Full wwPDB NMR Structure Validation Report (i)

Apr 21, 2024 – 12:21 PM EDT

PDB ID	:	2MLR
BMRB ID	:	7089
Title	:	Membrane Bilayer complex with Matrix Metalloproteinase-12 at its Alpha-face
Authors	:	Koppisetti, R.K.; Fulcher, Y.G.; Prior, S.H.; Lenoir, M.; Overduin, M.; Van Doren, S.R.
Deposited on	:	2014-03-04

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

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

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

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

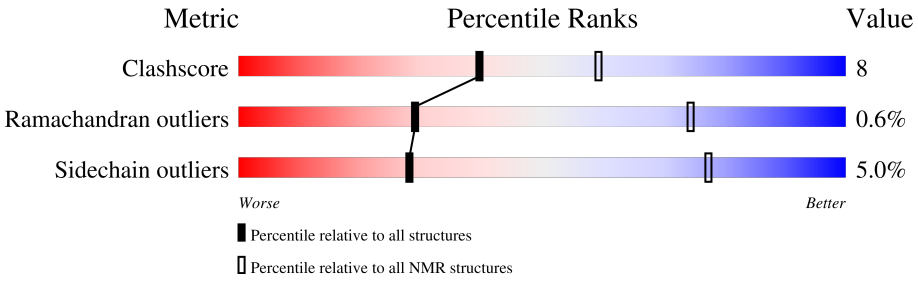
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance

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

The overall completeness of chemical shifts assignment is 81%.

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	164	79% 18%

2 Ensemble composition and analysis

This entry contains 14 models. Model 3 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:100-A:187, A:192-A:263 (160)	0.66	3

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	8, 9, 10, 11, 13
2	1, 2, 3, 4, 5
3	6, 7
4	12, 14

3 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8263 atoms, of which 1221 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Macrophage metalloelastase.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	164	2508	824	1221	225	234	4	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	219	ALA	GLU	engineered mutation	UNP P39900

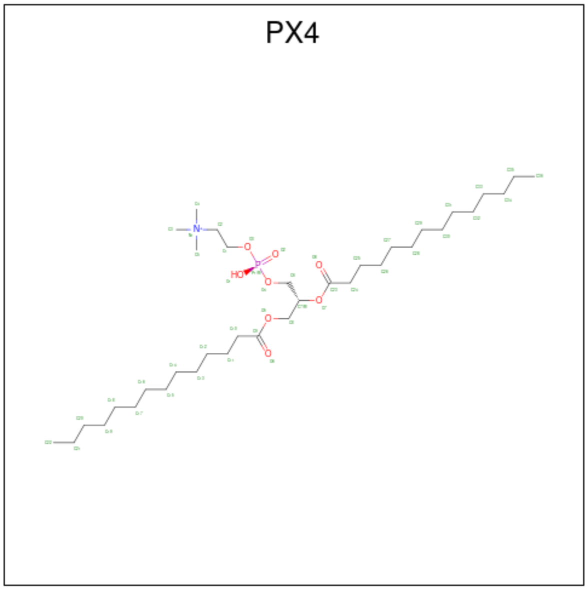
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
			Total	Zn
2	A	2	2	2

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	
			Total	Ca
3	A	3	3	3

- Molecule 4 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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4	A	1	Total 46	C 36	N 1	O 8	P 1
4	A	1	Total 46	C 36	N 1	O 8	P 1
4	A	1	Total 46	C 36	N 1	O 8	P 1
4	A	1	Total 46	C 36	N 1	O 8	P 1
4	A	1	Total 46	C 36	N 1	O 8	P 1
4	A	1	Total 46	C 36	N 1	O 8	P 1
4	A	1	Total 46	C 36	N 1	O 8	P 1
4	A	1	Total 46	C 36	N 1	O 8	P 1
4	A	1	Total 46	C 36	N 1	O 8	P 1
4	A	1	Total 46	C 36	N 1	O 8	P 1
4	A	1	Total 46	C 36	N 1	O 8	P 1
4	A	1	Total 46	C 36	N 1	O 8	P 1
4	A	1	Total 46	C 36	N 1	O 8	P 1

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Mol	Chain	Residues	Atoms				
4	A	1	Total	C	N	O	P
			46	36	1	8	1
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			46	36	1	8	1
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4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
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4	A	1	Total	C	N	O	P
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4	A	1	Total	C	N	O	P
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			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
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4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1

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Mol	Chain	Residues	Atoms				
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1

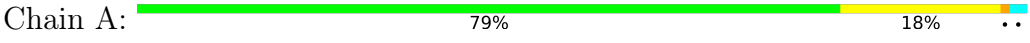
4 Residue-property plots

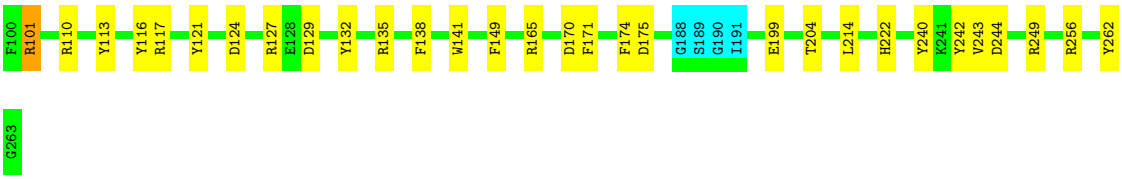
4.1 Average score per residue in the NMR ensemble

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: Macrophage metalloelastase

Chain A:





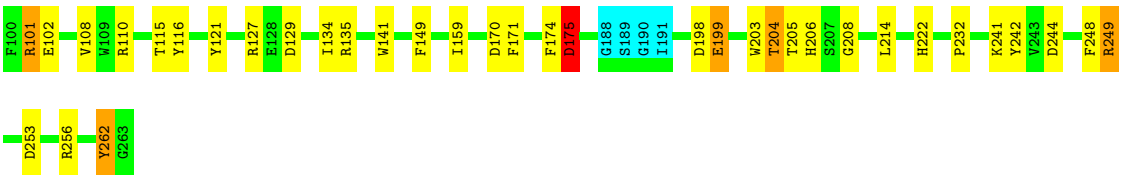
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Macrophage metalloelastase

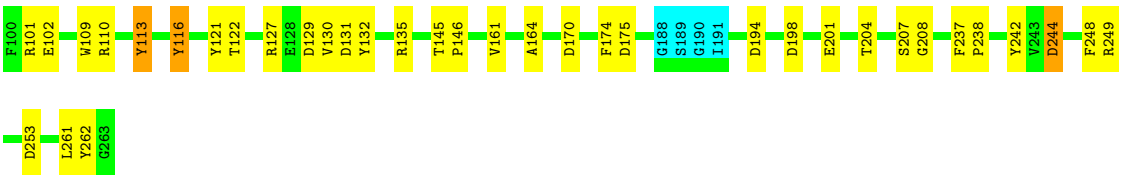
Chain A:



4.2.2 Score per residue for model 2

• Molecule 1: Macrophage metalloelastase

Chain A:



4.2.3 Score per residue for model 3 (medoid)

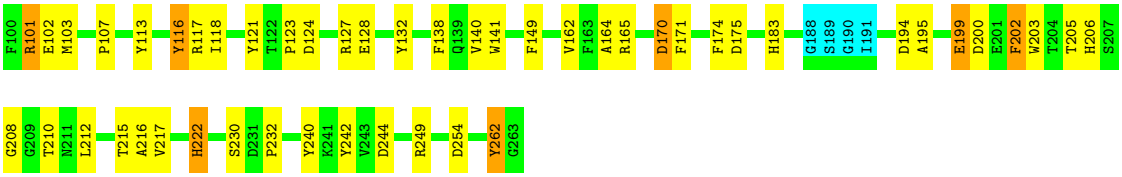
• Molecule 1: Macrophage metalloelastase

Chain A:

4.2.4 Score per residue for model 4

• Molecule 1: Macrophage metalloelastase

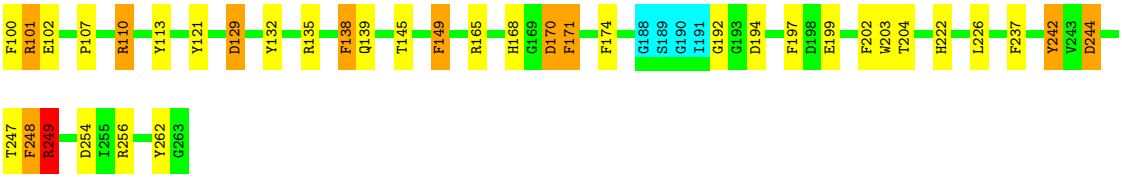
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: Macrophage metalloelastase

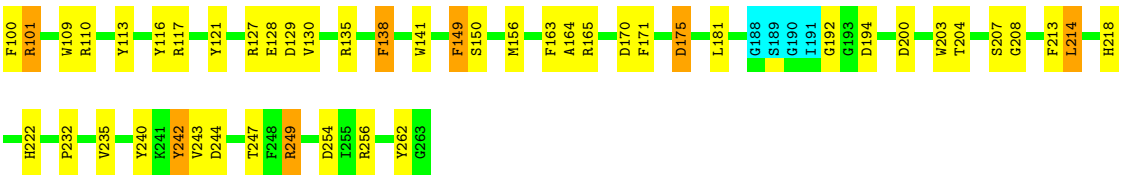
Chain A:



4.2.6 Score per residue for model 6

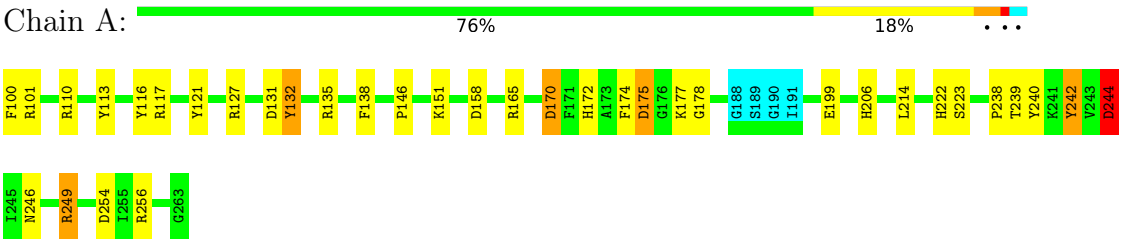
• Molecule 1: Macrophage metalloelastase

Chain A:



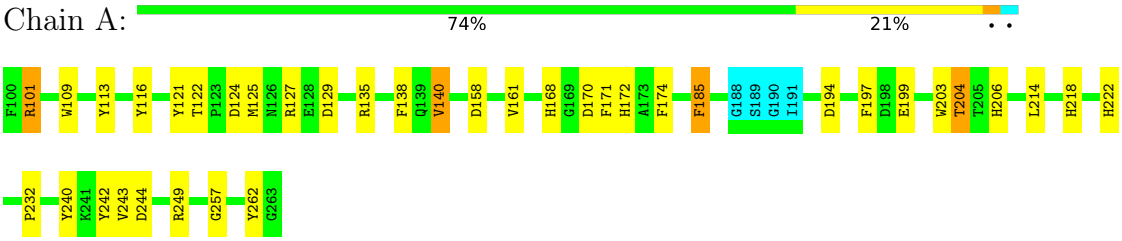
4.2.7 Score per residue for model 7

• Molecule 1: Macrophage metalloelastase



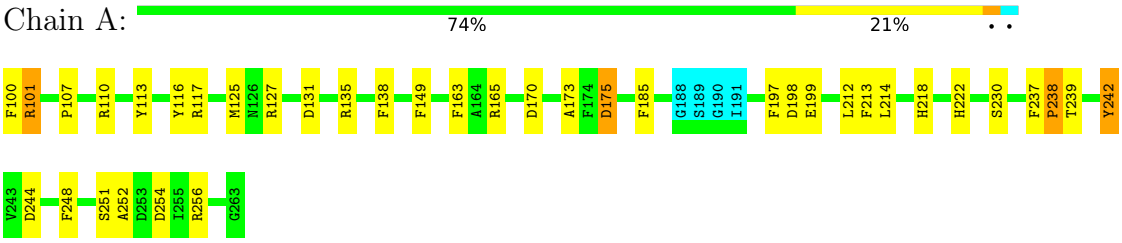
4.2.8 Score per residue for model 8

• Molecule 1: Macrophage metalloelastase



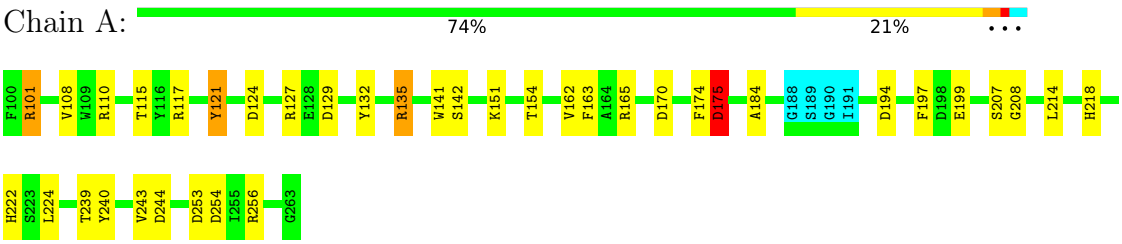
4.2.9 Score per residue for model 9

• Molecule 1: Macrophage metalloelastase



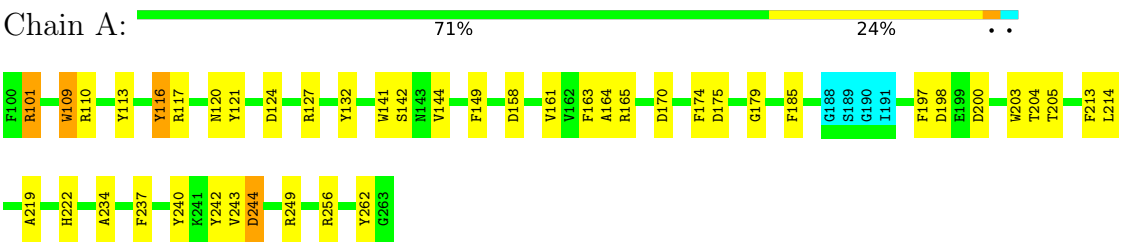
4.2.10 Score per residue for model 10

• Molecule 1: Macrophage metalloelastase



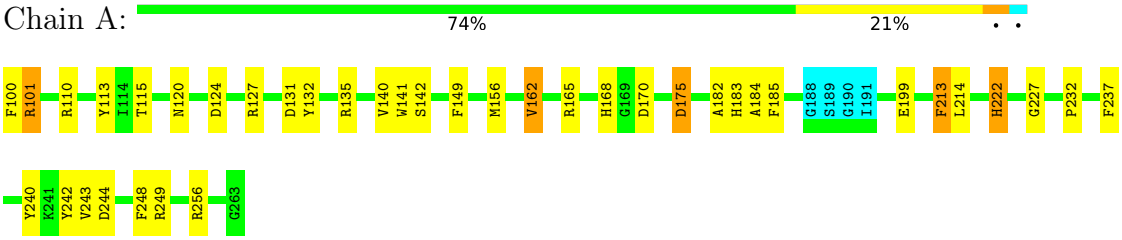
4.2.11 Score per residue for model 11

- Molecule 1: Macrophage metalloelastase



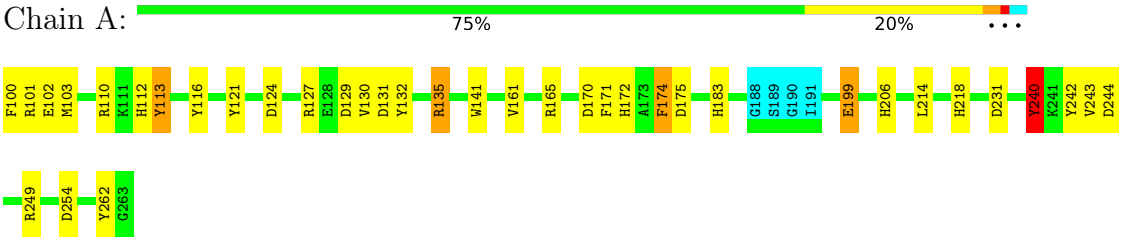
4.2.12 Score per residue for model 12

- Molecule 1: Macrophage metalloelastase



4.2.13 Score per residue for model 13

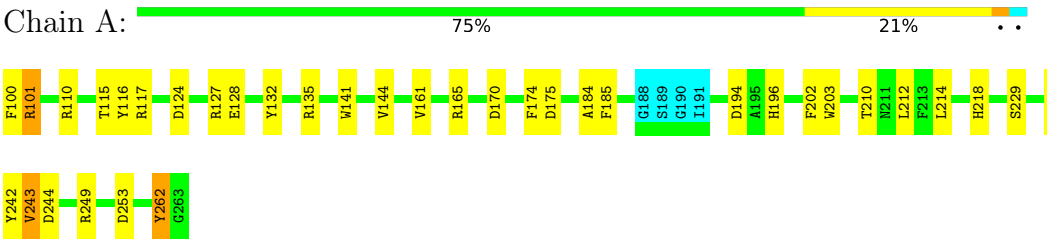
- Molecule 1: Macrophage metalloelastase



4.2.14 Score per residue for model 14

• Molecule 1: Macrophage metalloelastase

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 14 calculated structures, 14 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
GROMACS	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1762
Number of shifts mapped to atoms	1762
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	81%

6 Model quality

6.1 Standard geometry

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

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	0.58±0.01	0±0/1305 (0.0± 0.0%)	2.04±0.06	42±6/1768 (2.4± 0.4%)
All	All	0.58	0/18270 (0.0%)	2.05	584/24752 (2.4%)

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	5.1±1.9
All	All	0	71

There are no bond-length outliers.

