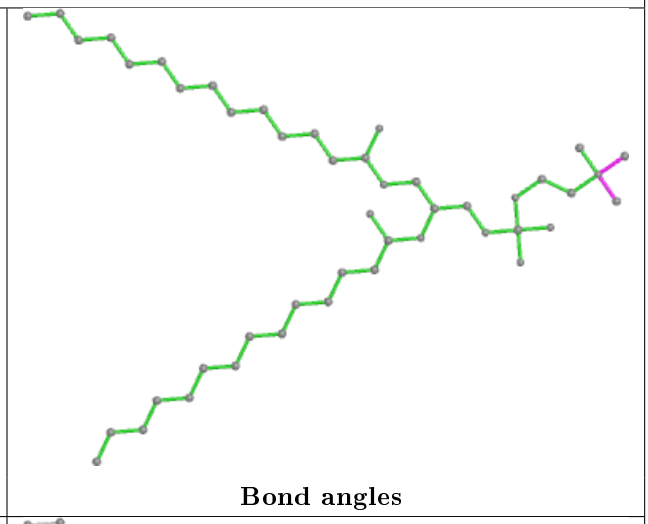
Ligand PX4 B 320



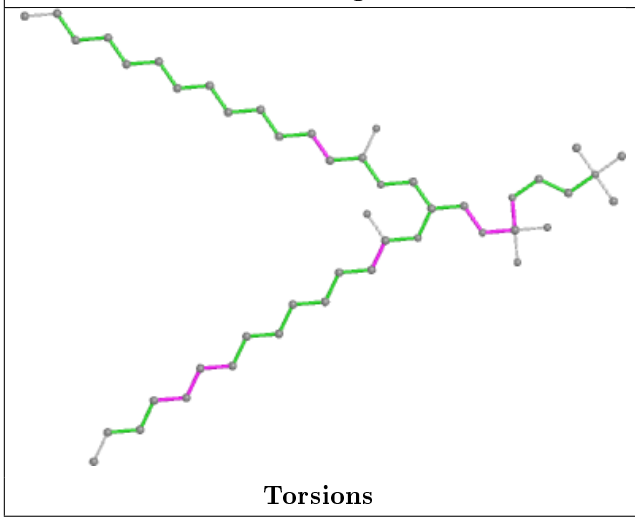
Ligand PX4 B 330



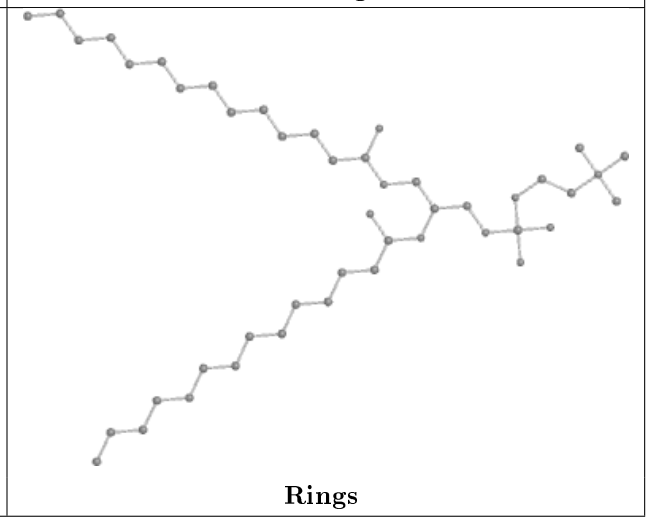
Bond lengths



Bond angles

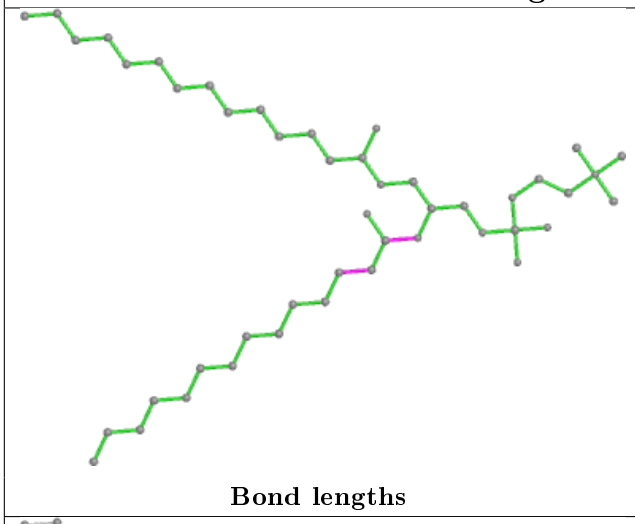


Torsions

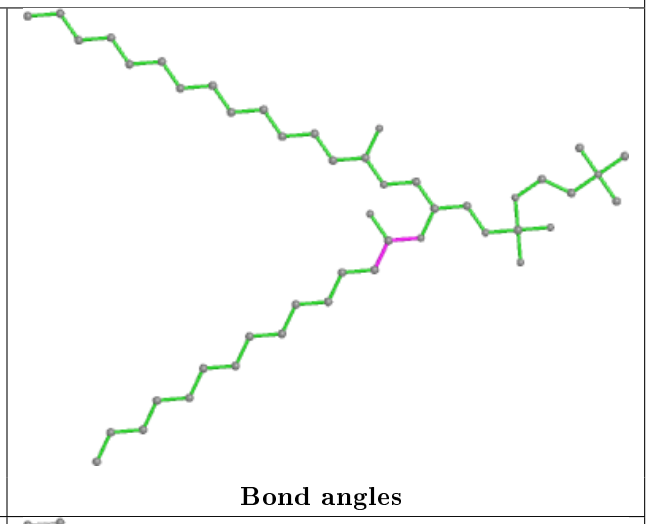


Rings

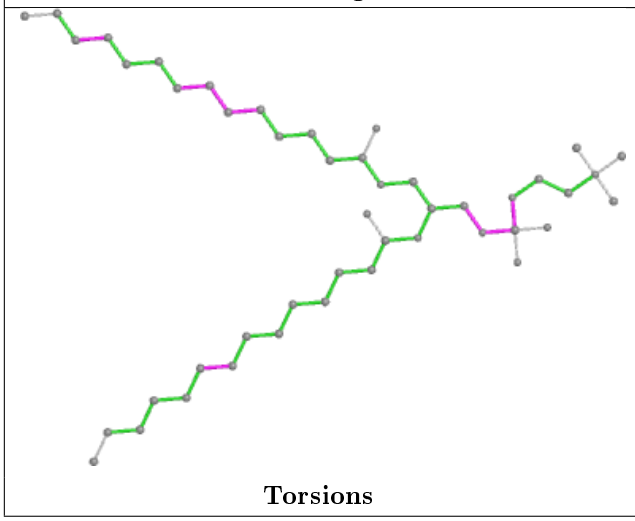
Ligand PX4 C 315



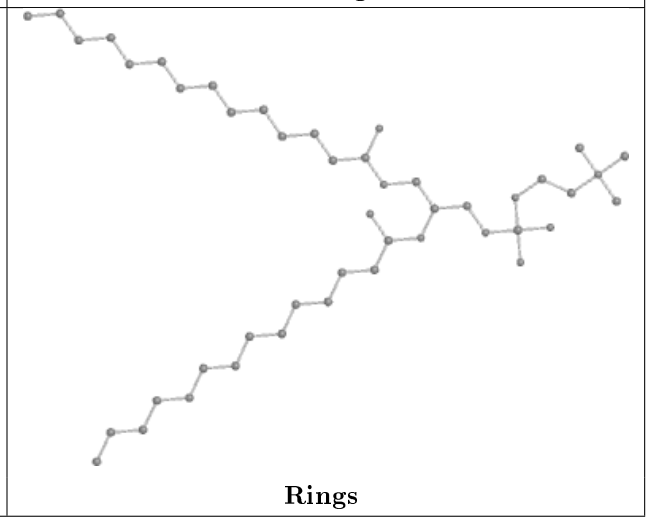
Bond lengths



Bond angles

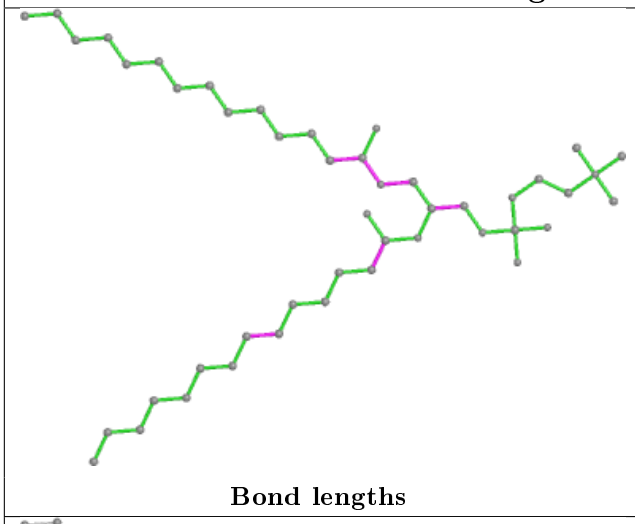


Torsions



Rings

Ligand PX4 C 316



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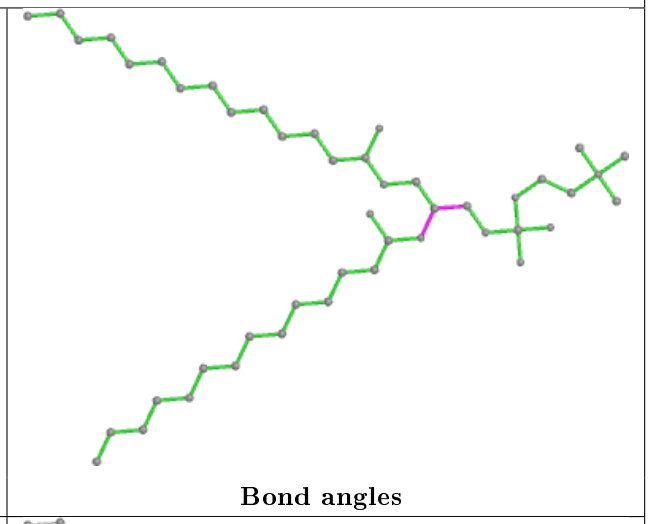
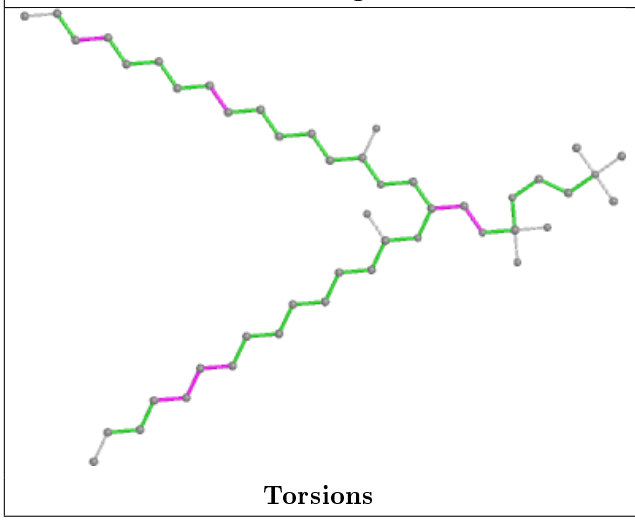
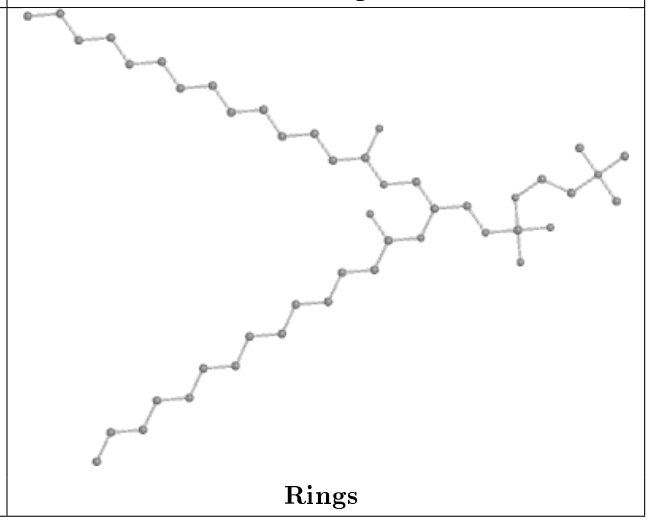