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
1	A	249	ARG	NE-CZ-NH1	19.17	129.88	120.30	11	6
1	A	127	ARG	NE-CZ-NH2	-18.79	110.91	120.30	11	8
1	A	165	ARG	NE-CZ-NH2	-18.12	111.24	120.30	5	4
1	A	262	TYR	CB-CG-CD2	-17.25	110.65	121.00	14	4
1	A	240	TYR	CB-CG-CD1	-14.90	112.06	121.00	6	5
1	A	110	ARG	NE-CZ-NH2	-14.86	112.87	120.30	13	6
1	A	174	PHE	CB-CG-CD1	-14.06	110.95	120.80	8	6
1	A	113	TYR	CB-CG-CD2	-14.02	112.59	121.00	2	3
1	A	165	ARG	NE-CZ-NH1	14.01	127.31	120.30	3	8
1	A	101	ARG	NE-CZ-NH2	-13.97	113.31	120.30	12	7
1	A	117	ARG	NE-CZ-NH2	-12.67	113.97	120.30	3	5
1	A	135	ARG	NE-CZ-NH2	-12.59	114.00	120.30	7	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	256	ARG	NE-CZ-NH2	-12.30	114.15	120.30	11	5
1	A	101	ARG	NE-CZ-NH1	12.20	126.40	120.30	4	6
1	A	127	ARG	NE-CZ-NH1	12.07	126.33	120.30	9	6
1	A	110	ARG	NE-CZ-NH1	-11.95	114.33	120.30	12	7
1	A	135	ARG	NE-CZ-NH1	11.80	126.20	120.30	13	6
1	A	248	PHE	CB-CG-CD1	-11.62	112.66	120.80	1	3
1	A	100	PHE	CB-CG-CD2	11.57	128.90	120.80	9	5
1	A	254	ASP	CB-CG-OD2	-11.53	107.92	118.30	10	6
1	A	117	ARG	NE-CZ-NH1	10.99	125.80	120.30	3	3
1	A	132	TYR	CB-CG-CD2	-10.80	114.52	121.00	10	4
1	A	256	ARG	NE-CZ-NH1	10.79	125.69	120.30	11	4
1	A	113	TYR	CG-CD1-CE1	-10.52	112.89	121.30	9	2
1	A	113	TYR	CD1-CE1-CZ	-10.37	110.46	119.80	5	2
1	A	213	PHE	CB-CG-CD1	-10.26	113.62	120.80	6	3
1	A	249	ARG	NE-CZ-NH2	-10.21	115.19	120.30	11	6
1	A	163	PHE	CB-CG-CD2	10.18	127.93	120.80	11	2
1	A	175	ASP	CB-CG-OD1	10.08	127.37	118.30	12	8
1	A	113	TYR	CB-CG-CD1	-10.07	114.96	121.00	9	7
1	A	199	GLU	OE1-CD-OE2	-10.05	111.24	123.30	4	2
1	A	175	ASP	CB-CG-OD2	10.01	127.31	118.30	11	4
1	A	170	ASP	CB-CG-OD1	9.97	127.27	118.30	14	11
1	A	124	ASP	CB-CG-OD1	9.87	127.18	118.30	10	6
1	A	185	PHE	CB-CG-CD2	-9.86	113.90	120.80	14	3
1	A	194	ASP	CB-CG-OD1	9.75	127.08	118.30	2	6
1	A	113	TYR	CG-CD2-CE2	-9.56	113.66	121.30	13	2
1	A	156	MET	CG-SD-CE	9.52	115.43	100.20	6	1
1	A	116	TYR	CB-CG-CD1	-9.48	115.31	121.00	11	4
1	A	262	TYR	CB-CG-CD1	9.38	126.63	121.00	14	4
1	A	121	TYR	CB-CG-CD2	9.29	126.57	121.00	10	5
1	A	100	PHE	CB-CG-CD1	-9.26	114.32	120.80	9	3
1	A	116	TYR	CG-CD1-CE1	-9.17	113.97	121.30	4	1
1	A	170	ASP	OD1-CG-OD2	-9.04	106.13	123.30	8	14
1	A	242	TYR	CB-CG-CD1	-9.02	115.59	121.00	2	5
1	A	132	TYR	CB-CG-CD1	8.98	126.39	121.00	10	4
1	A	204	THR	CA-CB-CG2	8.97	124.96	112.40	8	3
1	A	161	VAL	CA-CB-CG1	8.94	124.31	110.90	14	2
1	A	170	ASP	CB-CG-OD2	8.93	126.34	118.30	11	10
1	A	102	GLU	OE1-CD-OE2	-8.90	112.62	123.30	13	5
1	A	202	PHE	CB-CG-CD2	-8.86	114.60	120.80	5	2
1	A	121	TYR	CB-CG-CD1	-8.83	115.70	121.00	3	4
1	A	253	ASP	CB-CG-OD2	-8.44	110.70	118.30	14	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	163	PHE	CB-CG-CD1	-8.39	114.93	120.80	11	2
1	A	101	ARG	CD-NE-CZ	8.38	135.32	123.60	14	1
1	A	254	ASP	CB-CG-OD1	-8.36	110.78	118.30	5	3
1	A	194	ASP	CB-CG-OD2	8.35	125.82	118.30	8	3
1	A	138	PHE	CB-CG-CD1	8.31	126.62	120.80	5	4
1	A	262	TYR	CZ-CE2-CD2	-8.26	112.37	119.80	4	2
1	A	174	PHE	CB-CG-CD2	-8.15	115.09	120.80	2	4
1	A	248	PHE	CB-CG-CD2	-8.13	115.11	120.80	5	3
1	A	141	TRP	CD1-NE1-CE2	8.13	116.32	109.00	14	4
1	A	115	THR	CA-CB-CG2	8.11	123.76	112.40	1	3
1	A	231	ASP	CB-CG-OD1	-8.08	111.03	118.30	13	1
1	A	141	TRP	NE1-CE2-CD2	-7.98	99.32	107.30	14	3
1	A	203	TRP	CG-CD2-CE3	7.91	141.02	133.90	11	2
1	A	116	TYR	CB-CG-CD2	-7.88	116.27	121.00	3	5
1	A	141	TRP	NE1-CE2-CZ2	7.83	139.01	130.40	14	2
1	A	161	VAL	CA-CB-CG2	7.82	122.62	110.90	13	2
1	A	213	PHE	CB-CG-CD2	-7.77	115.36	120.80	9	3
1	A	238	PRO	N-CA-CB	7.76	112.61	103.30	2	3
1	A	237	PHE	CB-CG-CD2	7.72	126.20	120.80	11	1
1	A	131	ASP	CB-CG-OD2	-7.68	111.39	118.30	13	2
1	A	240	TYR	CB-CG-CD2	-7.67	116.40	121.00	8	3
1	A	140	VAL	CA-CB-CG1	7.62	122.33	110.90	4	3
1	A	185	PHE	CB-CG-CD1	7.59	126.11	120.80	14	2
1	A	116	TYR	CD1-CE1-CZ	7.50	126.55	119.80	4	2
1	A	129	ASP	CB-CG-OD1	7.49	125.04	118.30	5	6
1	A	138	PHE	CB-CG-CD2	-7.48	115.57	120.80	7	3
1	A	109	TRP	CD1-NE1-CE2	7.41	115.66	109.00	11	3
1	A	256	ARG	CD-NE-CZ	7.39	133.95	123.60	9	1
1	A	184	ALA	N-CA-CB	-7.39	99.75	110.10	12	2
1	A	203	TRP	CD1-NE1-CE2	7.39	115.65	109.00	1	3
1	A	232	PRO	N-CA-CB	7.29	112.05	103.30	1	3
1	A	135	ARG	CD-NE-CZ	7.25	133.75	123.60	14	2
1	A	197	PHE	CB-CG-CD2	-7.20	115.76	120.80	8	2
1	A	203	TRP	CD1-CG-CD2	7.18	112.04	106.30	5	2
1	A	210	THR	CA-CB-CG2	7.10	122.34	112.40	14	1
1	A	194	ASP	OD1-CG-OD2	-7.09	109.82	123.30	8	2
1	A	109	TRP	NE1-CE2-CD2	-7.07	100.23	107.30	11	3
1	A	262	TYR	CG-CD1-CE1	-7.07	115.64	121.30	6	1
1	A	253	ASP	CB-CG-OD1	7.06	124.66	118.30	10	3
1	A	197	PHE	CB-CG-CD1	7.04	125.73	120.80	8	3
1	A	149	PHE	CZ-CE2-CD2	-7.00	111.70	120.10	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	122	THR	CA-CB-CG2	6.95	122.13	112.40	8	1
1	A	127	ARG	NH1-CZ-NH2	6.94	127.04	119.40	11	2
1	A	132	TYR	CG-CD2-CE2	-6.93	115.75	121.30	11	2
1	A	244	ASP	CB-CG-OD1	-6.93	112.06	118.30	7	1
1	A	141	TRP	CB-CG-CD2	6.91	135.58	126.60	11	1
1	A	201	GLU	CB-CA-C	-6.90	96.60	110.40	2	1
1	A	222	HIS	CA-CB-CG	6.90	125.32	113.60	4	2
1	A	149	PHE	CB-CG-CD1	-6.89	115.98	120.80	9	4
1	A	171	PHE	CB-CG-CD2	-6.83	116.02	120.80	1	1
1	A	239	THR	N-CA-CB	-6.81	97.36	110.30	7	1
1	A	172	HIS	CA-CB-CG	6.79	125.15	113.60	7	2
1	A	235	VAL	CA-CB-CG1	6.78	121.06	110.90	14	2
1	A	242	TYR	CB-CG-CD2	-6.73	116.96	121.00	14	5
1	A	141	TRP	CB-CG-CD1	-6.61	118.40	127.00	11	1
1	A	101	ARG	NH1-CZ-NH2	6.58	126.63	119.40	6	2
1	A	158	ASP	CB-CG-OD2	-6.54	112.42	118.30	7	3
1	A	218	HIS	CA-CB-CG	6.54	124.71	113.60	13	5
1	A	239	THR	CA-CB-CG2	6.51	121.52	112.40	10	2
1	A	141	TRP	CZ3-CH2-CZ2	-6.48	113.83	121.60	6	2
1	A	175	ASP	OD1-CG-OD2	-6.47	111.01	123.30	12	6
1	A	131	ASP	CB-CG-OD1	6.45	124.10	118.30	9	3
1	A	240	TYR	CG-CD1-CE1	-6.45	116.14	121.30	6	3
1	A	164	ALA	CB-CA-C	6.43	119.75	110.10	4	2
1	A	168	HIS	C-N-CA	6.41	135.76	122.30	5	2
1	A	110	ARG	CD-NE-CZ	6.41	132.57	123.60	12	2
1	A	262	TYR	CG-CD2-CE2	-6.40	116.18	121.30	3	3
1	A	210	THR	O-C-N	-6.39	112.47	122.70	4	1
1	A	174	PHE	CG-CD2-CE2	-6.35	113.81	120.80	8	1
1	A	174	PHE	CD1-CG-CD2	6.33	126.52	118.30	11	2
1	A	227	GLY	N-CA-C	-6.28	97.41	113.10	12	1
1	A	248	PHE	CG-CD1-CE1	-6.25	113.92	120.80	9	1
1	A	117	ARG	CD-NE-CZ	6.25	132.34	123.60	6	2
1	A	130	VAL	CA-CB-CG1	6.23	120.24	110.90	13	2
1	A	151	LYS	C-N-CA	6.23	137.27	121.70	7	1
1	A	174	PHE	CB-CA-C	6.22	122.84	110.40	14	4
1	A	237	PHE	CB-CG-CD1	6.21	125.15	120.80	2	3
1	A	216	ALA	CB-CA-C	-6.21	100.79	110.10	4	1
1	A	158	ASP	CB-CG-OD1	-6.20	112.72	118.30	3	1
1	A	254	ASP	CA-CB-CG	6.18	126.99	113.40	4	1
1	A	183	HIS	CA-CB-CG	6.17	124.10	113.60	13	1
1	A	113	TYR	CZ-CE2-CD2	6.16	125.35	119.80	13	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	128	GLU	OE1-CD-OE2	-6.14	115.93	123.30	14	2
1	A	212	LEU	CB-CG-CD1	6.14	121.44	111.00	14	2
1	A	243	VAL	CA-CB-CG2	6.13	120.10	110.90	14	1
1	A	162	VAL	CA-CB-CG1	6.13	120.10	110.90	3	3
1	A	247	THR	O-C-N	-6.11	112.92	122.70	6	2
1	A	223	SER	N-CA-CB	-6.10	101.34	110.50	7	1
1	A	202	PHE	CB-CG-CD1	-6.05	116.56	120.80	14	1
1	A	116	TYR	CA-CB-CG	6.04	124.88	113.40	3	1
1	A	200	ASP	CB-CG-OD2	-6.03	112.87	118.30	6	1
1	A	200	ASP	CB-CG-OD1	6.03	123.73	118.30	4	1
1	A	175	ASP	CB-CA-C	6.01	122.42	110.40	4	1
1	A	165	ARG	CB-CA-C	5.97	122.35	110.40	9	2
1	A	116	TYR	CB-CA-C	5.97	122.34	110.40	6	1
1	A	150	SER	N-CA-CB	-5.96	101.56	110.50	6	1
1	A	231	ASP	CB-CG-OD2	5.95	123.65	118.30	13	1
1	A	229	SER	N-CA-CB	-5.91	101.63	110.50	14	1
1	A	135	ARG	NH1-CZ-NH2	5.89	125.89	119.40	12	1
1	A	165	ARG	NH1-CZ-NH2	5.88	125.86	119.40	5	1
1	A	205	THR	CA-CB-OG1	5.84	121.26	109.00	11	1
1	A	141	TRP	CE2-CD2-CG	5.82	111.95	107.30	14	3
1	A	149	PHE	CB-CG-CD2	-5.81	116.73	120.80	6	2
1	A	198	ASP	CB-CG-OD2	-5.80	113.08	118.30	1	2
1	A	132	TYR	CG-CD1-CE1	-5.79	116.67	121.30	2	1
1	A	219	ALA	N-CA-CB	-5.77	102.02	110.10	11	1
1	A	262	TYR	CA-CB-CG	5.77	124.36	113.40	1	1
1	A	102	GLU	N-CA-CB	-5.76	100.24	110.60	13	1
1	A	145	THR	CA-CB-CG2	5.73	120.43	112.40	5	1
1	A	130	VAL	CG1-CB-CG2	-5.71	101.77	110.90	2	1
1	A	124	ASP	CB-CG-OD2	5.68	123.41	118.30	4	2
1	A	109	TRP	CE2-CD2-CG	5.65	111.82	107.30	8	1
1	A	203	TRP	CG-CD1-NE1	-5.63	104.47	110.10	5	2
1	A	103	MET	N-CA-CB	-5.63	100.46	110.60	4	1
1	A	192	GLY	CA-C-N	5.62	127.43	116.20	5	1
1	A	249	ARG	NH1-CZ-NH2	-5.61	113.23	119.40	3	1
1	A	129	ASP	CB-CG-OD2	5.57	123.31	118.30	2	3
1	A	108	VAL	CA-CB-CG2	5.56	119.24	110.90	1	2
1	A	113	TYR	CD1-CG-CD2	5.56	124.01	117.90	9	1
1	A	168	HIS	CB-CA-C	5.56	121.51	110.40	12	1
1	A	171	PHE	CB-CG-CD1	-5.55	116.92	120.80	5	1
1	A	124	ASP	OD1-CG-OD2	-5.55	112.76	123.30	8	1
1	A	257	GLY	O-C-N	5.54	131.57	122.70	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	107	PRO	N-CD-CG	5.53	111.50	103.20	3	1
1	A	112	HIS	C-N-CA	5.52	135.50	121.70	13	1
1	A	226	LEU	CB-CG-CD2	5.51	120.37	111.00	5	1
1	A	163	PHE	CZ-CE2-CD2	-5.49	113.51	120.10	6	1
1	A	132	TYR	CD1-CG-CD2	5.48	123.93	117.90	14	1
1	A	107	PRO	C-N-CA	5.48	135.39	121.70	9	1
1	A	240	TYR	CD1-CG-CD2	5.47	123.92	117.90	6	1
1	A	125	MET	N-CA-CB	5.47	120.45	110.60	9	1
1	A	174	PHE	CG-CD1-CE1	5.44	126.79	120.80	4	2
1	A	150	SER	CB-CA-C	5.42	120.39	110.10	3	1
1	A	230	SER	N-CA-CB	-5.41	102.38	110.50	9	2
1	A	203	TRP	NE1-CE2-CZ2	5.41	136.35	130.40	8	1
1	A	128	GLU	O-C-N	-5.41	114.05	122.70	6	1
1	A	161	VAL	CG1-CB-CG2	-5.39	102.27	110.90	2	1
1	A	208	GLY	CA-C-O	-5.37	110.94	120.60	4	1
1	A	203	TRP	CA-CB-CG	5.37	123.90	113.70	6	1
1	A	123	PRO	C-N-CA	5.35	135.07	121.70	4	1
1	A	162	VAL	CB-CA-C	5.34	121.55	111.40	4	1
1	A	241	LYS	CB-CA-C	5.33	121.06	110.40	1	1
1	A	249	ARG	CD-NE-CZ	5.33	131.06	123.60	12	1
1	A	208	GLY	N-CA-C	-5.32	99.79	113.10	10	1
1	A	232	PRO	N-CD-CG	5.32	111.17	103.20	12	2
1	A	182	ALA	CB-CA-C	5.31	118.07	110.10	12	1
1	A	242	TYR	C-N-CA	5.30	134.95	121.70	13	2
1	A	132	TYR	CZ-CE2-CD2	5.30	124.57	119.80	11	1
1	A	149	PHE	CD1-CG-CD2	5.29	125.18	118.30	9	1
1	A	149	PHE	CG-CD1-CE1	-5.29	114.98	120.80	9	1
1	A	116	TYR	CG-CD2-CE2	-5.29	117.07	121.30	1	1
1	A	118	ILE	N-CA-C	-5.28	96.73	111.00	4	1
1	A	235	VAL	CG1-CB-CG2	-5.28	102.46	110.90	6	1
1	A	202	PHE	CG-CD2-CE2	-5.27	115.00	120.80	14	1
1	A	125	MET	CB-CA-C	5.24	120.88	110.40	8	1
1	A	144	VAL	CA-CB-CG2	5.24	118.76	110.90	14	2
1	A	129	ASP	N-CA-CB	5.24	120.03	110.60	3	1
1	A	240	TYR	CZ-CE2-CD2	-5.24	115.09	119.80	12	1
1	A	109	TRP	CB-CG-CD1	-5.23	120.20	127.00	2	1
1	A	240	TYR	C-N-CA	5.23	134.78	121.70	10	1
1	A	120	ASN	CB-CA-C	5.23	120.86	110.40	11	1
1	A	141	TRP	CH2-CZ2-CE2	5.22	122.62	117.40	6	2
1	A	251	SER	N-CA-CB	-5.21	102.68	110.50	9	1
1	A	165	ARG	CD-NE-CZ	5.20	130.88	123.60	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	163	PHE	CG-CD2-CE2	5.19	126.51	120.80	6	1
1	A	130	VAL	CA-CB-CG2	5.18	118.67	110.90	6	1
1	A	212	LEU	O-C-N	-5.17	114.42	122.70	4	1
1	A	215	THR	OG1-CB-CG2	-5.17	98.11	110.00	4	1
1	A	246	ASN	CB-CA-C	-5.15	100.10	110.40	7	1
1	A	256	ARG	C-N-CA	5.15	133.11	122.30	12	1
1	A	244	ASP	CB-CG-OD2	5.14	122.93	118.30	11	1
1	A	240	TYR	CG-CD2-CE2	-5.14	117.19	121.30	10	1
1	A	184	ALA	CB-CA-C	-5.14	102.39	110.10	14	1
1	A	101	ARG	C-N-CA	5.13	134.51	121.70	14	1
1	A	122	THR	N-CA-CB	-5.12	100.58	110.30	8	1
1	A	181	LEU	CB-CG-CD1	5.11	119.68	111.00	6	1
1	A	173	ALA	N-CA-CB	5.11	117.25	110.10	9	1
1	A	109	TRP	NE1-CE2-CZ2	5.11	136.02	130.40	11	2
1	A	154	THR	CA-CB-CG2	5.10	119.54	112.40	10	1
1	A	120	ASN	N-CA-CB	5.10	119.78	110.60	12	1
1	A	192	GLY	C-N-CA	5.09	132.99	122.30	6	1
1	A	242	TYR	CG-CD1-CE1	5.09	125.37	121.30	12	1
1	A	110	ARG	C-N-CA	5.08	134.40	121.70	7	1
1	A	121	TYR	CG-CD1-CE1	-5.08	117.24	121.30	11	1
1	A	164	ALA	O-C-N	-5.08	114.58	122.70	11	1
1	A	222	HIS	CG-ND1-CE1	-5.08	99.10	105.70	12	1
1	A	217	VAL	O-C-N	-5.08	114.58	122.70	4	1
1	A	199	GLU	CA-CB-CG	5.08	124.57	113.40	13	1
1	A	261	LEU	CB-CA-C	-5.06	100.59	110.20	2	1
1	A	206	HIS	CA-CB-CG	5.06	122.20	113.60	8	1
1	A	195	ALA	N-CA-CB	-5.05	103.03	110.10	4	1
1	A	174	PHE	C-N-CA	5.03	134.28	121.70	1	1
1	A	262	TYR	CB-CA-C	5.01	120.42	110.40	2	1
1	A	173	ALA	CB-CA-C	5.00	117.61	110.10	3	1
1	A	185	PHE	C-N-CA	5.00	132.80	122.30	9	1
1	A	234	ALA	C-N-CA	5.00	134.20	121.70	11	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	242	TYR	Sidechain,Peptide	7
1	A	121	TYR	Sidechain	5
1	A	204	THR	Peptide	5

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	262	TYR	Sidechain	5
1	A	240	TYR	Sidechain,Peptide	4
1	A	113	TYR	Sidechain	3
1	A	116	TYR	Mainchain,Sidechain	3
1	A	132	TYR	Sidechain	3
1	A	110	ARG	Sidechain	2
1	A	248	PHE	Sidechain,Peptide	2
1	A	185	PHE	Sidechain	2
1	A	135	ARG	Sidechain	2
1	A	197	PHE	Sidechain	2
1	A	159	ILE	Peptide	1
1	A	256	ARG	Sidechain	1
1	A	164	ALA	Peptide	1
1	A	199	GLU	Sidechain	1
1	A	202	PHE	Sidechain	1
1	A	222	HIS	Sidechain	1
1	A	249	ARG	Sidechain	1
1	A	171	PHE	Sidechain	1
1	A	206	HIS	Sidechain	1
1	A	172	HIS	Sidechain	1
1	A	117	ARG	Sidechain	1
1	A	163	PHE	Sidechain	1
1	A	252	ALA	Mainchain	1
1	A	101	ARG	Sidechain	1
1	A	151	LYS	Peptide	1
1	A	218	HIS	Sidechain	1
1	A	224	LEU	Mainchain	1
1	A	183	HIS	Sidechain	1
1	A	237	PHE	Sidechain	1
1	A	100	PHE	Sidechain	1
1	A	127	ARG	Mainchain	1
1	A	174	PHE	Peptide	1
1	A	196	HIS	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	1265	1199	1196	2±1
4	A	5750	0	9000	131±13
All	All	98280	16786	142744	1846