Bond angles

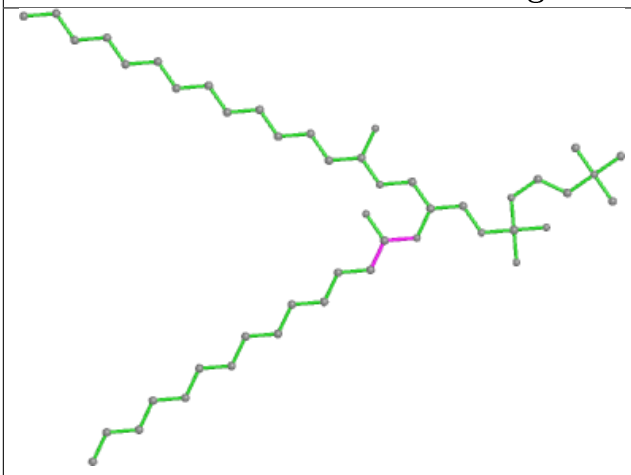


Torsions

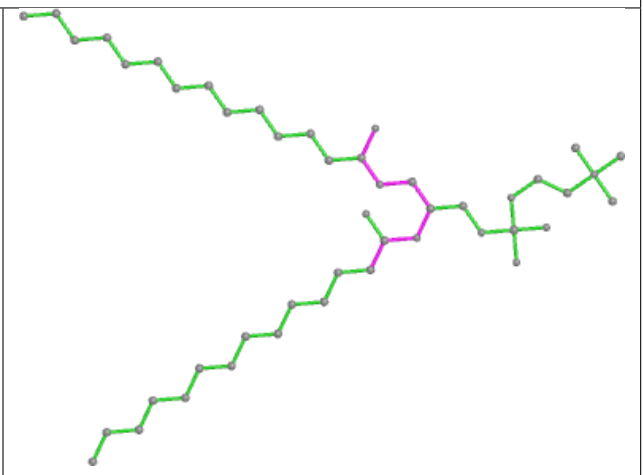


Rings

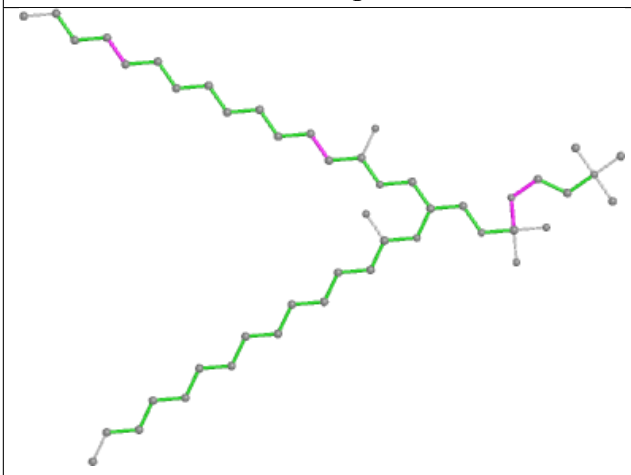
Ligand PX4 C 357



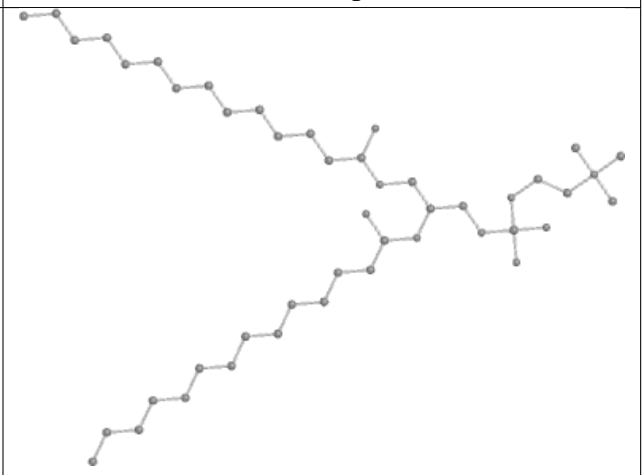
Bond lengths



Bond angles

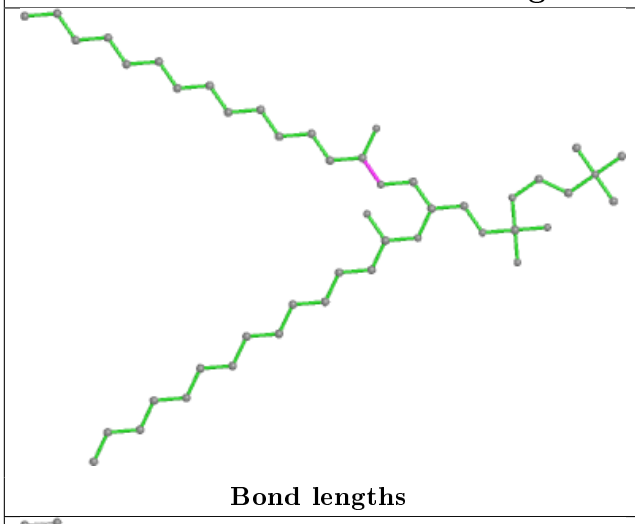


Torsions

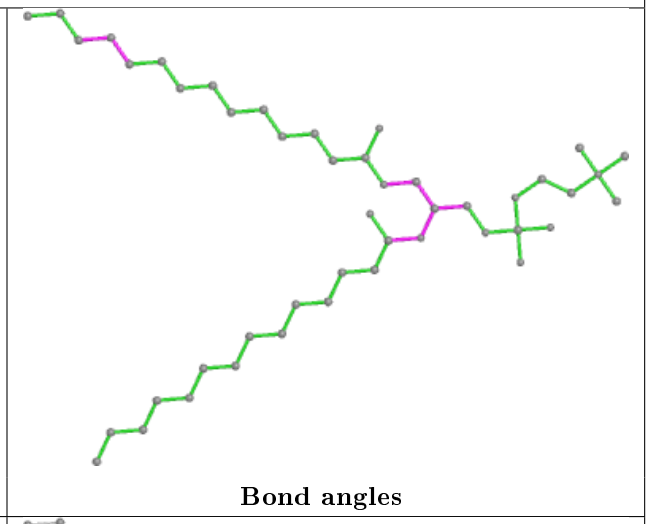


Rings

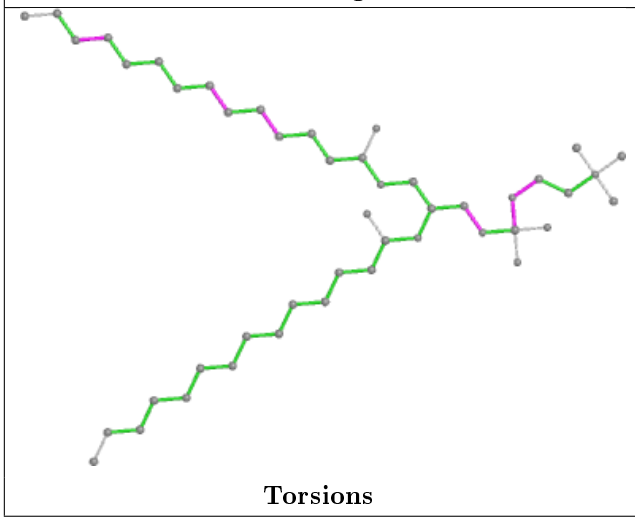
Ligand PX4 C 318



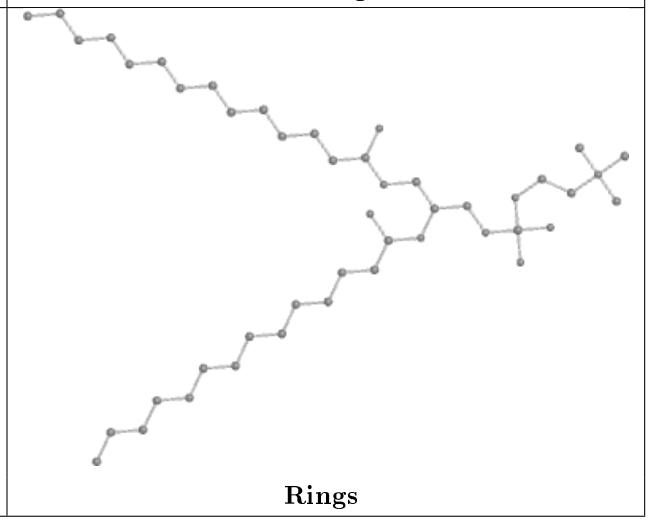
Bond lengths



Bond angles

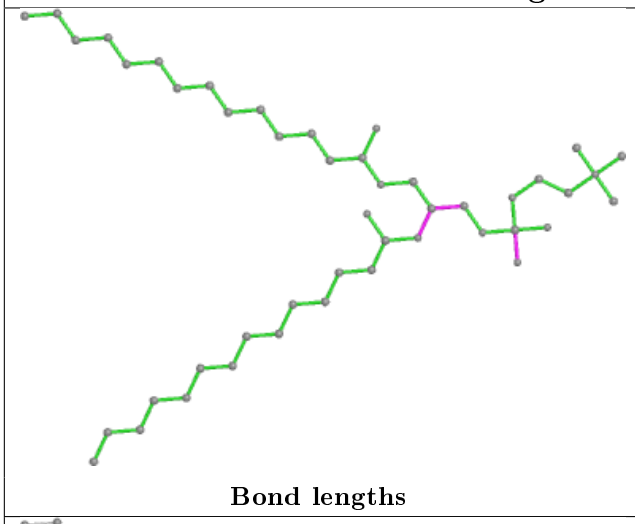


Torsions

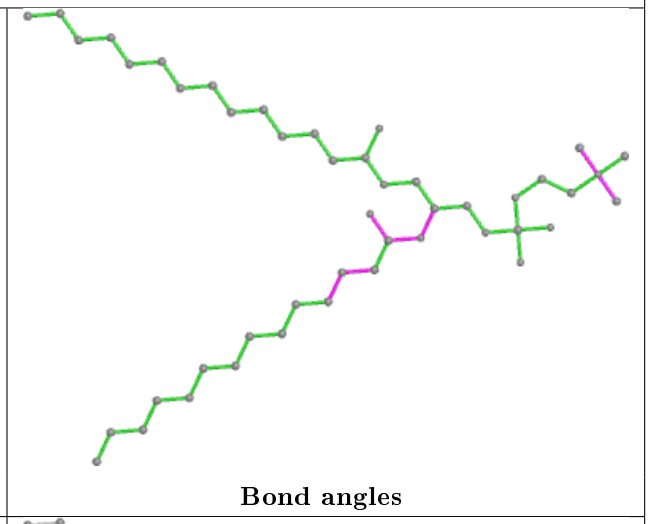


Rings

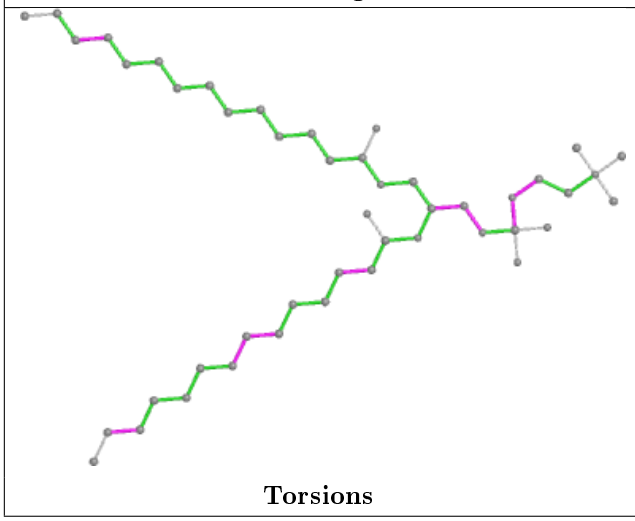
Ligand PX4 B 378



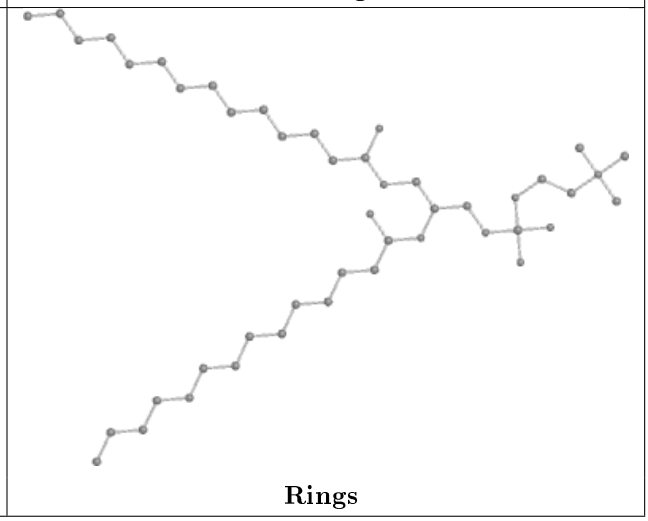
Bond lengths



Bond angles

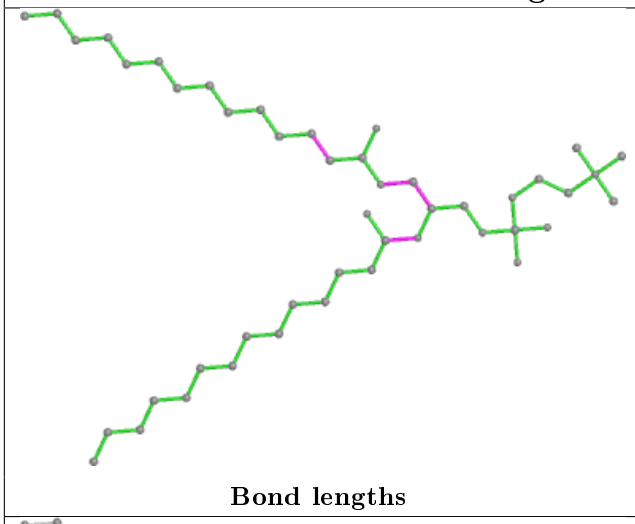


Torsions

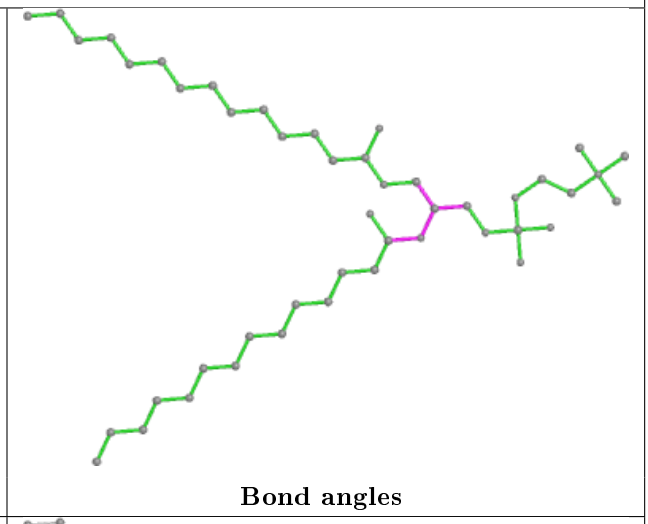


Rings

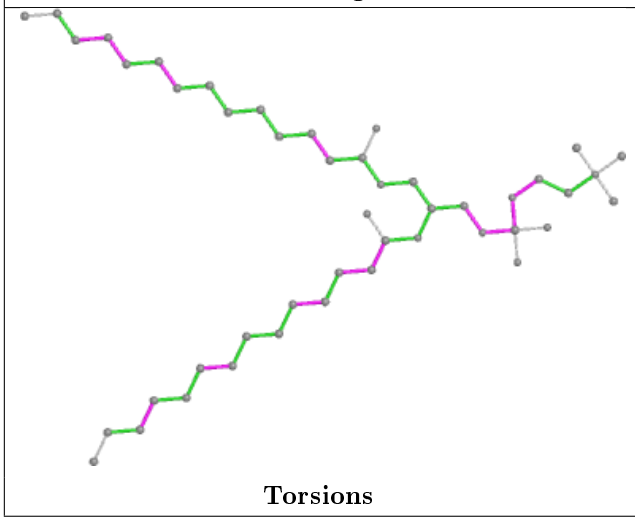
Ligand PX4 C 329



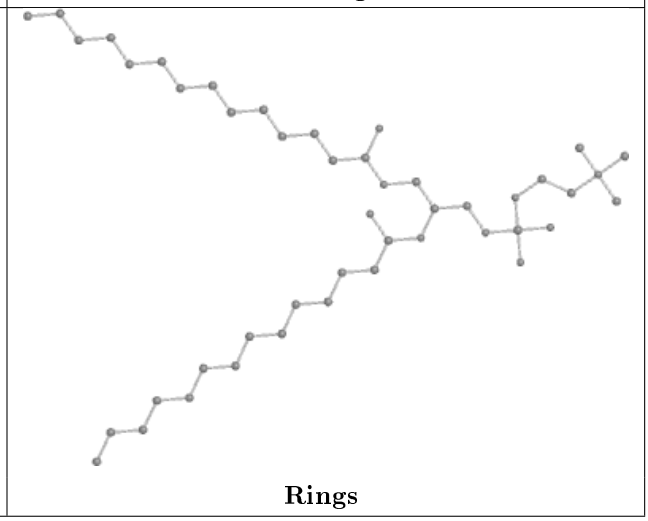
Bond lengths



Bond angles

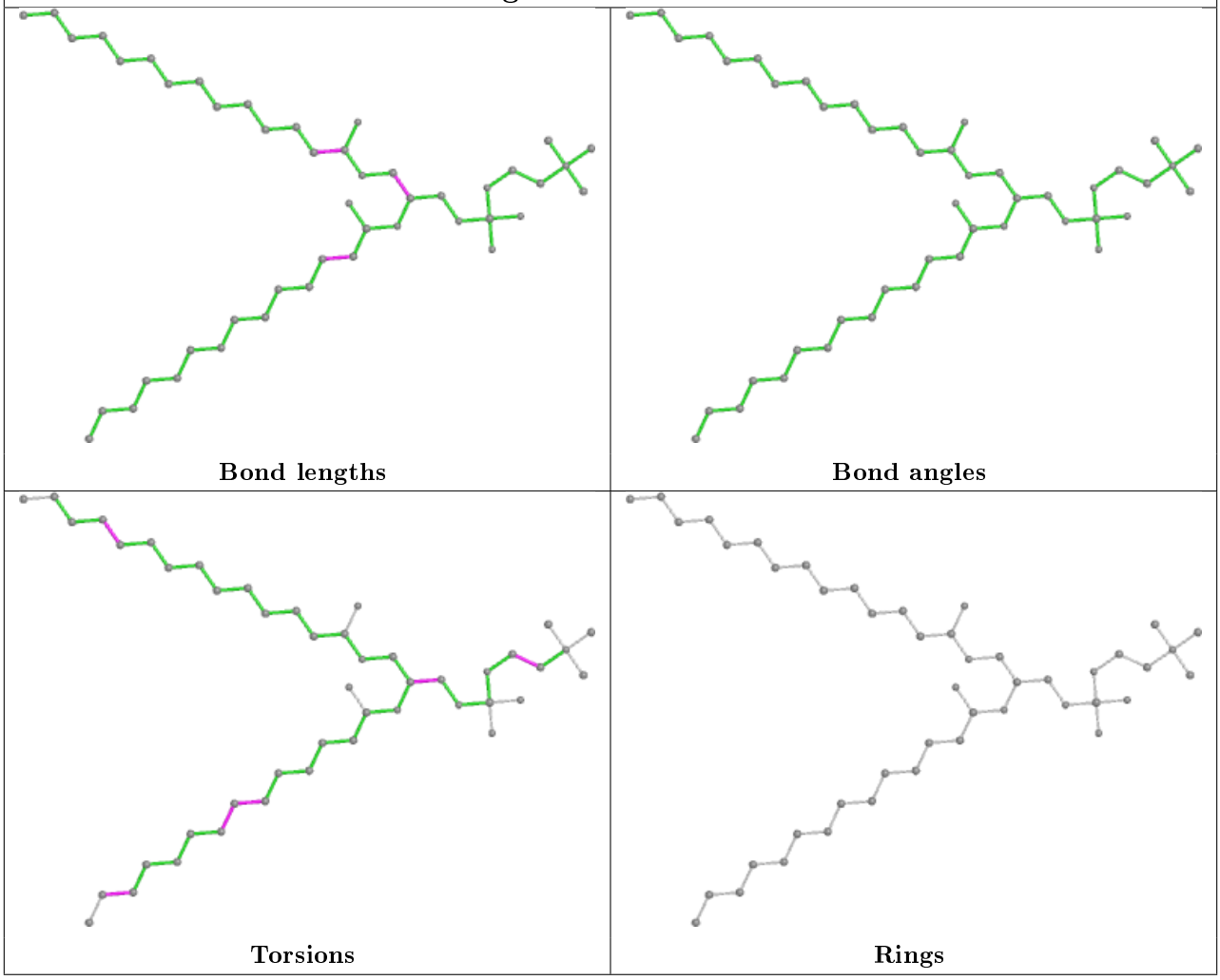


Torsions

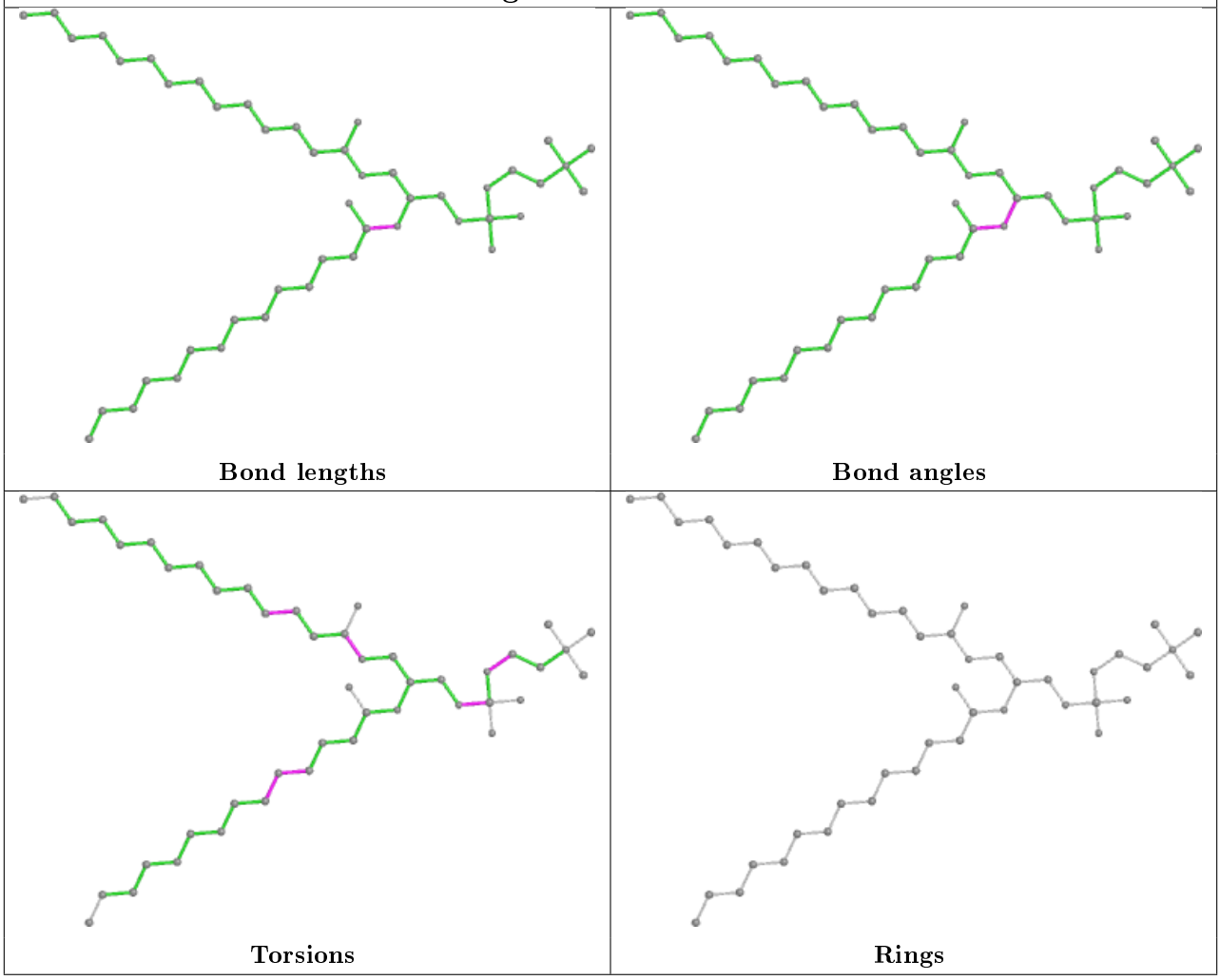


Rings

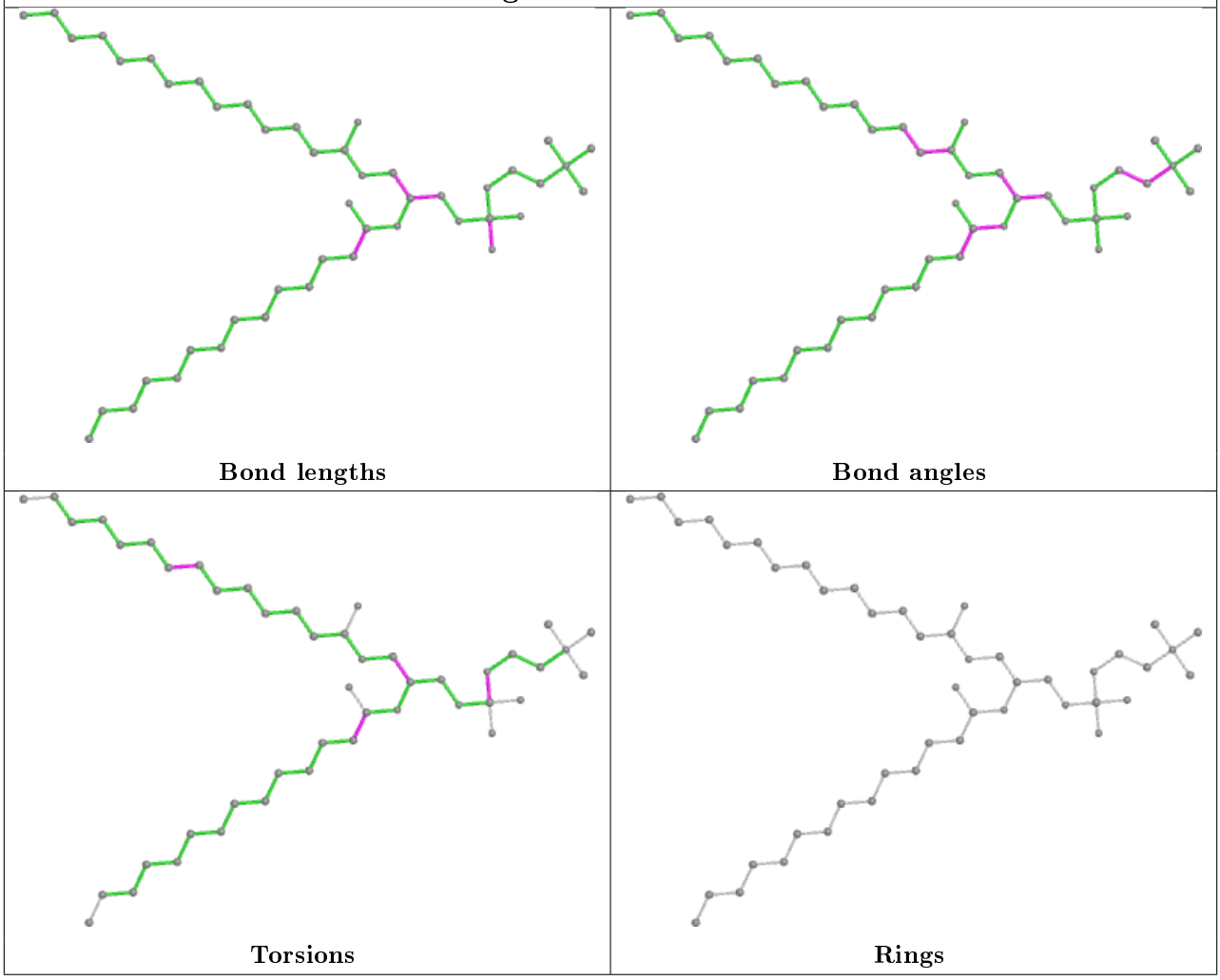
Ligand PX4 B 356



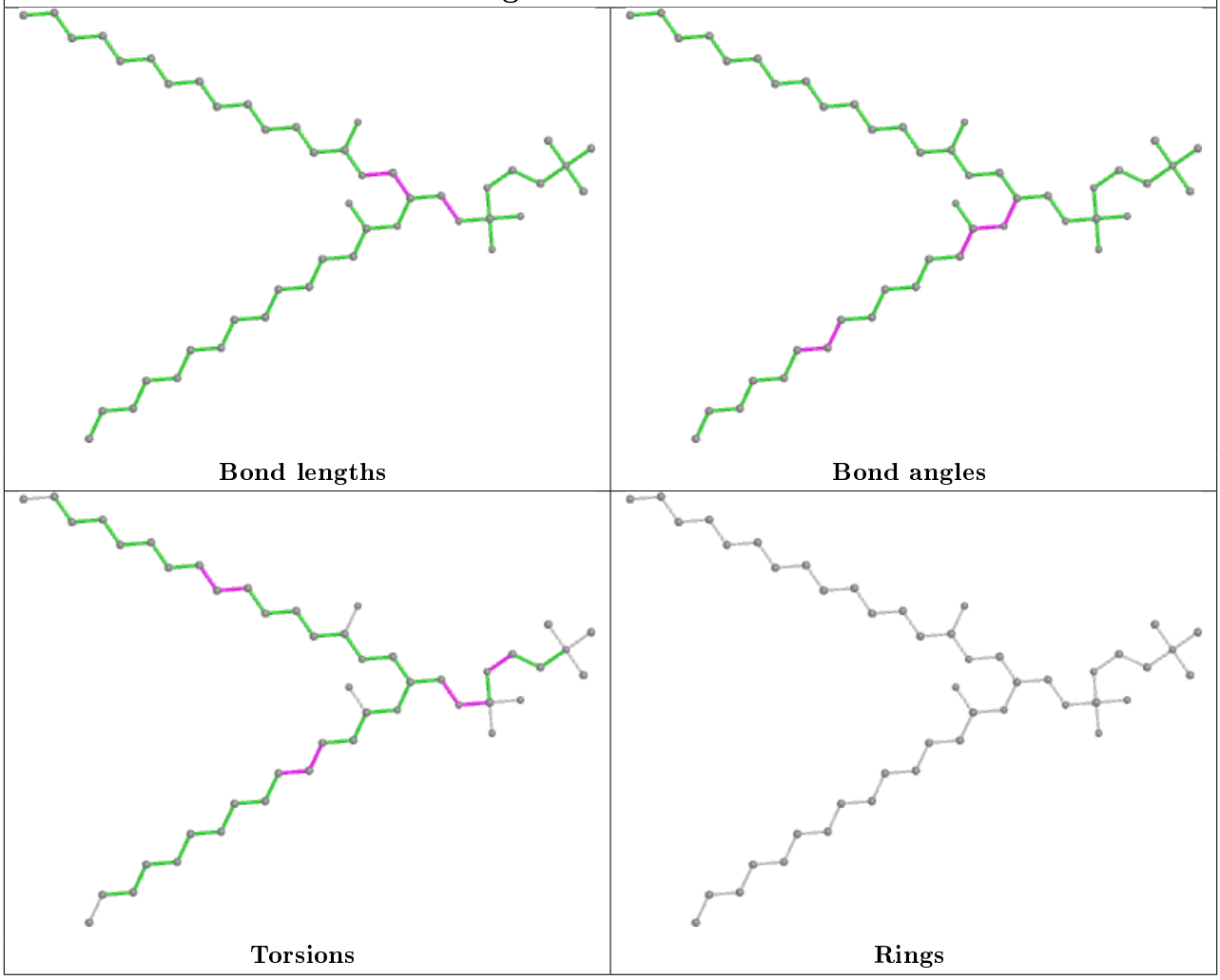
Ligand PX4 C 358



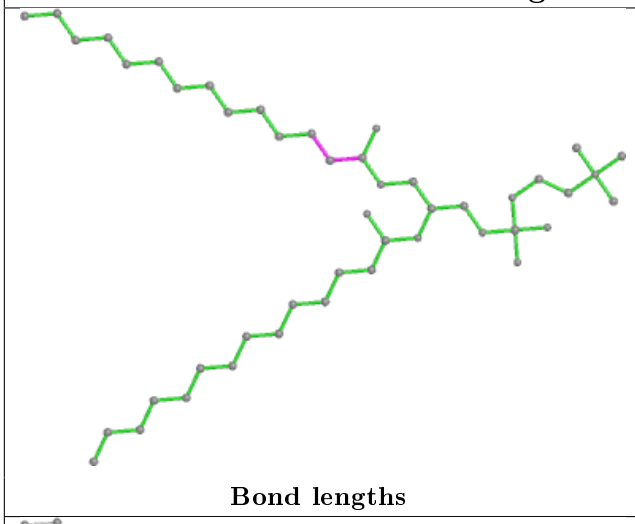
Ligand PX4 B 348



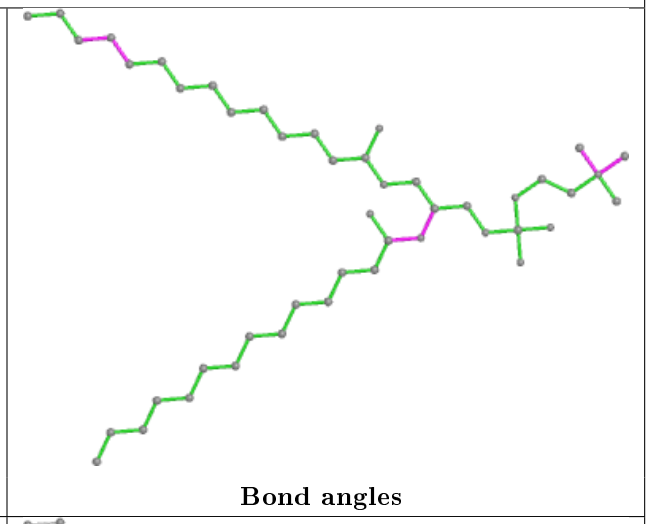
Ligand PX4 B 368



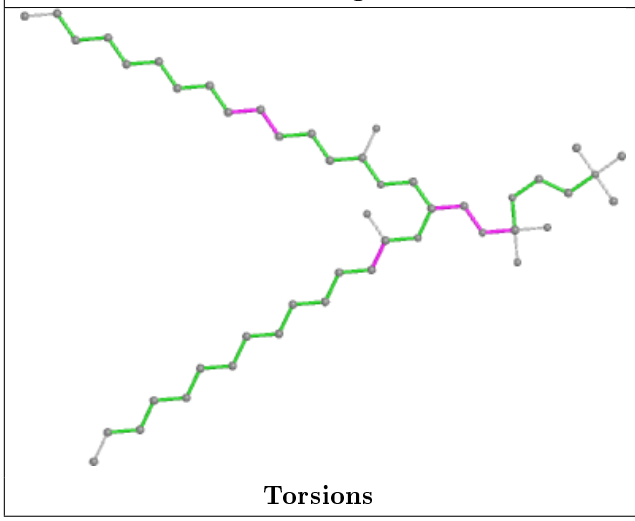