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 8.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:388:PX4:H39	4:A:411:PX4:H17	0.99	1.35	4	1
4:A:337:PX4:H47	4:A:353:PX4:H15	0.93	1.41	8	2
4:A:413:PX4:H24	4:A:430:PX4:H63	0.92	1.40	10	1
4:A:320:PX4:H20	4:A:359:PX4:H57	0.92	1.42	5	1
4:A:368:PX4:H22	4:A:369:PX4:H51	0.90	1.40	6	1
4:A:342:PX4:H24	4:A:352:PX4:H47	0.88	1.43	11	1
4:A:378:PX4:H16	4:A:417:PX4:H47	0.85	1.46	7	9
4:A:309:PX4:H59	4:A:324:PX4:H57	0.84	1.50	12	1
4:A:355:PX4:H48	4:A:356:PX4:H14	0.83	1.49	4	2
4:A:332:PX4:H61	4:A:349:PX4:H51	0.83	1.51	6	1
4:A:329:PX4:H70	4:A:382:PX4:H26	0.82	1.50	7	1
4:A:316:PX4:H20	4:A:364:PX4:H47	0.82	1.49	9	1
4:A:386:PX4:H28	4:A:394:PX4:H50	0.82	1.50	11	1
4:A:313:PX4:H18	4:A:318:PX4:H46	0.81	1.50	9	2
4:A:416:PX4:H21	4:A:425:PX4:H46	0.81	1.51	11	1
4:A:335:PX4:H21	4:A:343:PX4:H22	0.81	1.52	5	1
4:A:317:PX4:H17	4:A:325:PX4:H52	0.81	1.53	9	1
4:A:384:PX4:H60	4:A:385:PX4:H35	0.80	1.54	2	1
4:A:387:PX4:H47	4:A:411:PX4:H17	0.79	1.54	12	1
4:A:340:PX4:H31	4:A:340:PX4:H66	0.79	1.55	5	1
4:A:387:PX4:H24	4:A:394:PX4:H53	0.78	1.55	1	2
4:A:404:PX4:H34	4:A:419:PX4:H22	0.78	1.55	8	1
4:A:376:PX4:H54	4:A:385:PX4:H17	0.77	1.57	13	1
4:A:317:PX4:H47	4:A:342:PX4:H69	0.77	1.57	12	1
4:A:421:PX4:H31	4:A:422:PX4:H39	0.77	1.55	2	1
4:A:368:PX4:H25	4:A:425:PX4:H42	0.76	1.58	4	1
4:A:310:PX4:H16	4:A:363:PX4:H20	0.76	1.56	9	2
4:A:413:PX4:H50	4:A:422:PX4:H33	0.75	1.58	2	1
4:A:393:PX4:H22	4:A:394:PX4:H19	0.75	1.58	7	1
4:A:321:PX4:H20	4:A:354:PX4:H48	0.75	1.56	10	1
4:A:326:PX4:H50	4:A:351:PX4:H18	0.75	1.58	4	1
4:A:400:PX4:H51	4:A:409:PX4:H20	0.75	1.57	12	1
4:A:321:PX4:H41	4:A:354:PX4:H59	0.75	1.58	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:417:PX4:H31	4:A:426:PX4:H61	0.74	1.58	6	1
4:A:398:PX4:H16	4:A:407:PX4:H49	0.74	1.58	14	1
4:A:330:PX4:H22	4:A:335:PX4:H19	0.74	1.60	2	1
4:A:345:PX4:H48	4:A:353:PX4:H46	0.74	1.59	4	1
4:A:330:PX4:H60	4:A:357:PX4:H24	0.73	1.60	10	2
4:A:306:PX4:H23	4:A:321:PX4:H39	0.73	1.60	5	1
4:A:332:PX4:H31	4:A:332:PX4:H51	0.73	1.58	7	1
4:A:392:PX4:H18	4:A:393:PX4:H50	0.72	1.61	1	1
4:A:395:PX4:H53	4:A:405:PX4:H22	0.72	1.60	4	1
4:A:317:PX4:H17	4:A:325:PX4:H49	0.72	1.60	1	1
4:A:403:PX4:H10	4:A:427:PX4:H49	0.72	1.61	3	2
4:A:325:PX4:H30	4:A:334:PX4:H18	0.72	1.60	4	1
4:A:376:PX4:H50	4:A:385:PX4:H17	0.72	1.60	11	2
4:A:383:PX4:H65	4:A:399:PX4:H31	0.72	1.60	8	1
4:A:317:PX4:H46	4:A:324:PX4:H17	0.72	1.60	8	1
4:A:367:PX4:H28	4:A:424:PX4:H52	0.72	1.62	4	1
4:A:371:PX4:H59	4:A:379:PX4:H33	0.72	1.61	4	1
4:A:323:PX4:H68	4:A:367:PX4:H40	0.72	1.62	3	1
4:A:378:PX4:H63	4:A:417:PX4:H62	0.72	1.62	11	1
4:A:321:PX4:H38	4:A:328:PX4:H57	0.72	1.61	13	1
4:A:385:PX4:H52	4:A:386:PX4:H26	0.71	1.61	14	1
4:A:383:PX4:H61	4:A:399:PX4:H29	0.71	1.60	6	1
4:A:402:PX4:H38	4:A:404:PX4:H62	0.71	1.59	14	1
4:A:376:PX4:H64	4:A:392:PX4:H29	0.71	1.60	5	1
4:A:387:PX4:H65	4:A:411:PX4:H54	0.71	1.63	8	1
4:A:409:PX4:H33	4:A:410:PX4:H46	0.71	1.60	2	1
4:A:332:PX4:H43	4:A:363:PX4:H72	0.71	1.63	12	1
4:A:402:PX4:H60	4:A:413:PX4:H41	0.71	1.63	7	1
4:A:363:PX4:H1	4:A:364:PX4:H20	0.71	1.61	11	1
4:A:391:PX4:H64	4:A:408:PX4:H55	0.71	1.63	7	1
4:A:321:PX4:H38	4:A:412:PX4:H43	0.70	1.62	14	1
4:A:370:PX4:H19	4:A:403:PX4:H17	0.70	1.63	11	2
4:A:419:PX4:H49	4:A:427:PX4:H49	0.70	1.63	13	1
4:A:308:PX4:H62	4:A:311:PX4:H41	0.70	1.64	13	1
4:A:325:PX4:H31	4:A:332:PX4:H25	0.70	1.63	11	1
4:A:306:PX4:H56	4:A:321:PX4:H55	0.69	1.64	13	1
4:A:384:PX4:H42	4:A:385:PX4:H43	0.69	1.62	8	1
4:A:317:PX4:H16	4:A:351:PX4:H24	0.69	1.64	14	1
4:A:408:PX4:H17	4:A:415:PX4:H20	0.69	1.64	8	1
4:A:322:PX4:H50	4:A:336:PX4:H27	0.69	1.63	1	1
4:A:332:PX4:H33	4:A:347:PX4:H62	0.69	1.64	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:374:PX4:H49	4:A:382:PX4:H46	0.69	1.62	8	2
4:A:358:PX4:H23	4:A:363:PX4:H53	0.69	1.64	9	1
4:A:315:PX4:H17	4:A:316:PX4:H49	0.69	1.64	13	1
4:A:360:PX4:H70	4:A:419:PX4:H41	0.69	1.62	4	1
4:A:399:PX4:H63	4:A:399:PX4:H29	0.69	1.64	2	1
4:A:368:PX4:H17	4:A:369:PX4:H53	0.69	1.63	9	1
4:A:331:PX4:H58	4:A:339:PX4:H22	0.69	1.63	4	1
4:A:396:PX4:H38	4:A:402:PX4:H41	0.69	1.64	12	1
4:A:422:PX4:H36	4:A:423:PX4:H23	0.68	1.65	5	1
4:A:388:PX4:H54	4:A:395:PX4:H30	0.68	1.65	12	1
4:A:368:PX4:H47	4:A:369:PX4:H56	0.68	1.63	1	1
4:A:429:PX4:H55	4:A:429:PX4:H30	0.68	1.63	11	1
4:A:337:PX4:H50	4:A:353:PX4:H21	0.68	1.64	4	1
4:A:328:PX4:H70	4:A:412:PX4:H70	0.68	1.65	13	1
4:A:395:PX4:H55	4:A:404:PX4:H46	0.68	1.66	1	1
4:A:416:PX4:H55	4:A:418:PX4:H30	0.68	1.66	12	1
4:A:388:PX4:H38	4:A:411:PX4:H46	0.68	1.65	5	1
4:A:306:PX4:H14	4:A:321:PX4:H28	0.68	1.66	12	1
4:A:316:PX4:H14	4:A:320:PX4:H22	0.68	1.64	10	1
4:A:378:PX4:H51	4:A:418:PX4:H50	0.68	1.65	13	1
4:A:376:PX4:H67	4:A:385:PX4:H30	0.68	1.64	2	1
4:A:391:PX4:H40	4:A:408:PX4:H42	0.67	1.66	2	1
4:A:370:PX4:H22	4:A:403:PX4:H17	0.67	1.65	9	2
4:A:306:PX4:H20	4:A:329:PX4:H52	0.67	1.66	9	1
4:A:346:PX4:H22	4:A:354:PX4:H21	0.67	1.65	9	1
4:A:331:PX4:H63	4:A:340:PX4:H71	0.67	1.67	14	1
4:A:330:PX4:H44	4:A:344:PX4:H45	0.67	1.66	12	1
4:A:312:PX4:H16	4:A:359:PX4:H5	0.67	1.64	14	1
4:A:384:PX4:H2	4:A:385:PX4:H18	0.67	1.66	1	4
4:A:331:PX4:H33	4:A:340:PX4:H69	0.67	1.66	3	1
4:A:315:PX4:H42	4:A:425:PX4:H31	0.67	1.67	4	1
4:A:332:PX4:H25	4:A:390:PX4:H41	0.67	1.67	6	1
4:A:308:PX4:H38	4:A:311:PX4:H69	0.67	1.65	12	1
4:A:417:PX4:H19	4:A:426:PX4:H24	0.67	1.66	12	1
4:A:424:PX4:H53	4:A:425:PX4:H22	0.66	1.67	2	1
4:A:331:PX4:H35	4:A:397:PX4:H44	0.66	1.66	7	1
4:A:395:PX4:H49	4:A:396:PX4:H24	0.66	1.67	14	1
4:A:350:PX4:H56	4:A:364:PX4:H37	0.66	1.66	3	1
4:A:371:PX4:H61	4:A:372:PX4:H27	0.66	1.68	4	1
4:A:306:PX4:H56	4:A:361:PX4:H59	0.66	1.66	5	1
4:A:311:PX4:H53	4:A:316:PX4:H20	0.66	1.68	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:378:PX4:H56	4:A:417:PX4:H58	0.66	1.68	8	2
4:A:313:PX4:H49	4:A:328:PX4:H17	0.65	1.65	4	1
4:A:326:PX4:H28	4:A:350:PX4:H24	0.65	1.68	5	1
4:A:391:PX4:H28	4:A:414:PX4:H46	0.65	1.69	5	1
4:A:311:PX4:H65	4:A:359:PX4:H71	0.65	1.66	7	1
4:A:383:PX4:H50	4:A:399:PX4:H17	0.65	1.67	8	1
4:A:380:PX4:H56	4:A:387:PX4:H50	0.65	1.68	11	1
4:A:311:PX4:H10	4:A:359:PX4:H51	0.65	1.68	2	1
4:A:373:PX4:H26	4:A:381:PX4:H53	0.65	1.68	9	1
4:A:345:PX4:H40	4:A:345:PX4:H64	0.65	1.69	4	1
4:A:321:PX4:H50	4:A:354:PX4:H27	0.65	1.66	6	1
4:A:316:PX4:H51	4:A:320:PX4:H27	0.65	1.69	12	1
4:A:417:PX4:H31	4:A:426:PX4:H37	0.65	1.67	13	1
4:A:387:PX4:H16	4:A:394:PX4:H9	0.65	1.69	2	1
4:A:356:PX4:H10	4:A:356:PX4:H16	0.65	1.68	8	1
4:A:333:PX4:H56	4:A:341:PX4:H54	0.65	1.68	12	1
4:A:382:PX4:H19	4:A:428:PX4:H23	0.64	1.69	1	1
4:A:388:PX4:H20	4:A:411:PX4:H14	0.64	1.70	3	1
4:A:421:PX4:H22	4:A:422:PX4:H26	0.64	1.68	6	1
4:A:306:PX4:H18	4:A:322:PX4:H51	0.64	1.69	13	1
4:A:317:PX4:H55	4:A:324:PX4:H31	0.64	1.69	14	1
4:A:354:PX4:H50	4:A:360:PX4:H55	0.64	1.69	4	1
4:A:371:PX4:H20	4:A:379:PX4:H21	0.64	1.68	14	1
4:A:385:PX4:H71	4:A:392:PX4:H30	0.64	1.69	5	1
4:A:326:PX4:O8	4:A:351:PX4:H17	0.64	1.91	6	1
4:A:314:PX4:H34	4:A:356:PX4:H33	0.64	1.67	7	1
4:A:403:PX4:H7	4:A:427:PX4:H52	0.64	1.68	9	1
4:A:418:PX4:H42	4:A:422:PX4:H59	0.64	1.68	1	1
4:A:307:PX4:H60	4:A:349:PX4:H45	0.64	1.69	14	1
4:A:360:PX4:H44	4:A:412:PX4:H60	0.64	1.69	4	1
4:A:335:PX4:H48	4:A:343:PX4:H21	0.64	1.67	11	1
4:A:406:PX4:H48	4:A:421:PX4:H53	0.64	1.69	12	1
4:A:311:PX4:H52	4:A:320:PX4:H24	0.64	1.68	5	1
4:A:317:PX4:H48	4:A:342:PX4:H54	0.64	1.69	5	1
4:A:391:PX4:H43	4:A:394:PX4:H34	0.64	1.70	5	1
4:A:371:PX4:H16	4:A:379:PX4:H20	0.64	1.70	14	2
4:A:391:PX4:H48	4:A:408:PX4:H16	0.64	1.69	2	3
4:A:306:PX4:H38	4:A:321:PX4:H43	0.64	1.68	12	1
4:A:403:PX4:H47	4:A:427:PX4:H48	0.64	1.68	12	1
4:A:345:PX4:H37	4:A:353:PX4:H64	0.64	1.68	1	1
4:A:395:PX4:H19	4:A:398:PX4:H54	0.64	1.68	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:387:PX4:H46	4:A:388:PX4:H37	0.64	1.68	6	1
4:A:308:PX4:H34	4:A:314:PX4:H58	0.64	1.70	8	1
4:A:404:PX4:H34	4:A:419:PX4:H48	0.63	1.70	3	1
4:A:409:PX4:H41	4:A:410:PX4:H24	0.63	1.70	4	1
4:A:404:PX4:H39	4:A:419:PX4:H30	0.63	1.68	9	1
4:A:385:PX4:H32	4:A:386:PX4:H32	0.63	1.70	7	1
4:A:350:PX4:H50	4:A:363:PX4:H51	0.63	1.68	11	2
4:A:421:PX4:H39	4:A:423:PX4:H33	0.63	1.68	11	1
4:A:404:PX4:H49	4:A:413:PX4:H21	0.63	1.68	5	1
4:A:424:PX4:H48	4:A:425:PX4:H21	0.63	1.70	9	1
4:A:313:PX4:H22	4:A:318:PX4:H51	0.63	1.70	11	1
4:A:324:PX4:H48	4:A:341:PX4:H3	0.63	1.69	8	1
4:A:322:PX4:H17	4:A:336:PX4:H23	0.63	1.70	11	1
4:A:355:PX4:H72	4:A:356:PX4:H53	0.63	1.70	3	1
4:A:428:PX4:H61	4:A:430:PX4:H29	0.63	1.71	7	1
4:A:410:PX4:H62	4:A:426:PX4:H37	0.63	1.69	4	1
4:A:382:PX4:H22	4:A:428:PX4:H32	0.63	1.68	5	1
4:A:320:PX4:H17	4:A:359:PX4:H56	0.63	1.71	7	1
4:A:408:PX4:H47	4:A:415:PX4:H21	0.63	1.70	9	1
4:A:395:PX4:H47	4:A:396:PX4:H20	0.63	1.71	12	1
4:A:363:PX4:H20	4:A:364:PX4:H33	0.63	1.69	1	1
4:A:372:PX4:H38	4:A:378:PX4:H42	0.63	1.70	13	1
4:A:311:PX4:H50	4:A:316:PX4:H19	0.63	1.71	14	1
4:A:325:PX4:H24	4:A:340:PX4:H53	0.63	1.70	5	1
4:A:362:PX4:O2	4:A:362:PX4:H13	0.62	1.93	11	1
4:A:370:PX4:H54	4:A:411:PX4:H50	0.62	1.71	12	1
4:A:308:PX4:H22	4:A:364:PX4:H14	0.62	1.71	3	1
4:A:320:PX4:H68	4:A:417:PX4:H72	0.62	1.71	1	1
4:A:353:PX4:H39	4:A:366:PX4:H26	0.62	1.70	1	1
4:A:375:PX4:H55	4:A:429:PX4:H41	0.62	1.70	5	1
4:A:377:PX4:H4	4:A:418:PX4:H49	0.62	1.71	6	1
4:A:309:PX4:H40	4:A:372:PX4:H45	0.62	1.69	11	1
4:A:317:PX4:H55	4:A:324:PX4:H20	0.62	1.70	2	1
4:A:331:PX4:H66	4:A:373:PX4:H45	0.62	1.71	13	1
4:A:378:PX4:H21	4:A:417:PX4:H48	0.62	1.72	3	1
4:A:337:PX4:H58	4:A:353:PX4:H27	0.62	1.69	5	1
4:A:330:PX4:H64	4:A:357:PX4:H28	0.62	1.71	10	1
4:A:395:PX4:H63	4:A:421:PX4:H20	0.62	1.70	9	1
4:A:317:PX4:H63	4:A:325:PX4:H59	0.62	1.71	5	1
4:A:326:PX4:H17	4:A:351:PX4:O8	0.62	1.95	14	2
4:A:389:PX4:H69	4:A:397:PX4:H45	0.62	1.71	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:345:PX4:H29	4:A:362:PX4:H65	0.62	1.71	12	1
4:A:354:PX4:H39	4:A:362:PX4:H33	0.62	1.70	8	1
4:A:378:PX4:H22	4:A:417:PX4:H48	0.62	1.69	8	1
4:A:405:PX4:H17	4:A:406:PX4:H54	0.62	1.70	1	2
4:A:331:PX4:H28	4:A:347:PX4:H49	0.62	1.71	4	1
4:A:307:PX4:H28	4:A:349:PX4:H23	0.62	1.71	14	1
4:A:426:PX4:H64	4:A:426:PX4:H38	0.61	1.72	1	1
4:A:317:PX4:H16	4:A:342:PX4:H52	0.61	1.70	5	1
4:A:329:PX4:H18	4:A:336:PX4:H53	0.61	1.69	8	1
4:A:314:PX4:H57	4:A:364:PX4:H53	0.61	1.71	9	1
4:A:417:PX4:O6	4:A:417:PX4:H4	0.61	1.95	5	1
4:A:306:PX4:H15	4:A:321:PX4:H42	0.61	1.70	10	1
4:A:369:PX4:H38	4:A:378:PX4:H68	0.61	1.72	14	1
4:A:380:PX4:H18	4:A:381:PX4:H15	0.61	1.71	4	3
4:A:376:PX4:H46	4:A:385:PX4:H17	0.61	1.71	10	1
4:A:316:PX4:H34	4:A:320:PX4:H37	0.61	1.71	3	1
4:A:391:PX4:H62	4:A:408:PX4:H52	0.61	1.72	4	1
4:A:320:PX4:H54	4:A:359:PX4:H26	0.61	1.70	6	1
4:A:307:PX4:H52	4:A:321:PX4:H59	0.61	1.72	13	1
4:A:403:PX4:H53	4:A:403:PX4:H32	0.61	1.73	12	1
4:A:376:PX4:H40	4:A:399:PX4:H64	0.61	1.73	1	1
4:A:368:PX4:H52	4:A:369:PX4:H64	0.61	1.73	3	1
4:A:386:PX4:O6	4:A:394:PX4:H18	0.61	1.94	7	1
4:A:398:PX4:H16	4:A:407:PX4:H48	0.61	1.72	9	1
4:A:423:PX4:H48	4:A:425:PX4:H18	0.61	1.73	12	1
4:A:369:PX4:H31	4:A:377:PX4:H62	0.61	1.73	13	1
4:A:360:PX4:H2	4:A:366:PX4:H16	0.61	1.71	6	2
4:A:380:PX4:H67	4:A:387:PX4:H65	0.61	1.73	12	1
4:A:306:PX4:H66	4:A:362:PX4:H45	0.61	1.71	10	1
1:A:214:LEU:HD12	1:A:240:TYR:CE1	0.61	2.30	13	1
4:A:347:PX4:H19	4:A:348:PX4:H14	0.61	1.72	13	1
4:A:367:PX4:H49	4:A:428:PX4:H51	0.60	1.73	1	1
4:A:391:PX4:H55	4:A:408:PX4:H55	0.60	1.72	3	1
4:A:317:PX4:H17	4:A:325:PX4:H46	0.60	1.73	7	2
4:A:371:PX4:H20	4:A:372:PX4:H17	0.60	1.71	7	1
4:A:406:PX4:O1	4:A:414:PX4:H9	0.60	1.95	8	1
4:A:363:PX4:H24	4:A:364:PX4:H37	0.60	1.71	1	1
4:A:329:PX4:H24	4:A:336:PX4:H60	0.60	1.73	3	1
4:A:393:PX4:O2	4:A:394:PX4:H17	0.60	1.96	10	2
4:A:347:PX4:H30	4:A:348:PX4:H19	0.60	1.72	14	1
4:A:404:PX4:H70	4:A:430:PX4:H65	0.60	1.73	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:306:PX4:H23	4:A:328:PX4:H54	0.60	1.73	13	1
4:A:325:PX4:H45	4:A:407:PX4:H29	0.60	1.72	7	1
4:A:371:PX4:H14	4:A:379:PX4:H20	0.60	1.71	11	1
4:A:401:PX4:H46	4:A:426:PX4:H56	0.60	1.72	13	1
4:A:398:PX4:H30	4:A:407:PX4:H18	0.60	1.72	10	1
4:A:350:PX4:H67	4:A:358:PX4:H33	0.60	1.71	3	1
4:A:378:PX4:H20	4:A:410:PX4:H52	0.60	1.73	12	2
4:A:395:PX4:H64	4:A:406:PX4:H56	0.60	1.72	1	2
1:A:244:ASP:OD2	4:A:349:PX4:H9	0.60	1.96	7	2
4:A:348:PX4:H11	4:A:355:PX4:O2	0.60	1.95	5	2
4:A:311:PX4:H60	4:A:311:PX4:H29	0.60	1.74	9	1
4:A:321:PX4:H26	4:A:360:PX4:H61	0.60	1.72	12	1
4:A:327:PX4:H20	4:A:328:PX4:H16	0.60	1.72	7	2
4:A:381:PX4:H51	4:A:396:PX4:H46	0.60	1.73	14	1
4:A:380:PX4:H52	4:A:387:PX4:H49	0.60	1.73	6	1
4:A:315:PX4:H55	4:A:323:PX4:H46	0.59	1.74	1	1
4:A:400:PX4:H71	4:A:426:PX4:H43	0.59	1.73	2	1
4:A:328:PX4:H72	4:A:374:PX4:H43	0.59	1.74	5	1
4:A:424:PX4:H47	4:A:429:PX4:H21	0.59	1.74	2	1
4:A:347:PX4:H64	4:A:356:PX4:H56	0.59	1.72	3	1
4:A:422:PX4:H35	4:A:423:PX4:H32	0.59	1.74	3	1
4:A:413:PX4:O2	4:A:430:PX4:H18	0.59	1.96	3	1
4:A:347:PX4:H35	4:A:348:PX4:H24	0.59	1.73	4	1
4:A:403:PX4:H2	4:A:427:PX4:H46	0.59	1.73	14	1
4:A:316:PX4:O6	4:A:364:PX4:H12	0.59	1.98	3	1
4:A:335:PX4:H28	4:A:343:PX4:H56	0.59	1.74	6	1
4:A:331:PX4:H31	4:A:340:PX4:H56	0.59	1.73	8	1
4:A:371:PX4:H54	4:A:379:PX4:H25	0.59	1.73	11	1
4:A:306:PX4:H29	4:A:329:PX4:H51	0.59	1.73	3	1
4:A:350:PX4:H60	4:A:364:PX4:H41	0.59	1.73	3	1
4:A:416:PX4:H58	4:A:423:PX4:H60	0.59	1.74	6	1
4:A:388:PX4:O6	4:A:395:PX4:H5	0.59	1.97	8	2
4:A:351:PX4:H50	4:A:358:PX4:H55	0.59	1.74	10	1
4:A:330:PX4:H25	4:A:343:PX4:H54	0.59	1.75	14	1
4:A:342:PX4:H24	4:A:352:PX4:C24	0.59	2.24	11	1
4:A:345:PX4:H33	4:A:362:PX4:H69	0.59	1.73	12	1
4:A:400:PX4:H46	4:A:408:PX4:H64	0.59	1.74	12	1
4:A:393:PX4:H45	4:A:394:PX4:H37	0.59	1.72	5	1
4:A:369:PX4:H20	4:A:377:PX4:H51	0.59	1.75	14	1
4:A:327:PX4:H57	4:A:327:PX4:H26	0.59	1.73	1	1
4:A:421:PX4:H44	4:A:428:PX4:H58	0.59	1.74	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:371:PX4:H34	4:A:377:PX4:H36	0.59	1.74	5	1
4:A:375:PX4:H65	4:A:412:PX4:H38	0.59	1.74	9	1
4:A:334:PX4:H42	4:A:391:PX4:H43	0.58	1.75	2	1
4:A:416:PX4:H49	4:A:425:PX4:H57	0.58	1.75	9	1
4:A:347:PX4:H34	4:A:348:PX4:H22	0.58	1.73	14	1
4:A:383:PX4:H63	4:A:399:PX4:H67	0.58	1.74	3	1
4:A:312:PX4:H61	4:A:359:PX4:H33	0.58	1.73	6	1
4:A:377:PX4:H72	4:A:425:PX4:H68	0.58	1.74	6	1
4:A:409:PX4:H51	4:A:415:PX4:H21	0.58	1.74	8	1
4:A:350:PX4:H9	4:A:358:PX4:O6	0.58	1.99	12	2
4:A:337:PX4:H71	4:A:353:PX4:H62	0.58	1.75	10	1
4:A:354:PX4:H51	4:A:360:PX4:H18	0.58	1.74	4	1
4:A:360:PX4:H62	4:A:360:PX4:H25	0.58	1.73	4	1
4:A:377:PX4:H34	4:A:379:PX4:H27	0.58	1.76	7	1
4:A:404:PX4:O2	4:A:413:PX4:H17	0.58	1.97	7	1
4:A:428:PX4:H52	4:A:430:PX4:H53	0.58	1.75	7	1
4:A:308:PX4:H24	4:A:364:PX4:H22	0.58	1.74	12	1
4:A:382:PX4:H69	4:A:412:PX4:H71	0.58	1.75	13	1
4:A:375:PX4:H42	4:A:424:PX4:H69	0.58	1.76	2	1
4:A:395:PX4:H67	4:A:406:PX4:H56	0.58	1.75	2	1
4:A:378:PX4:H20	4:A:410:PX4:H48	0.58	1.75	13	1
4:A:307:PX4:H56	4:A:362:PX4:H23	0.58	1.75	14	1
4:A:412:PX4:H55	4:A:427:PX4:H22	0.58	1.75	3	1
4:A:363:PX4:H24	4:A:365:PX4:H22	0.58	1.75	13	2
4:A:350:PX4:H54	4:A:415:PX4:H43	0.58	1.76	7	1
4:A:392:PX4:H66	4:A:415:PX4:H39	0.58	1.75	8	1
4:A:374:PX4:H31	4:A:427:PX4:H20	0.58	1.74	10	1
4:A:314:PX4:H34	4:A:362:PX4:H16	0.58	1.75	3	1
4:A:354:PX4:H60	4:A:360:PX4:H63	0.58	1.76	7	1
4:A:318:PX4:H53	4:A:359:PX4:H25	0.58	1.75	2	1
4:A:316:PX4:H61	4:A:323:PX4:H70	0.58	1.76	12	1
4:A:410:PX4:H51	4:A:426:PX4:H25	0.58	1.74	3	1
4:A:351:PX4:H28	4:A:352:PX4:H26	0.58	1.76	4	1
4:A:329:PX4:H69	4:A:382:PX4:H41	0.58	1.75	8	1
4:A:382:PX4:H21	4:A:428:PX4:H29	0.58	1.76	9	1
4:A:400:PX4:H17	4:A:408:PX4:H61	0.58	1.76	12	1
4:A:395:PX4:H49	4:A:396:PX4:H20	0.58	1.74	13	1
4:A:388:PX4:H20	4:A:411:PX4:H19	0.58	1.74	1	1
4:A:348:PX4:H5	4:A:355:PX4:O3	0.58	1.99	3	1
4:A:370:PX4:H35	4:A:403:PX4:H67	0.58	1.75	3	1
4:A:326:PX4:H16	4:A:351:PX4:H16	0.58	1.76	4	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:317:PX4:H60	4:A:325:PX4:H68	0.58	1.76	9	1
4:A:323:PX4:H55	4:A:323:PX4:H34	0.58	1.74	9	1
4:A:314:PX4:H49	4:A:364:PX4:H18	0.58	1.75	10	2
4:A:372:PX4:H62	4:A:379:PX4:H61	0.57	1.75	2	1
4:A:403:PX4:H50	4:A:404:PX4:H28	0.57	1.75	8	1
4:A:409:PX4:H29	4:A:425:PX4:H71	0.57	1.76	8	1
4:A:393:PX4:H11	4:A:401:PX4:H16	0.57	1.75	11	1
4:A:332:PX4:H67	4:A:349:PX4:H57	0.57	1.76	12	1
4:A:410:PX4:H58	4:A:426:PX4:H32	0.57	1.76	4	1
4:A:352:PX4:H20	4:A:358:PX4:H15	0.57	1.75	9	1
4:A:340:PX4:H66	4:A:397:PX4:H31	0.57	1.74	11	1
4:A:402:PX4:H15	4:A:404:PX4:H14	0.57	1.75	2	1
4:A:349:PX4:H17	4:A:356:PX4:H21	0.57	1.76	7	2
4:A:337:PX4:H63	4:A:353:PX4:H56	0.57	1.77	8	1
4:A:420:PX4:H72	4:A:426:PX4:H40	0.57	1.76	8	1
4:A:391:PX4:H62	4:A:400:PX4:H32	0.57	1.76	9	1
4:A:378:PX4:H30	4:A:417:PX4:H56	0.57	1.76	10	1
4:A:367:PX4:O2	4:A:424:PX4:H1	0.57	1.99	3	1
4:A:334:PX4:H69	4:A:352:PX4:H32	0.57	1.77	6	1
4:A:400:PX4:H28	4:A:408:PX4:H52	0.57	1.75	7	1
4:A:318:PX4:H27	4:A:327:PX4:H56	0.57	1.75	12	1
4:A:319:PX4:H39	4:A:324:PX4:H37	0.57	1.77	14	1
4:A:333:PX4:H39	4:A:375:PX4:H28	0.57	1.76	1	1
4:A:393:PX4:H46	4:A:401:PX4:H19	0.57	1.75	4	1
4:A:330:PX4:H21	4:A:335:PX4:H22	0.57	1.75	12	1
4:A:352:PX4:H33	4:A:358:PX4:H64	0.57	1.74	4	1
4:A:388:PX4:H17	4:A:396:PX4:H22	0.57	1.75	8	1
4:A:334:PX4:H37	4:A:407:PX4:H43	0.57	1.75	12	1
4:A:351:PX4:H62	4:A:358:PX4:H30	0.57	1.76	13	1
4:A:331:PX4:H11	4:A:340:PX4:O1	0.57	1.99	2	1
4:A:314:PX4:H69	4:A:350:PX4:H55	0.57	1.77	5	1
4:A:326:PX4:H47	4:A:334:PX4:H56	0.57	1.77	8	1
4:A:376:PX4:H52	4:A:385:PX4:H21	0.57	1.77	8	1
4:A:342:PX4:O2	4:A:352:PX4:H4	0.57	1.99	14	1
4:A:345:PX4:H15	4:A:353:PX4:H16	0.57	1.76	2	1
4:A:344:PX4:H28	4:A:348:PX4:H21	0.57	1.76	3	1
4:A:337:PX4:H17	4:A:345:PX4:H46	0.57	1.76	4	2
4:A:320:PX4:H20	4:A:359:PX4:C29	0.57	2.26	5	1
4:A:371:PX4:H56	4:A:378:PX4:H62	0.57	1.75	5	1
4:A:312:PX4:H65	4:A:359:PX4:H37	0.57	1.76	6	1
4:A:311:PX4:H70	4:A:312:PX4:H69	0.56	1.77	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:424:PX4:H17	4:A:429:PX4:O6	0.56	2.00	3	1
4:A:380:PX4:H67	4:A:388:PX4:H62	0.56	1.77	10	1
4:A:367:PX4:H47	4:A:428:PX4:H48	0.56	1.76	11	1
4:A:349:PX4:H56	4:A:350:PX4:H30	0.56	1.77	12	1
4:A:362:PX4:H38	4:A:430:PX4:H69	0.56	1.76	12	1
4:A:375:PX4:H10	4:A:375:PX4:H14	0.56	1.77	14	1
1:A:207:SER:O	4:A:321:PX4:H4	0.56	2.00	2	1
4:A:317:PX4:H31	4:A:326:PX4:H62	0.56	1.76	5	1
4:A:360:PX4:H33	4:A:366:PX4:H64	0.56	1.76	5	1
4:A:391:PX4:H21	4:A:392:PX4:H47	0.56	1.78	5	1
4:A:393:PX4:H20	4:A:401:PX4:H16	0.56	1.77	5	2
4:A:400:PX4:H59	4:A:426:PX4:H40	0.56	1.76	6	1
4:A:336:PX4:H70	4:A:382:PX4:H42	0.56	1.76	8	1
4:A:371:PX4:H68	4:A:379:PX4:H41	0.56	1.76	9	1
4:A:329:PX4:H26	4:A:336:PX4:H60	0.56	1.75	11	1
4:A:373:PX4:H31	4:A:381:PX4:H30	0.56	1.77	11	1
4:A:309:PX4:H63	4:A:316:PX4:H65	0.56	1.77	14	1
4:A:318:PX4:H27	4:A:359:PX4:H23	0.56	1.76	2	1
4:A:388:PX4:H23	4:A:402:PX4:H16	0.56	1.75	3	1
4:A:320:PX4:C10	4:A:359:PX4:H57	0.56	2.25	5	1
4:A:315:PX4:H29	4:A:361:PX4:H24	0.56	1.77	4	1
4:A:429:PX4:H33	4:A:429:PX4:H53	0.56	1.77	9	1
4:A:318:PX4:H64	4:A:318:PX4:H43	0.56	1.78	11	1
4:A:379:PX4:H58	4:A:420:PX4:H31	0.56	1.78	11	1
4:A:310:PX4:H20	4:A:365:PX4:H21	0.56	1.76	14	1
4:A:313:PX4:H58	4:A:327:PX4:H23	0.56	1.78	2	1
4:A:320:PX4:H19	4:A:359:PX4:H59	0.56	1.77	14	1
4:A:352:PX4:O8	4:A:365:PX4:H11	0.56	2.00	1	1
4:A:316:PX4:H48	4:A:320:PX4:H26	0.56	1.77	3	1
4:A:332:PX4:H56	4:A:349:PX4:H48	0.56	1.76	3	1
4:A:402:PX4:H3	4:A:404:PX4:O1	0.56	2.01	3	1
4:A:307:PX4:H65	4:A:349:PX4:H28	0.56	1.76	11	1
4:A:369:PX4:H56	4:A:416:PX4:H69	0.56	1.78	9	1
4:A:400:PX4:H53	4:A:410:PX4:H50	0.56	1.78	12	1
4:A:408:PX4:H43	4:A:414:PX4:H64	0.56	1.76	12	1
4:A:338:PX4:H71	4:A:395:PX4:H40	0.56	1.78	13	1
4:A:389:PX4:H30	4:A:397:PX4:H54	0.55	1.79	4	1
4:A:358:PX4:H19	4:A:363:PX4:H49	0.55	1.77	3	1
1:A:177:LYS:O	4:A:354:PX4:H13	0.55	2.01	7	1
4:A:337:PX4:H62	4:A:366:PX4:H53	0.55	1.77	8	1
4:A:377:PX4:H16	4:A:418:PX4:H7	0.55	1.78	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:309:PX4:H55	4:A:324:PX4:H53	0.55	1.77	12	1
4:A:381:PX4:H29	4:A:386:PX4:H58	0.55	1.77	12	1
4:A:330:PX4:H19	4:A:338:PX4:H19	0.55	1.77	1	1
4:A:380:PX4:H66	4:A:411:PX4:H22	0.55	1.77	2	1
4:A:375:PX4:H58	4:A:382:PX4:H71	0.55	1.78	6	1
4:A:395:PX4:H36	4:A:397:PX4:H61	0.55	1.76	6	1
4:A:347:PX4:H69	4:A:407:PX4:H68	0.55	1.77	11	1
4:A:349:PX4:H54	4:A:355:PX4:H34	0.55	1.76	11	1
4:A:412:PX4:H20	4:A:428:PX4:H46	0.55	1.77	11	1
4:A:337:PX4:H55	4:A:353:PX4:H47	0.55	1.77	10	1
4:A:326:PX4:H18	4:A:334:PX4:H72	0.55	1.79	11	1
4:A:360:PX4:H47	4:A:366:PX4:H46	0.55	1.77	11	1
4:A:341:PX4:H34	4:A:399:PX4:H69	0.55	1.78	14	1
4:A:399:PX4:H25	4:A:399:PX4:H59	0.55	1.77	2	1
4:A:392:PX4:H35	4:A:399:PX4:H56	0.55	1.77	10	1
4:A:313:PX4:H64	4:A:328:PX4:H68	0.55	1.77	1	1
4:A:412:PX4:H19	4:A:428:PX4:H54	0.55	1.79	5	1
4:A:354:PX4:H56	4:A:360:PX4:H59	0.55	1.77	7	1
4:A:338:PX4:H34	4:A:357:PX4:H27	0.55	1.78	9	1
4:A:357:PX4:H29	4:A:365:PX4:H62	0.55	1.78	14	1
4:A:416:PX4:H25	4:A:422:PX4:H56	0.55	1.77	6	1
4:A:367:PX4:H2	4:A:428:PX4:O8	0.55	2.02	14	1
4:A:375:PX4:H68	4:A:428:PX4:H54	0.55	1.78	14	1
4:A:329:PX4:H46	4:A:336:PX4:H18	0.55	1.78	2	1
4:A:346:PX4:H70	4:A:357:PX4:H31	0.55	1.77	6	1
4:A:369:PX4:H38	4:A:416:PX4:H63	0.55	1.78	11	1
4:A:306:PX4:H49	4:A:321:PX4:H22	0.55	1.77	1	1
4:A:373:PX4:H20	4:A:381:PX4:H18	0.55	1.78	1	1
4:A:316:PX4:H36	4:A:364:PX4:H55	0.55	1.78	3	1
4:A:360:PX4:H45	4:A:404:PX4:H41	0.55	1.78	9	1
4:A:385:PX4:H45	4:A:386:PX4:H45	0.55	1.78	10	1
4:A:314:PX4:H46	4:A:364:PX4:H18	0.55	1.79	11	1
4:A:317:PX4:H51	4:A:324:PX4:H17	0.55	1.79	11	1
4:A:395:PX4:H19	4:A:396:PX4:H14	0.55	1.79	12	1
4:A:348:PX4:H69	4:A:355:PX4:H27	0.55	1.79	14	1
4:A:416:PX4:H30	4:A:423:PX4:H30	0.55	1.79	2	1
4:A:392:PX4:H60	4:A:408:PX4:H31	0.55	1.78	7	1
4:A:392:PX4:O6	4:A:392:PX4:H2	0.55	2.02	9	1
4:A:307:PX4:H31	4:A:364:PX4:H57	0.54	1.79	1	1
4:A:332:PX4:H17	4:A:356:PX4:H7	0.54	1.78	2	1
4:A:408:PX4:H72	4:A:426:PX4:H69	0.54	1.79	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:382:PX4:H45	4:A:428:PX4:H43	0.54	1.78	8	1
4:A:339:PX4:H32	4:A:339:PX4:H50	0.54	1.78	9	1
4:A:389:PX4:H63	4:A:397:PX4:H35	0.54	1.78	14	1
4:A:355:PX4:H52	4:A:356:PX4:H14	0.54	1.77	1	1
4:A:318:PX4:O2	4:A:359:PX4:H14	0.54	2.03	5	1
4:A:321:PX4:H71	4:A:322:PX4:H33	0.54	1.79	8	1
4:A:383:PX4:H57	4:A:407:PX4:H24	0.54	1.80	9	1
4:A:380:PX4:H32	4:A:381:PX4:H59	0.54	1.77	3	1
4:A:416:PX4:H20	4:A:422:PX4:H48	0.54	1.80	4	1
4:A:330:PX4:H25	4:A:343:PX4:H51	0.54	1.77	6	1
4:A:323:PX4:H55	4:A:424:PX4:H70	0.54	1.77	6	1
4:A:307:PX4:H43	4:A:311:PX4:H43	0.54	1.78	12	1
4:A:372:PX4:H51	4:A:420:PX4:H19	0.54	1.78	3	1
4:A:308:PX4:H54	4:A:364:PX4:H31	0.54	1.79	4	1
4:A:403:PX4:H61	4:A:427:PX4:H62	0.54	1.78	6	1
4:A:383:PX4:H54	4:A:407:PX4:H20	0.54	1.78	9	1
4:A:404:PX4:H21	4:A:419:PX4:H10	0.54	1.79	9	1
4:A:317:PX4:H21	4:A:342:PX4:H68	0.54	1.78	10	1
4:A:325:PX4:H53	4:A:334:PX4:H36	0.54	1.78	12	1
4:A:332:PX4:O8	4:A:347:PX4:H52	0.54	2.03	13	1
4:A:428:PX4:H70	4:A:430:PX4:H32	0.54	1.79	1	1
4:A:331:PX4:H56	4:A:339:PX4:H22	0.54	1.80	2	1
4:A:351:PX4:H67	4:A:358:PX4:H36	0.54	1.79	2	1
4:A:354:PX4:H28	4:A:362:PX4:H17	0.54	1.79	5	1
4:A:372:PX4:H58	4:A:379:PX4:H57	0.54	1.80	5	1
4:A:386:PX4:H25	4:A:394:PX4:H20	0.54	1.79	9	1
4:A:338:PX4:H59	4:A:348:PX4:H57	0.54	1.78	12	1
4:A:369:PX4:H21	4:A:377:PX4:H56	0.54	1.78	1	1
4:A:419:PX4:H63	4:A:427:PX4:H60	0.54	1.80	2	1
4:A:327:PX4:H19	4:A:329:PX4:H23	0.54	1.78	5	1
4:A:373:PX4:H25	4:A:397:PX4:H15	0.54	1.79	7	1
4:A:406:PX4:H12	4:A:406:PX4:H15	0.54	1.80	9	1
4:A:423:PX4:H13	4:A:430:PX4:H46	0.54	1.80	10	1
4:A:377:PX4:H51	4:A:418:PX4:H52	0.54	1.79	13	1
4:A:416:PX4:H48	4:A:425:PX4:H49	0.54	1.79	14	1
4:A:307:PX4:H4	4:A:322:PX4:O8	0.54	2.03	3	1
4:A:384:PX4:O2	4:A:385:PX4:H18	0.54	2.03	8	2
4:A:372:PX4:H52	4:A:420:PX4:H21	0.54	1.80	4	1
4:A:370:PX4:H23	4:A:427:PX4:H59	0.54	1.80	9	1
4:A:308:PX4:H43	4:A:425:PX4:H68	0.54	1.79	13	1
1:A:208:GLY:HA3	4:A:307:PX4:H15	0.53	1.80	2	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:391:PX4:H23	4:A:414:PX4:H51	0.53	1.80	1	1
4:A:409:PX4:H16	4:A:410:PX4:H8	0.53	1.80	4	1
4:A:412:PX4:H48	4:A:419:PX4:H22	0.53	1.80	4	2
4:A:381:PX4:H57	4:A:397:PX4:H46	0.53	1.80	6	1
4:A:412:PX4:H54	4:A:427:PX4:H22	0.53	1.79	6	1
4:A:367:PX4:H22	4:A:424:PX4:H16	0.53	1.79	7	1
4:A:340:PX4:H63	4:A:397:PX4:H30	0.53	1.81	10	1
4:A:381:PX4:H62	4:A:381:PX4:H35	0.53	1.79	11	1
4:A:337:PX4:H64	4:A:345:PX4:H63	0.53	1.78	1	1
4:A:378:PX4:H49	4:A:410:PX4:H23	0.53	1.80	6	1
4:A:307:PX4:H29	4:A:361:PX4:H28	0.53	1.80	8	1
4:A:317:PX4:H26	4:A:334:PX4:H40	0.53	1.80	9	1
4:A:400:PX4:H51	4:A:409:PX4:H21	0.53	1.80	9	1
4:A:393:PX4:H66	4:A:399:PX4:H69	0.53	1.79	12	1