Ligand PX4 B 318



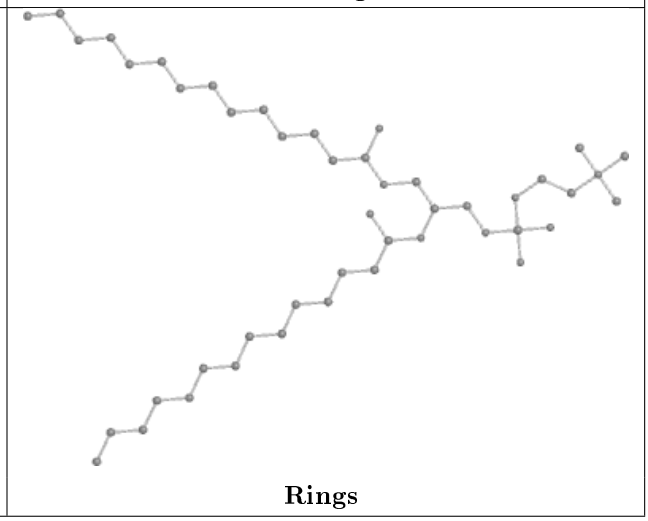
Bond lengths



Bond angles

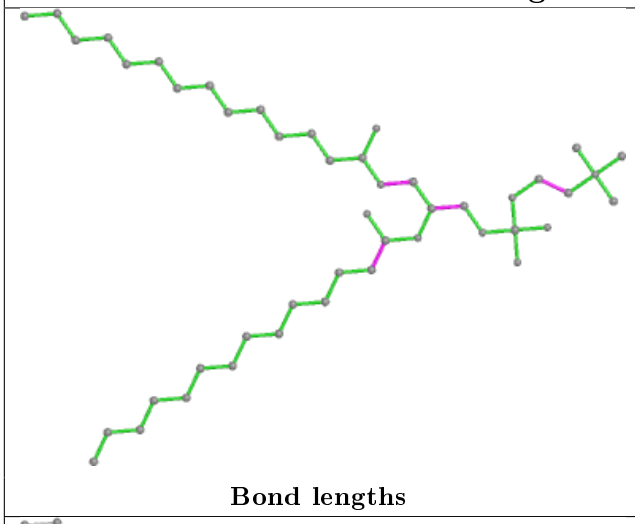


Torsions

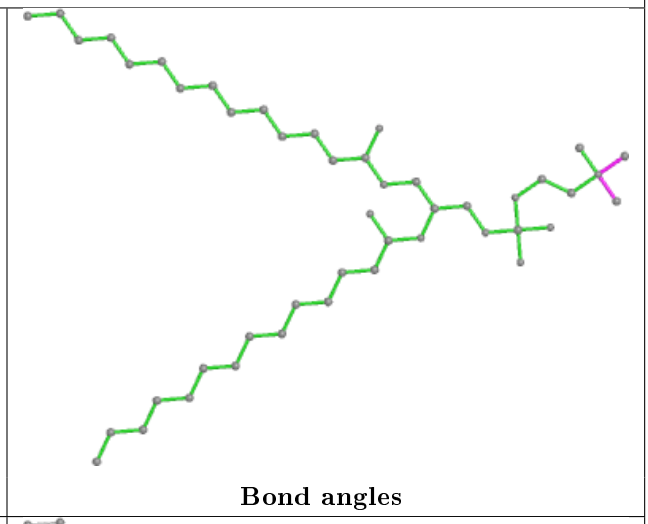


Rings

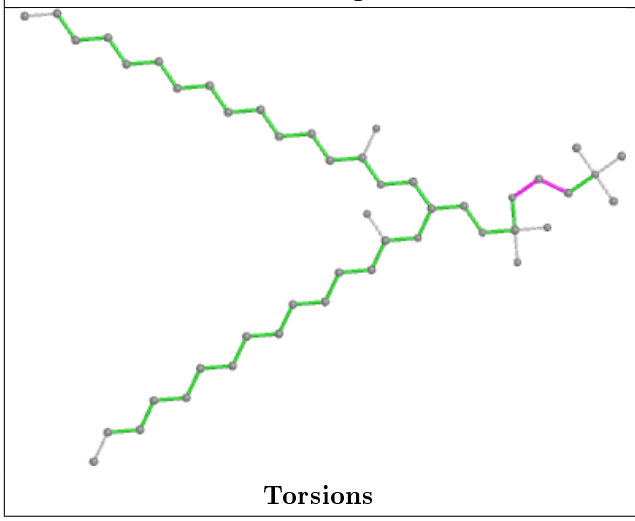
Ligand PX4 C 365



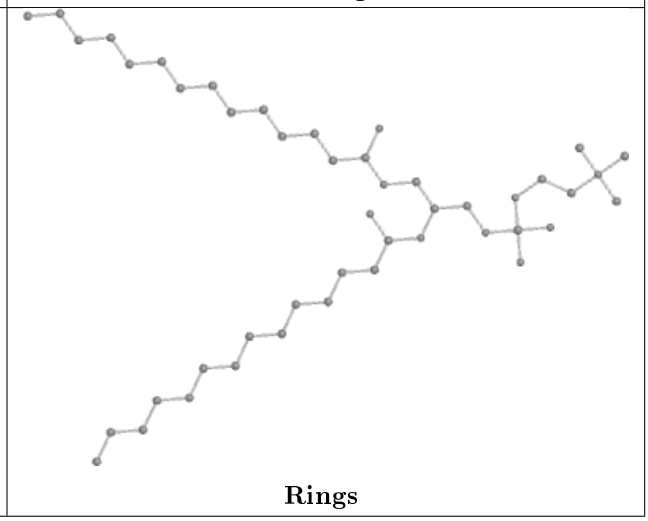
Bond lengths



Bond angles

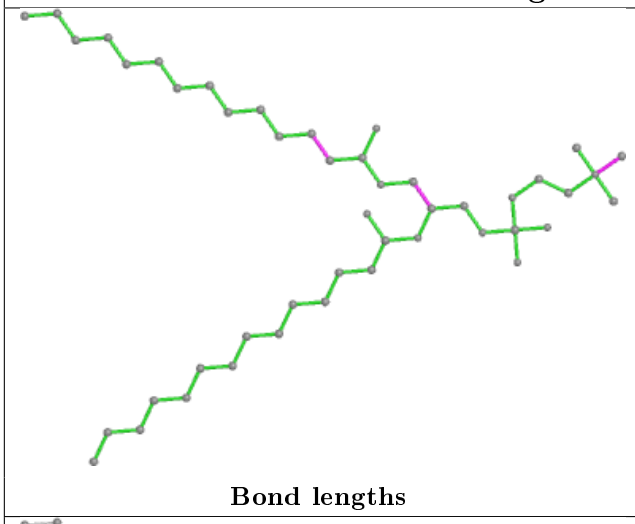


Torsions

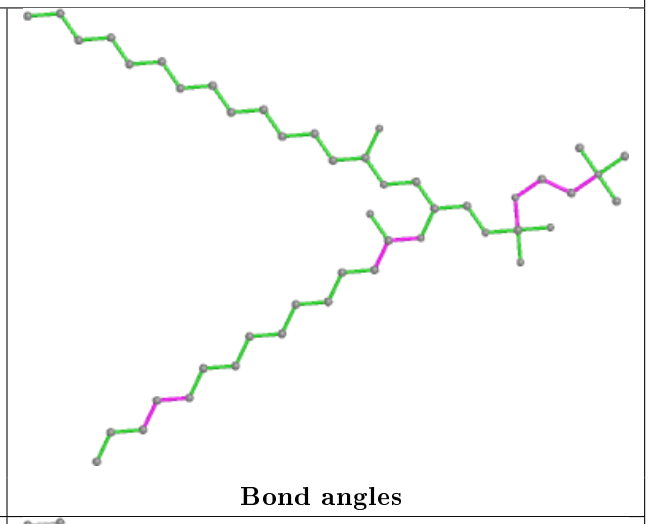


Rings

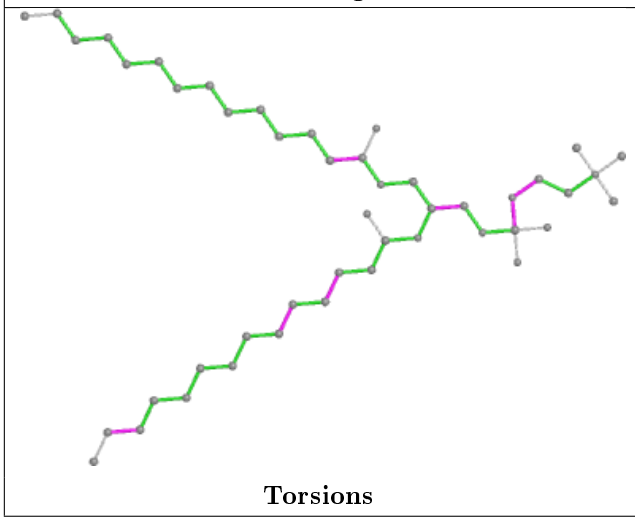
Ligand PX4 C 346



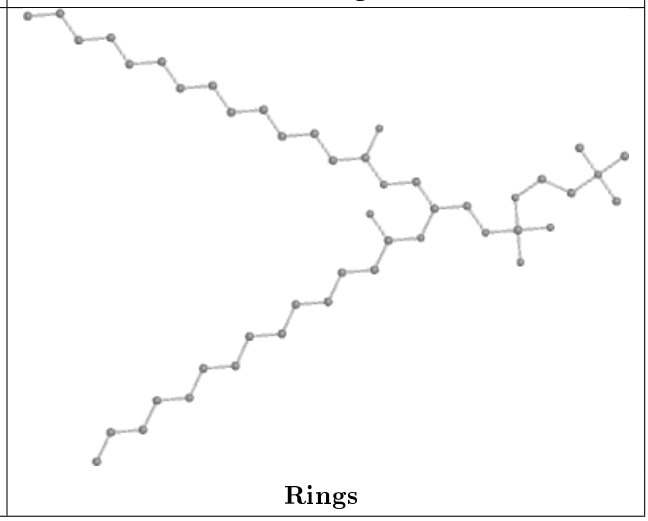
Bond lengths



Bond angles

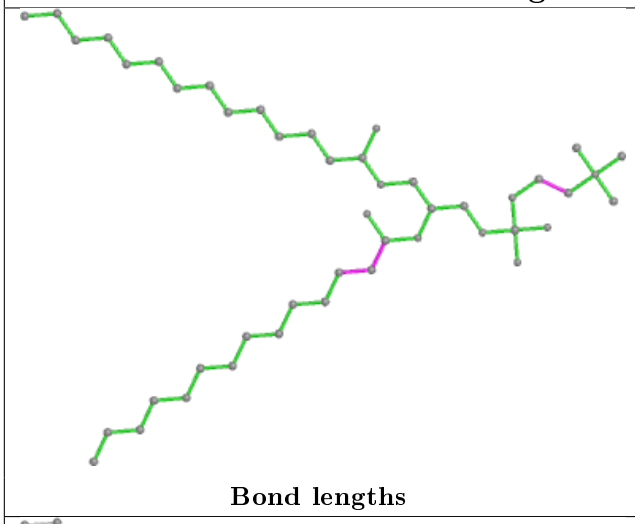


Torsions

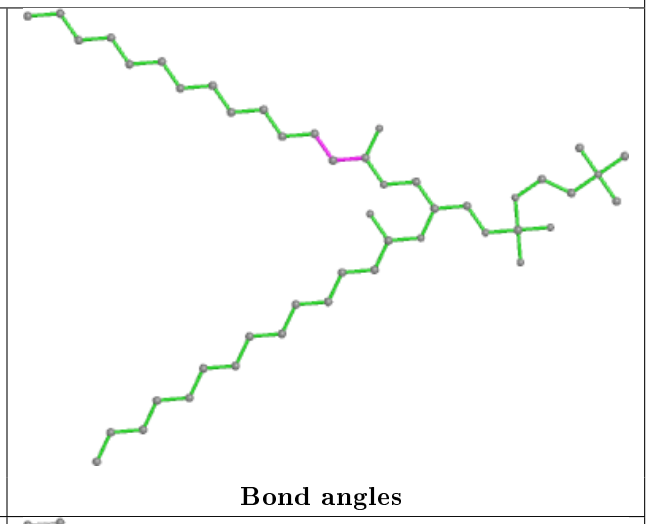


Rings

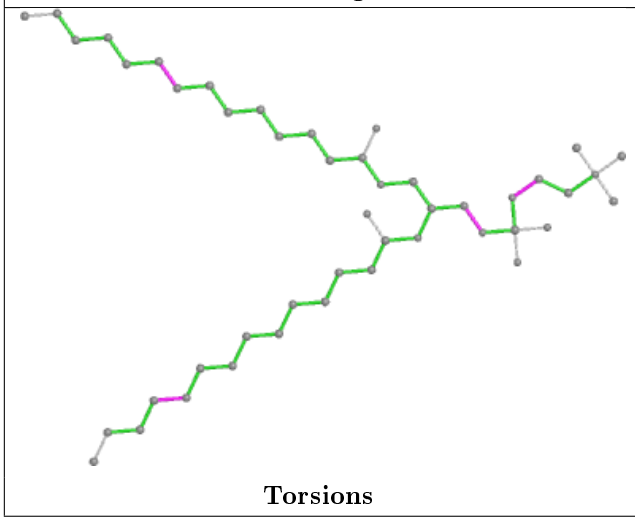
Ligand PX4 C 326



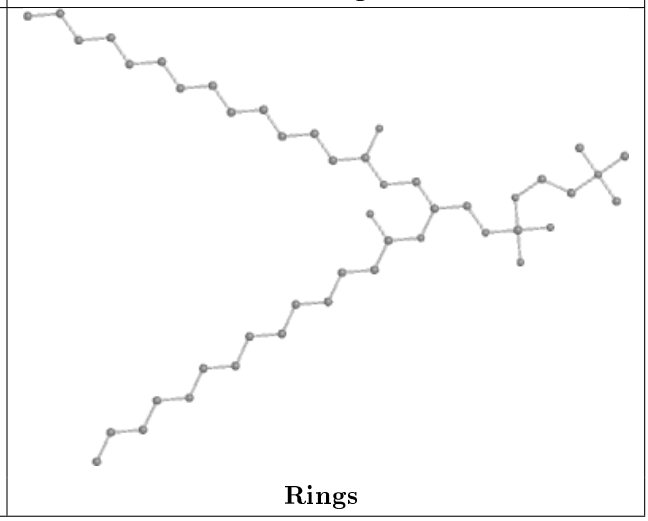
Bond lengths



Bond angles

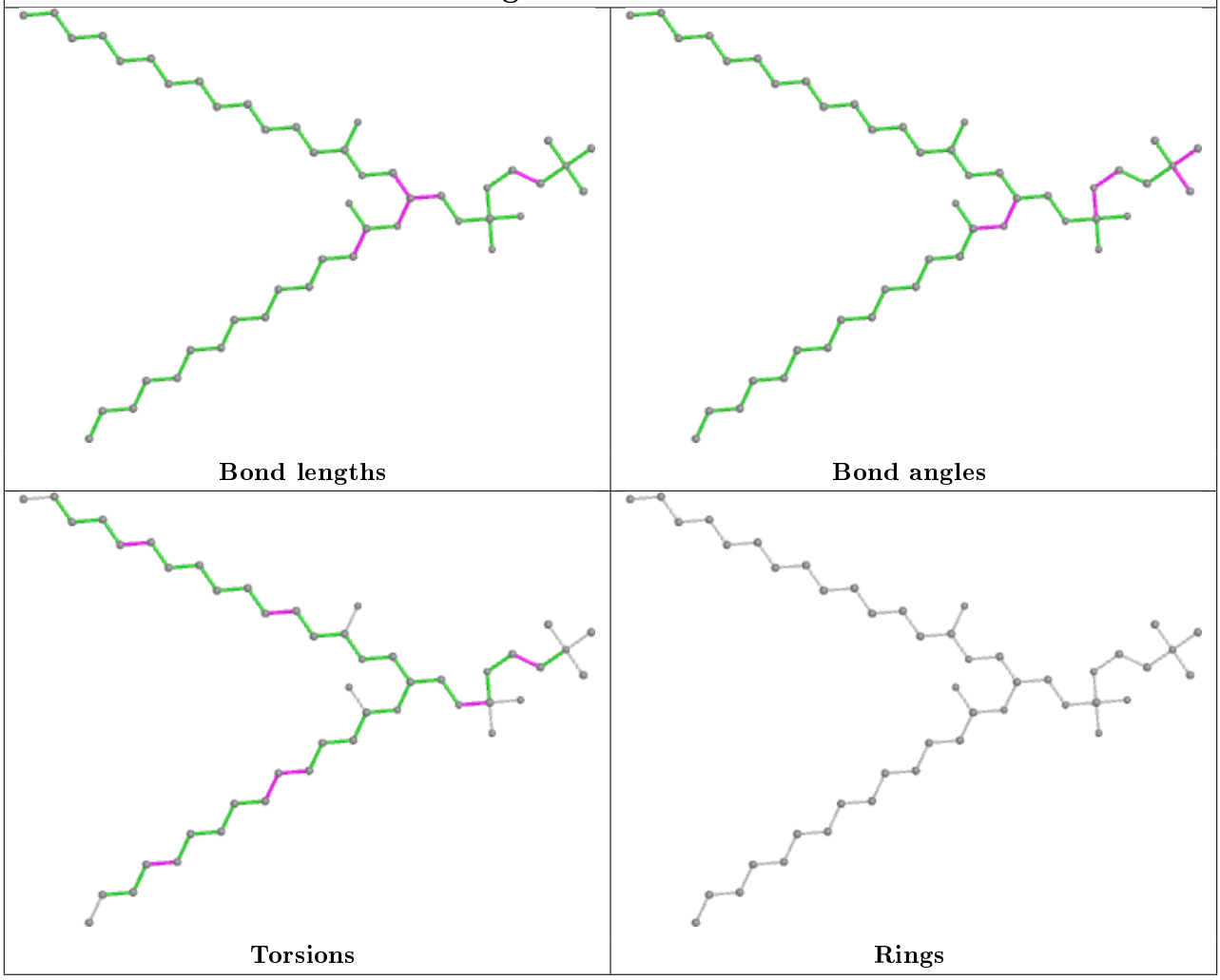


Torsions

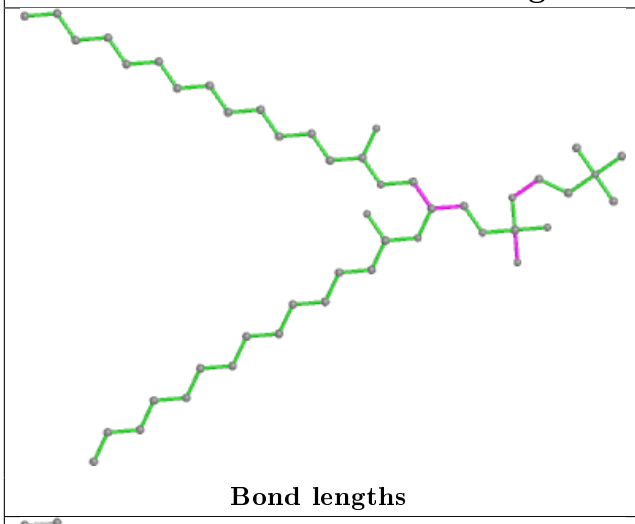


Rings

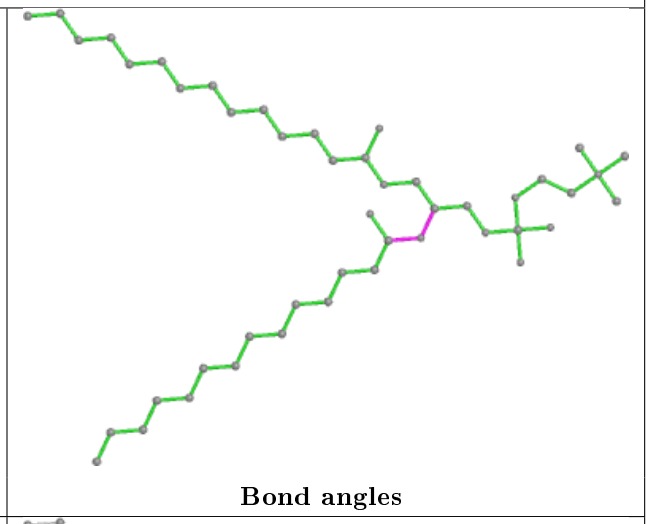
Ligand PX4 B 327



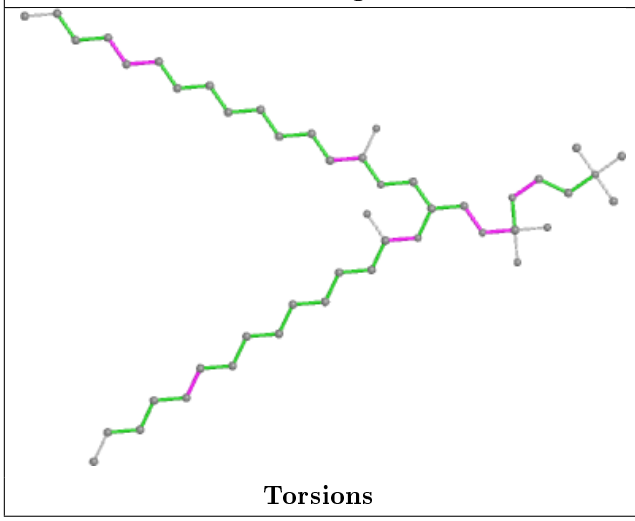
Ligand PX4 B 399



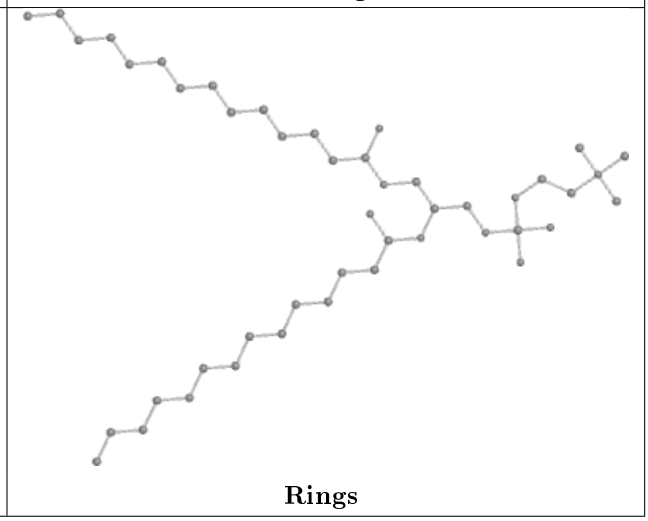
Bond lengths



Bond angles

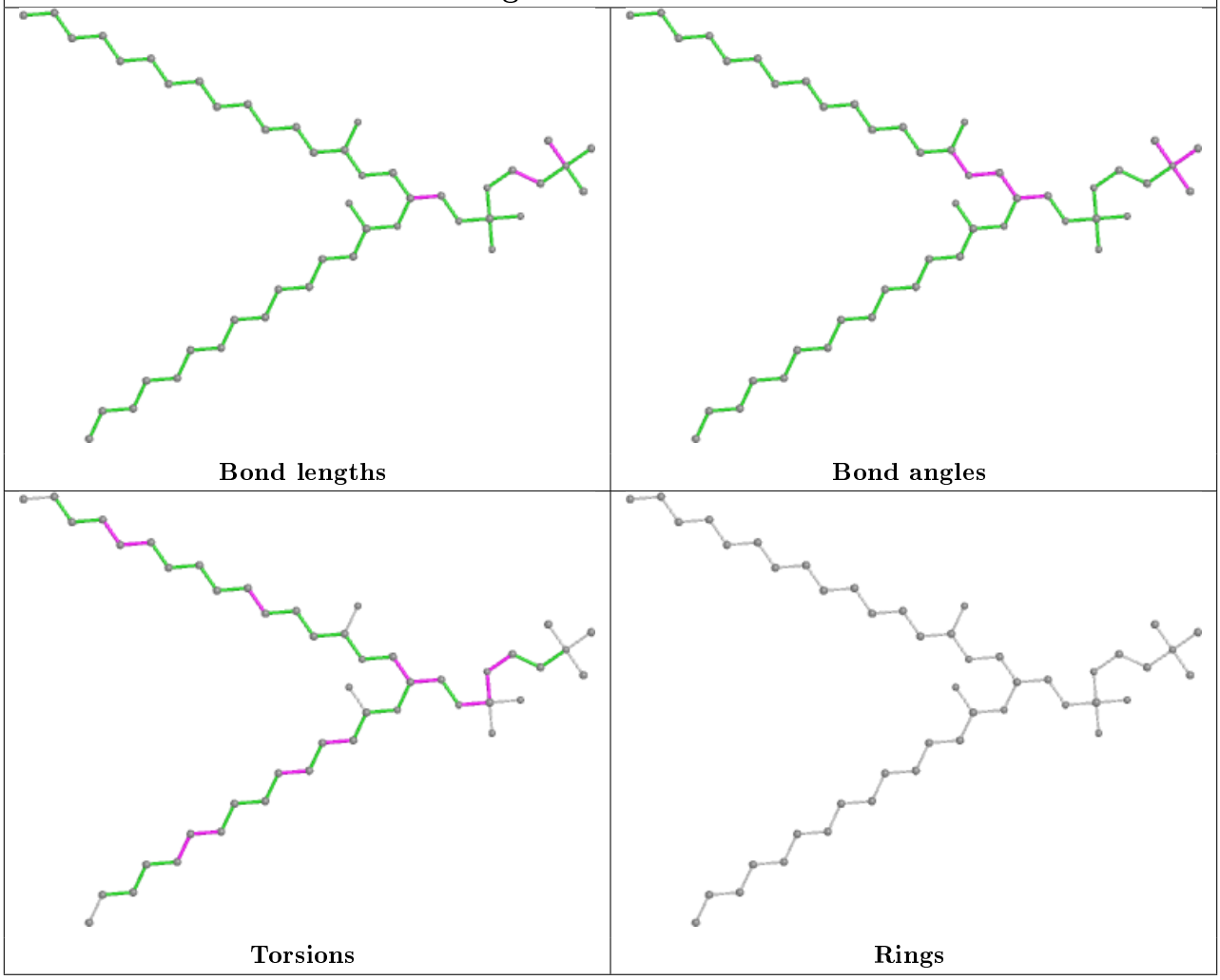


Torsions

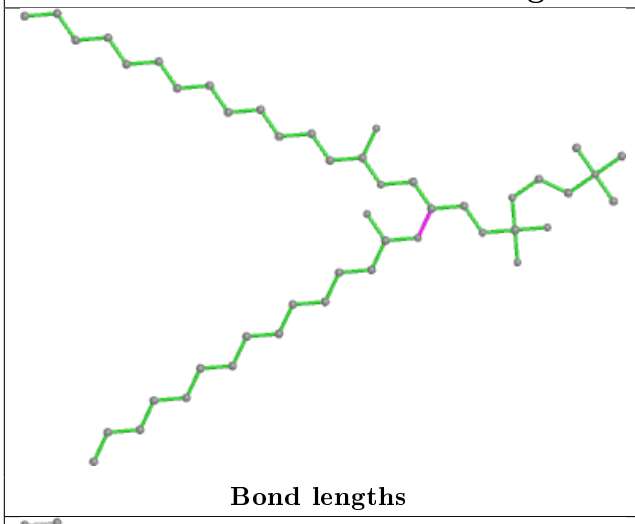


Rings

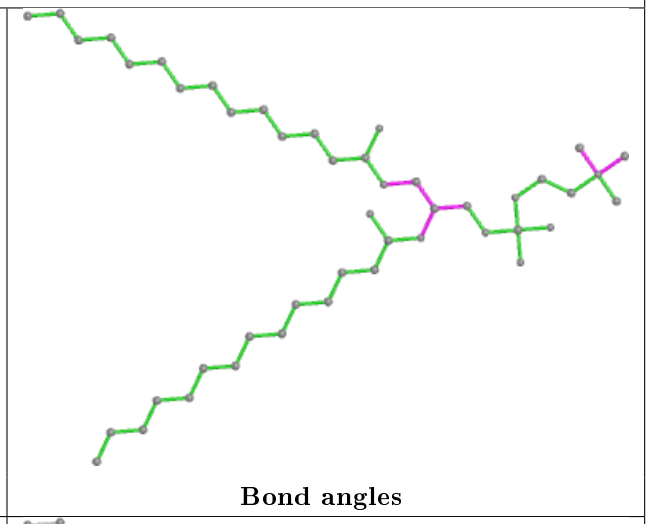
Ligand PX4 B 359



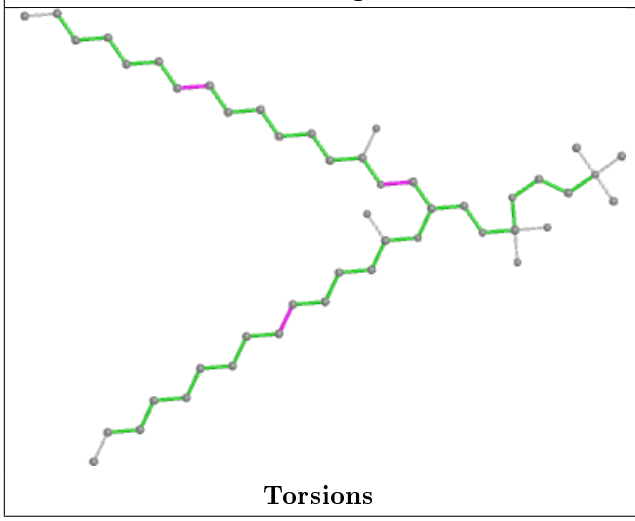
Ligand PX4 A 637



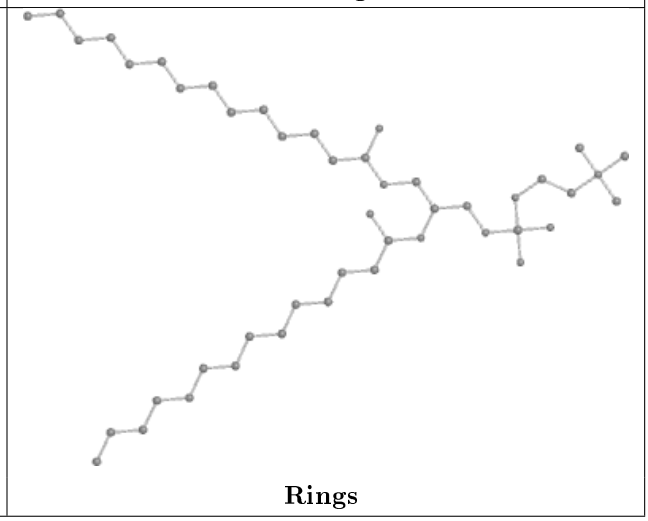