4:A:332:PX4:H44	4:A:389:PX4:H57	0.53	1.79	13	1
4:A:371:PX4:H21	4:A:379:PX4:H20	0.53	1.80	13	1
4:A:328:PX4:H55	4:A:329:PX4:H47	0.53	1.79	1	1
4:A:421:PX4:H4	4:A:422:PX4:O6	0.53	2.03	1	1
4:A:311:PX4:O2	4:A:359:PX4:H13	0.53	2.03	5	1
4:A:406:PX4:H27	4:A:415:PX4:H59	0.53	1.80	7	1
4:A:430:PX4:H71	4:A:430:PX4:H28	0.53	1.79	11	1
4:A:329:PX4:H66	4:A:375:PX4:H35	0.53	1.79	1	1
4:A:352:PX4:H48	4:A:358:PX4:H50	0.53	1.79	3	1
4:A:367:PX4:H59	4:A:424:PX4:H21	0.53	1.81	4	1
4:A:311:PX4:H43	4:A:425:PX4:H68	0.53	1.78	5	1
4:A:311:PX4:H17	4:A:359:PX4:H51	0.53	1.79	6	2
4:A:389:PX4:H48	4:A:390:PX4:H49	0.53	1.79	5	2
4:A:363:PX4:H70	4:A:392:PX4:H66	0.53	1.81	7	1
4:A:388:PX4:H58	4:A:397:PX4:H54	0.53	1.78	9	1
4:A:345:PX4:H37	4:A:403:PX4:H45	0.53	1.80	14	1
4:A:384:PX4:H19	4:A:385:PX4:H23	0.53	1.79	1	1
4:A:386:PX4:H35	4:A:394:PX4:H36	0.53	1.81	3	1
4:A:429:PX4:H15	4:A:429:PX4:H10	0.53	1.80	3	1
4:A:395:PX4:H44	4:A:398:PX4:H69	0.53	1.81	4	1
4:A:345:PX4:H44	4:A:402:PX4:H67	0.53	1.81	6	1
4:A:388:PX4:H18	4:A:411:PX4:O2	0.53	2.04	6	1
4:A:350:PX4:H68	4:A:351:PX4:H58	0.53	1.81	2	1
4:A:308:PX4:H16	4:A:311:PX4:H20	0.53	1.78	5	1
4:A:338:PX4:H32	4:A:348:PX4:H33	0.53	1.81	6	1
4:A:395:PX4:H58	4:A:404:PX4:H48	0.53	1.79	6	1
4:A:398:PX4:H38	4:A:414:PX4:H47	0.53	1.80	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:391:PX4:H49	4:A:408:PX4:H16	0.53	1.80	7	1
4:A:317:PX4:H20	4:A:351:PX4:O6	0.53	2.04	11	1
4:A:351:PX4:H66	4:A:358:PX4:H32	0.53	1.79	3	1
4:A:311:PX4:H48	4:A:320:PX4:H21	0.53	1.79	4	1
4:A:325:PX4:H15	4:A:341:PX4:H17	0.53	1.79	5	1
4:A:358:PX4:H29	4:A:363:PX4:H26	0.53	1.79	10	1
4:A:345:PX4:H42	4:A:388:PX4:H40	0.53	1.79	12	1
4:A:370:PX4:H69	4:A:411:PX4:H65	0.53	1.80	2	1
4:A:307:PX4:H37	4:A:423:PX4:H39	0.53	1.78	4	1
4:A:416:PX4:H51	4:A:418:PX4:H26	0.53	1.79	4	1
4:A:329:PX4:H30	4:A:336:PX4:H68	0.53	1.79	8	1
4:A:310:PX4:H65	4:A:312:PX4:H52	0.53	1.80	9	1
4:A:361:PX4:H34	4:A:423:PX4:H35	0.53	1.80	12	1
4:A:400:PX4:H28	4:A:426:PX4:H59	0.53	1.81	12	1
4:A:410:PX4:H16	4:A:418:PX4:H28	0.53	1.80	12	1
4:A:376:PX4:H26	4:A:399:PX4:H48	0.53	1.81	4	1
4:A:309:PX4:H51	4:A:316:PX4:H48	0.53	1.80	5	1
4:A:335:PX4:H31	4:A:343:PX4:H55	0.53	1.79	11	1
4:A:405:PX4:H22	4:A:406:PX4:H61	0.53	1.79	13	1
4:A:392:PX4:H68	4:A:400:PX4:H45	0.53	1.80	1	1
4:A:311:PX4:H60	4:A:311:PX4:H24	0.53	1.81	6	1
4:A:337:PX4:H40	4:A:338:PX4:H47	0.53	1.79	10	1
4:A:347:PX4:H20	4:A:348:PX4:H14	0.52	1.81	6	1
4:A:367:PX4:H64	4:A:375:PX4:H57	0.52	1.80	7	1
4:A:413:PX4:H61	4:A:430:PX4:H42	0.52	1.81	9	1
4:A:349:PX4:H58	4:A:356:PX4:H42	0.52	1.80	10	1
4:A:398:PX4:H39	4:A:414:PX4:H31	0.52	1.81	10	1
4:A:412:PX4:H12	4:A:419:PX4:O1	0.52	2.04	12	1
4:A:314:PX4:H53	4:A:364:PX4:H18	0.52	1.81	1	1
4:A:337:PX4:H56	4:A:345:PX4:H59	0.52	1.81	5	1
4:A:389:PX4:H32	4:A:397:PX4:H22	0.52	1.82	6	1
4:A:306:PX4:H47	4:A:322:PX4:H50	0.52	1.81	7	1
4:A:398:PX4:H21	4:A:407:PX4:H49	0.52	1.80	10	1
4:A:346:PX4:H19	4:A:354:PX4:H28	0.52	1.80	1	1
4:A:361:PX4:H26	4:A:364:PX4:H54	0.52	1.81	3	1
4:A:315:PX4:H10	4:A:315:PX4:O6	0.52	2.04	4	1
4:A:326:PX4:H48	4:A:334:PX4:H35	0.52	1.79	5	1
4:A:407:PX4:H30	4:A:414:PX4:H61	0.52	1.81	11	1
4:A:311:PX4:H44	4:A:314:PX4:H65	0.52	1.82	13	1
4:A:388:PX4:H49	4:A:396:PX4:H21	0.52	1.81	12	1
4:A:313:PX4:H56	4:A:327:PX4:H27	0.52	1.82	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:415:PX4:H56	4:A:422:PX4:H53	0.52	1.81	13	1
4:A:410:PX4:H67	4:A:417:PX4:H37	0.52	1.81	14	1
4:A:310:PX4:H34	4:A:365:PX4:H34	0.52	1.81	3	1
4:A:329:PX4:H56	4:A:336:PX4:H35	0.52	1.82	6	2
4:A:314:PX4:H33	4:A:362:PX4:O8	0.52	2.04	9	1
4:A:325:PX4:H55	4:A:334:PX4:H40	0.52	1.81	11	1
4:A:400:PX4:H46	4:A:409:PX4:H23	0.52	1.81	1	1
4:A:340:PX4:H22	4:A:341:PX4:H63	0.52	1.81	2	1
4:A:405:PX4:H51	4:A:406:PX4:H51	0.52	1.81	3	1
4:A:308:PX4:H21	4:A:311:PX4:H55	0.52	1.82	7	1
4:A:329:PX4:H60	4:A:336:PX4:H40	0.52	1.82	8	1
4:A:313:PX4:H28	4:A:366:PX4:H21	0.52	1.81	9	1
4:A:404:PX4:H21	4:A:413:PX4:H30	0.52	1.81	10	1
4:A:393:PX4:H71	4:A:414:PX4:H53	0.52	1.81	11	1
4:A:340:PX4:H59	4:A:340:PX4:H36	0.52	1.79	12	1
4:A:307:PX4:H45	4:A:422:PX4:H39	0.52	1.80	13	1
4:A:317:PX4:H21	4:A:326:PX4:H53	0.52	1.81	13	1
4:A:390:PX4:H1	4:A:399:PX4:O6	0.52	2.05	13	1
4:A:354:PX4:H69	4:A:360:PX4:H27	0.52	1.81	2	1
4:A:405:PX4:H55	4:A:406:PX4:H51	0.52	1.82	2	1
4:A:312:PX4:H29	4:A:365:PX4:H24	0.52	1.82	3	1
4:A:348:PX4:H52	4:A:355:PX4:H67	0.52	1.81	5	1
4:A:306:PX4:H61	4:A:362:PX4:H37	0.52	1.82	9	1
4:A:342:PX4:H29	4:A:352:PX4:H60	0.52	1.82	9	1
4:A:331:PX4:H38	4:A:340:PX4:H40	0.52	1.82	10	1
4:A:380:PX4:H6	4:A:381:PX4:O1	0.52	2.04	11	1
4:A:383:PX4:H71	4:A:399:PX4:H67	0.52	1.80	5	1
4:A:419:PX4:H67	4:A:427:PX4:H69	0.52	1.81	5	1
4:A:370:PX4:H19	4:A:427:PX4:H55	0.52	1.82	9	1
4:A:410:PX4:H16	4:A:418:PX4:H31	0.52	1.81	10	1
4:A:310:PX4:H60	4:A:312:PX4:H53	0.52	1.82	4	2
4:A:371:PX4:H56	4:A:372:PX4:H23	0.52	1.82	4	1
4:A:341:PX4:H39	4:A:399:PX4:H72	0.52	1.81	5	1
4:A:306:PX4:H43	4:A:328:PX4:H67	0.52	1.82	8	1
4:A:327:PX4:H14	4:A:328:PX4:O2	0.52	2.05	7	1
4:A:308:PX4:H27	4:A:316:PX4:H27	0.52	1.81	8	1
4:A:361:PX4:H39	4:A:364:PX4:H65	0.52	1.81	9	1
4:A:314:PX4:H26	4:A:356:PX4:H25	0.52	1.82	12	1
4:A:313:PX4:H61	4:A:329:PX4:H25	0.52	1.81	13	1
4:A:354:PX4:H65	4:A:360:PX4:H20	0.51	1.81	1	1
4:A:409:PX4:H67	4:A:415:PX4:H33	0.51	1.81	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:377:PX4:H71	4:A:425:PX4:H19	0.51	1.81	8	1
4:A:324:PX4:H66	4:A:341:PX4:H32	0.51	1.82	9	1
4:A:393:PX4:H23	4:A:401:PX4:H16	0.51	1.81	4	1
4:A:421:PX4:H71	4:A:422:PX4:H32	0.51	1.81	4	1
4:A:321:PX4:H28	4:A:412:PX4:H41	0.51	1.80	5	1
4:A:387:PX4:H47	4:A:411:PX4:H54	0.51	1.80	5	1
4:A:360:PX4:H31	4:A:419:PX4:H42	0.51	1.80	7	1
4:A:338:PX4:H67	4:A:348:PX4:H58	0.51	1.82	10	1
4:A:416:PX4:H45	4:A:422:PX4:H67	0.51	1.81	12	1
4:A:368:PX4:H10	4:A:369:PX4:O2	0.51	2.05	1	1
4:A:360:PX4:H43	4:A:403:PX4:H65	0.51	1.82	3	1
4:A:323:PX4:H38	4:A:361:PX4:H54	0.51	1.82	6	1
4:A:350:PX4:H51	4:A:363:PX4:H62	0.51	1.82	8	1
4:A:380:PX4:H60	4:A:380:PX4:H32	0.51	1.80	12	1
4:A:398:PX4:H44	4:A:415:PX4:H27	0.51	1.82	14	1
4:A:308:PX4:H27	4:A:311:PX4:H31	0.51	1.81	4	1
4:A:347:PX4:H56	4:A:356:PX4:H58	0.51	1.83	4	1
4:A:400:PX4:H59	4:A:410:PX4:H62	0.51	1.82	5	1
4:A:417:PX4:H31	4:A:426:PX4:H66	0.51	1.83	7	1
4:A:404:PX4:H15	4:A:413:PX4:H20	0.51	1.81	1	1
4:A:378:PX4:H29	4:A:420:PX4:H57	0.51	1.82	4	1
4:A:322:PX4:H49	4:A:336:PX4:H25	0.51	1.83	9	1
4:A:393:PX4:H18	4:A:401:PX4:H20	0.51	1.83	12	1
4:A:402:PX4:H21	4:A:404:PX4:H67	0.51	1.83	14	1
4:A:345:PX4:H15	4:A:353:PX4:H14	0.51	1.81	4	2
4:A:358:PX4:H23	4:A:363:PX4:H55	0.51	1.83	12	1
4:A:363:PX4:H71	4:A:392:PX4:H66	0.51	1.82	3	1
4:A:349:PX4:H26	4:A:356:PX4:H38	0.51	1.83	11	1
4:A:392:PX4:H57	4:A:401:PX4:H29	0.51	1.81	13	1
4:A:312:PX4:H31	4:A:365:PX4:H46	0.51	1.82	14	1
4:A:314:PX4:H47	4:A:350:PX4:H43	0.51	1.82	14	1
4:A:346:PX4:H68	4:A:362:PX4:H72	0.51	1.82	14	1
4:A:372:PX4:H34	4:A:420:PX4:H29	0.51	1.82	14	1
4:A:346:PX4:H19	4:A:354:PX4:H31	0.51	1.82	3	1
4:A:311:PX4:O1	4:A:359:PX4:H3	0.51	2.06	5	2
4:A:355:PX4:H36	4:A:356:PX4:H41	0.51	1.81	4	1
4:A:372:PX4:H23	4:A:417:PX4:H46	0.51	1.83	8	1
4:A:306:PX4:H22	4:A:321:PX4:H35	0.51	1.82	9	1
4:A:306:PX4:H60	4:A:362:PX4:H38	0.51	1.83	10	1
4:A:321:PX4:H56	4:A:361:PX4:H54	0.51	1.82	10	1
4:A:318:PX4:H53	4:A:328:PX4:H22	0.51	1.81	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:333:PX4:H14	4:A:340:PX4:H1	0.51	1.82	11	1
4:A:316:PX4:H20	4:A:364:PX4:H14	0.51	1.81	12	1
4:A:343:PX4:H33	4:A:344:PX4:H30	0.51	1.83	12	1
4:A:378:PX4:H59	4:A:410:PX4:H26	0.51	1.82	12	1
4:A:309:PX4:H3	4:A:320:PX4:O1	0.51	2.05	13	1
4:A:409:PX4:O6	4:A:410:PX4:H5	0.51	2.06	13	1
4:A:410:PX4:H42	4:A:418:PX4:H42	0.51	1.82	14	1
4:A:354:PX4:H49	4:A:360:PX4:H49	0.51	1.83	4	1
4:A:410:PX4:H16	4:A:418:PX4:H29	0.51	1.81	6	1
4:A:333:PX4:H54	4:A:341:PX4:H54	0.51	1.83	11	1
4:A:319:PX4:H51	4:A:324:PX4:H16	0.51	1.83	1	1
4:A:395:PX4:H24	4:A:396:PX4:H64	0.51	1.83	4	1
4:A:320:PX4:H51	4:A:359:PX4:H25	0.51	1.81	8	1
4:A:388:PX4:H51	4:A:396:PX4:H48	0.51	1.81	10	1
4:A:390:PX4:H57	4:A:429:PX4:H60	0.51	1.82	11	1
4:A:400:PX4:H20	4:A:426:PX4:H50	0.51	1.82	12	1
4:A:327:PX4:H16	4:A:328:PX4:O6	0.50	2.05	5	1
4:A:313:PX4:H20	4:A:360:PX4:H15	0.50	1.82	7	1
4:A:344:PX4:H25	4:A:344:PX4:H60	0.50	1.83	14	1
4:A:363:PX4:H47	4:A:364:PX4:H37	0.50	1.81	14	1
1:A:206:HIS:ND1	4:A:314:PX4:H1	0.50	2.21	13	3
4:A:307:PX4:H42	4:A:350:PX4:H45	0.50	1.82	2	1
4:A:402:PX4:H21	4:A:403:PX4:H21	0.50	1.82	3	1
4:A:388:PX4:H29	4:A:411:PX4:H24	0.50	1.83	5	1
4:A:310:PX4:H48	4:A:365:PX4:H20	0.50	1.81	7	1
4:A:413:PX4:H63	4:A:430:PX4:H36	0.50	1.82	7	1
4:A:337:PX4:H39	4:A:338:PX4:H51	0.50	1.83	9	1
4:A:345:PX4:H70	4:A:370:PX4:H39	0.50	1.83	10	1
4:A:369:PX4:H19	4:A:418:PX4:H15	0.50	1.83	10	1
4:A:308:PX4:H18	4:A:311:PX4:O8	0.50	2.06	14	2
4:A:403:PX4:H3	4:A:427:PX4:H48	0.50	1.83	11	1
4:A:412:PX4:H47	4:A:419:PX4:H14	0.50	1.84	12	1
4:A:346:PX4:H12	4:A:360:PX4:H46	0.50	1.82	13	1
4:A:370:PX4:H17	4:A:403:PX4:O1	0.50	2.06	4	1
4:A:352:PX4:H61	4:A:358:PX4:H57	0.50	1.82	9	1
4:A:311:PX4:O4	4:A:359:PX4:H6	0.50	2.05	13	1
4:A:363:PX4:H25	4:A:365:PX4:H26	0.50	1.83	13	1
4:A:378:PX4:H35	4:A:410:PX4:H60	0.50	1.83	13	1
4:A:416:PX4:H53	4:A:418:PX4:H30	0.50	1.84	13	1
4:A:368:PX4:H32	4:A:425:PX4:H42	0.50	1.81	3	1
4:A:347:PX4:H35	4:A:348:PX4:H28	0.50	1.83	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:394:PX4:O8	4:A:394:PX4:H9	0.50	2.07	14	1
4:A:407:PX4:H9	4:A:414:PX4:H48	0.50	1.83	14	1
4:A:421:PX4:H13	4:A:423:PX4:O6	0.50	2.07	1	1
4:A:383:PX4:H46	4:A:399:PX4:H50	0.50	1.83	3	1
4:A:316:PX4:H65	4:A:320:PX4:H40	0.50	1.83	5	1
4:A:378:PX4:H50	4:A:418:PX4:H51	0.50	1.81	9	1
4:A:388:PX4:H24	4:A:402:PX4:O8	0.50	2.05	11	1
4:A:374:PX4:H22	4:A:428:PX4:H20	0.50	1.82	14	1
4:A:307:PX4:H34	4:A:307:PX4:H67	0.50	1.84	2	1
4:A:384:PX4:H56	4:A:385:PX4:H32	0.50	1.82	3	1
4:A:409:PX4:H54	4:A:422:PX4:H62	0.50	1.82	3	1
4:A:408:PX4:H18	4:A:408:PX4:H2	0.50	1.84	6	1
4:A:422:PX4:H38	4:A:423:PX4:H40	0.50	1.83	6	1
1:A:237:PHE:CD1	1:A:238:PRO:HD2	0.50	2.42	9	1
4:A:392:PX4:H27	4:A:393:PX4:H61	0.50	1.84	9	1
4:A:402:PX4:H4	4:A:404:PX4:O2	0.50	2.06	11	2
4:A:395:PX4:H42	4:A:405:PX4:H36	0.50	1.81	13	1
4:A:400:PX4:H30	4:A:401:PX4:H57	0.50	1.83	1	1
4:A:408:PX4:H17	4:A:415:PX4:O6	0.50	2.07	1	1
4:A:369:PX4:H18	4:A:425:PX4:H9	0.50	1.82	4	1
4:A:416:PX4:H24	4:A:422:PX4:H17	0.50	1.83	10	1
4:A:345:PX4:H46	4:A:346:PX4:H56	0.50	1.84	12	1
4:A:371:PX4:H35	4:A:371:PX4:H68	0.50	1.83	12	1
4:A:322:PX4:O2	4:A:333:PX4:H9	0.50	2.07	13	1
4:A:321:PX4:H24	4:A:354:PX4:H53	0.50	1.81	2	2
4:A:306:PX4:H19	4:A:321:PX4:H42	0.50	1.84	6	1
4:A:380:PX4:H49	4:A:381:PX4:H13	0.50	1.83	12	1
4:A:338:PX4:H17	4:A:348:PX4:H17	0.49	1.84	1	1
4:A:356:PX4:H32	4:A:362:PX4:H27	0.49	1.82	1	1
4:A:395:PX4:H58	4:A:404:PX4:H50	0.49	1.83	1	1
4:A:308:PX4:H40	4:A:316:PX4:H41	0.49	1.84	4	1
4:A:428:PX4:H63	4:A:430:PX4:H32	0.49	1.84	8	1
4:A:400:PX4:H68	4:A:410:PX4:H67	0.49	1.84	10	1
4:A:409:PX4:H51	4:A:415:PX4:C11	0.49	2.36	8	1
4:A:306:PX4:H22	4:A:322:PX4:H57	0.49	1.84	1	1
4:A:347:PX4:H22	4:A:348:PX4:H56	0.49	1.83	5	1
4:A:393:PX4:H3	4:A:401:PX4:O2	0.49	2.08	5	1
4:A:374:PX4:H18	4:A:382:PX4:O7	0.49	2.06	8	1
4:A:390:PX4:H62	4:A:397:PX4:H42	0.49	1.84	9	1
4:A:312:PX4:H29	4:A:365:PX4:H22	0.49	1.84	12	1
4:A:421:PX4:H67	4:A:423:PX4:H45	0.49	1.83	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:393:PX4:H37	4:A:401:PX4:H70	0.49	1.84	7	1
4:A:308:PX4:O6	4:A:364:PX4:H3	0.49	2.07	12	1
4:A:372:PX4:H20	4:A:420:PX4:H16	0.49	1.84	13	2
4:A:317:PX4:H14	4:A:351:PX4:H20	0.49	1.85	5	1
4:A:337:PX4:H9	4:A:357:PX4:H2	0.49	1.84	11	1
4:A:316:PX4:H51	4:A:320:PX4:C14	0.49	2.37	12	1
4:A:312:PX4:H35	4:A:365:PX4:H46	0.49	1.83	13	1
4:A:377:PX4:H42	4:A:379:PX4:H56	0.49	1.84	13	1
4:A:313:PX4:H65	4:A:360:PX4:H70	0.49	1.85	1	1
4:A:316:PX4:H29	4:A:361:PX4:H25	0.49	1.85	2	1
4:A:347:PX4:H21	4:A:348:PX4:H55	0.49	1.83	3	1
4:A:369:PX4:H20	4:A:377:PX4:H46	0.49	1.85	4	1
4:A:326:PX4:O6	4:A:363:PX4:H61	0.49	2.07	8	1
4:A:326:PX4:H19	4:A:334:PX4:H55	0.49	1.83	4	1
4:A:335:PX4:O6	4:A:343:PX4:H14	0.49	2.08	5	1
4:A:419:PX4:H42	4:A:427:PX4:H41	0.49	1.83	5	1
4:A:390:PX4:O1	4:A:399:PX4:H12	0.49	2.08	6	1
4:A:348:PX4:H35	4:A:380:PX4:H42	0.49	1.83	7	1