Bond lengths



Bond angles

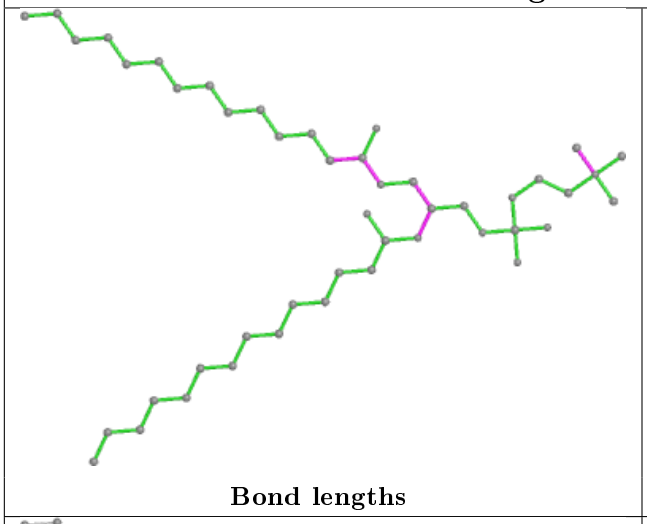


Torsions

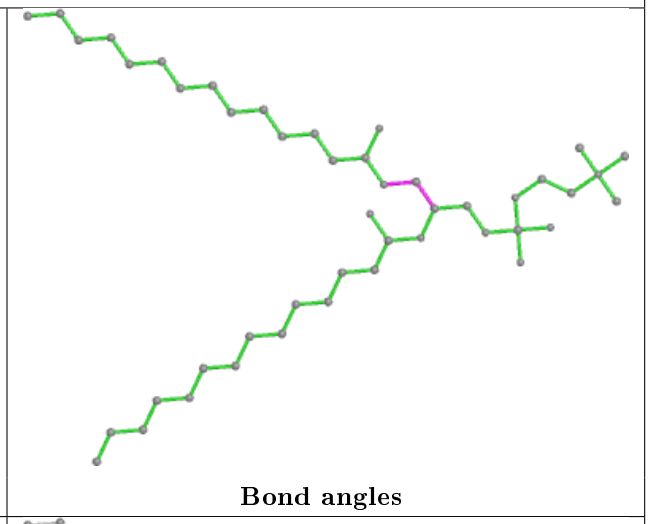


Rings

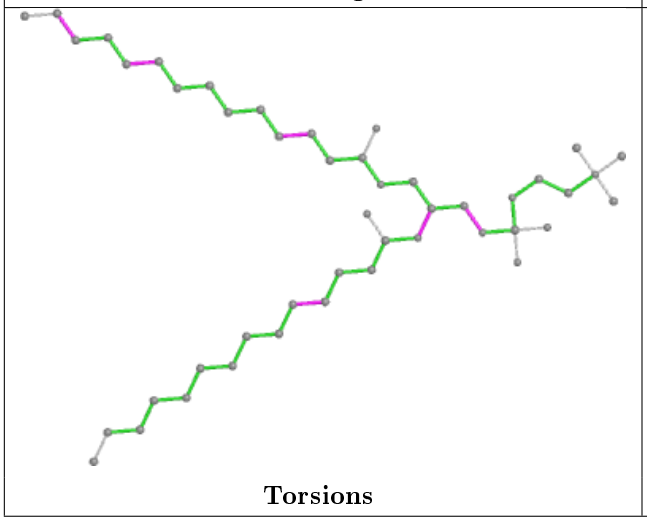
Ligand PX4 B 396



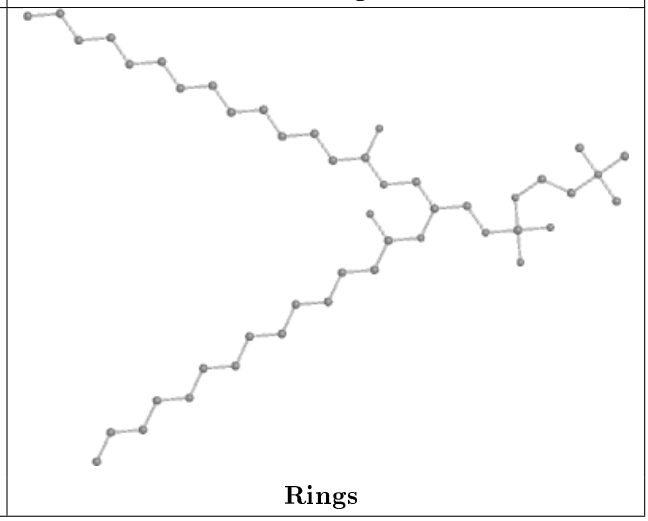
Bond lengths



Bond angles

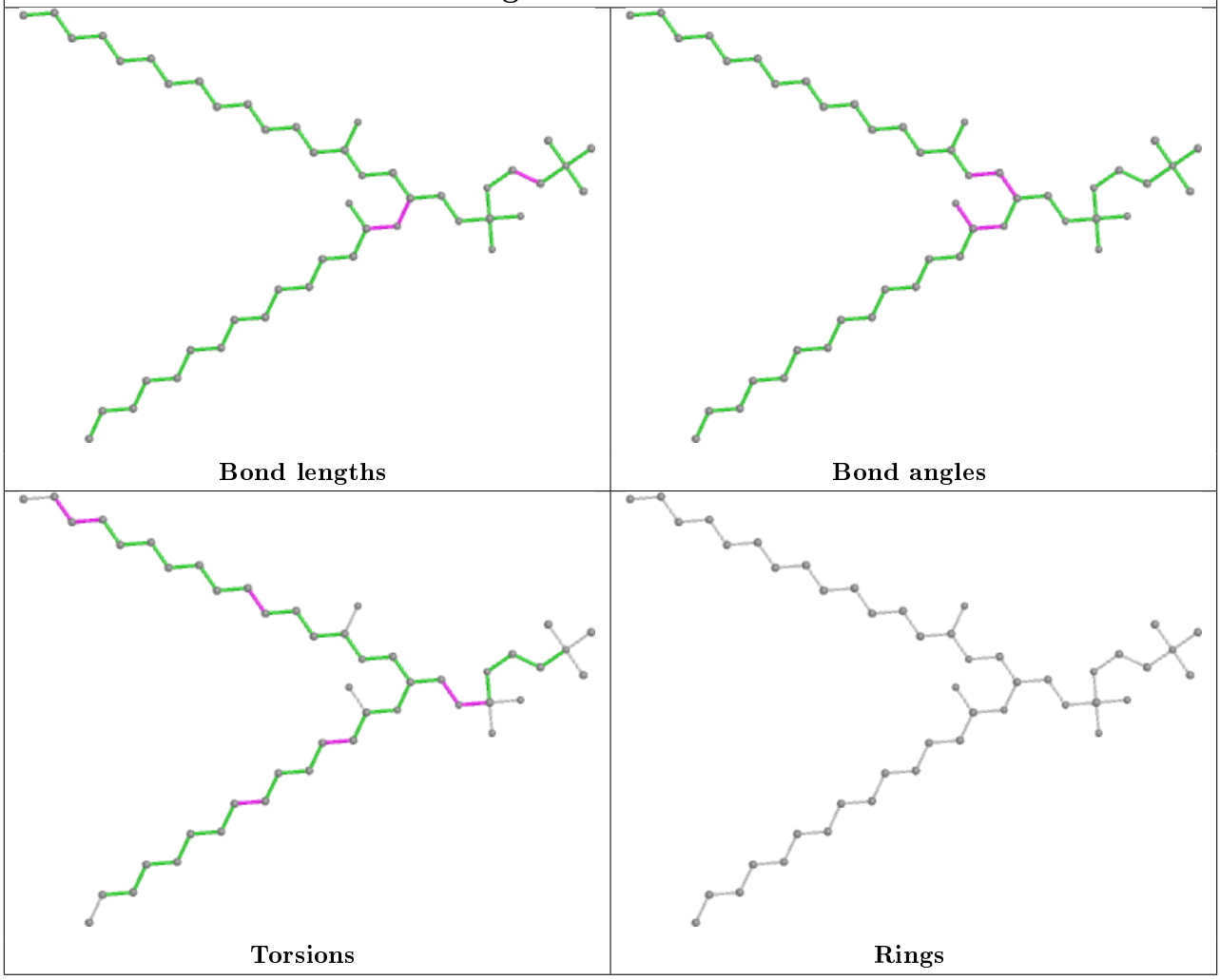


Torsions

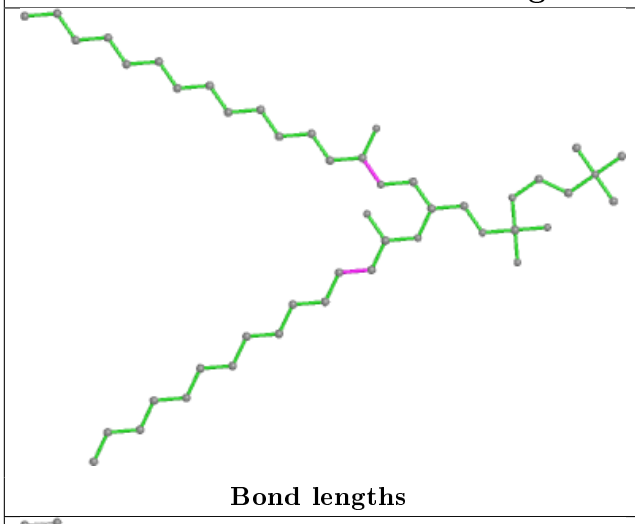


Rings

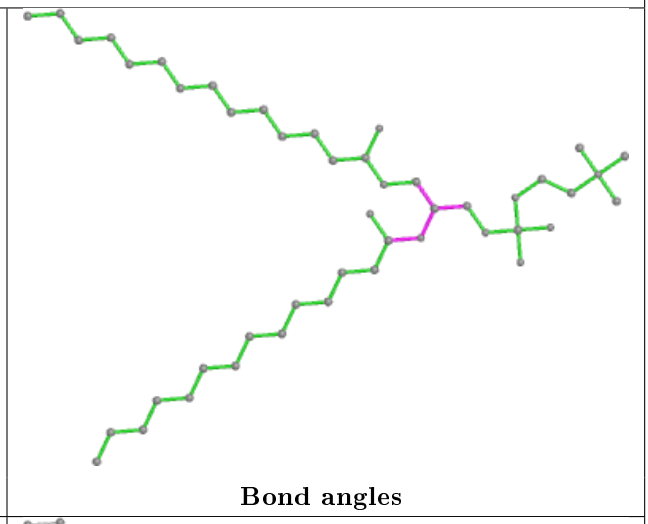
Ligand PX4 C 348



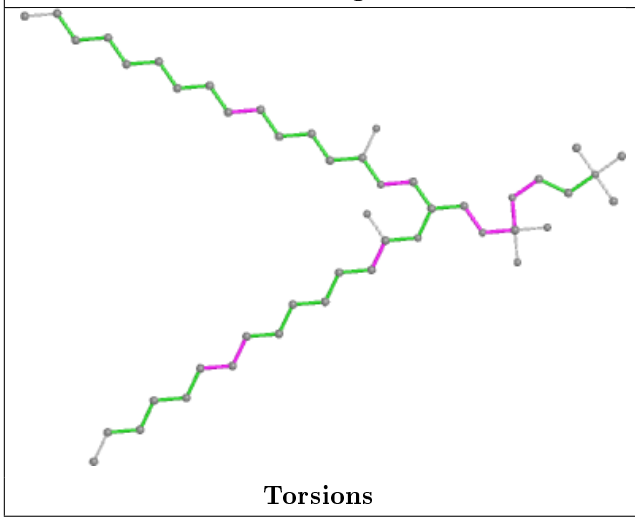
Ligand PX4 C 334



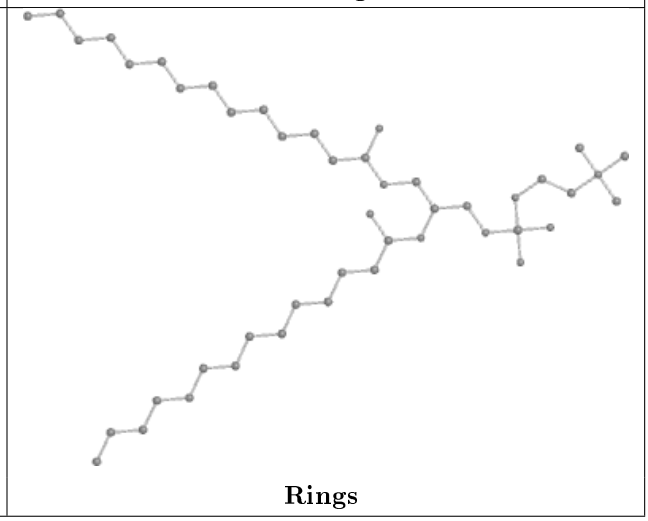
Bond lengths



Bond angles

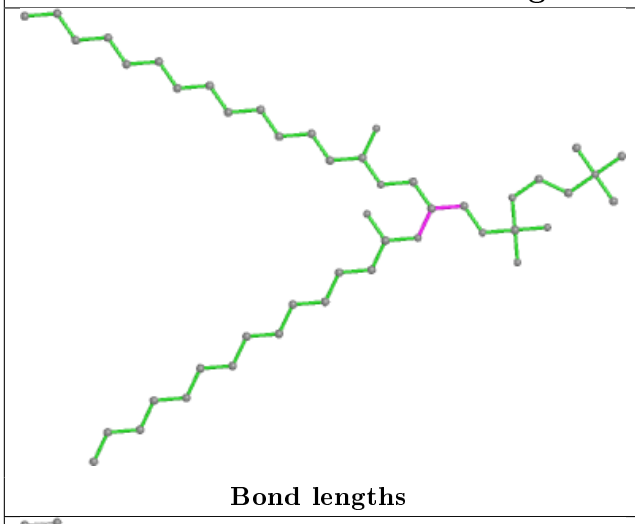


Torsions

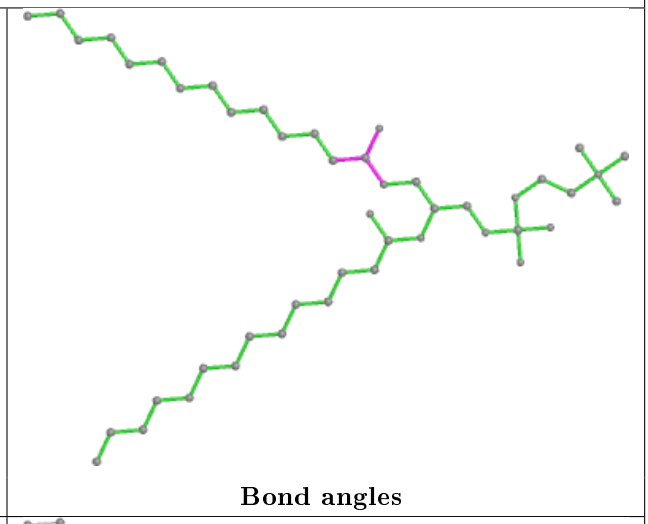


Rings

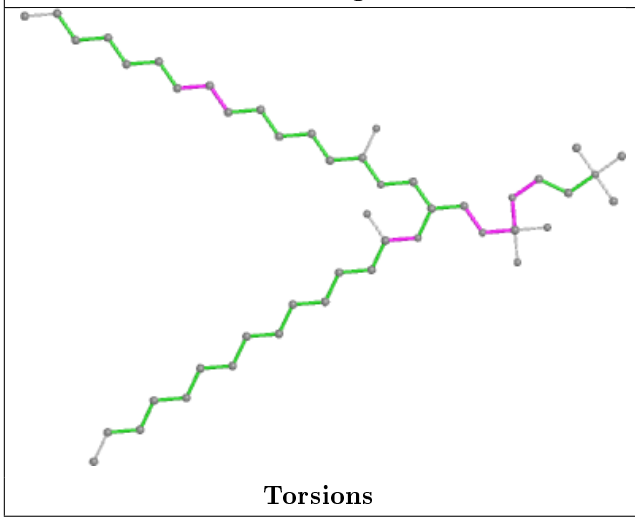
Ligand PX4 B 397



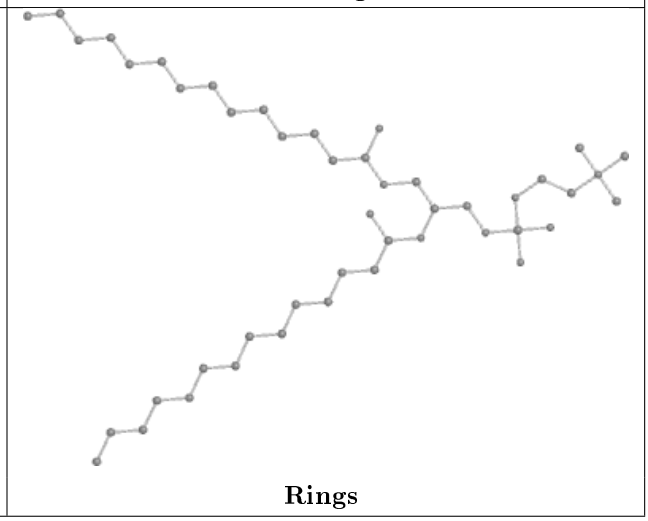
Bond lengths



Bond angles

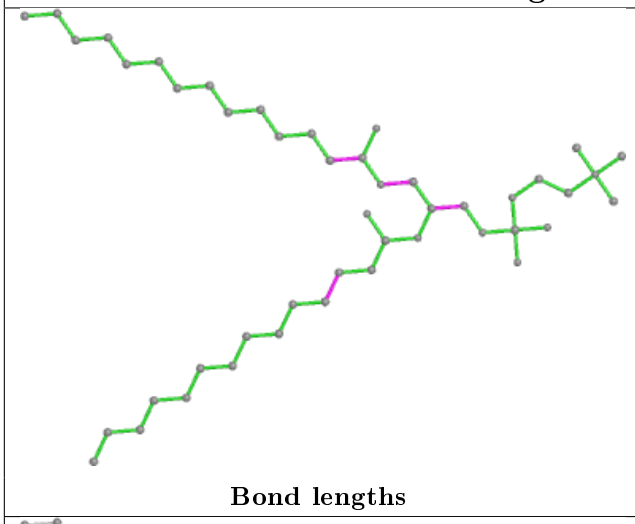


Torsions

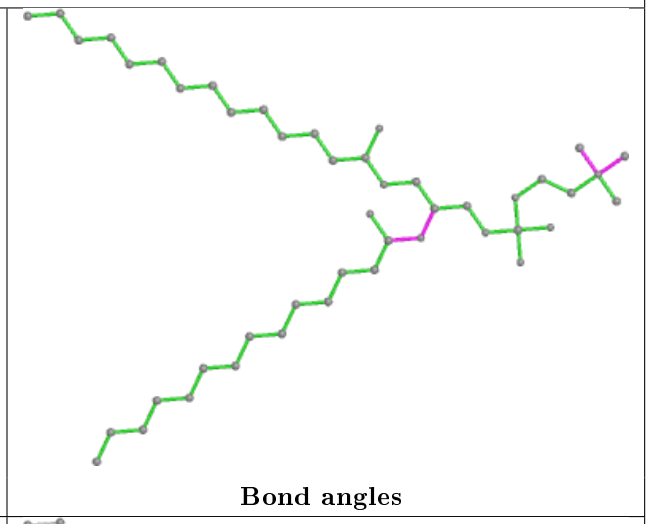


Rings

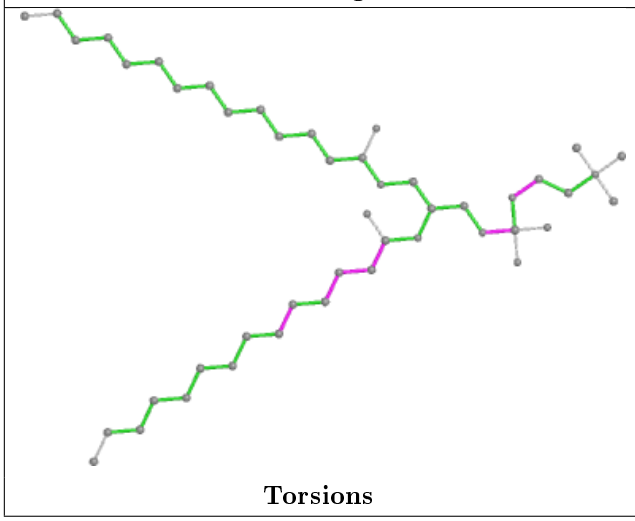
Ligand PX4 B 366



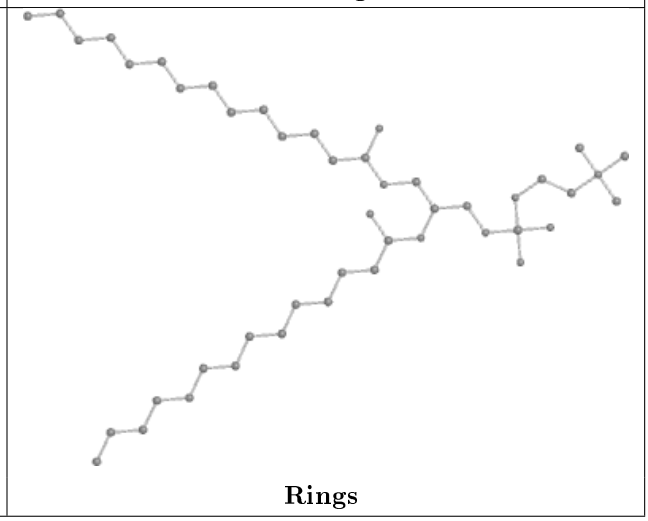
Bond lengths



Bond angles

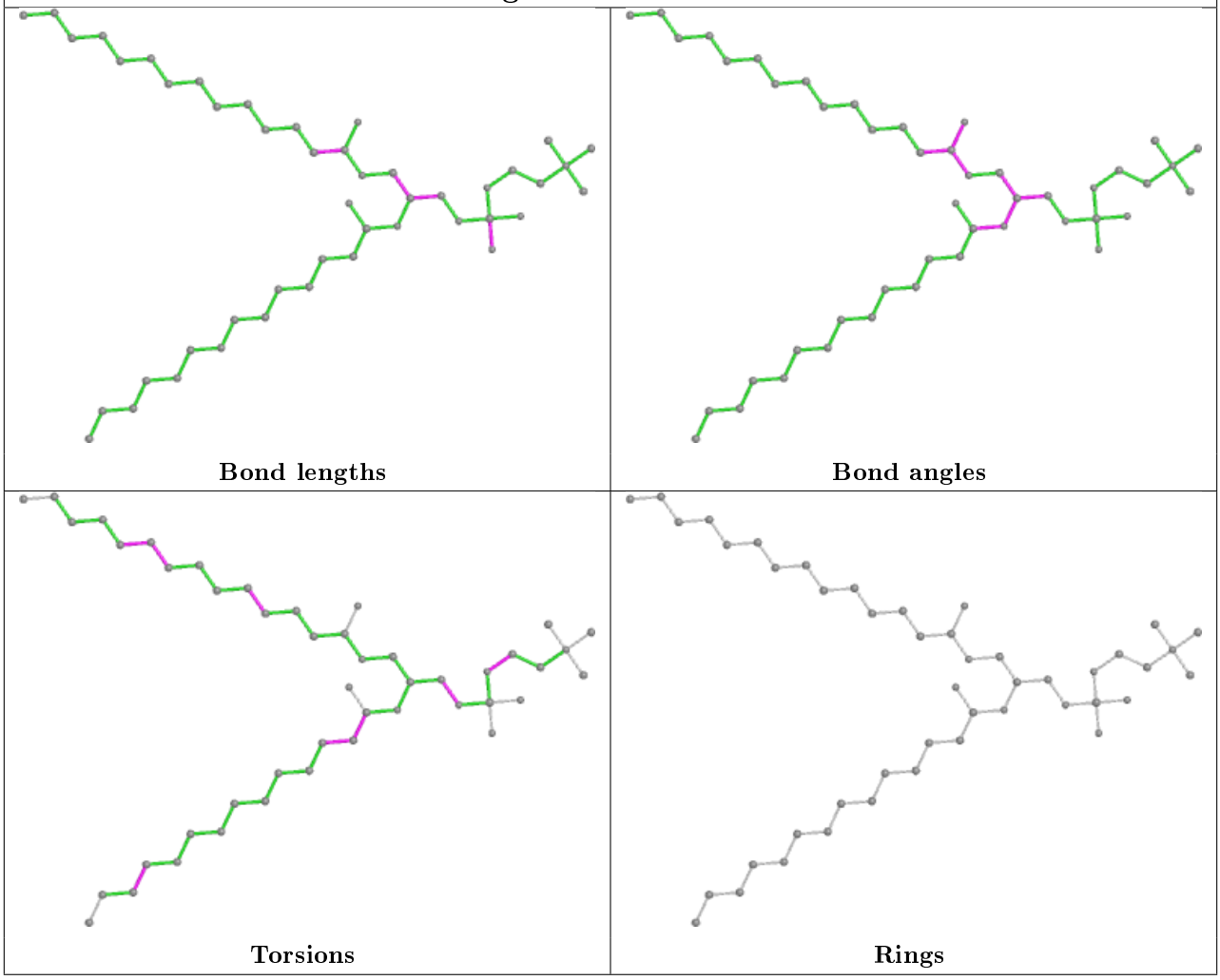


Torsions

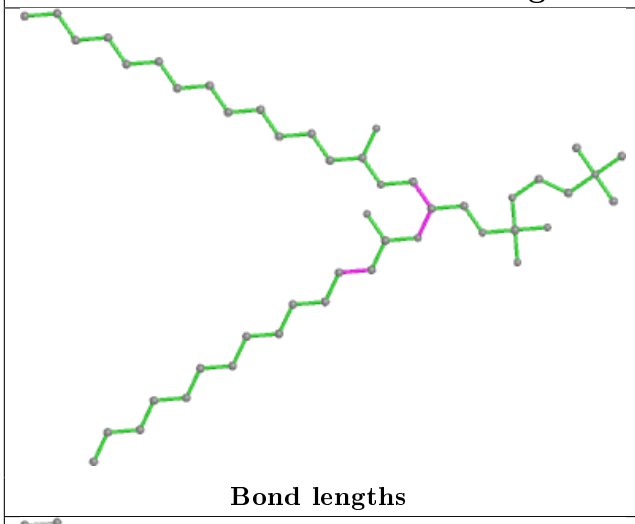


Rings

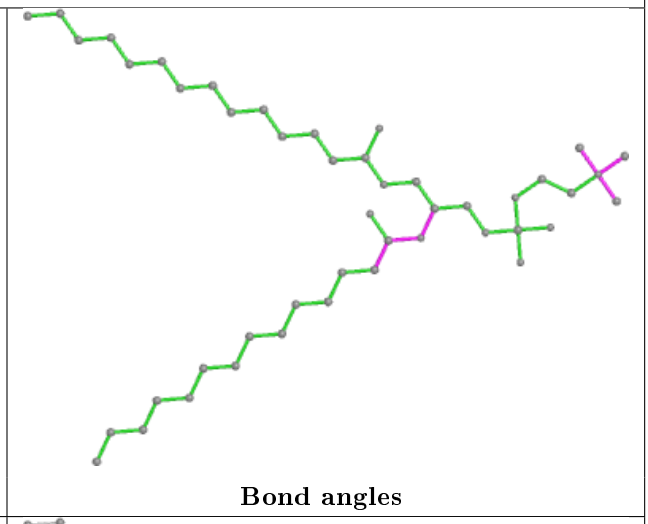
Ligand PX4 B 312



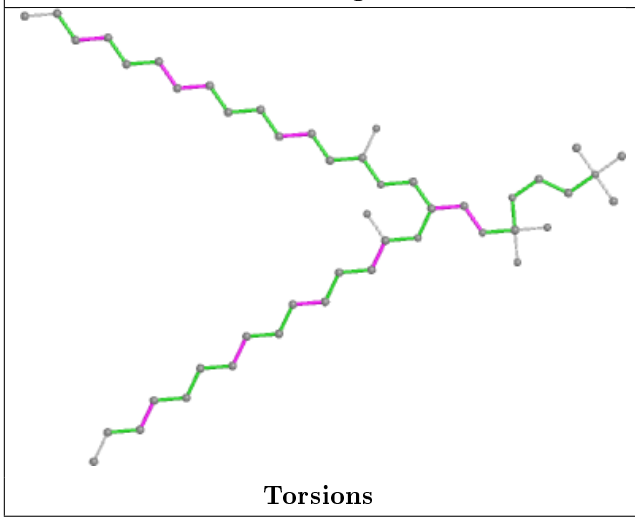
Ligand PX4 B 324



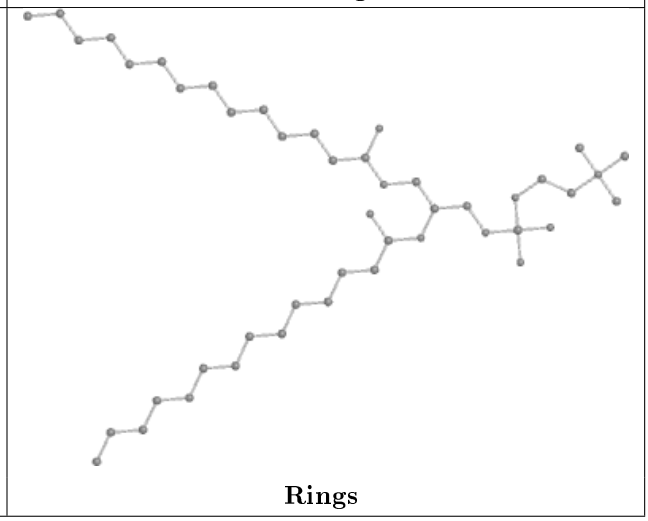
Bond lengths



Bond angles