4:A:306:PX4:H59	4:A:361:PX4:H57	0.49	1.84	8	1
4:A:340:PX4:H42	4:A:389:PX4:H27	0.49	1.84	9	1
4:A:345:PX4:O1	4:A:346:PX4:H9	0.49	2.08	9	1
4:A:332:PX4:H53	4:A:356:PX4:H47	0.49	1.84	5	1
4:A:392:PX4:H70	4:A:415:PX4:H33	0.49	1.84	7	1
4:A:344:PX4:H56	4:A:347:PX4:H33	0.49	1.84	10	1
4:A:408:PX4:H4	4:A:414:PX4:O2	0.49	2.07	10	2
4:A:406:PX4:H23	4:A:415:PX4:H22	0.49	1.85	13	1
4:A:312:PX4:H25	4:A:365:PX4:H20	0.49	1.84	3	1
4:A:332:PX4:H52	4:A:347:PX4:H65	0.49	1.85	3	1
4:A:313:PX4:H51	4:A:354:PX4:H66	0.49	1.85	5	1
4:A:337:PX4:H42	4:A:347:PX4:H30	0.49	1.84	7	1
4:A:395:PX4:H19	4:A:396:PX4:H15	0.49	1.85	8	1
4:A:337:PX4:H31	4:A:338:PX4:H28	0.49	1.84	10	1
4:A:337:PX4:H48	4:A:345:PX4:H51	0.49	1.82	12	1
4:A:393:PX4:H32	4:A:401:PX4:H53	0.49	1.83	12	1
4:A:313:PX4:H15	4:A:360:PX4:C9	0.49	2.38	14	1
4:A:405:PX4:H64	4:A:406:PX4:H67	0.49	1.85	3	1
4:A:415:PX4:H56	4:A:421:PX4:H68	0.49	1.83	3	1
4:A:385:PX4:H49	4:A:393:PX4:H52	0.49	1.84	5	1
4:A:400:PX4:H39	4:A:401:PX4:H35	0.49	1.84	5	1
4:A:421:PX4:H26	4:A:423:PX4:H22	0.49	1.85	7	1
4:A:319:PX4:H17	4:A:324:PX4:O4	0.49	2.08	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:400:PX4:H57	4:A:408:PX4:H72	0.49	1.85	8	1
4:A:326:PX4:H69	4:A:393:PX4:H62	0.49	1.83	9	1
4:A:344:PX4:H52	4:A:347:PX4:H27	0.49	1.84	9	1
4:A:361:PX4:H37	4:A:423:PX4:H36	0.49	1.84	9	1
4:A:387:PX4:H47	4:A:411:PX4:C8	0.49	2.34	12	1
4:A:321:PX4:H34	4:A:322:PX4:H58	0.49	1.83	13	1
4:A:335:PX4:H1	4:A:344:PX4:O6	0.48	2.08	4	1
4:A:376:PX4:H59	4:A:385:PX4:H57	0.48	1.84	5	1
4:A:385:PX4:H23	4:A:386:PX4:H28	0.48	1.85	5	1
4:A:355:PX4:H54	4:A:356:PX4:H47	0.48	1.85	8	1
4:A:367:PX4:H18	4:A:424:PX4:O3	0.48	2.08	8	1
4:A:373:PX4:O2	4:A:382:PX4:H9	0.48	2.08	12	1
4:A:316:PX4:H64	4:A:323:PX4:H69	0.48	1.84	14	1
4:A:376:PX4:H61	4:A:392:PX4:H32	0.48	1.85	14	1
4:A:308:PX4:H19	4:A:311:PX4:H52	0.48	1.85	2	1
4:A:322:PX4:H56	4:A:336:PX4:H31	0.48	1.85	3	1
4:A:404:PX4:H48	4:A:413:PX4:O6	0.48	2.08	4	1
4:A:406:PX4:H28	4:A:421:PX4:H63	0.48	1.86	5	1
4:A:385:PX4:H28	4:A:386:PX4:H28	0.48	1.85	7	1
4:A:369:PX4:H32	4:A:410:PX4:H21	0.48	1.83	2	1
4:A:332:PX4:H43	4:A:407:PX4:H61	0.48	1.85	3	1
4:A:372:PX4:H25	4:A:420:PX4:H50	0.48	1.84	4	1
4:A:421:PX4:H40	4:A:423:PX4:H53	0.48	1.85	7	1
4:A:311:PX4:H31	4:A:364:PX4:H27	0.48	1.86	11	1
4:A:307:PX4:H71	4:A:349:PX4:H45	0.48	1.84	1	1
4:A:376:PX4:H60	4:A:392:PX4:H25	0.48	1.84	5	1
4:A:316:PX4:H24	4:A:364:PX4:H47	0.48	1.86	8	1
4:A:320:PX4:H71	4:A:378:PX4:H40	0.48	1.85	8	1
4:A:357:PX4:H71	4:A:357:PX4:H29	0.48	1.84	10	1
4:A:345:PX4:H20	4:A:346:PX4:H15	0.48	1.85	11	1
4:A:307:PX4:H22	4:A:321:PX4:H64	0.48	1.83	13	1
4:A:378:PX4:H2	4:A:410:PX4:O6	0.48	2.09	13	1
4:A:389:PX4:H51	4:A:390:PX4:H24	0.48	1.85	13	1
4:A:400:PX4:H40	4:A:401:PX4:H45	0.48	1.85	1	1
4:A:309:PX4:H65	4:A:320:PX4:H36	0.48	1.85	2	1
4:A:326:PX4:H21	4:A:350:PX4:H17	0.48	1.85	9	1
4:A:349:PX4:H38	4:A:421:PX4:H42	0.48	1.85	10	1
4:A:400:PX4:H46	4:A:409:PX4:H20	0.48	1.85	10	1
4:A:346:PX4:H50	4:A:362:PX4:H56	0.48	1.86	11	1
4:A:354:PX4:H24	4:A:362:PX4:H17	0.48	1.84	11	1
4:A:310:PX4:O6	4:A:365:PX4:H11	0.48	2.08	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:400:PX4:H60	4:A:410:PX4:H54	0.48	1.85	13	1
4:A:331:PX4:O6	4:A:340:PX4:H4	0.48	2.08	1	1
4:A:330:PX4:C11	4:A:335:PX4:H19	0.48	2.36	2	1
4:A:393:PX4:H42	4:A:401:PX4:H40	0.48	1.84	2	1
4:A:353:PX4:H70	4:A:412:PX4:H37	0.48	1.86	5	1
4:A:377:PX4:H60	4:A:416:PX4:H62	0.48	1.85	5	1
4:A:388:PX4:H23	4:A:396:PX4:H30	0.48	1.84	11	1
4:A:392:PX4:H67	4:A:408:PX4:H36	0.48	1.84	12	1
4:A:369:PX4:H18	4:A:425:PX4:H1	0.48	1.86	1	1
4:A:395:PX4:H48	4:A:405:PX4:H19	0.48	1.86	12	2
4:A:358:PX4:H27	4:A:363:PX4:H26	0.48	1.86	2	1
1:A:242:TYR:CD1	4:A:314:PX4:H19	0.48	2.43	4	1
4:A:337:PX4:H30	4:A:338:PX4:H48	0.48	1.86	5	1
4:A:319:PX4:H21	4:A:324:PX4:H19	0.48	1.84	6	1
4:A:374:PX4:H29	4:A:427:PX4:H31	0.48	1.86	7	1
4:A:390:PX4:H62	4:A:397:PX4:C21	0.48	2.38	9	1
4:A:337:PX4:H50	4:A:353:PX4:H25	0.48	1.84	10	1
1:A:145:THR:HB	1:A:146:PRO:HD2	0.48	1.85	2	1
4:A:318:PX4:O2	4:A:359:PX4:H18	0.48	2.07	4	1
4:A:323:PX4:H26	4:A:333:PX4:H17	0.48	1.85	4	1
4:A:331:PX4:H18	4:A:340:PX4:H21	0.48	1.84	5	1
4:A:346:PX4:H51	4:A:355:PX4:H14	0.48	1.85	6	1
4:A:406:PX4:H18	4:A:415:PX4:O1	0.48	2.09	11	1
4:A:326:PX4:H49	4:A:351:PX4:H18	0.48	1.84	1	1
4:A:307:PX4:H49	4:A:321:PX4:H56	0.48	1.86	5	1
4:A:348:PX4:H55	4:A:388:PX4:H71	0.48	1.84	6	1
4:A:315:PX4:H45	4:A:425:PX4:H27	0.48	1.85	7	1
4:A:326:PX4:H20	4:A:350:PX4:H48	0.48	1.86	8	1
4:A:404:PX4:H53	4:A:413:PX4:H24	0.48	1.86	14	1
4:A:416:PX4:H10	4:A:416:PX4:O3	0.48	2.09	1	1
4:A:347:PX4:H13	4:A:348:PX4:O1	0.48	2.08	6	3
4:A:404:PX4:H59	4:A:430:PX4:H40	0.48	1.86	4	1
4:A:351:PX4:C5	4:A:352:PX4:H24	0.48	2.39	9	1
4:A:325:PX4:H62	4:A:334:PX4:H45	0.48	1.86	11	1
4:A:321:PX4:H15	4:A:354:PX4:H15	0.48	1.85	12	1
4:A:337:PX4:H22	4:A:337:PX4:H8	0.48	1.85	12	1
4:A:421:PX4:H30	4:A:423:PX4:H19	0.48	1.86	12	1
4:A:373:PX4:H60	4:A:381:PX4:H25	0.47	1.85	3	1
4:A:357:PX4:H39	4:A:402:PX4:H41	0.47	1.84	4	1
4:A:308:PX4:O1	4:A:311:PX4:H14	0.47	2.10	7	1
4:A:349:PX4:H30	4:A:356:PX4:H38	0.47	1.86	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:424:PX4:H69	4:A:429:PX4:H67	0.47	1.86	7	1
4:A:325:PX4:H17	4:A:341:PX4:H47	0.47	1.85	14	1
4:A:388:PX4:H17	4:A:396:PX4:O6	0.47	2.09	1	2
4:A:331:PX4:H14	4:A:347:PX4:H14	0.47	1.86	5	1
4:A:421:PX4:H30	4:A:430:PX4:H19	0.47	1.84	5	1
4:A:402:PX4:O2	4:A:402:PX4:H10	0.47	2.09	7	1
4:A:413:PX4:H50	4:A:430:PX4:H23	0.47	1.86	7	1
4:A:338:PX4:H68	4:A:396:PX4:H38	0.47	1.85	2	1
4:A:314:PX4:H61	4:A:364:PX4:H71	0.47	1.86	7	1
4:A:351:PX4:H55	4:A:358:PX4:H52	0.47	1.86	7	1
4:A:322:PX4:H25	4:A:361:PX4:H48	0.47	1.86	10	2
4:A:326:PX4:H35	4:A:350:PX4:H52	0.47	1.86	10	1
4:A:335:PX4:H24	4:A:344:PX4:H24	0.47	1.86	11	1
4:A:332:PX4:H3	4:A:356:PX4:O3	0.47	2.08	14	1
4:A:367:PX4:H28	4:A:423:PX4:H50	0.47	1.85	14	1
4:A:376:PX4:H68	4:A:385:PX4:H63	0.47	1.87	14	1
4:A:368:PX4:H1	4:A:369:PX4:O2	0.47	2.09	1	1
4:A:421:PX4:H5	4:A:423:PX4:O1	0.47	2.09	3	2
4:A:372:PX4:H55	4:A:379:PX4:H53	0.47	1.86	2	1
4:A:398:PX4:H40	4:A:414:PX4:H32	0.47	1.86	6	1
4:A:310:PX4:H48	4:A:312:PX4:H21	0.47	1.86	10	1
4:A:311:PX4:H69	4:A:320:PX4:H44	0.47	1.86	10	1
4:A:342:PX4:H54	4:A:351:PX4:H29	0.47	1.86	11	2
4:A:345:PX4:H19	4:A:346:PX4:H19	0.47	1.86	11	1
4:A:405:PX4:H54	4:A:414:PX4:H30	0.47	1.86	11	1
4:A:378:PX4:H52	4:A:410:PX4:H26	0.47	1.87	13	1
4:A:355:PX4:H20	4:A:362:PX4:H51	0.47	1.86	14	1
4:A:325:PX4:H17	4:A:341:PX4:H17	0.47	1.87	1	1
4:A:326:PX4:H51	4:A:334:PX4:H40	0.47	1.87	3	1
4:A:351:PX4:H56	4:A:358:PX4:H56	0.47	1.86	3	1
1:A:205:THR:O	4:A:314:PX4:H9	0.47	2.09	4	1
4:A:317:PX4:O1	4:A:351:PX4:H20	0.47	2.09	4	1
4:A:338:PX4:H70	4:A:362:PX4:H44	0.47	1.86	4	1
4:A:325:PX4:H14	4:A:325:PX4:H12	0.47	1.87	5	1
4:A:412:PX4:H5	4:A:427:PX4:O1	0.47	2.10	7	1
4:A:399:PX4:O1	4:A:407:PX4:H7	0.47	2.10	9	1
4:A:400:PX4:H47	4:A:426:PX4:H26	0.47	1.85	12	1
4:A:361:PX4:H31	4:A:367:PX4:H42	0.47	1.84	1	1
4:A:417:PX4:H64	4:A:420:PX4:H60	0.47	1.86	4	1
4:A:340:PX4:H47	4:A:341:PX4:H61	0.47	1.87	7	1
4:A:405:PX4:O2	4:A:406:PX4:H12	0.47	2.09	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:424:PX4:H48	4:A:425:PX4:H22	0.47	1.86	7	1
4:A:358:PX4:H20	4:A:363:PX4:H18	0.47	1.86	14	2
4:A:316:PX4:H61	4:A:323:PX4:C36	0.47	2.38	12	1
4:A:306:PX4:H29	4:A:336:PX4:H31	0.47	1.87	1	1
4:A:319:PX4:H12	4:A:342:PX4:O2	0.47	2.09	1	1
4:A:359:PX4:H44	4:A:372:PX4:H40	0.47	1.87	2	1
4:A:336:PX4:H36	4:A:361:PX4:H67	0.47	1.86	4	1
4:A:349:PX4:O6	4:A:349:PX4:H12	0.47	2.09	4	1
4:A:306:PX4:H70	4:A:349:PX4:H35	0.47	1.86	5	1
4:A:308:PX4:H54	4:A:364:PX4:H30	0.47	1.85	5	1
4:A:310:PX4:H54	4:A:312:PX4:H22	0.47	1.87	5	1
4:A:322:PX4:H40	4:A:361:PX4:H54	0.47	1.84	5	1
4:A:346:PX4:H29	4:A:354:PX4:H19	0.47	1.86	5	1
4:A:395:PX4:H59	4:A:405:PX4:H42	0.47	1.84	5	1
4:A:345:PX4:O1	4:A:346:PX4:H13	0.47	2.08	6	1
4:A:360:PX4:H3	4:A:366:PX4:O4	0.47	2.10	6	1
4:A:403:PX4:H52	4:A:419:PX4:H55	0.47	1.86	6	1
1:A:214:LEU:H	1:A:214:LEU:HD23	0.47	1.69	7	1
4:A:390:PX4:H60	4:A:390:PX4:H29	0.47	1.86	7	1
4:A:309:PX4:O6	4:A:320:PX4:H4	0.47	2.09	9	1
4:A:358:PX4:H38	4:A:365:PX4:H34	0.47	1.86	9	1
4:A:396:PX4:H63	4:A:398:PX4:H50	0.47	1.86	9	1
4:A:400:PX4:O2	4:A:426:PX4:H14	0.47	2.09	9	1
4:A:346:PX4:H46	4:A:355:PX4:O1	0.47	2.10	10	1
4:A:388:PX4:H52	4:A:411:PX4:H28	0.47	1.87	11	1
4:A:405:PX4:H9	4:A:405:PX4:O6	0.47	2.10	11	1
4:A:335:PX4:H48	4:A:343:PX4:H22	0.47	1.86	12	1
4:A:391:PX4:H64	4:A:409:PX4:H62	0.47	1.87	13	1
4:A:402:PX4:H37	4:A:413:PX4:H36	0.47	1.86	13	1
4:A:331:PX4:H69	4:A:347:PX4:H42	0.47	1.85	14	1
4:A:381:PX4:H52	4:A:388:PX4:H46	0.47	1.86	14	1
4:A:392:PX4:H51	4:A:408:PX4:H24	0.47	1.85	14	1
4:A:323:PX4:H43	4:A:424:PX4:H27	0.47	1.86	1	1
4:A:413:PX4:H66	4:A:422:PX4:H41	0.47	1.87	1	1
4:A:389:PX4:H21	4:A:396:PX4:H71	0.47	1.87	5	1
4:A:315:PX4:H28	4:A:322:PX4:H40	0.47	1.87	9	1
4:A:400:PX4:H48	4:A:410:PX4:H46	0.47	1.87	10	1
4:A:412:PX4:H27	4:A:413:PX4:H38	0.47	1.84	10	1
4:A:376:PX4:H23	4:A:399:PX4:H49	0.47	1.86	11	1
4:A:371:PX4:H71	4:A:378:PX4:H62	0.47	1.87	14	1
4:A:326:PX4:H36	4:A:349:PX4:H71	0.47	1.87	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:307:PX4:H64	4:A:321:PX4:H67	0.47	1.87	4	1
4:A:369:PX4:H32	4:A:377:PX4:H61	0.47	1.86	4	1
4:A:375:PX4:H68	4:A:419:PX4:H32	0.47	1.86	4	1
4:A:334:PX4:H41	4:A:408:PX4:H41	0.47	1.87	5	1
4:A:350:PX4:H49	4:A:363:PX4:H50	0.47	1.87	5	1
4:A:398:PX4:H16	4:A:407:PX4:H46	0.47	1.85	7	1
4:A:400:PX4:H17	4:A:408:PX4:H53	0.47	1.85	7	1
4:A:312:PX4:H28	4:A:365:PX4:H46	0.47	1.85	8	1
4:A:355:PX4:H61	4:A:355:PX4:H17	0.47	1.85	9	1
4:A:408:PX4:H72	4:A:426:PX4:H57	0.47	1.87	9	1
4:A:391:PX4:H41	4:A:408:PX4:H39	0.47	1.85	10	1
4:A:371:PX4:H39	4:A:420:PX4:H36	0.47	1.86	11	1
4:A:332:PX4:H37	4:A:390:PX4:H39	0.47	1.86	14	1
4:A:402:PX4:H51	4:A:404:PX4:H47	0.47	1.87	3	1
4:A:388:PX4:H34	4:A:402:PX4:H24	0.47	1.87	4	1
4:A:416:PX4:H57	4:A:423:PX4:H64	0.47	1.86	9	1
4:A:322:PX4:H25	4:A:361:PX4:H46	0.47	1.85	13	1
4:A:419:PX4:O8	4:A:427:PX4:H17	0.47	2.09	13	1
4:A:308:PX4:H62	4:A:363:PX4:H21	0.46	1.87	1	1
4:A:368:PX4:O2	4:A:369:PX4:H4	0.46	2.09	2	1
4:A:345:PX4:H20	4:A:346:PX4:H47	0.46	1.86	5	1
4:A:349:PX4:H41	4:A:422:PX4:H45	0.46	1.87	7	1
4:A:372:PX4:H26	4:A:378:PX4:H34	0.46	1.87	9	1
4:A:342:PX4:H19	4:A:352:PX4:H23	0.46	1.87	10	1
4:A:404:PX4:H41	4:A:412:PX4:H64	0.46	1.88	10	1
4:A:370:PX4:H68	4:A:403:PX4:H23	0.46	1.88	13	1
4:A:358:PX4:H31	4:A:364:PX4:H43	0.46	1.85	14	1
4:A:325:PX4:H47	4:A:341:PX4:H22	0.46	1.87	2	1
4:A:393:PX4:H38	4:A:401:PX4:H36	0.46	1.86	2	1
4:A:382:PX4:H59	4:A:428:PX4:H21	0.46	1.88	3	1
4:A:310:PX4:H71	4:A:311:PX4:H20	0.46	1.85	7	1
4:A:400:PX4:H31	4:A:426:PX4:H58	0.46	1.87	8	1
4:A:392:PX4:H18	4:A:393:PX4:H47	0.46	1.87	11	2
4:A:353:PX4:H27	4:A:366:PX4:H14	0.46	1.86	10	1
4:A:380:PX4:H52	4:A:387:PX4:H46	0.46	1.87	11	1
4:A:386:PX4:H29	4:A:387:PX4:H26	0.46	1.86	12	1
4:A:400:PX4:H29	4:A:401:PX4:H31	0.46	1.87	13	1
4:A:322:PX4:H38	4:A:413:PX4:H68	0.46	1.88	2	1
4:A:355:PX4:H40	4:A:356:PX4:H35	0.46	1.87	3	1
4:A:395:PX4:H35	4:A:397:PX4:H64	0.46	1.86	3	1
4:A:310:PX4:H72	4:A:311:PX4:H67	0.46	1.87	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:424:PX4:H40	4:A:429:PX4:H68	0.46	1.88	6	1
4:A:404:PX4:H15	4:A:413:PX4:O6	0.46	2.11	9	1
4:A:310:PX4:H63	4:A:311:PX4:H21	0.46	1.87	10	1
4:A:378:PX4:H19	4:A:410:PX4:H27	0.46	1.87	12	1
4:A:315:PX4:H5	4:A:361:PX4:O6	0.46	2.11	14	1
4:A:392:PX4:H49	4:A:393:PX4:H50	0.46	1.88	14	1
4:A:404:PX4:H69	4:A:412:PX4:H45	0.46	1.87	1	1
4:A:371:PX4:H60	4:A:378:PX4:H66	0.46	1.87	5	1
4:A:331:PX4:H42	4:A:397:PX4:H30	0.46	1.88	6	1
4:A:315:PX4:H17	4:A:316:PX4:H54	0.46	1.87	7	1
4:A:353:PX4:O6	4:A:366:PX4:H3	0.46	2.10	8	1
4:A:383:PX4:H59	4:A:399:PX4:H17	0.46	1.87	9	1
4:A:398:PX4:H19	4:A:407:PX4:H19	0.46	1.86	9	1
4:A:330:PX4:H30	4:A:338:PX4:H29	0.46	1.87	10	1
4:A:390:PX4:H61	4:A:397:PX4:H36	0.46	1.87	10	1
4:A:315:PX4:H21	4:A:316:PX4:H32	0.46	1.88	12	1
4:A:407:PX4:H18	4:A:414:PX4:H49	0.46	1.85	12	1
4:A:410:PX4:H60	4:A:417:PX4:H62	0.46	1.87	14	1
4:A:322:PX4:H24	4:A:361:PX4:H48	0.46	1.85	2	1
4:A:347:PX4:H43	4:A:348:PX4:H31	0.46	1.86	3	1
4:A:378:PX4:H17	4:A:410:PX4:H22	0.46	1.86	3	1
4:A:378:PX4:H42	4:A:410:PX4:H71	0.46	1.85	5	1
4:A:321:PX4:H68	4:A:361:PX4:H49	0.46	1.88	7	1