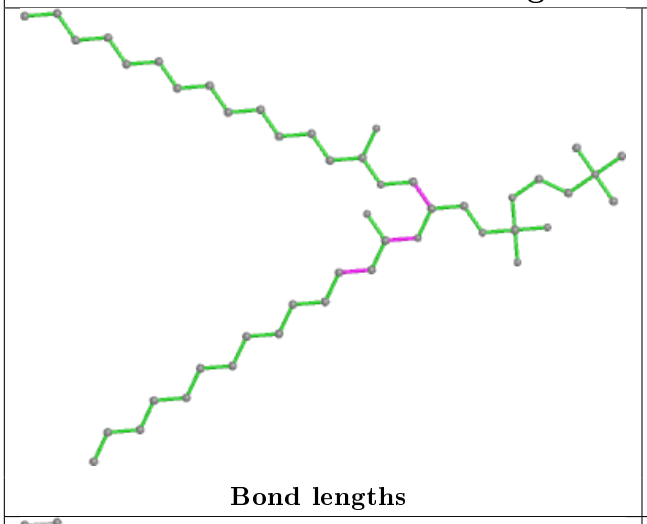


Torsions

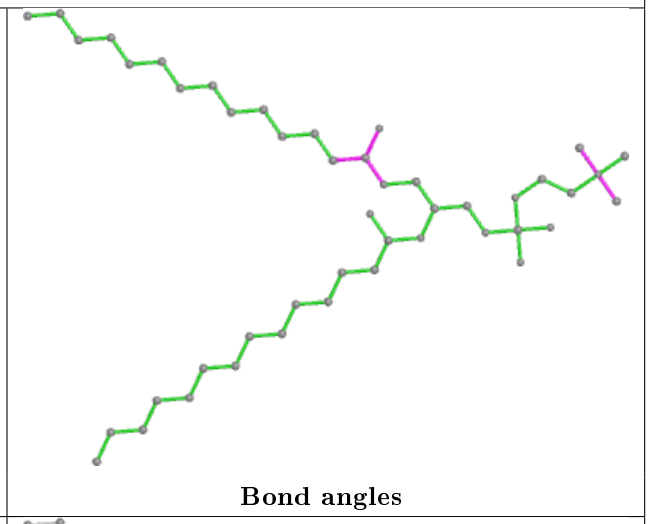


Rings

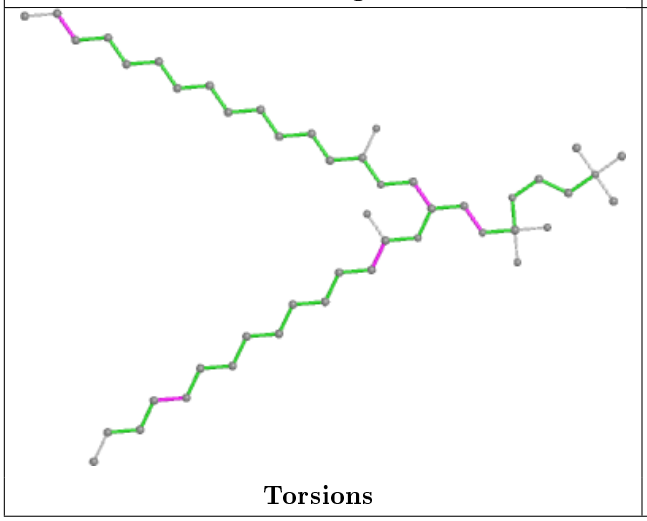
Ligand PX4 A 643



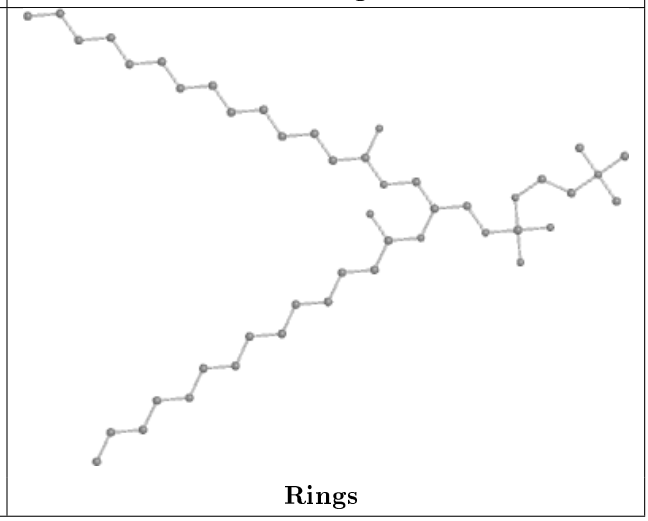
Bond lengths



Bond angles

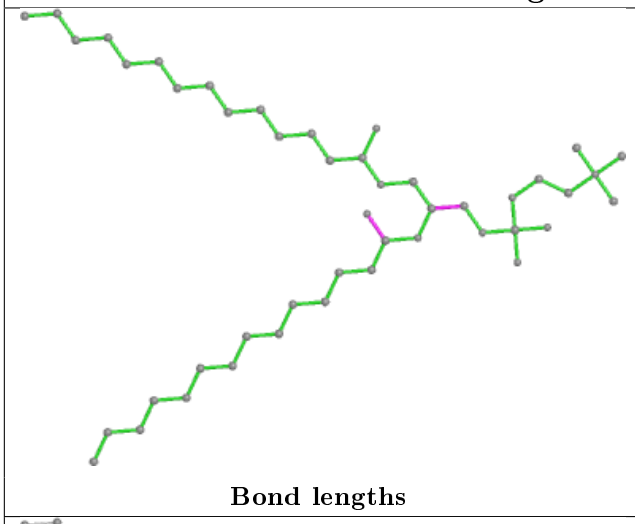


Torsions

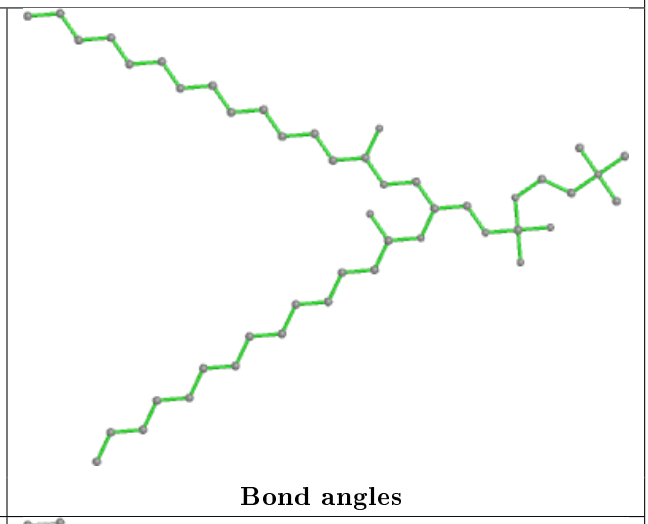


Rings

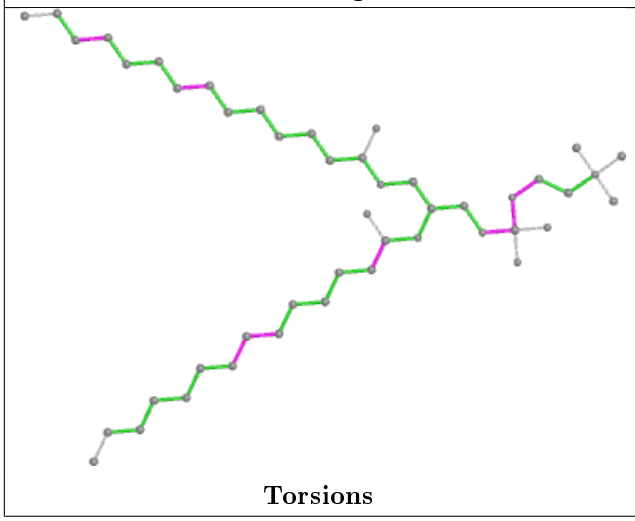
Ligand PX4 A 616



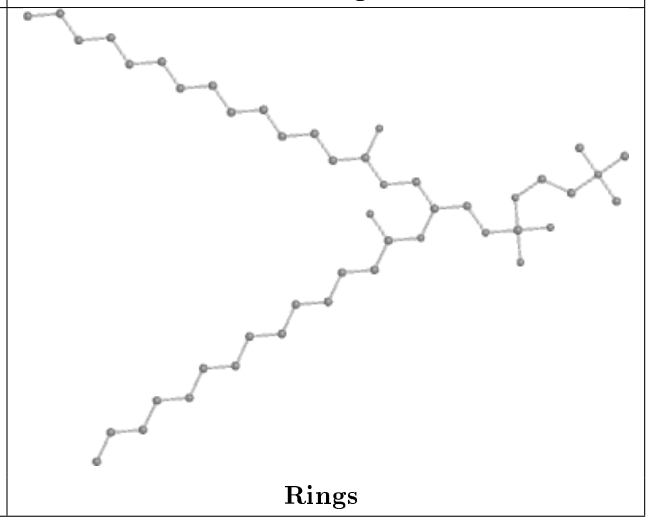
Bond lengths



Bond angles

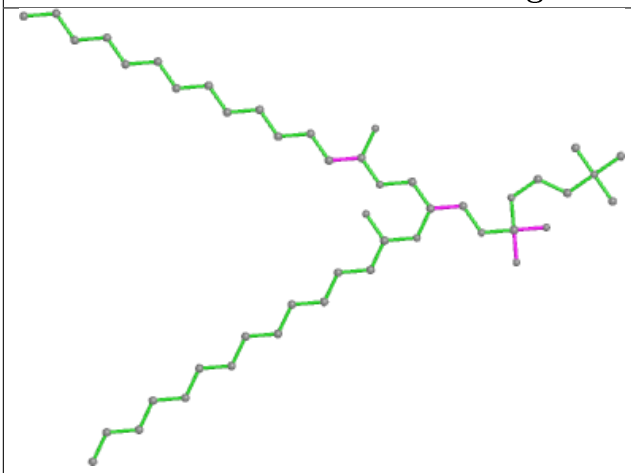


Torsions

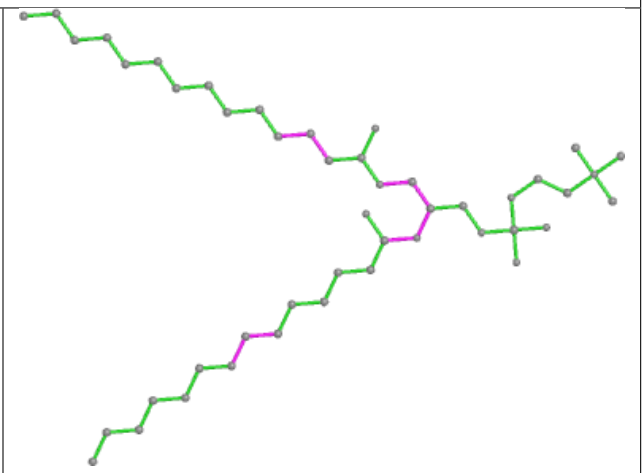


Rings

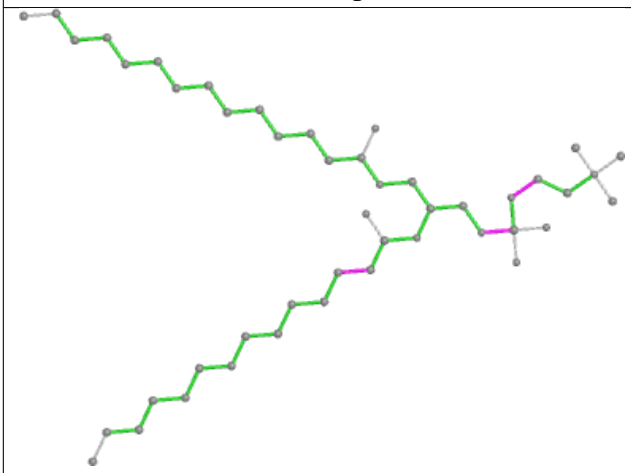
Ligand PX4 A 632



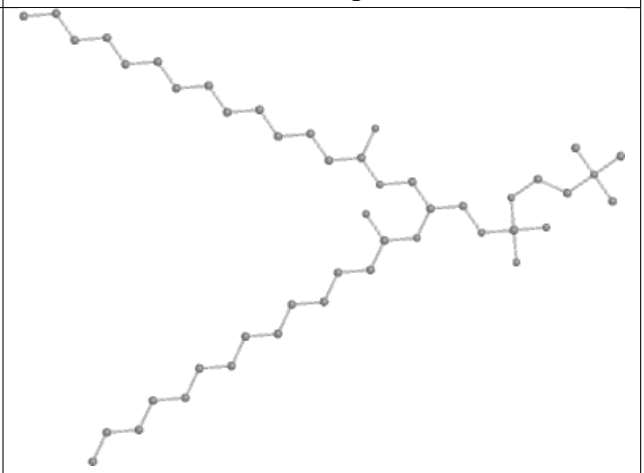
Bond lengths



Bond angles

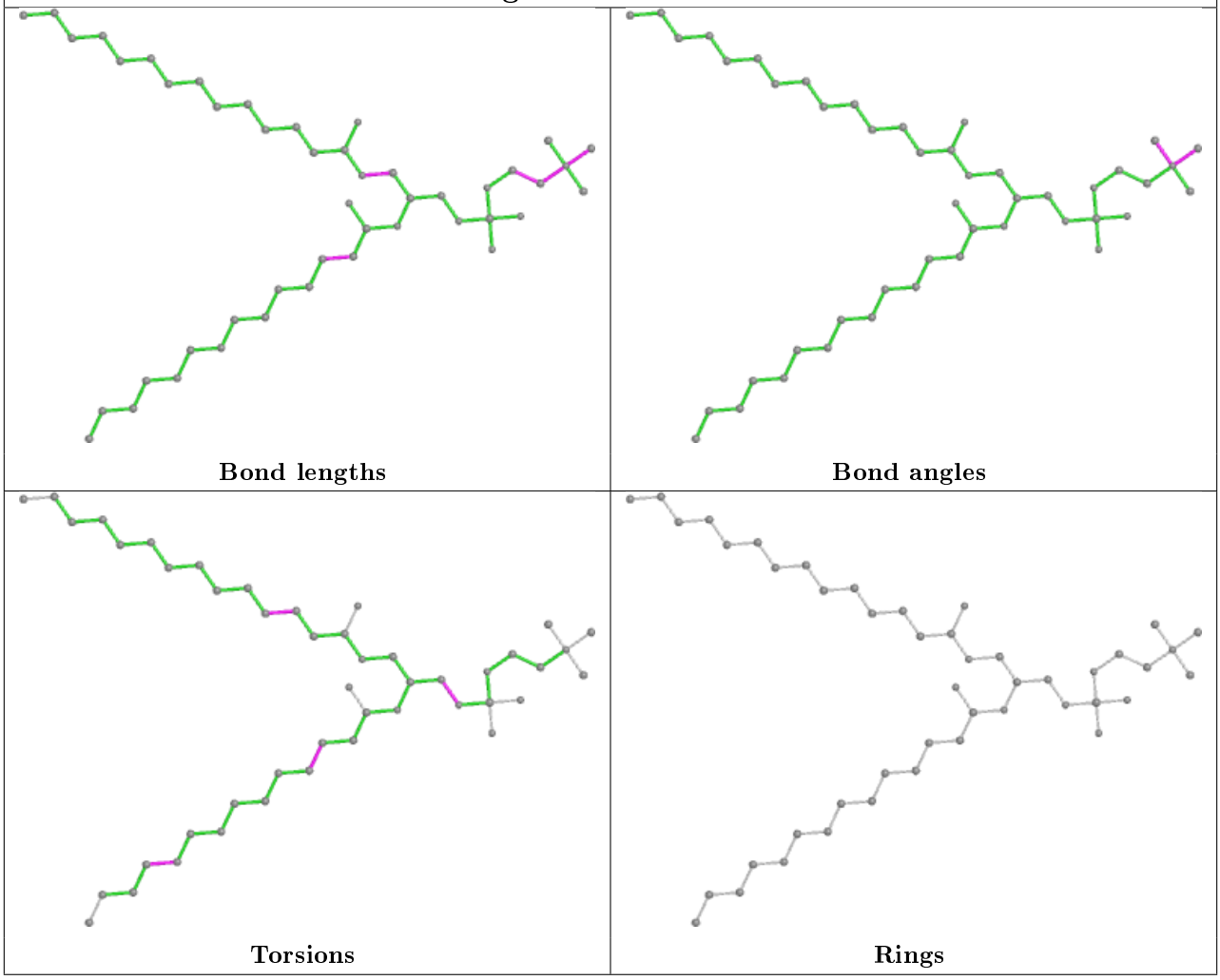


Torsions

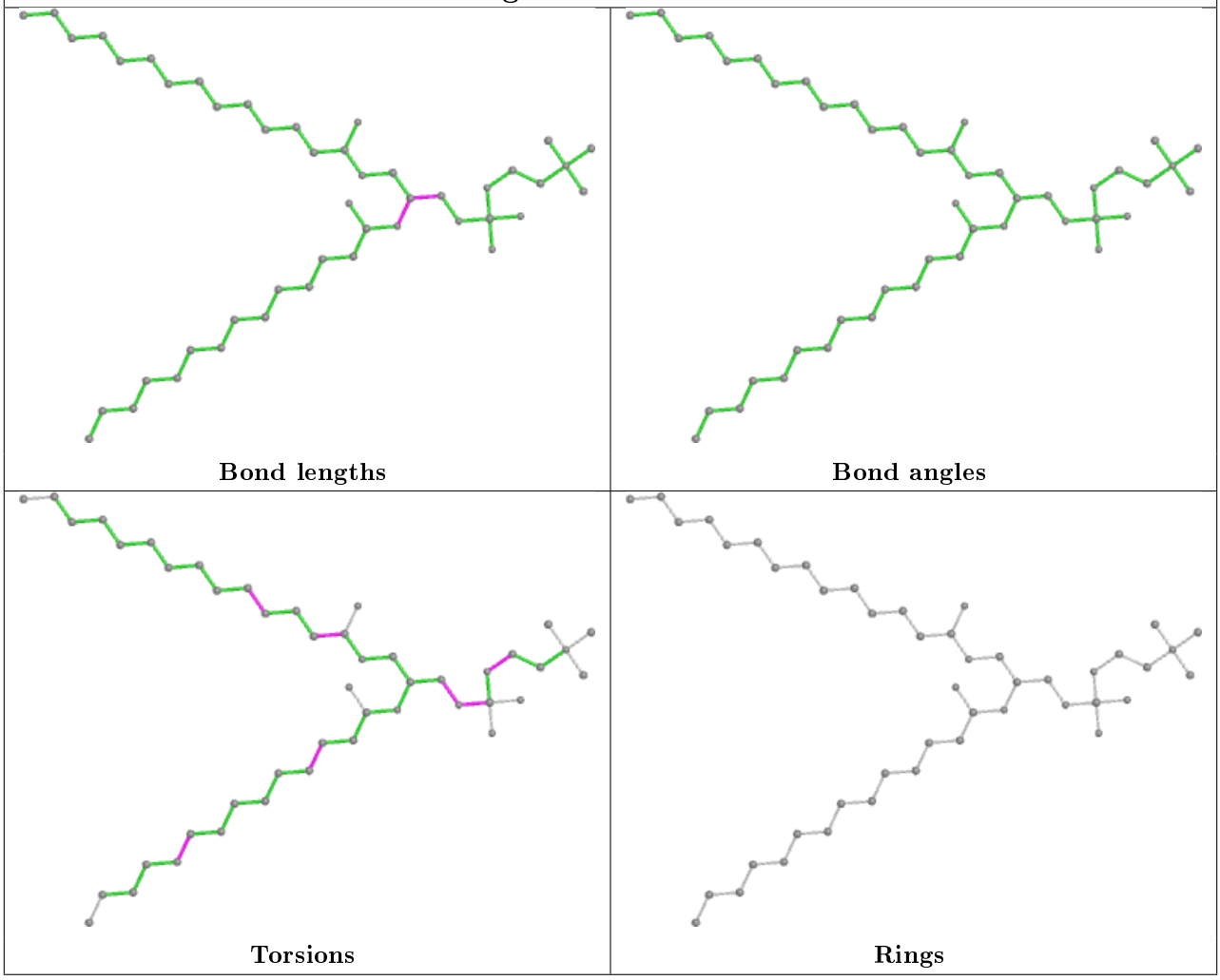


Rings

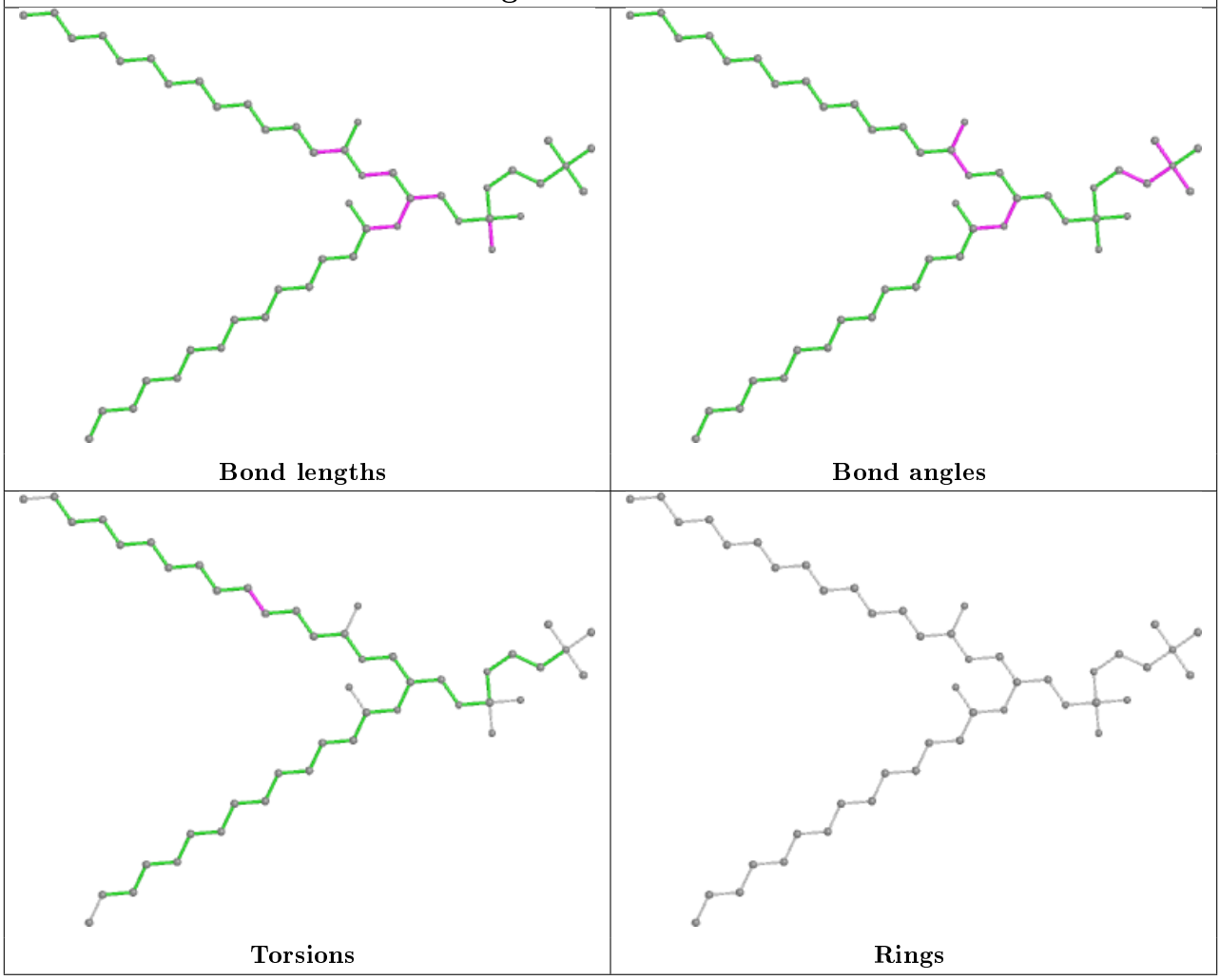
Ligand PX4 B 371



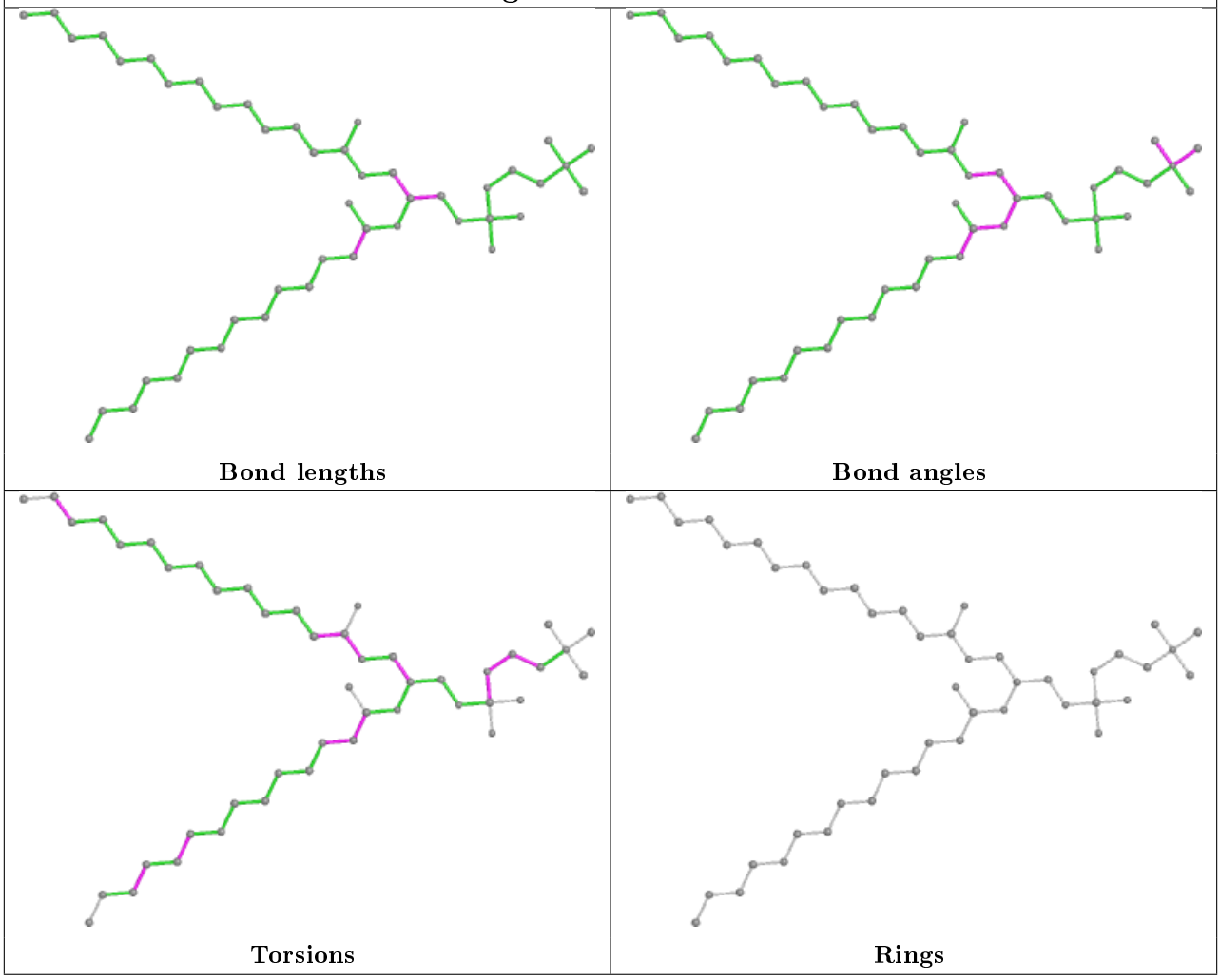
Ligand PX4 B 310



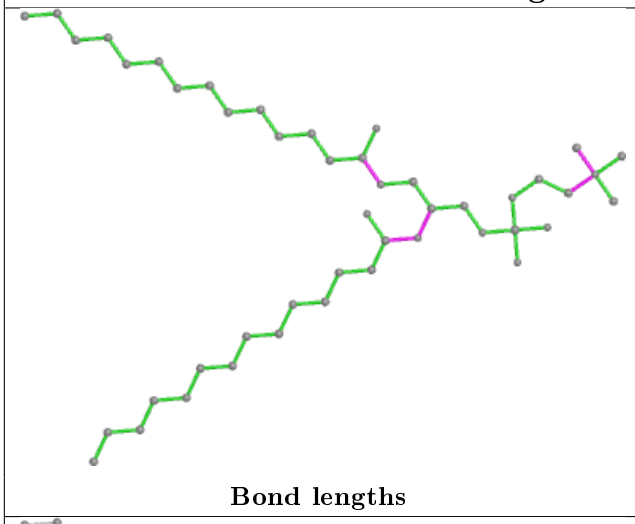
Ligand PX4 A 610



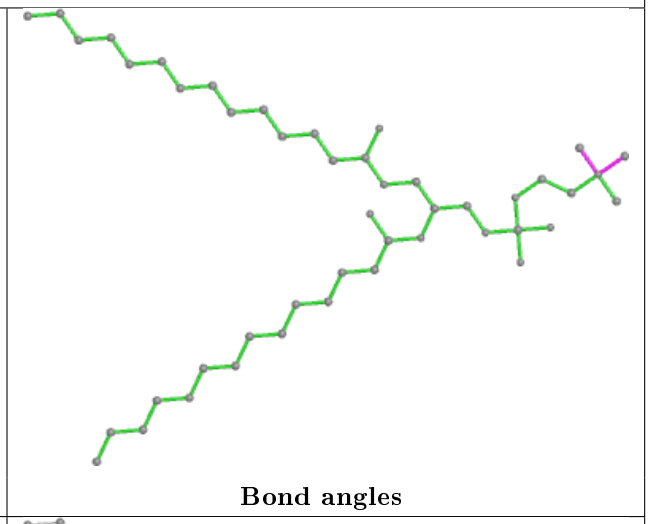
Ligand PX4 C 345



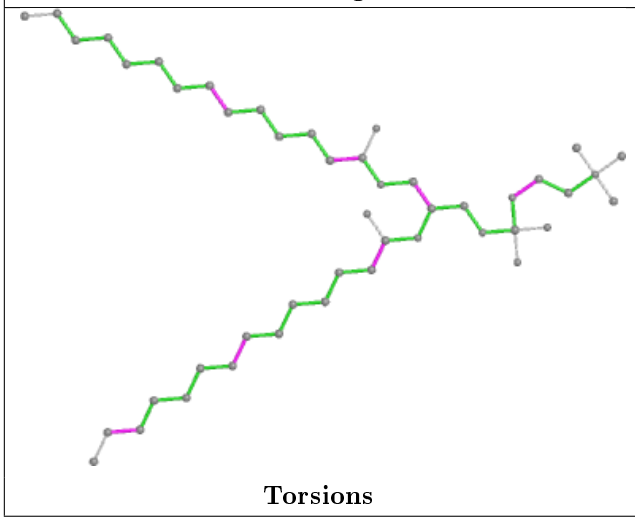
Ligand PX4 C 307



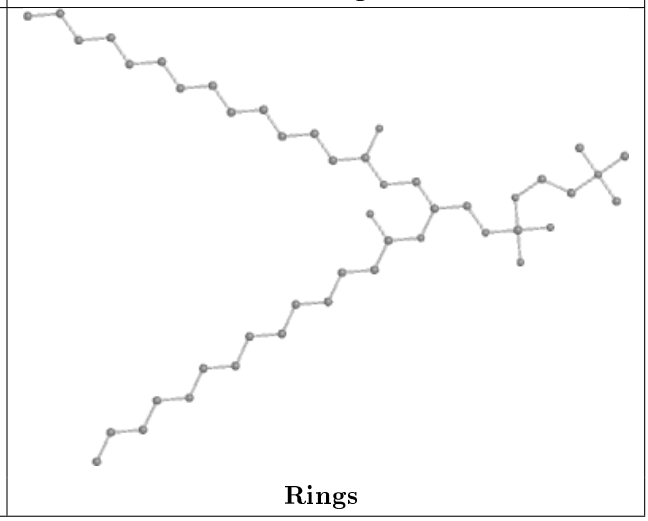
Bond lengths



Bond angles

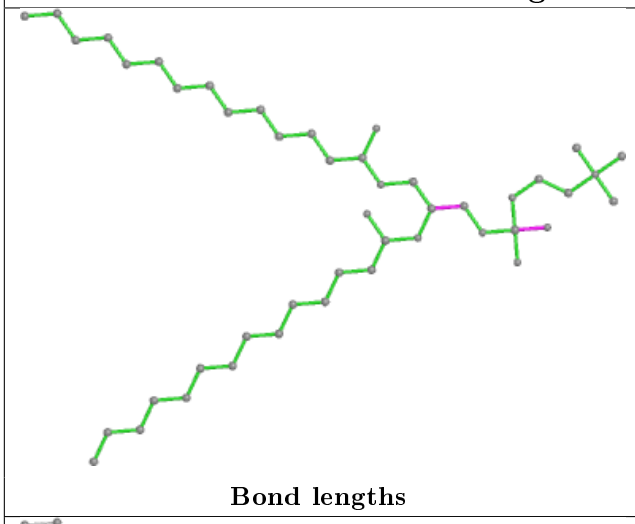


Torsions

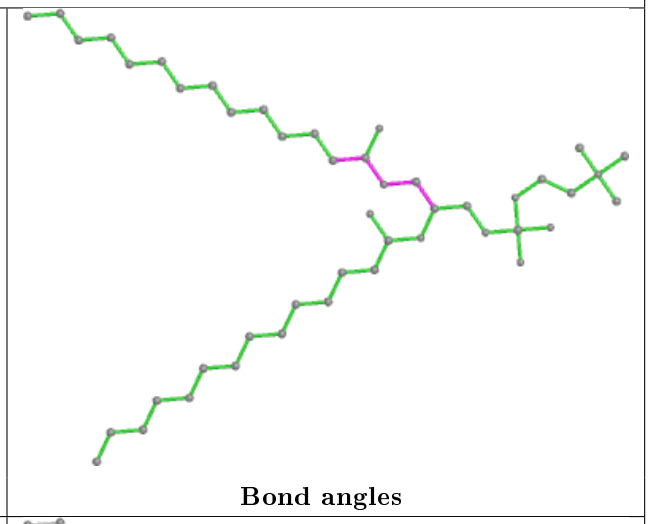


Rings

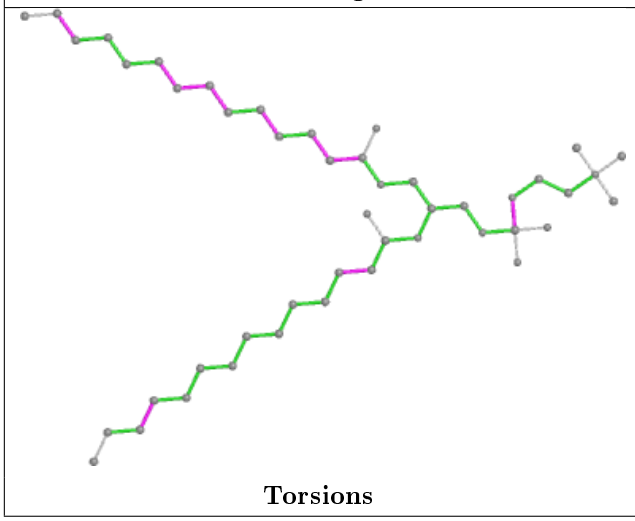
Ligand PX4 C 310