4:A:417:PX4:H20	4:A:426:PX4:H23	0.46	1.87	7	1
4:A:349:PX4:H56	4:A:350:PX4:H28	0.46	1.86	10	1
4:A:321:PX4:H70	4:A:423:PX4:H41	0.46	1.88	12	1
4:A:307:PX4:H39	4:A:349:PX4:H69	0.46	1.86	13	1
4:A:391:PX4:H29	4:A:414:PX4:H46	0.46	1.87	13	1
4:A:367:PX4:H25	4:A:424:PX4:H26	0.46	1.87	1	1
4:A:350:PX4:H69	4:A:351:PX4:H69	0.46	1.87	3	1
4:A:331:PX4:H28	4:A:347:PX4:C25	0.46	2.40	4	1
4:A:387:PX4:H14	4:A:387:PX4:H6	0.46	1.86	6	1
4:A:402:PX4:H18	4:A:404:PX4:H20	0.46	1.85	6	1
4:A:347:PX4:H72	4:A:356:PX4:H65	0.46	1.87	9	1
4:A:307:PX4:H55	4:A:362:PX4:H27	0.46	1.86	11	1
4:A:349:PX4:H64	4:A:405:PX4:H70	0.46	1.87	11	1
4:A:369:PX4:H25	4:A:418:PX4:H25	0.46	1.87	11	1
4:A:346:PX4:H30	4:A:353:PX4:H65	0.46	1.86	13	1
4:A:421:PX4:H43	4:A:423:PX4:H41	0.46	1.87	7	1
4:A:331:PX4:H29	4:A:347:PX4:H52	0.46	1.87	8	1
4:A:337:PX4:H47	4:A:353:PX4:C6	0.46	2.29	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:340:PX4:H36	4:A:397:PX4:H65	0.46	1.85	9	1
4:A:313:PX4:C19	4:A:337:PX4:H64	0.46	2.41	10	1
4:A:423:PX4:H55	4:A:425:PX4:H28	0.46	1.88	10	1
4:A:308:PX4:H52	4:A:363:PX4:H24	0.46	1.86	12	1
4:A:321:PX4:H61	4:A:361:PX4:H46	0.46	1.88	12	1
4:A:340:PX4:H65	4:A:340:PX4:H28	0.46	1.86	13	1
4:A:407:PX4:O6	4:A:407:PX4:H7	0.46	2.11	1	1
4:A:396:PX4:H63	4:A:398:PX4:H51	0.46	1.88	11	1
4:A:337:PX4:H65	4:A:353:PX4:H40	0.46	1.86	12	1
4:A:383:PX4:H20	4:A:392:PX4:H27	0.46	1.85	12	1
4:A:313:PX4:H60	4:A:327:PX4:H31	0.46	1.87	13	1
4:A:390:PX4:H57	4:A:397:PX4:H35	0.46	1.86	13	1
4:A:330:PX4:H13	4:A:338:PX4:O6	0.46	2.11	5	1
4:A:317:PX4:H42	4:A:342:PX4:H72	0.46	1.88	6	1
4:A:391:PX4:H17	4:A:408:PX4:H2	0.46	1.88	7	1
4:A:344:PX4:H31	4:A:348:PX4:H25	0.46	1.88	8	1
4:A:392:PX4:H68	4:A:408:PX4:H35	0.46	1.88	8	1
4:A:367:PX4:H48	4:A:428:PX4:H50	0.46	1.86	9	1
4:A:392:PX4:H29	4:A:393:PX4:H61	0.46	1.88	11	1
4:A:357:PX4:H43	4:A:358:PX4:H44	0.46	1.86	13	1
4:A:325:PX4:H42	4:A:334:PX4:H59	0.46	1.87	14	1
4:A:340:PX4:H37	4:A:397:PX4:H29	0.46	1.88	1	1
4:A:370:PX4:H42	4:A:403:PX4:H38	0.46	1.86	1	1
4:A:402:PX4:H20	4:A:411:PX4:O8	0.46	2.11	1	1
4:A:332:PX4:H29	4:A:347:PX4:H66	0.46	1.87	5	1
4:A:311:PX4:H51	4:A:359:PX4:H59	0.46	1.86	7	1
4:A:362:PX4:H26	4:A:413:PX4:H72	0.46	1.88	7	1
4:A:388:PX4:H14	4:A:396:PX4:H18	0.46	1.88	7	1
4:A:338:PX4:H47	4:A:348:PX4:C23	0.46	2.41	8	1
4:A:382:PX4:H60	4:A:412:PX4:H64	0.46	1.88	8	1
4:A:398:PX4:H32	4:A:414:PX4:H55	0.46	1.86	8	1
4:A:311:PX4:H20	4:A:311:PX4:H55	0.46	1.88	10	1
4:A:398:PX4:H48	4:A:407:PX4:H57	0.46	1.86	12	1
4:A:404:PX4:H26	4:A:419:PX4:H9	0.45	1.87	3	1
4:A:409:PX4:H64	4:A:415:PX4:H60	0.45	1.88	4	1
4:A:334:PX4:H33	4:A:407:PX4:H38	0.45	1.88	9	1
4:A:330:PX4:C4	4:A:330:PX4:H19	0.45	2.41	10	1
4:A:410:PX4:O2	4:A:416:PX4:H3	0.45	2.10	14	2
4:A:326:PX4:H55	4:A:408:PX4:H44	0.45	1.87	11	1
4:A:391:PX4:H16	4:A:392:PX4:H46	0.45	1.88	12	1
4:A:312:PX4:H32	4:A:357:PX4:H55	0.45	1.88	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:361:PX4:H19	4:A:364:PX4:H46	0.45	1.87	14	1
4:A:323:PX4:H4	4:A:333:PX4:O2	0.45	2.11	3	1
4:A:308:PX4:H21	4:A:311:PX4:H49	0.45	1.88	7	1
4:A:308:PX4:H16	4:A:311:PX4:C9	0.45	2.41	7	1
4:A:316:PX4:H48	4:A:320:PX4:H21	0.45	1.87	7	1
4:A:317:PX4:H51	4:A:341:PX4:H19	0.45	1.87	8	1
4:A:360:PX4:H43	4:A:382:PX4:H64	0.45	1.88	8	1
4:A:380:PX4:H62	4:A:388:PX4:H42	0.45	1.88	9	1
4:A:421:PX4:H7	4:A:422:PX4:O6	0.45	2.11	9	1
4:A:413:PX4:H35	4:A:419:PX4:H27	0.45	1.87	10	1
4:A:333:PX4:H33	4:A:389:PX4:H45	0.45	1.88	11	1
4:A:367:PX4:H16	4:A:424:PX4:H14	0.45	1.87	14	1
4:A:403:PX4:H46	4:A:419:PX4:H51	0.45	1.88	1	1
4:A:383:PX4:O4	4:A:392:PX4:H1	0.45	2.10	3	1
4:A:393:PX4:H31	4:A:394:PX4:C11	0.45	2.41	3	1
4:A:354:PX4:H63	4:A:360:PX4:H63	0.45	1.88	4	1
4:A:422:PX4:H3	4:A:423:PX4:O2	0.45	2.10	4	1
4:A:331:PX4:C21	4:A:397:PX4:H30	0.45	2.41	6	1
4:A:391:PX4:H48	4:A:392:PX4:H46	0.45	1.87	8	1
4:A:351:PX4:H12	4:A:352:PX4:H24	0.45	1.88	9	1
4:A:345:PX4:C36	4:A:370:PX4:H39	0.45	2.41	10	1
4:A:390:PX4:H1	4:A:399:PX4:H18	0.45	1.88	12	1
4:A:317:PX4:H59	4:A:319:PX4:H56	0.45	1.88	14	1
4:A:348:PX4:H55	4:A:388:PX4:H70	0.45	1.88	1	1
4:A:405:PX4:H47	4:A:406:PX4:H48	0.45	1.88	4	1
4:A:307:PX4:H37	4:A:416:PX4:H42	0.45	1.88	5	1
4:A:310:PX4:H70	4:A:359:PX4:H59	0.45	1.88	5	1
4:A:313:PX4:H21	4:A:366:PX4:H18	0.45	1.88	5	1
4:A:331:PX4:H40	4:A:340:PX4:H63	0.45	1.88	5	1
4:A:337:PX4:H48	4:A:345:PX4:H49	0.45	1.88	6	1
4:A:328:PX4:H47	4:A:329:PX4:H28	0.45	1.89	9	1
4:A:380:PX4:H20	4:A:381:PX4:H48	0.45	1.89	9	1
4:A:348:PX4:H59	4:A:362:PX4:H54	0.45	1.89	13	1
4:A:338:PX4:H66	4:A:395:PX4:H38	0.45	1.89	4	1
4:A:381:PX4:H59	4:A:397:PX4:H47	0.45	1.87	7	1
4:A:369:PX4:H21	4:A:377:PX4:H71	0.45	1.87	10	1
4:A:323:PX4:H36	4:A:424:PX4:H67	0.45	1.87	4	1
4:A:313:PX4:H42	4:A:403:PX4:H62	0.45	1.87	5	1
4:A:421:PX4:H24	4:A:423:PX4:H19	0.45	1.87	5	1
4:A:307:PX4:H5	4:A:321:PX4:H48	0.45	1.87	8	1
4:A:412:PX4:O8	4:A:428:PX4:H17	0.45	2.11	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:349:PX4:O1	4:A:350:PX4:H14	0.45	2.11	10	1
4:A:391:PX4:H46	4:A:401:PX4:O6	0.45	2.12	11	1
4:A:378:PX4:H19	4:A:410:PX4:C14	0.45	2.42	12	1
4:A:371:PX4:H58	4:A:379:PX4:H32	0.45	1.89	13	1
4:A:375:PX4:H50	4:A:428:PX4:H14	0.45	1.88	13	1
4:A:322:PX4:H22	4:A:323:PX4:H19	0.45	1.89	1	1
4:A:393:PX4:H56	4:A:401:PX4:H35	0.45	1.89	1	1
4:A:313:PX4:H42	4:A:403:PX4:H66	0.45	1.89	2	1
4:A:368:PX4:H37	4:A:418:PX4:H72	0.45	1.89	4	1
4:A:416:PX4:H27	4:A:423:PX4:H24	0.45	1.87	7	1
4:A:312:PX4:H62	4:A:320:PX4:H67	0.45	1.87	11	1
4:A:373:PX4:O6	4:A:397:PX4:H12	0.45	2.12	11	1
4:A:419:PX4:H18	4:A:419:PX4:H12	0.45	1.87	11	1
4:A:391:PX4:H40	4:A:392:PX4:H56	0.45	1.88	13	1
1:A:214:LEU:HD11	1:A:243:VAL:H	0.45	1.71	14	1
4:A:373:PX4:H36	4:A:381:PX4:H45	0.45	1.88	2	1
4:A:316:PX4:H25	4:A:320:PX4:H33	0.45	1.88	3	1
4:A:394:PX4:H34	4:A:401:PX4:H39	0.45	1.89	3	1
4:A:331:PX4:H53	4:A:340:PX4:H34	0.45	1.87	4	1
4:A:402:PX4:H57	4:A:404:PX4:H60	0.45	1.88	4	1
4:A:342:PX4:H27	4:A:358:PX4:H58	0.45	1.89	5	1
1:A:243:VAL:HG12	4:A:356:PX4:H23	0.45	1.88	6	1
4:A:331:PX4:H43	4:A:389:PX4:H29	0.45	1.88	6	1
4:A:367:PX4:H17	4:A:428:PX4:H54	0.45	1.88	9	1
4:A:330:PX4:H21	4:A:338:PX4:H22	0.45	1.87	10	1
4:A:370:PX4:H28	4:A:403:PX4:H57	0.45	1.89	1	1
4:A:306:PX4:H14	4:A:321:PX4:O6	0.45	2.12	3	1
4:A:337:PX4:H53	4:A:353:PX4:H25	0.45	1.89	4	1
4:A:398:PX4:H67	4:A:405:PX4:H57	0.45	1.88	6	1
4:A:378:PX4:H16	4:A:417:PX4:C24	0.45	2.33	7	1
4:A:330:PX4:H7	4:A:330:PX4:H19	0.45	1.87	11	1
4:A:310:PX4:H17	4:A:365:PX4:O5	0.45	2.11	13	1
4:A:392:PX4:H25	4:A:393:PX4:H66	0.45	1.87	13	1
4:A:417:PX4:H24	4:A:426:PX4:H26	0.45	1.89	4	1
4:A:383:PX4:H31	4:A:383:PX4:H24	0.45	1.89	5	1
4:A:384:PX4:H61	4:A:384:PX4:H34	0.45	1.89	5	1
4:A:369:PX4:H52	4:A:425:PX4:H21	0.45	1.89	11	1
4:A:350:PX4:H1	4:A:358:PX4:O2	0.45	2.12	12	1
4:A:389:PX4:O2	4:A:398:PX4:H4	0.45	2.12	14	1
4:A:383:PX4:H66	4:A:399:PX4:H69	0.44	1.89	1	1
4:A:380:PX4:H26	4:A:381:PX4:H36	0.44	1.87	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:412:PX4:H23	4:A:413:PX4:H31	0.44	1.89	9	1
4:A:347:PX4:H10	4:A:348:PX4:O1	0.44	2.13	10	1
4:A:352:PX4:H52	4:A:358:PX4:H50	0.44	1.89	10	1
4:A:322:PX4:H62	4:A:412:PX4:H42	0.44	1.88	11	1
4:A:369:PX4:H44	4:A:418:PX4:H68	0.44	1.87	11	1
4:A:398:PX4:H15	4:A:398:PX4:H13	0.44	1.90	11	1
4:A:306:PX4:H59	4:A:361:PX4:H54	0.44	1.89	13	1
4:A:406:PX4:H25	4:A:415:PX4:H22	0.44	1.88	14	1
4:A:311:PX4:H53	4:A:359:PX4:H56	0.44	1.89	5	1
4:A:319:PX4:H26	4:A:324:PX4:H24	0.44	1.88	5	1
4:A:347:PX4:H9	4:A:347:PX4:H19	0.44	1.89	6	1
4:A:367:PX4:H48	4:A:424:PX4:H19	0.44	1.88	6	1
4:A:317:PX4:O2	4:A:325:PX4:H10	0.44	2.12	7	1
4:A:334:PX4:O6	4:A:334:PX4:H3	0.44	2.12	7	1
4:A:389:PX4:H30	4:A:396:PX4:H60	0.44	1.89	8	1
4:A:398:PX4:H45	4:A:414:PX4:H21	0.44	1.89	9	1
4:A:353:PX4:H20	4:A:366:PX4:H2	0.44	1.88	10	1
4:A:313:PX4:H47	4:A:328:PX4:H17	0.44	1.90	11	1
4:A:410:PX4:H66	4:A:426:PX4:H41	0.44	1.89	12	1
4:A:375:PX4:H21	4:A:429:PX4:H45	0.44	1.88	1	1
4:A:307:PX4:H51	4:A:362:PX4:H22	0.44	1.90	6	1
4:A:396:PX4:H31	4:A:411:PX4:H34	0.44	1.90	8	1
4:A:318:PX4:H18	4:A:328:PX4:H19	0.44	1.88	11	1
4:A:419:PX4:H60	4:A:427:PX4:H58	0.44	1.89	11	1
4:A:423:PX4:H16	4:A:425:PX4:O8	0.44	2.12	13	1
4:A:337:PX4:H15	4:A:353:PX4:O1	0.44	2.13	1	2
4:A:311:PX4:H6	4:A:311:PX4:O3	0.44	2.10	2	1
4:A:377:PX4:H10	4:A:418:PX4:O8	0.44	2.13	2	1
4:A:400:PX4:H47	4:A:409:PX4:H23	0.44	1.89	3	1
4:A:422:PX4:H34	4:A:423:PX4:H45	0.44	1.88	6	1
4:A:321:PX4:H68	4:A:322:PX4:H30	0.44	1.90	9	1
4:A:387:PX4:H54	4:A:388:PX4:H38	0.44	1.89	10	1
4:A:370:PX4:H26	4:A:427:PX4:H57	0.44	1.89	11	1
4:A:402:PX4:H54	4:A:404:PX4:H59	0.44	1.89	11	1
4:A:329:PX4:H67	4:A:424:PX4:H40	0.44	1.90	14	1
4:A:369:PX4:O1	4:A:425:PX4:H4	0.44	2.13	12	3
4:A:342:PX4:H29	4:A:351:PX4:H30	0.44	1.89	3	1
4:A:337:PX4:H52	4:A:345:PX4:H55	0.44	1.88	7	2
4:A:319:PX4:H66	4:A:324:PX4:H58	0.44	1.88	9	1
4:A:405:PX4:H53	4:A:414:PX4:H33	0.44	1.89	9	1
4:A:326:PX4:H66	4:A:399:PX4:H65	0.44	1.88	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:380:PX4:H46	4:A:387:PX4:H20	0.44	1.89	11	1
4:A:345:PX4:H35	4:A:346:PX4:H37	0.44	1.89	12	1
4:A:389:PX4:H48	4:A:398:PX4:H17	0.44	1.89	12	1
4:A:320:PX4:H54	4:A:359:PX4:H30	0.44	1.90	13	1
4:A:338:PX4:H55	4:A:348:PX4:H53	0.44	1.90	14	1
4:A:412:PX4:H27	4:A:430:PX4:H60	0.44	1.89	14	1
4:A:310:PX4:O6	4:A:365:PX4:H4	0.44	2.12	1	1
4:A:391:PX4:H25	4:A:393:PX4:H64	0.44	1.89	1	1
4:A:400:PX4:C24	4:A:409:PX4:H23	0.44	2.42	2	1
4:A:315:PX4:H5	4:A:364:PX4:O8	0.44	2.11	7	1
4:A:355:PX4:H38	4:A:356:PX4:H44	0.44	1.88	7	1
4:A:389:PX4:H30	4:A:396:PX4:C31	0.44	2.42	8	1
4:A:390:PX4:H30	4:A:398:PX4:H19	0.44	1.89	8	1
4:A:321:PX4:H37	4:A:354:PX4:H59	0.44	1.90	9	1
1:A:207:SER:O	4:A:321:PX4:H6	0.44	2.13	10	1
4:A:331:PX4:H44	4:A:340:PX4:H71	0.44	1.89	3	1
4:A:315:PX4:H20	4:A:320:PX4:H28	0.44	1.89	4	1
4:A:333:PX4:H61	4:A:368:PX4:H72	0.44	1.90	4	1
4:A:338:PX4:H64	4:A:411:PX4:H36	0.44	1.89	4	1
4:A:346:PX4:H39	4:A:354:PX4:H31	0.44	1.89	5	1
4:A:393:PX4:H14	4:A:394:PX4:C9	0.44	2.43	8	1
4:A:391:PX4:H58	4:A:401:PX4:H36	0.44	1.89	13	1
4:A:402:PX4:H36	4:A:403:PX4:H35	0.44	1.89	1	1
4:A:318:PX4:H24	4:A:320:PX4:H46	0.44	1.90	2	1
4:A:393:PX4:O6	4:A:394:PX4:H15	0.44	2.13	2	1
4:A:406:PX4:H35	4:A:414:PX4:H32	0.44	1.90	3	1
4:A:392:PX4:H35	4:A:399:PX4:H61	0.44	1.89	4	1
4:A:322:PX4:H34	4:A:361:PX4:H22	0.44	1.88	6	1
4:A:400:PX4:H38	4:A:401:PX4:H38	0.44	1.87	7	1
4:A:344:PX4:H37	4:A:347:PX4:H45	0.44	1.90	8	1
4:A:377:PX4:H16	4:A:418:PX4:C3	0.44	2.42	8	1
4:A:403:PX4:H9	4:A:427:PX4:O8	0.44	2.13	8	1
4:A:312:PX4:H25	4:A:363:PX4:H32	0.44	1.90	9	1
4:A:393:PX4:H41	4:A:394:PX4:H40	0.44	1.89	10	1
4:A:338:PX4:H17	4:A:348:PX4:O6	0.44	2.13	13	1
4:A:358:PX4:H22	4:A:363:PX4:H53	0.44	1.89	13	1
4:A:310:PX4:H23	4:A:358:PX4:H49	0.44	1.89	14	1
4:A:313:PX4:H57	4:A:327:PX4:H21	0.44	1.87	14	1
4:A:323:PX4:H16	4:A:333:PX4:H51	0.44	1.90	1	1
4:A:382:PX4:H52	4:A:428:PX4:H28	0.44	1.88	3	1
4:A:413:PX4:H69	4:A:428:PX4:H70	0.44	1.88	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:367:PX4:H46	4:A:428:PX4:H47	0.44	1.90	7	1
4:A:314:PX4:H69	4:A:364:PX4:H45	0.44	1.89	10	1
4:A:326:PX4:H57	4:A:334:PX4:H34	0.44	1.90	11	1
4:A:352:PX4:H32	4:A:358:PX4:H62	0.44	1.90	14	1
4:A:370:PX4:H34	4:A:403:PX4:H67	0.44	1.90	14	1
4:A:340:PX4:H62	4:A:341:PX4:H66	0.43	1.90	1	1
4:A:351:PX4:O7	4:A:352:PX4:H23	0.43	2.13	2	1
4:A:416:PX4:O1	4:A:422:PX4:H10	0.43	2.13	2	1
4:A:351:PX4:H8	4:A:352:PX4:O1	0.43	2.13	4	1
4:A:308:PX4:H44	4:A:311:PX4:H70	0.43	1.90	12	1
4:A:318:PX4:H35	4:A:327:PX4:H65	0.43	1.89	12	1
4:A:330:PX4:H52	4:A:338:PX4:H24	0.43	1.90	12	1
4:A:417:PX4:H28	4:A:426:PX4:H32	0.43	1.90	12	1
4:A:312:PX4:H69	4:A:359:PX4:H37	0.43	1.89	13	1
4:A:321:PX4:H67	4:A:361:PX4:H24	0.43	1.90	13	1
4:A:376:PX4:H66	4:A:385:PX4:H30	0.43	1.90	13	1
4:A:374:PX4:H32	4:A:427:PX4:H23	0.43	1.90	14	1
4:A:330:PX4:H63	4:A:338:PX4:H42	0.43	1.88	2	1
4:A:361:PX4:H40	4:A:423:PX4:H66	0.43	1.90	3	1
4:A:312:PX4:H44	4:A:365:PX4:H68	0.43	1.89	5	1
4:A:393:PX4:H45	4:A:401:PX4:H45	0.43	1.90	6	1
4:A:310:PX4:H43	4:A:365:PX4:H37	0.43	1.90	7	1
4:A:328:PX4:H20	4:A:328:PX4:H25	0.43	1.38	8	1
4:A:416:PX4:O8	4:A:418:PX4:H40	0.43	2.13	8	1
4:A:346:PX4:H46	4:A:362:PX4:H46	0.43	1.90	12	1
4:A:311:PX4:H5	4:A:320:PX4:O4	0.43	2.13	13	1
4:A:326:PX4:H37	4:A:350:PX4:H32	0.43	1.89	1	1
1:A:244:ASP:OD2	4:A:349:PX4:H3	0.43	2.14	2	1
4:A:378:PX4:H23	4:A:378:PX4:H29	0.43	1.63	2	1
4:A:418:PX4:O1	4:A:425:PX4:H5	0.43	2.13	3	1
4:A:347:PX4:O4	4:A:348:PX4:H6	0.43	2.13	5	1
4:A:386:PX4:H38	4:A:394:PX4:H67	0.43	1.89	10	1
4:A:430:PX4:H44	4:A:430:PX4:H38	0.43	1.51	11	1
4:A:395:PX4:H43	4:A:405:PX4:H40	0.43	1.89	13	1
4:A:315:PX4:H10	4:A:316:PX4:O6	0.43	2.13	2	1
4:A:334:PX4:H69	4:A:352:PX4:H37	0.43	1.89	2	1
4:A:389:PX4:H33	4:A:397:PX4:H21	0.43	1.90	2	1
4:A:418:PX4:H36	4:A:418:PX4:H41	0.43	1.56	5	1
4:A:341:PX4:H58	4:A:390:PX4:H72	0.43	1.89	7	1
4:A:320:PX4:H32	4:A:359:PX4:H63	0.43	1.90	8	1
4:A:307:PX4:H61	4:A:362:PX4:H27	0.43	1.91	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:378:PX4:O1	4:A:417:PX4:H17	0.43	2.12	10	1
4:A:314:PX4:H31	4:A:356:PX4:H28	0.43	1.90	11	1
4:A:363:PX4:H30	4:A:363:PX4:H35	0.43	1.61	6	1
4:A:306:PX4:H56	4:A:306:PX4:H51	0.43	1.58	7	1
4:A:331:PX4:H51	4:A:347:PX4:H22	0.43	1.91	8	1
4:A:410:PX4:O2	4:A:416:PX4:H10	0.43	2.14	9	1
4:A:387:PX4:H5	4:A:411:PX4:O3	0.43	2.13	12	1
4:A:314:PX4:H71	4:A:409:PX4:H31	0.43	1.90	13	1
4:A:341:PX4:H72	4:A:397:PX4:H35	0.43	1.89	1	1
4:A:369:PX4:H29	4:A:378:PX4:H51	0.43	1.89	1	1
4:A:314:PX4:H37	4:A:362:PX4:H16	0.43	1.90	4	1
4:A:333:PX4:H53	4:A:341:PX4:H57	0.43	1.89	5	1
1:A:178:GLY:HA3	4:A:354:PX4:H1	0.43	1.89	7	1
4:A:376:PX4:H19	4:A:383:PX4:H19	0.43	1.90	7	1
4:A:374:PX4:H8	4:A:427:PX4:H20	0.43	1.91	8	1
4:A:338:PX4:H70	4:A:395:PX4:H38	0.43	1.90	10	1
4:A:352:PX4:O8	4:A:365:PX4:H3	0.43	2.13	10	1
4:A:407:PX4:O6	4:A:414:PX4:H49	0.43	2.13	10	1
4:A:342:PX4:C12	4:A:352:PX4:H47	0.43	2.31	11	1
4:A:374:PX4:H58	4:A:382:PX4:H50	0.43	1.91	11	1
4:A:410:PX4:H51	4:A:426:PX4:H33	0.43	1.90	11	1
4:A:423:PX4:H55	4:A:425:PX4:H27	0.43	1.90	11	1
4:A:316:PX4:H47	4:A:320:PX4:H23	0.43	1.90	12	1
4:A:393:PX4:H30	4:A:400:PX4:H31	0.43	1.91	13	1
4:A:412:PX4:H36	4:A:419:PX4:H28	0.43	1.90	2	1
4:A:309:PX4:H28	4:A:309:PX4:H62	0.43	1.89	3	1
4:A:331:PX4:H17	4:A:340:PX4:H5	0.43	1.89	3	1
4:A:346:PX4:O6	4:A:362:PX4:H15	0.43	2.14	3	1
4:A:384:PX4:O1	4:A:385:PX4:H10	0.43	2.13	4	1
4:A:349:PX4:H65	4:A:406:PX4:H68	0.43	1.88	5	1
4:A:412:PX4:H58	4:A:427:PX4:H30	0.43	1.90	5	1
4:A:325:PX4:H49	4:A:341:PX4:H19	0.43	1.89	6	1
4:A:345:PX4:H19	4:A:346:PX4:H22	0.43	1.90	6	1
4:A:387:PX4:H56	4:A:387:PX4:H50	0.43	1.43	6	1
4:A:391:PX4:H26	4:A:392:PX4:H46	0.43	1.89	6	1
4:A:395:PX4:O1	4:A:396:PX4:H17	0.43	2.14	7	1
4:A:333:PX4:H14	4:A:340:PX4:O2	0.43	2.14	9	1
4:A:353:PX4:H35	4:A:366:PX4:H22	0.43	1.91	10	1
4:A:334:PX4:H56	4:A:334:PX4:H51	0.43	1.42	11	1
4:A:356:PX4:H62	4:A:397:PX4:H71	0.43	1.90	11	1
4:A:330:PX4:H31	4:A:348:PX4:H30	0.43	1.89	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:333:PX4:H30	4:A:339:PX4:H28	0.43	1.90	14	1
4:A:398:PX4:H21	4:A:407:PX4:H46	0.43	1.91	14	1
4:A:326:PX4:H47	4:A:334:PX4:H60	0.43	1.90	1	1
4:A:373:PX4:H28	4:A:381:PX4:H57	0.43	1.91	1	1
4:A:381:PX4:H16	4:A:388:PX4:H12	0.43	1.90	2	1
4:A:308:PX4:H14	4:A:311:PX4:O8	0.43	2.14	3	1
4:A:350:PX4:H61	4:A:363:PX4:H23	0.43	1.89	3	1
4:A:330:PX4:H5	4:A:344:PX4:H16	0.43	1.91	4	1
4:A:314:PX4:H33	4:A:362:PX4:H16	0.43	1.89	7	1
4:A:403:PX4:H3	4:A:427:PX4:H49	0.43	1.90	7	1
1:A:116:TYR:CD1	1:A:138:PHE:CE2	0.43	3.06	8	1
4:A:326:PX4:H61	4:A:334:PX4:H35	0.43	1.89	10	1
4:A:345:PX4:H71	4:A:403:PX4:H36	0.43	1.91	10	1
4:A:391:PX4:H23	4:A:392:PX4:H14	0.43	1.89	10	1
4:A:314:PX4:H44	4:A:355:PX4:H46	0.43	1.90	11	1
4:A:339:PX4:H68	4:A:339:PX4:H62	0.43	1.44	13	1
4:A:391:PX4:H37	4:A:393:PX4:H72	0.43	1.89	13	1
4:A:395:PX4:H9	4:A:411:PX4:O2	0.43	2.14	14	1
4:A:325:PX4:H28	4:A:407:PX4:H41	0.43	1.90	1	1
4:A:379:PX4:H65	4:A:379:PX4:H71	0.43	1.55	2	1
4:A:371:PX4:H46	4:A:371:PX4:H16	0.43	1.75	3	2
4:A:378:PX4:H19	4:A:426:PX4:H28	0.43	1.90	3	1
4:A:354:PX4:H65	4:A:360:PX4:H24	0.43	1.89	5	1
4:A:327:PX4:O3	4:A:327:PX4:H10	0.43	2.14	6	1
4:A:376:PX4:H36	4:A:376:PX4:H42	0.43	1.68	6	1
4:A:386:PX4:H17	4:A:394:PX4:O8	0.43	2.13	6	1
4:A:403:PX4:H32	4:A:404:PX4:H21	0.43	1.91	7	1
4:A:337:PX4:H45	4:A:338:PX4:H52	0.43	1.91	8	1
4:A:325:PX4:H32	4:A:332:PX4:H28	0.43	1.90	9	1
4:A:335:PX4:H42	4:A:343:PX4:H64	0.43	1.89	10	1
4:A:412:PX4:H51	4:A:419:PX4:H16	0.43	1.91	12	1
4:A:404:PX4:H71	4:A:404:PX4:H19	0.43	1.89	13	1
4:A:403:PX4:H47	4:A:427:PX4:H47	0.43	1.90	1	1
4:A:314:PX4:H71	4:A:364:PX4:H39	0.43	1.91	2	1
4:A:314:PX4:H38	4:A:355:PX4:H57	0.43	1.91	3	1
4:A:372:PX4:H54	4:A:379:PX4:H53	0.43	1.90	5	1
1:A:207:SER:O	4:A:321:PX4:H9	0.43	2.13	6	1
4:A:328:PX4:H56	4:A:354:PX4:H72	0.43	1.90	7	1
4:A:314:PX4:H47	4:A:349:PX4:H19	0.43	1.91	8	1
4:A:377:PX4:H72	4:A:425:PX4:O2	0.43	2.13	8	1
4:A:367:PX4:H20	4:A:424:PX4:H16	0.43	1.91	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:353:PX4:H58	4:A:360:PX4:H61	0.43	1.91	11	1
4:A:393:PX4:H17	4:A:401:PX4:H22	0.43	1.91	11	1
4:A:419:PX4:H60	4:A:427:PX4:H25	0.42	1.91	1	1
4:A:395:PX4:H62	4:A:413:PX4:O8	0.42	2.14	2	1
4:A:418:PX4:H40	4:A:418:PX4:H33	0.42	1.61	3	1
4:A:378:PX4:H23	4:A:378:PX4:H30	0.42	1.54	4	1
4:A:388:PX4:H63	4:A:397:PX4:H63	0.42	1.89	4	1
4:A:320:PX4:H17	4:A:359:PX4:C29	0.42	2.43	7	1
4:A:335:PX4:H41	4:A:335:PX4:H36	0.42	1.61	7	1
4:A:348:PX4:H67	4:A:348:PX4:H60	0.42	1.52	9	1
4:A:316:PX4:O2	4:A:364:PX4:H12	0.42	2.13	12	1
4:A:398:PX4:H41	4:A:415:PX4:H20	0.42	1.90	1	1
4:A:317:PX4:H55	4:A:324:PX4:C10	0.42	2.42	2	1
4:A:344:PX4:H45	4:A:344:PX4:H37	0.42	1.62	3	1
4:A:412:PX4:H17	4:A:419:PX4:H20	0.42	1.89	5	1
4:A:315:PX4:H3	4:A:361:PX4:O1	0.42	2.14	6	1
4:A:342:PX4:H52	4:A:351:PX4:H27	0.42	1.91	8	1
4:A:349:PX4:H16	4:A:350:PX4:H30	0.42	1.90	9	1
4:A:331:PX4:H28	4:A:347:PX4:H51	0.42	1.91	11	1
4:A:308:PX4:H66	4:A:308:PX4:H61	0.42	1.59	12	1
4:A:308:PX4:H34	4:A:311:PX4:H65	0.42	1.89	12	1
4:A:330:PX4:C22	4:A:344:PX4:H45	0.42	2.40	12	1
4:A:376:PX4:H62	4:A:385:PX4:H30	0.42	1.90	12	1
4:A:354:PX4:H22	4:A:362:PX4:H21	0.42	1.90	13	1
4:A:392:PX4:H10	4:A:392:PX4:O6	0.42	2.13	13	1
4:A:369:PX4:H58	4:A:424:PX4:H50	0.42	1.91	1	1
4:A:380:PX4:O4	4:A:381:PX4:H15	0.42	2.14	4	1
4:A:310:PX4:H16	4:A:363:PX4:O6	0.42	2.14	5	1
4:A:314:PX4:H15	4:A:314:PX4:O8	0.42	2.13	5	1
4:A:429:PX4:H27	4:A:429:PX4:H54	0.42	1.91	7	1
4:A:378:PX4:H60	4:A:410:PX4:H70	0.42	1.90	8	1
4:A:333:PX4:H16	4:A:340:PX4:H15	0.42	1.90	9	1
4:A:351:PX4:H54	4:A:358:PX4:H22	0.42	1.90	9	1
4:A:314:PX4:H26	4:A:314:PX4:H19	0.42	1.66	10	1
4:A:361:PX4:C33	4:A:412:PX4:H40	0.42	2.44	11	1
4:A:423:PX4:H57	4:A:423:PX4:H26	0.42	1.91	11	1
4:A:317:PX4:H1	4:A:317:PX4:O6	0.42	2.14	13	1
4:A:310:PX4:H36	4:A:351:PX4:H65	0.42	1.91	14	1
4:A:332:PX4:H28	4:A:334:PX4:H53	0.42	1.90	14	1
4:A:316:PX4:H71	4:A:333:PX4:H67	0.42	1.92	2	1
4:A:381:PX4:H40	4:A:381:PX4:H61	0.42	1.91	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:355:PX4:H55	4:A:355:PX4:H49	0.42	1.69	4	1
4:A:357:PX4:H66	4:A:357:PX4:H61	0.42	1.65	5	1
4:A:382:PX4:H22	4:A:428:PX4:C16	0.42	2.42	5	1
4:A:416:PX4:H48	4:A:425:PX4:H48	0.42	1.91	5	1
4:A:332:PX4:H66	4:A:349:PX4:H67	0.42	1.91	8	1
4:A:320:PX4:H21	4:A:359:PX4:H60	0.42	1.91	9	1
4:A:361:PX4:H29	4:A:361:PX4:H24	0.42	1.61	9	1
4:A:391:PX4:H67	4:A:401:PX4:H33	0.42	1.91	9	1
4:A:358:PX4:H70	4:A:401:PX4:H37	0.42	1.91	10	1
4:A:356:PX4:H35	4:A:356:PX4:H42	0.42	1.71	11	1
4:A:346:PX4:H25	4:A:354:PX4:H31	0.42	1.90	12	1
4:A:412:PX4:H20	4:A:428:PX4:H49	0.42	1.90	14	1
4:A:415:PX4:H11	4:A:422:PX4:H16	0.42	1.91	1	1
4:A:418:PX4:H34	4:A:425:PX4:H56	0.42	1.91	1	1
4:A:335:PX4:H6	4:A:344:PX4:O6	0.42	2.13	2	1
4:A:356:PX4:H42	4:A:405:PX4:H60	0.42	1.91	3	1
4:A:381:PX4:H54	4:A:388:PX4:H57	0.42	1.90	3	1
4:A:307:PX4:H16	4:A:307:PX4:H46	0.42	1.64	4	1
4:A:406:PX4:O1	4:A:414:PX4:H3	0.42	2.15	4	1
4:A:308:PX4:H16	4:A:311:PX4:C10	0.42	2.44	5	1
4:A:356:PX4:O3	4:A:356:PX4:H16	0.42	2.15	5	1
4:A:424:PX4:H17	4:A:429:PX4:H21	0.42	1.92	6	1
4:A:312:PX4:H59	4:A:359:PX4:H30	0.42	1.91	7	1
4:A:325:PX4:H64	4:A:341:PX4:H35	0.42	1.90	7	1
4:A:412:PX4:H24	4:A:430:PX4:H58	0.42	1.92	9	1
4:A:315:PX4:O3	4:A:361:PX4:H4	0.42	2.15	10	1
4:A:369:PX4:H48	4:A:377:PX4:H67	0.42	1.91	10	1
4:A:387:PX4:H17	4:A:411:PX4:H61	0.42	1.90	10	1
4:A:334:PX4:H27	4:A:334:PX4:H22	0.42	1.65	11	1
4:A:387:PX4:H17	4:A:411:PX4:H57	0.42	1.91	12	1
4:A:395:PX4:H27	4:A:405:PX4:H28	0.42	1.91	13	1
4:A:330:PX4:H49	4:A:343:PX4:H46	0.42	1.91	14	1
4:A:317:PX4:H66	4:A:342:PX4:H66	0.42	1.91	2	1
4:A:406:PX4:H33	4:A:414:PX4:H34	0.42	1.91	2	1
4:A:372:PX4:H29	4:A:420:PX4:H55	0.42	1.92	4	1
4:A:404:PX4:H54	4:A:405:PX4:H39	0.42	1.91	5	1
4:A:367:PX4:O6	4:A:423:PX4:H11	0.42	2.15	6	1
4:A:326:PX4:H44	4:A:416:PX4:H41	0.42	1.91	8	1
4:A:350:PX4:O2	4:A:363:PX4:H7	0.42	2.14	8	1
4:A:354:PX4:H50	4:A:360:PX4:H18	0.42	1.90	11	1
4:A:337:PX4:H20	4:A:346:PX4:H63	0.42	1.92	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:384:PX4:H3	4:A:385:PX4:H18	0.42	1.91	14	1
4:A:326:PX4:O6	4:A:350:PX4:H5	0.42	2.14	6	1
4:A:342:PX4:H37	4:A:352:PX4:H33	0.42	1.90	9	1
4:A:346:PX4:O4	4:A:362:PX4:H11	0.42	2.15	10	1
4:A:381:PX4:H53	4:A:397:PX4:H46	0.42	1.90	10	1
4:A:382:PX4:H22	4:A:428:PX4:H34	0.42	1.92	10	1
4:A:391:PX4:H71	4:A:415:PX4:H45	0.42	1.92	10	1
4:A:406:PX4:H17	4:A:414:PX4:H22	0.42	1.92	10	1
4:A:334:PX4:H29	4:A:414:PX4:H69	0.42	1.91	11	1
4:A:338:PX4:H68	4:A:348:PX4:H58	0.42	1.90	11	1
4:A:349:PX4:O6	4:A:349:PX4:H7	0.42	2.15	11	1
4:A:332:PX4:H25	4:A:334:PX4:H49	0.42	1.90	14	1
4:A:321:PX4:H47	4:A:354:PX4:H20	0.42	1.91	2	1
4:A:371:PX4:H36	4:A:379:PX4:H60	0.42	1.91	3	1
4:A:375:PX4:H19	4:A:429:PX4:H45	0.42	1.90	3	1
4:A:391:PX4:H66	4:A:408:PX4:H57	0.42	1.92	4	1
4:A:402:PX4:H33	4:A:402:PX4:H28	0.42	1.57	4	1
4:A:307:PX4:H58	4:A:314:PX4:H17	0.42	1.92	5	1
4:A:337:PX4:O6	4:A:345:PX4:H49	0.42	2.15	5	1
4:A:347:PX4:H56	4:A:356:PX4:H56	0.42	1.92	5	1
4:A:416:PX4:H17	4:A:425:PX4:O8	0.42	2.14	5	1
4:A:344:PX4:H27	4:A:348:PX4:H21	0.42	1.92	6	1
4:A:398:PX4:H40	4:A:414:PX4:C16	0.42	2.45	6	1
4:A:384:PX4:H30	4:A:384:PX4:H57	0.42	1.91	7	1
4:A:370:PX4:H36	4:A:402:PX4:H40	0.42	1.92	8	1
4:A:331:PX4:H62	4:A:397:PX4:H59	0.42	1.92	10	1
4:A:333:PX4:O8	4:A:340:PX4:H15	0.42	2.15	11	1
4:A:338:PX4:H65	4:A:338:PX4:H58	0.42	1.68	13	1
4:A:367:PX4:O1	4:A:423:PX4:H3	0.42	2.15	2	1
4:A:354:PX4:H30	4:A:362:PX4:H17	0.42	1.90	3	1
4:A:372:PX4:H61	4:A:379:PX4:H59	0.42	1.91	3	1
4:A:353:PX4:H35	4:A:353:PX4:H41	0.42	1.58	4	1
4:A:375:PX4:H3	4:A:429:PX4:H17	0.42	1.91	4	1
4:A:382:PX4:H14	4:A:382:PX4:O6	0.42	2.14	4	1
4:A:337:PX4:H43	4:A:380:PX4:H39	0.42	1.91	6	1
4:A:324:PX4:H23	4:A:342:PX4:H55	0.42	1.91	7	1
4:A:388:PX4:H28	4:A:411:PX4:H16	0.42	1.91	7	1
4:A:363:PX4:H47	4:A:364:PX4:H33	0.42	1.91	9	1
4:A:395:PX4:H70	4:A:421:PX4:H58	0.42	1.91	10	1
4:A:403:PX4:H52	4:A:403:PX4:H47	0.42	1.50	11	1
4:A:408:PX4:H50	4:A:409:PX4:H19	0.42	1.92	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:308:PX4:H7	4:A:308:PX4:O3	0.42	2.15	12	1
4:A:318:PX4:H56	4:A:328:PX4:H33	0.42	1.90	12	1
4:A:335:PX4:H17	4:A:343:PX4:O1	0.42	2.15	12	1
4:A:317:PX4:H41	4:A:385:PX4:H65	0.42	1.92	13	1
4:A:325:PX4:H62	4:A:342:PX4:H70	0.42	1.90	13	1
4:A:332:PX4:H54	4:A:407:PX4:H70	0.42	1.90	13	1
4:A:391:PX4:H17	4:A:408:PX4:O5	0.42	2.15	13	1
4:A:424:PX4:H47	4:A:429:PX4:H19	0.42	1.91	1	1
4:A:372:PX4:H29	4:A:420:PX4:H26	0.42	1.91	2	1
4:A:306:PX4:H40	4:A:329:PX4:H40	0.42	1.91	3	1
4:A:316:PX4:H34	4:A:320:PX4:C19	0.42	2.43	3	1
4:A:376:PX4:H26	4:A:399:PX4:C25	0.42	2.45	4	1
4:A:333:PX4:H23	4:A:340:PX4:H24	0.42	1.91	5	1
4:A:364:PX4:H69	4:A:364:PX4:H62	0.42	1.69	5	1
4:A:334:PX4:C35	4:A:352:PX4:H32	0.42	2.45	6	1
4:A:350:PX4:H36	4:A:415:PX4:H71	0.42	1.92	6	1
4:A:383:PX4:H13	4:A:399:PX4:O1	0.42	2.15	6	1
4:A:395:PX4:H40	4:A:397:PX4:H65	0.42	1.92	6	1
4:A:398:PX4:H48	4:A:405:PX4:H49	0.42	1.92	6	1
4:A:373:PX4:H22	4:A:397:PX4:O3	0.42	2.14	7	1
4:A:322:PX4:C27	4:A:336:PX4:H32	0.42	2.45	10	1
4:A:354:PX4:H32	4:A:354:PX4:H25	0.42	1.63	10	1
4:A:388:PX4:H6	4:A:396:PX4:O8	0.42	2.15	12	1
4:A:413:PX4:H17	4:A:430:PX4:C8	0.42	2.45	12	1
4:A:424:PX4:H55	4:A:424:PX4:H48	0.42	1.64	13	1
4:A:308:PX4:H69	4:A:426:PX4:H70	0.42	1.91	14	1
4:A:371:PX4:O8	4:A:377:PX4:H3	0.41	2.15	1	1
4:A:378:PX4:H28	4:A:420:PX4:H57	0.41	1.92	1	1
4:A:398:PX4:H51	4:A:405:PX4:C23	0.41	2.45	4	1
4:A:405:PX4:H58	4:A:414:PX4:H26	0.41	1.91	4	1
4:A:318:PX4:H39	4:A:359:PX4:H36	0.41	1.92	5	1
4:A:393:PX4:H10	4:A:393:PX4:O6	0.41	2.14	9	1
4:A:340:PX4:H35	4:A:397:PX4:H60	0.41	1.91	10	1
4:A:363:PX4:H57	