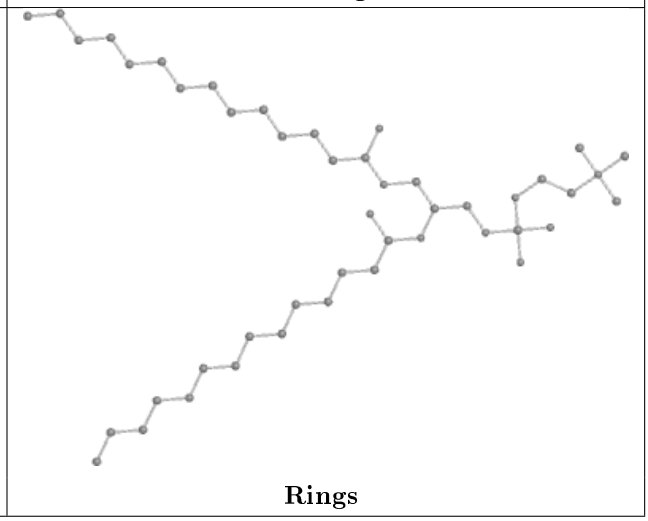
Bond lengths



Bond angles

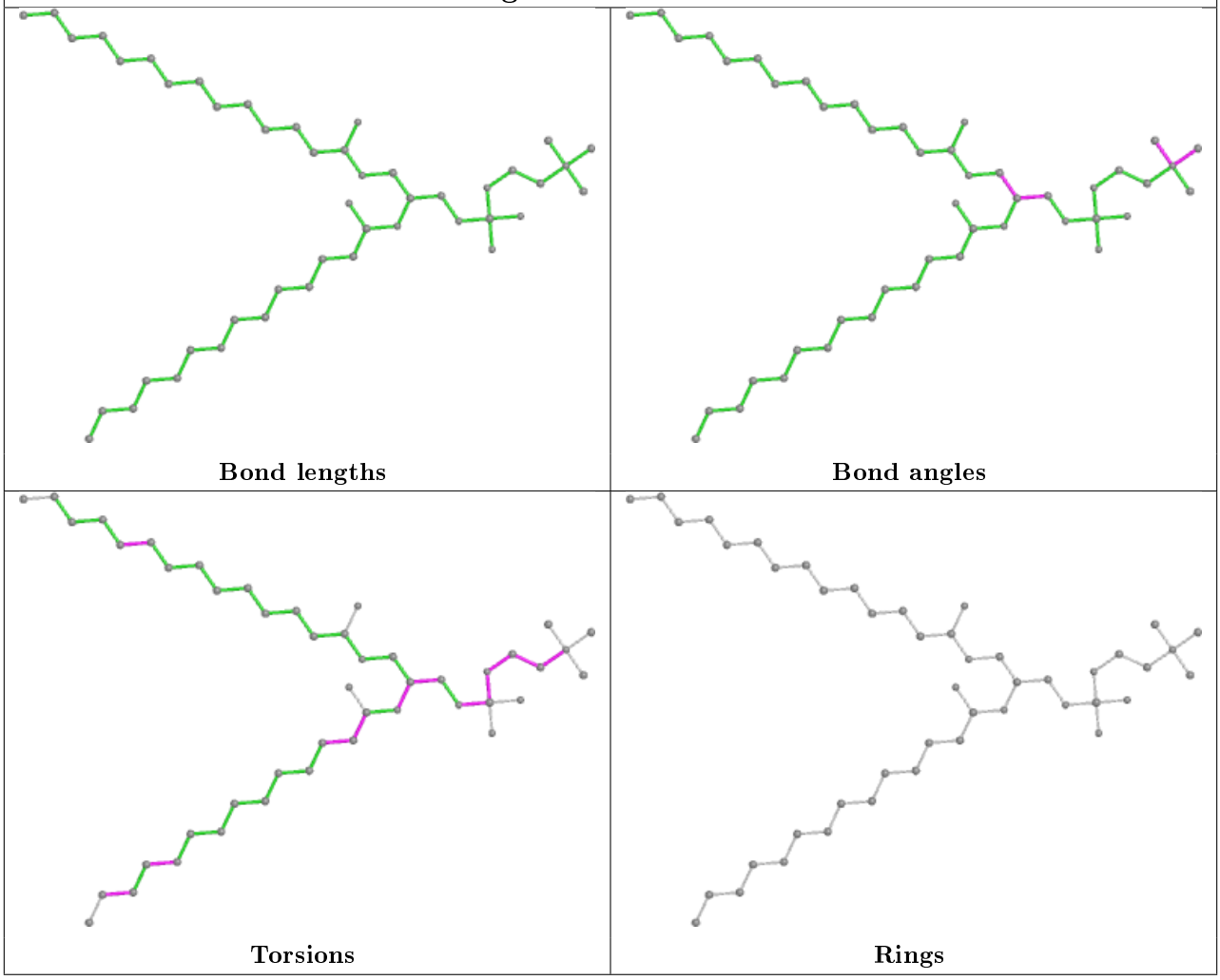


Torsions

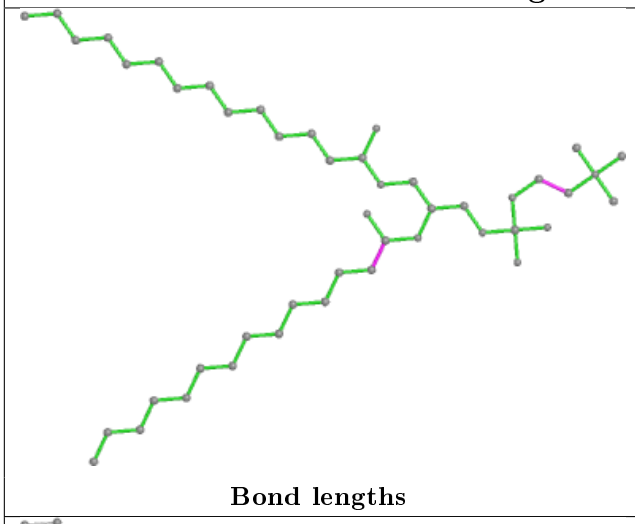


Rings

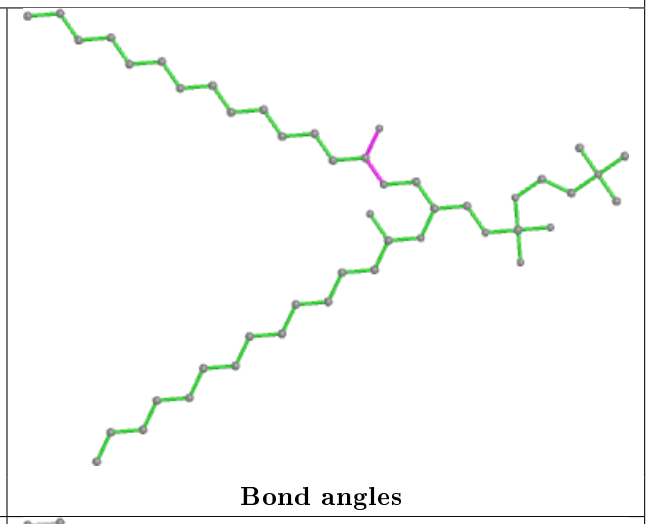
Ligand PX4 A 615



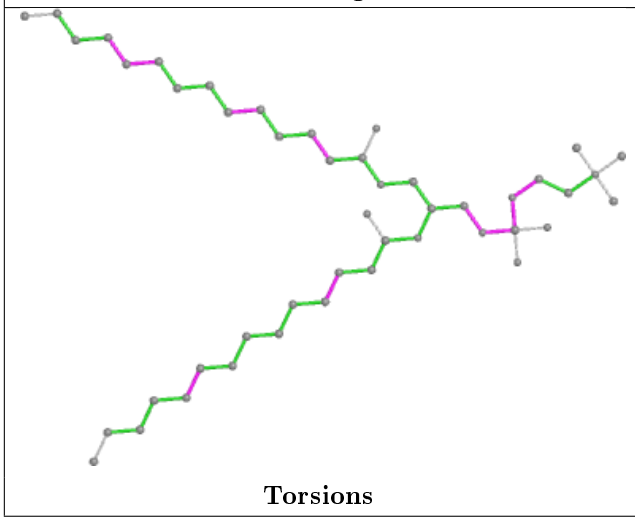
Ligand PX4 C 352



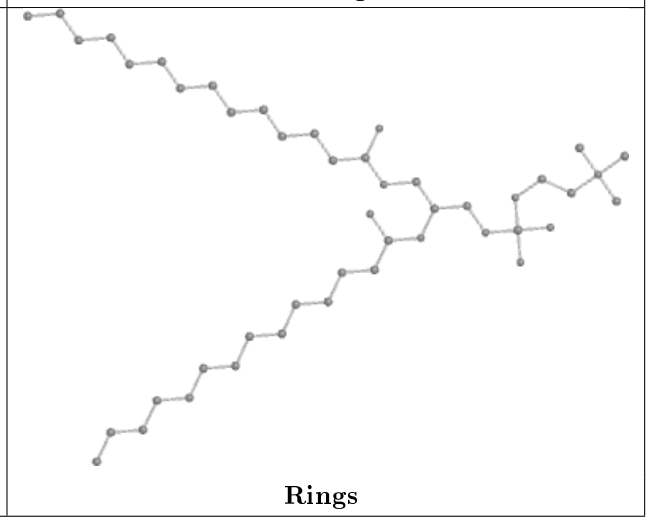
Bond lengths



Bond angles

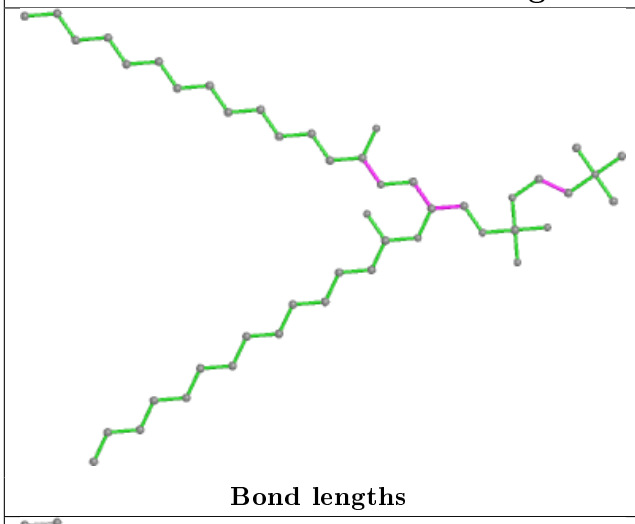


Torsions

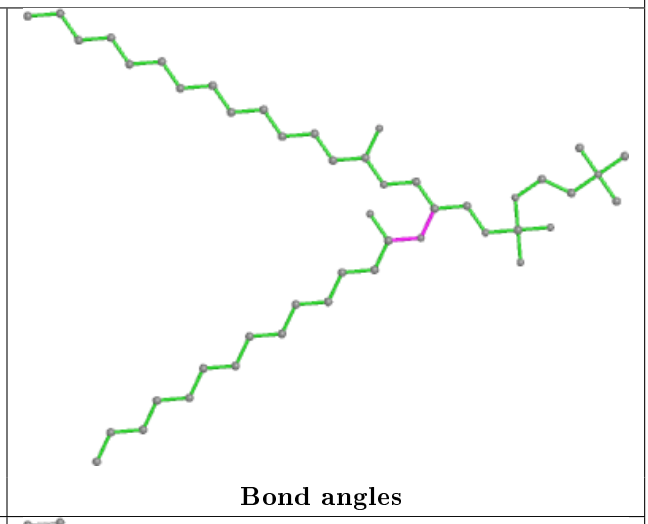


Rings

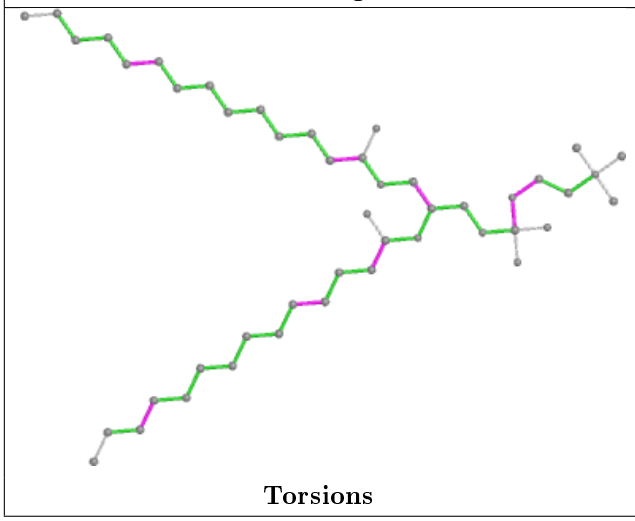
Ligand PX4 C 304



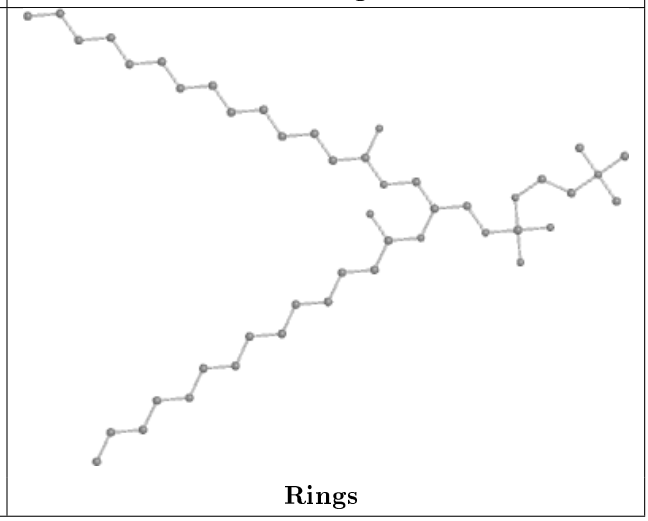
Bond lengths



Bond angles

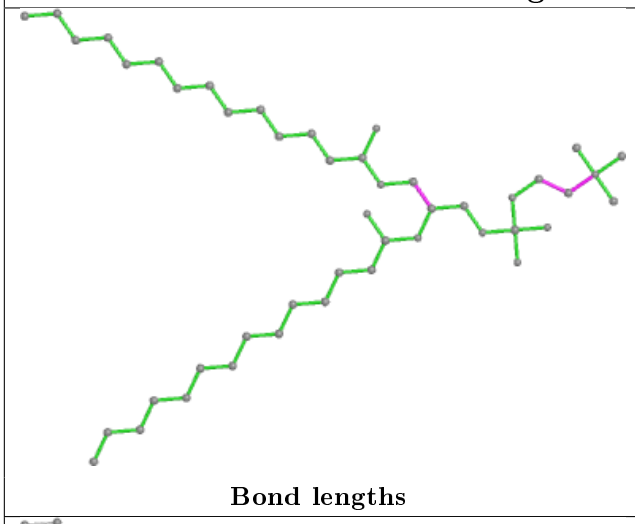


Torsions

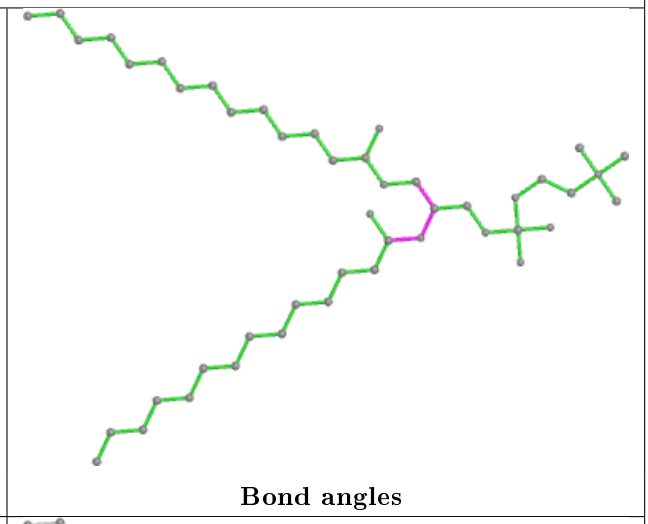


Rings

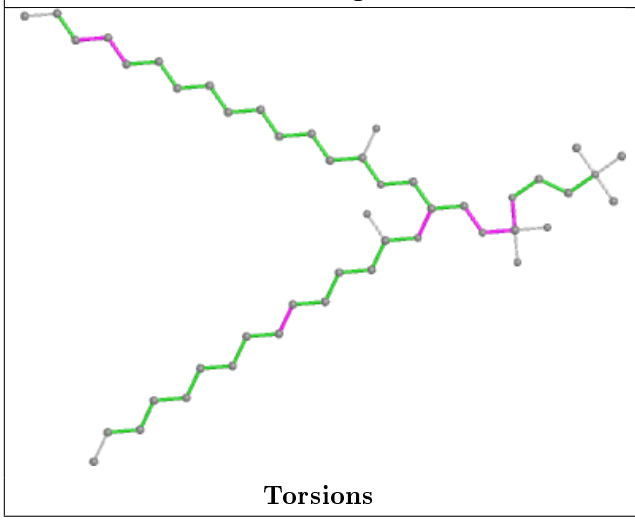
Ligand PX4 A 606



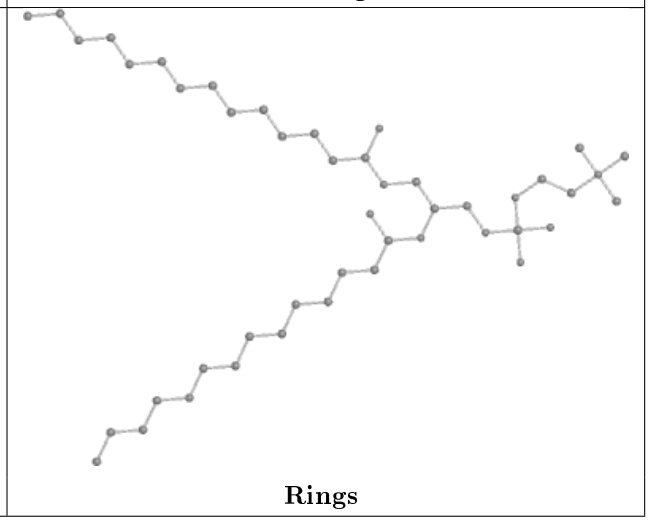
Bond lengths



Bond angles

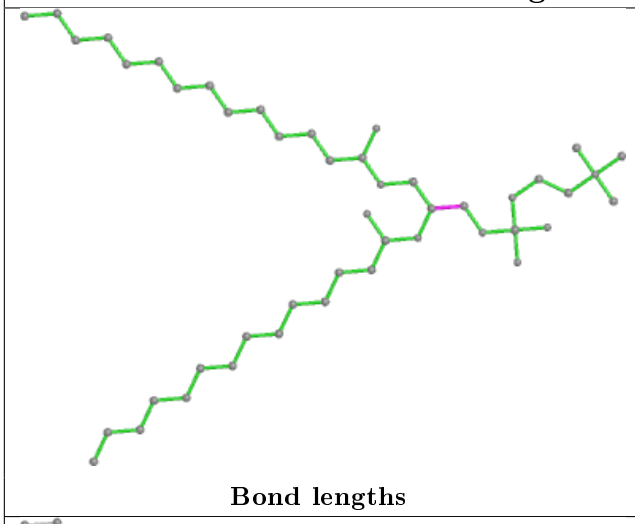


Torsions

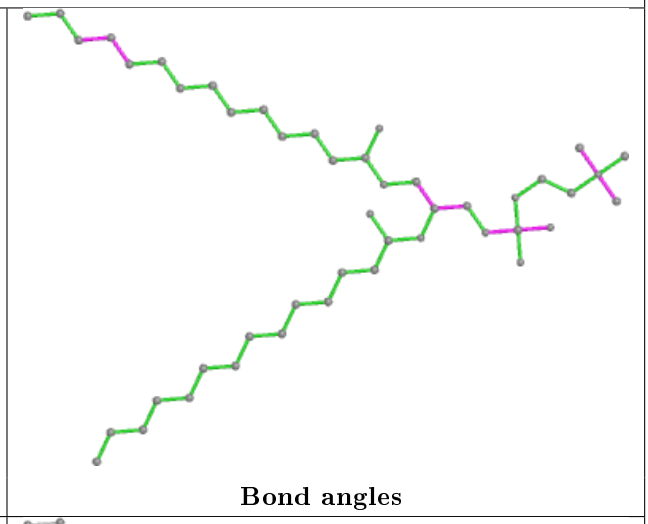


Rings

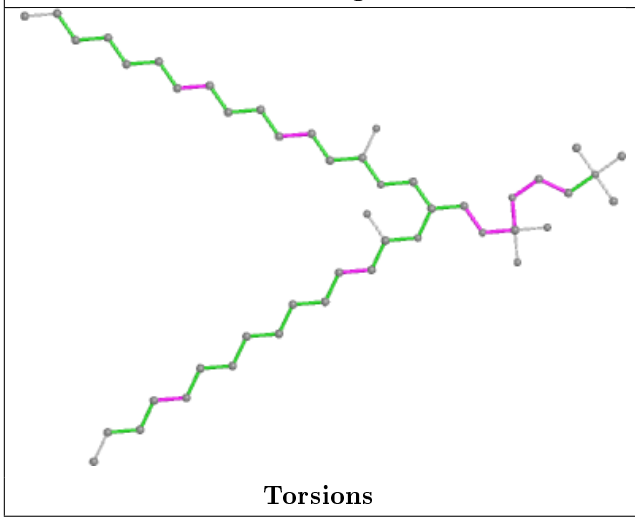
Ligand PX4 B 400



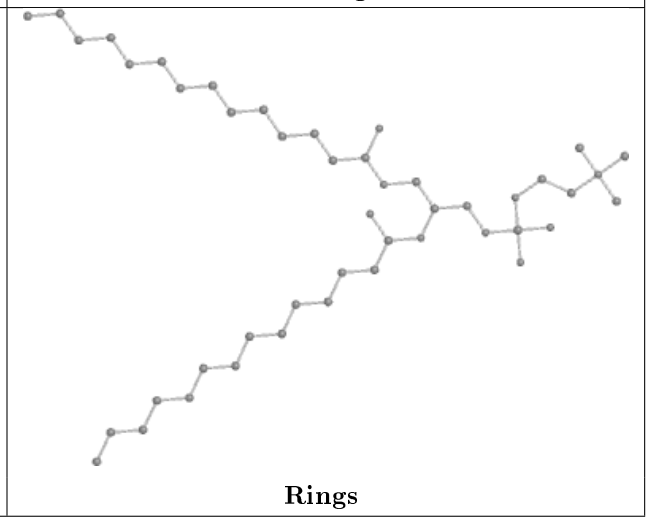
Bond lengths



Bond angles

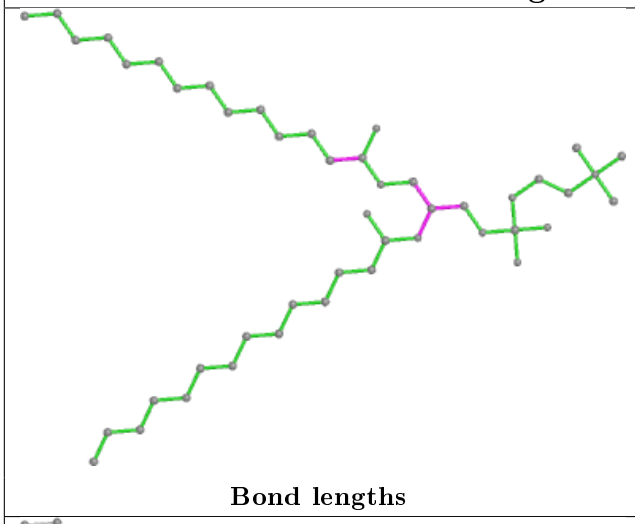


Torsions

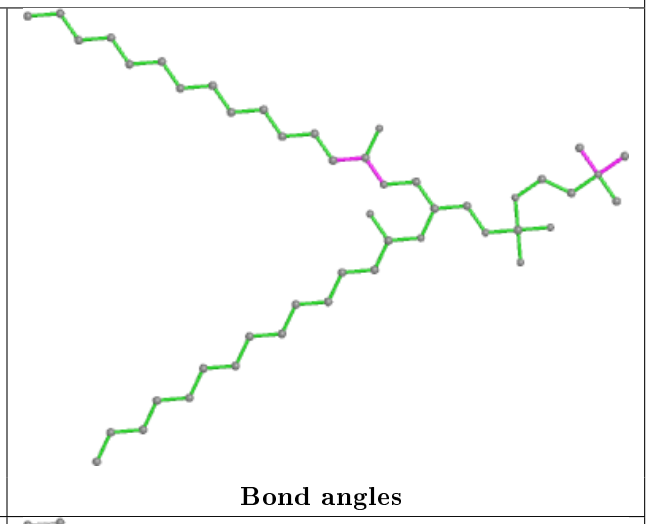


Rings

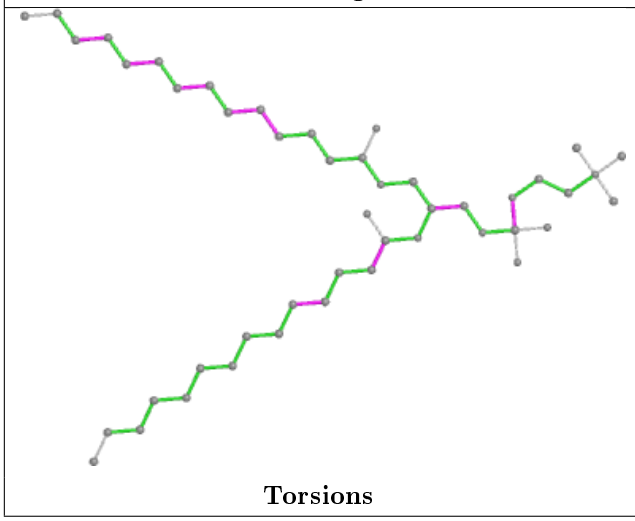
Ligand PX4 B 309



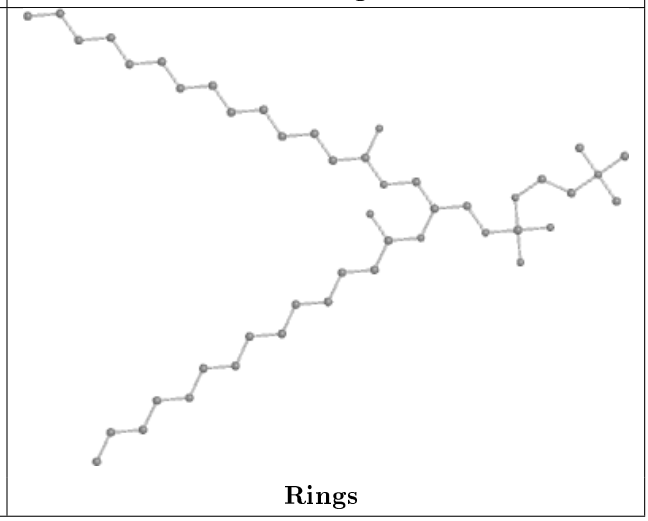
Bond lengths



Bond angles

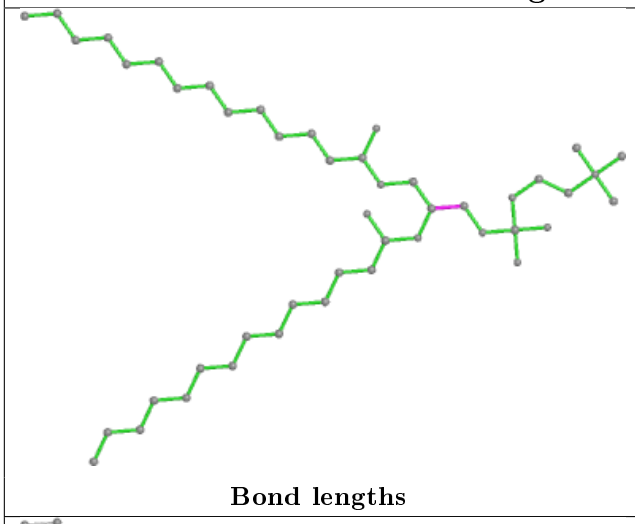


Torsions

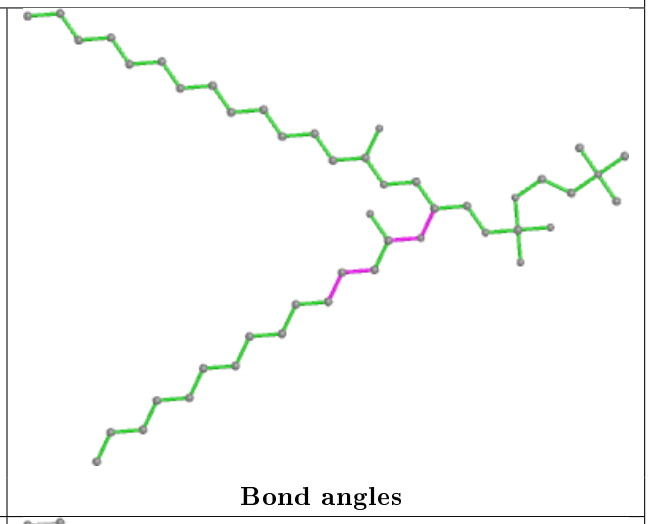


Rings

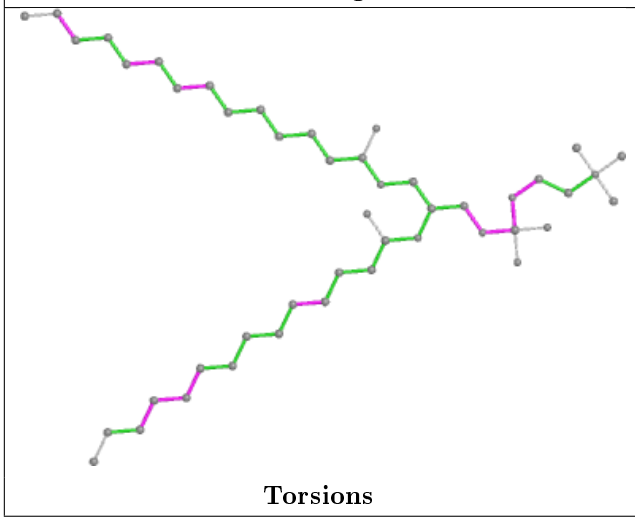
Ligand PX4 C 361



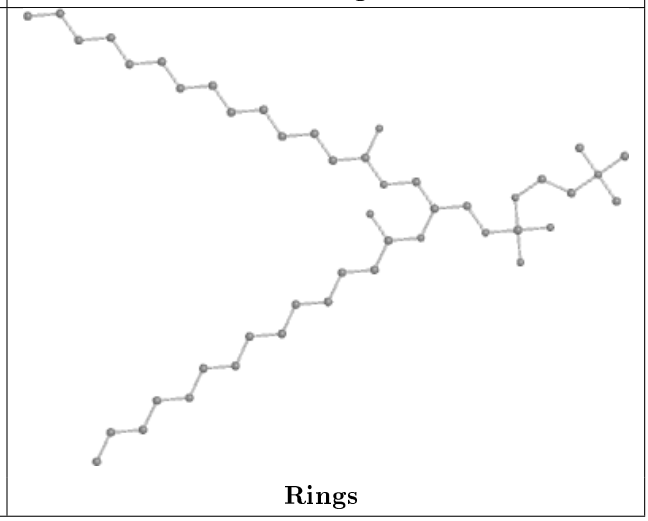
Bond lengths



Bond angles

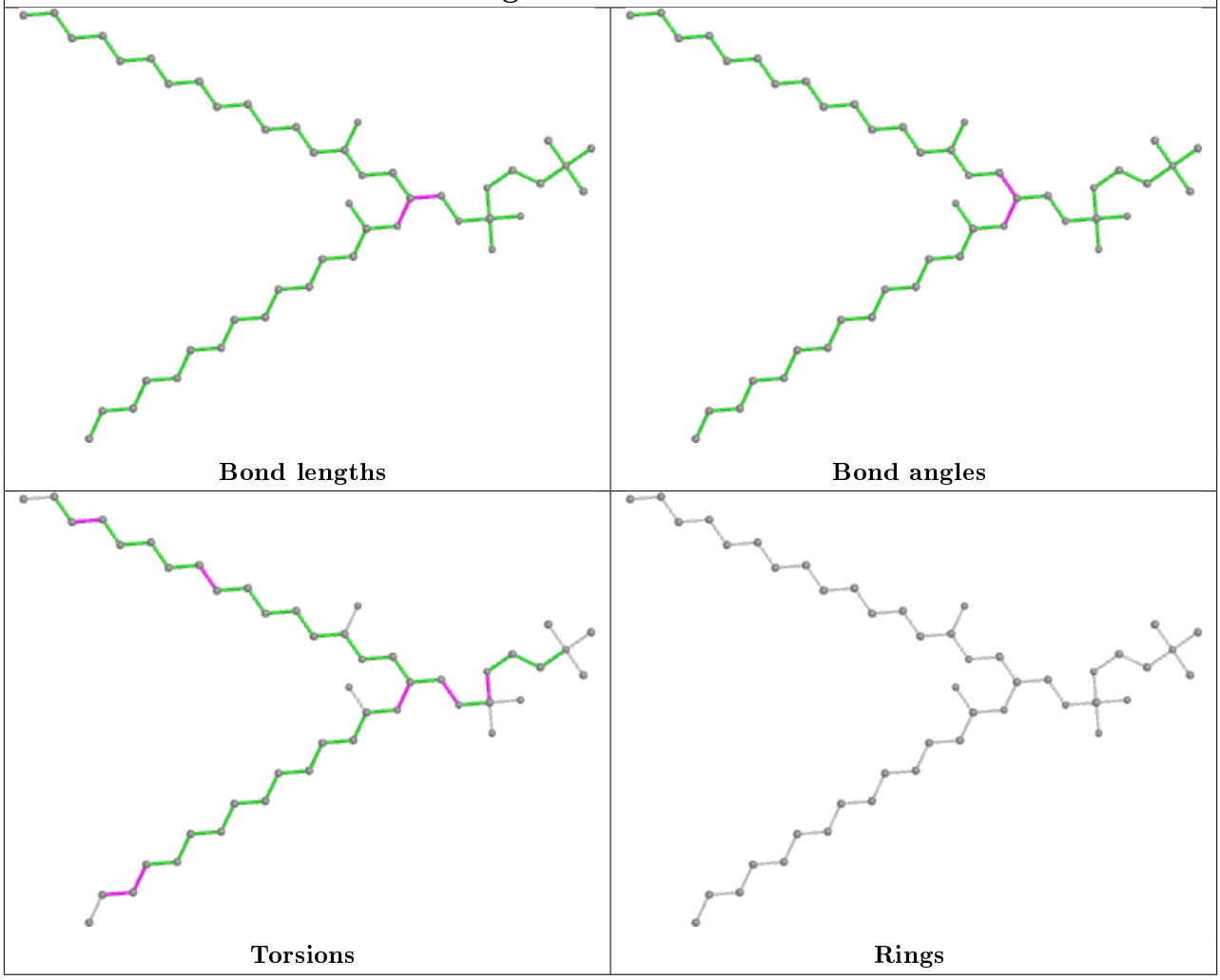


Torsions

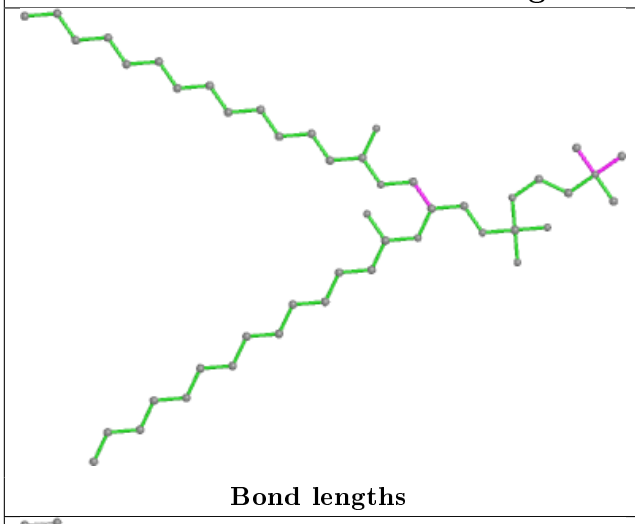


Rings

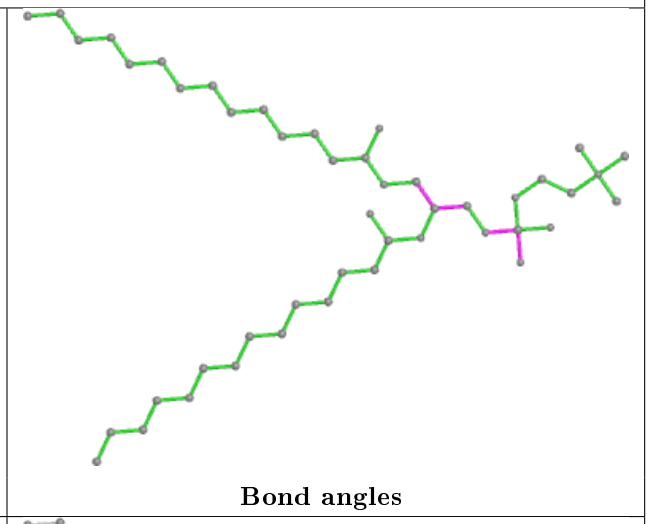
Ligand PX4 B 302



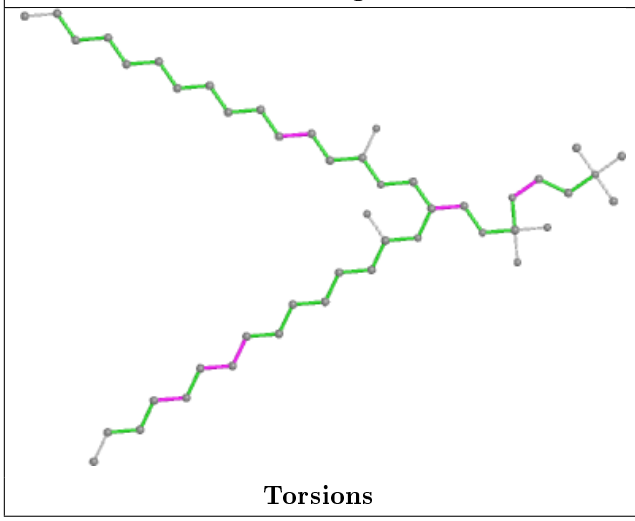
Ligand PX4 B 392



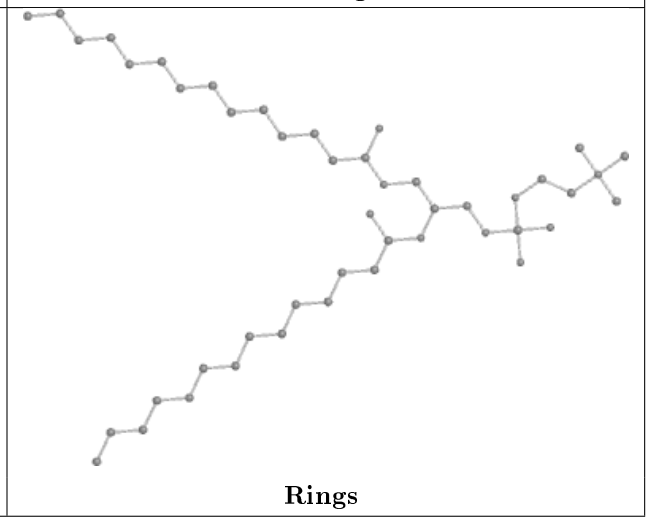
Bond lengths



Bond angles

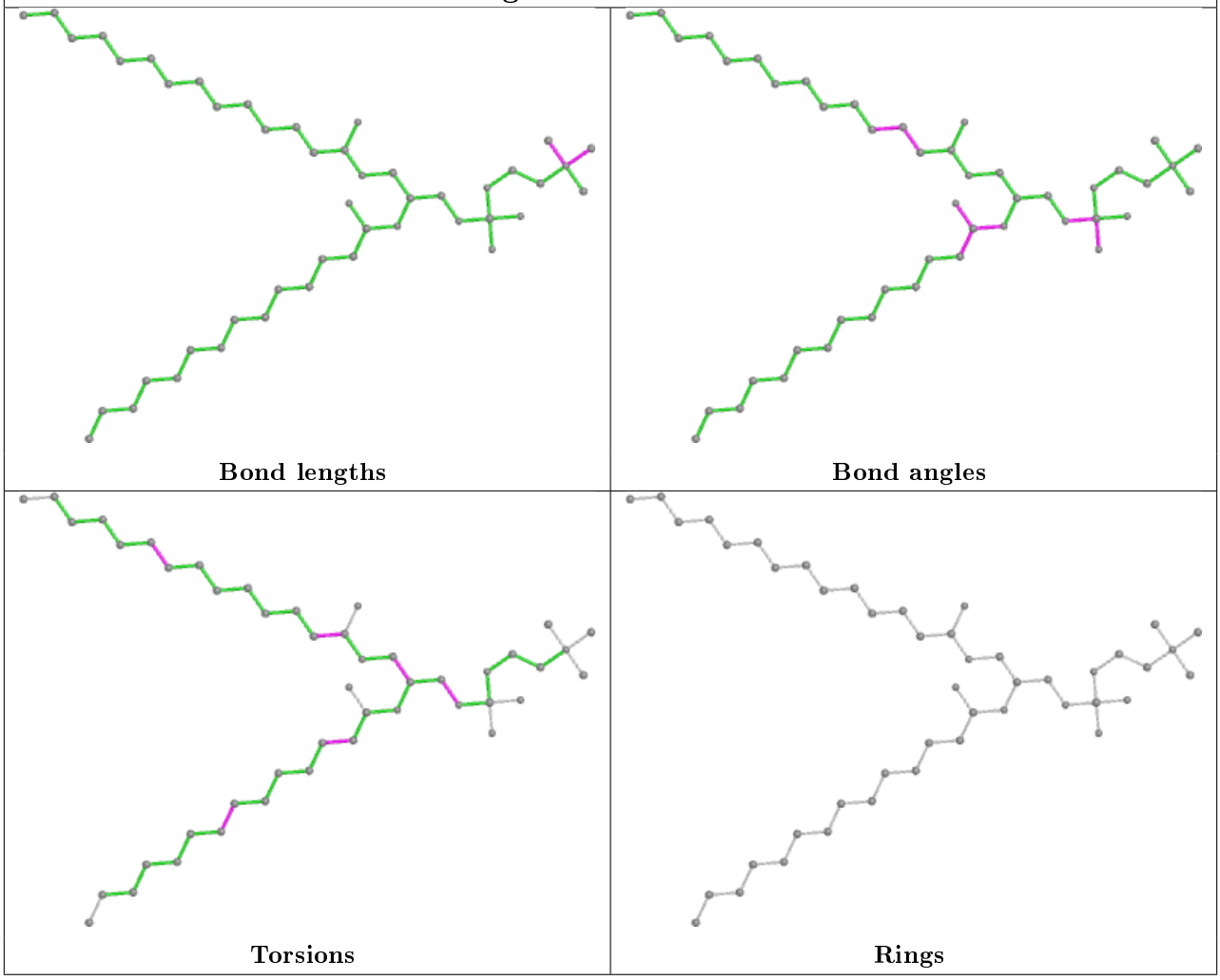


Torsions

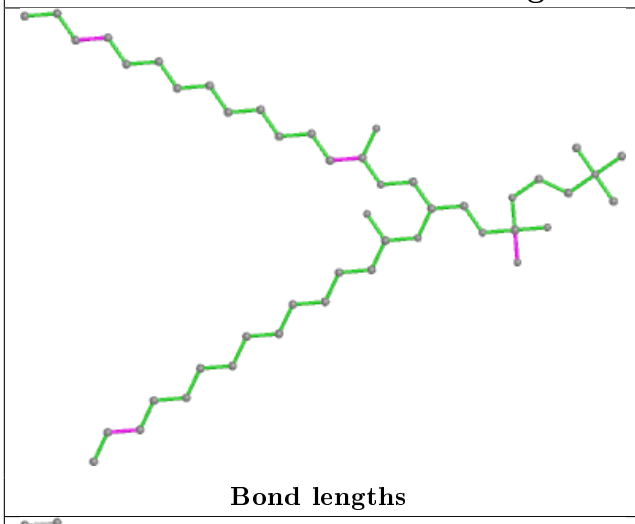


Rings

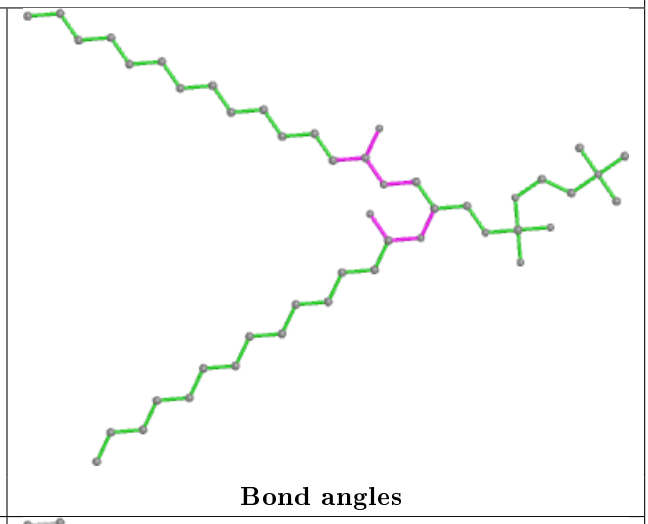
Ligand PX4 B 381



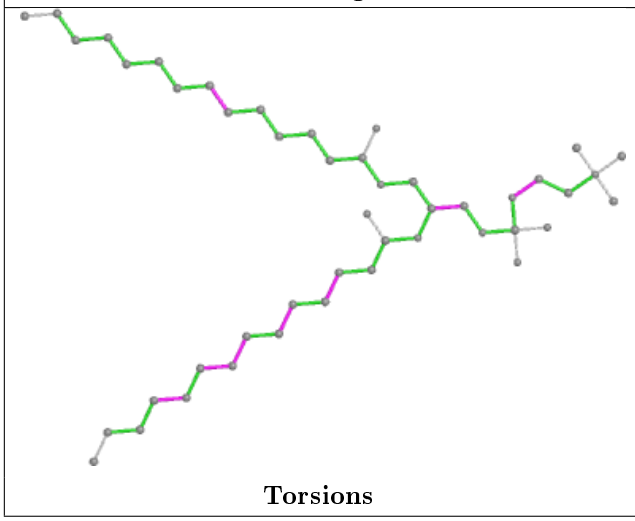
Ligand PX4 A 647



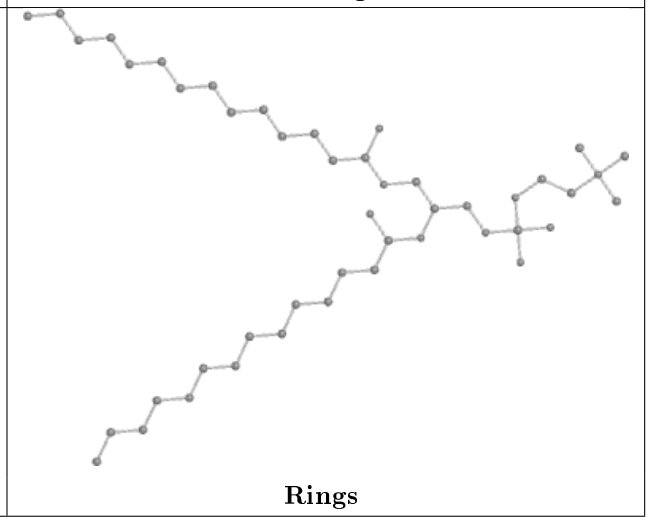
Bond lengths



Bond angles

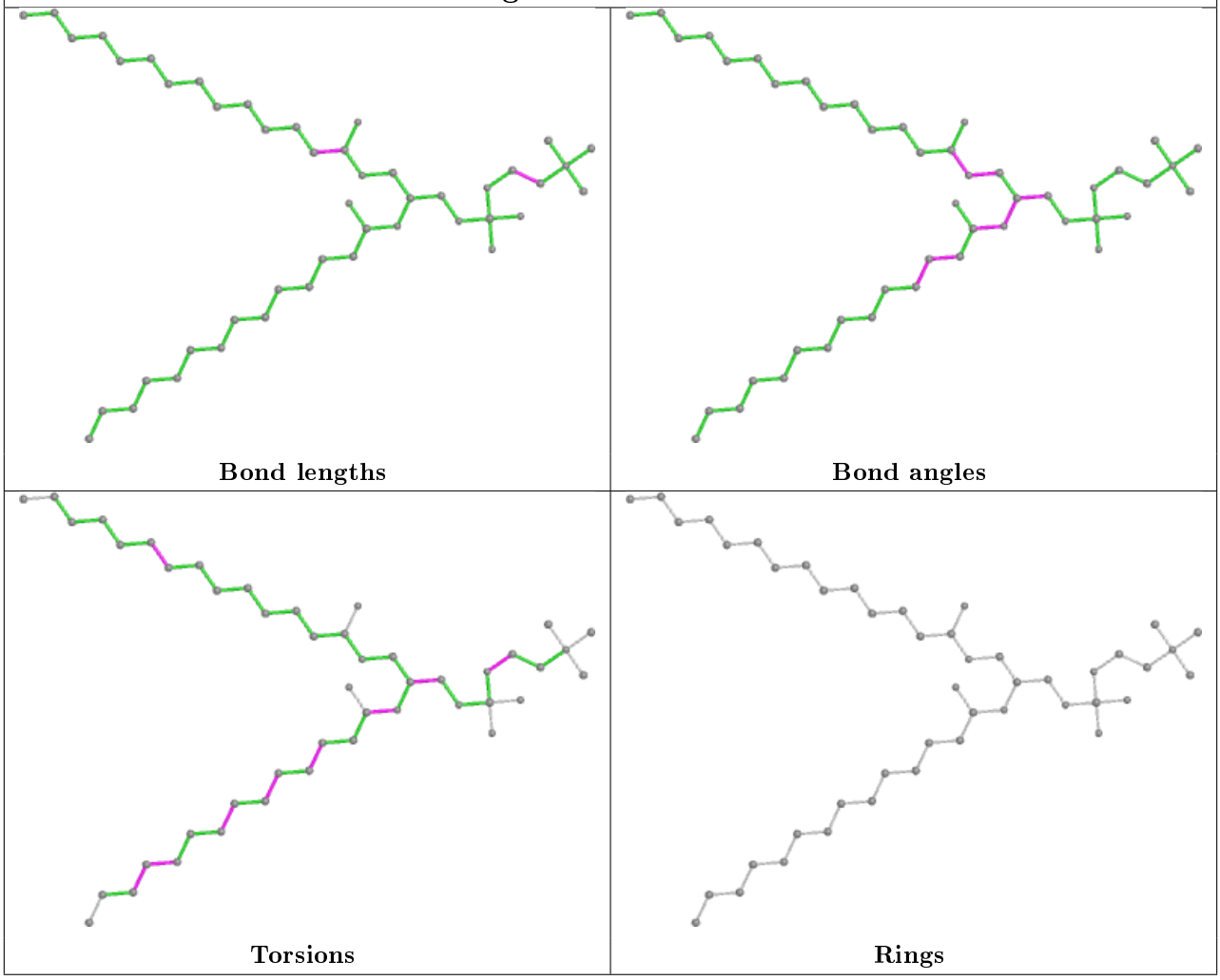


Torsions

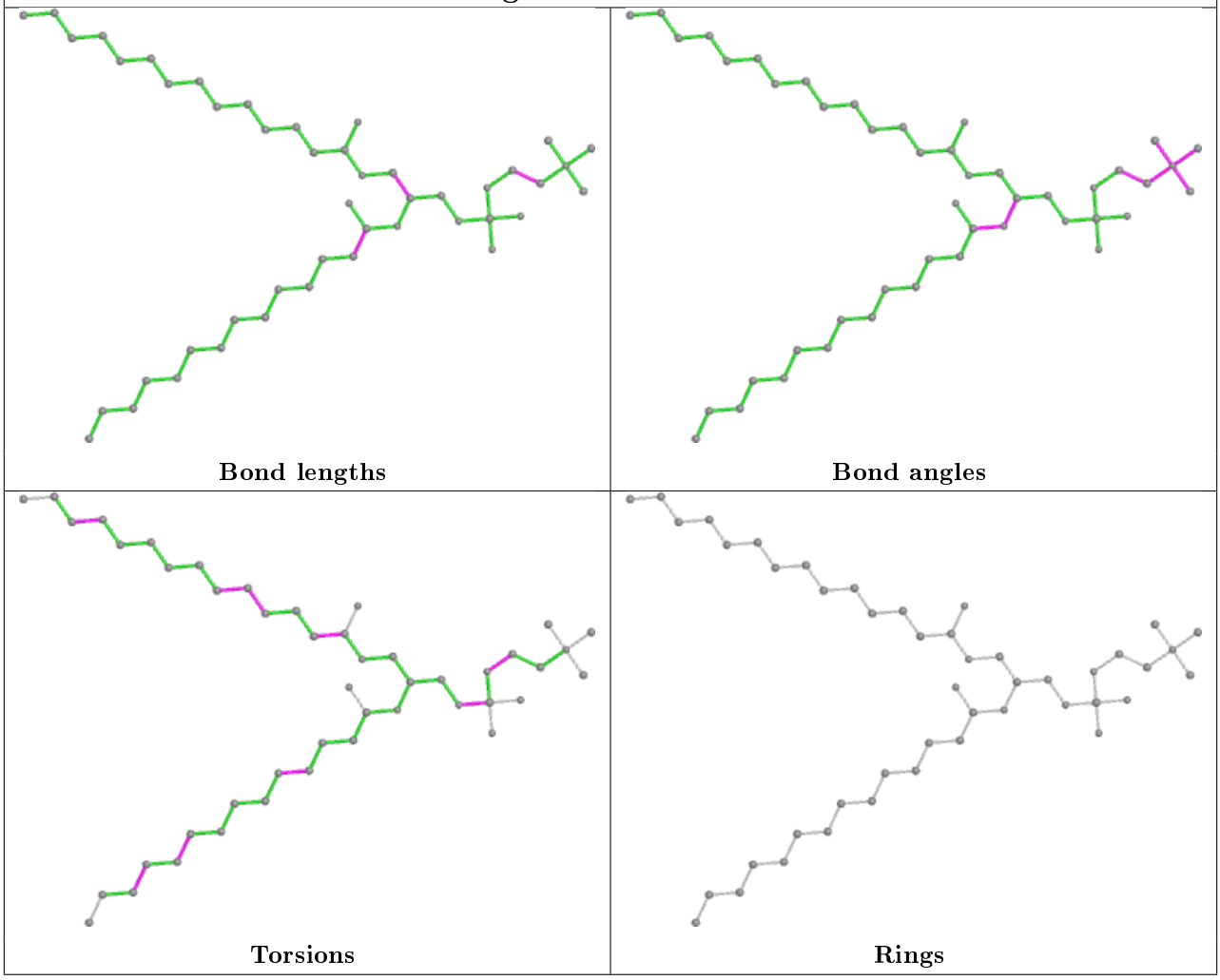


Rings

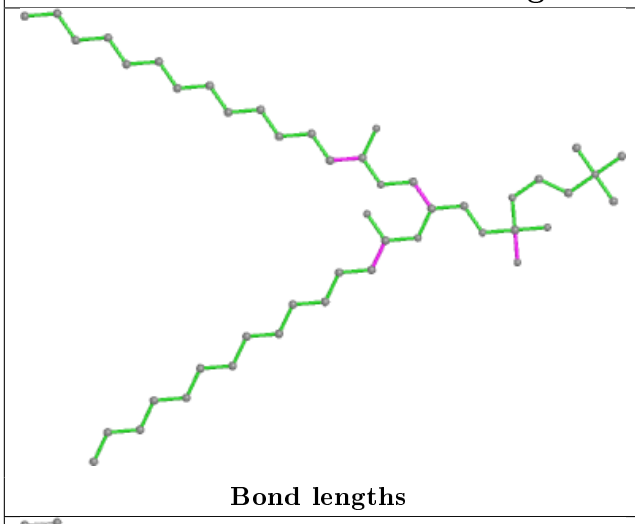
Ligand PX4 B 351



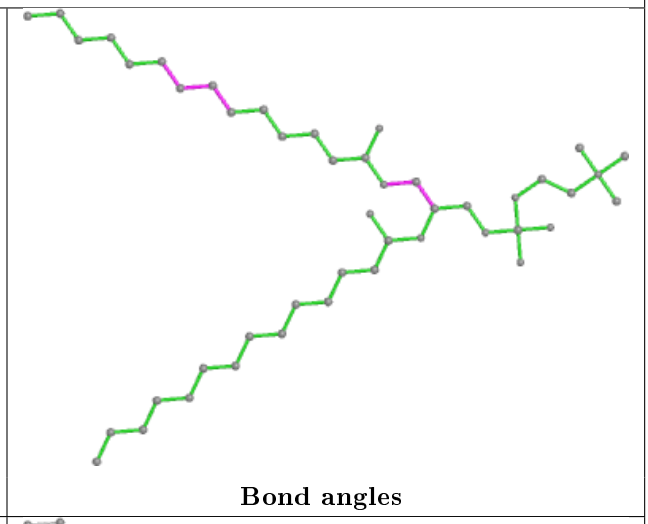
Ligand PX4 B 315



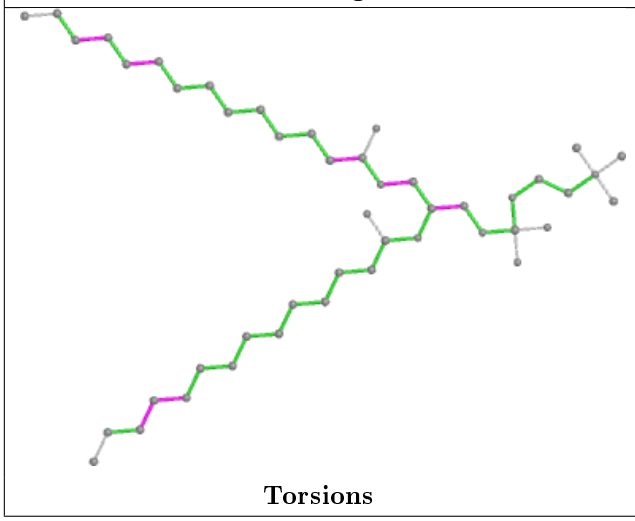
Ligand PX4 A 646



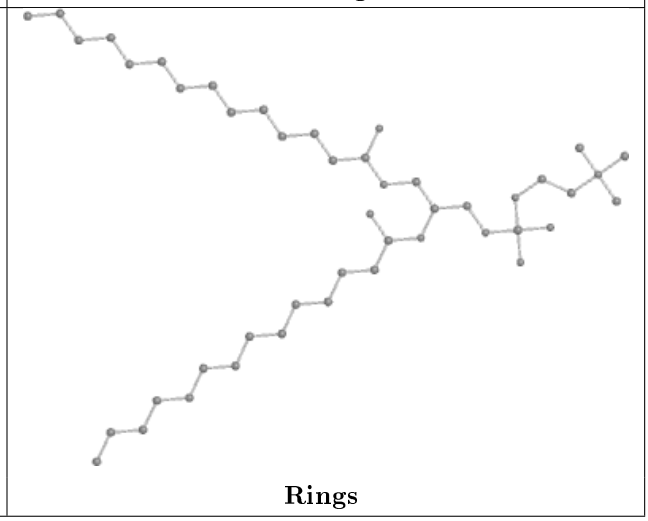
Bond lengths



Bond angles

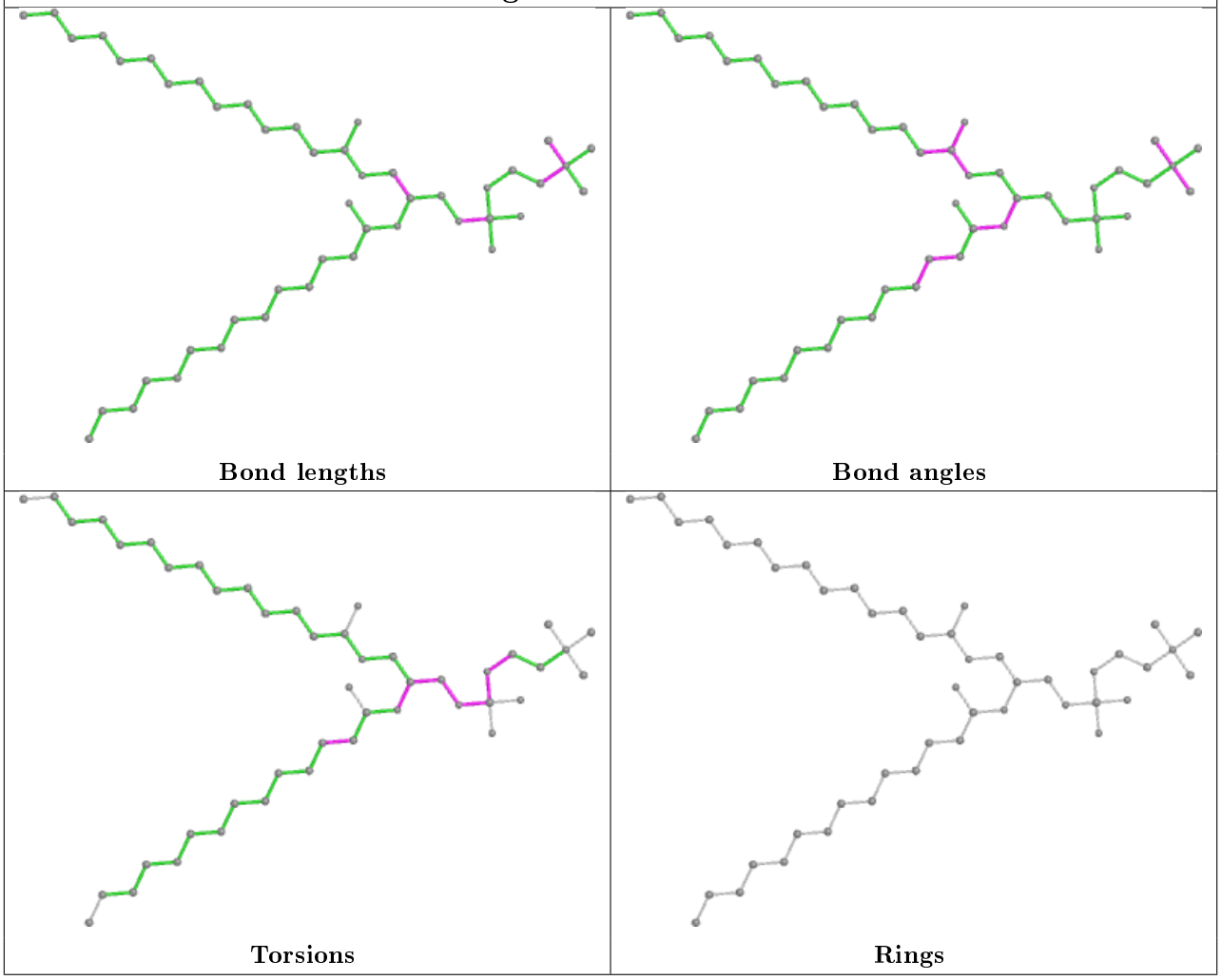


Torsions



Rings

Ligand PX4 C 324



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 3% for the well-defined parts and 3% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *showstar5.txt*

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	324
Number of shifts mapped to atoms	324
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	0	—	None (insufficient data)
$^{13}C_{\beta}$	0	—	None (insufficient data)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	92	1.12 ± 0.47	Should be applied

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 3%, i.e. 262 atoms were assigned a chemical shift out of a possible 8156. 0 out of 99 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	184/3030 (6%)	92/1206 (8%)	0/1236 (0%)	92/588 (16%)
Sidechain	78/4413 (2%)	35/2615 (1%)	43/1561 (3%)	0/237 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	0/713 (0%)	0/377 (0%)	0/310 (0%)	0/26 (0%)
Overall	262/8156 (3%)	127/4198 (3%)	43/3107 (1%)	92/851 (11%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 3%, i.e. 262 atoms were assigned a chemical shift out of a possible 8156. 0 out of 99 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	184/3030 (6%)	92/1206 (8%)	0/1236 (0%)	92/588 (16%)
Sidechain	78/4413 (2%)	35/2615 (1%)	43/1561 (3%)	0/237 (0%)
Aromatic	0/713 (0%)	0/377 (0%)	0/310 (0%)	0/26 (0%)
Overall	262/8156 (3%)	127/4198 (3%)	43/3107 (1%)	92/851 (11%)

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.

Random coil index (RCI) for chain A: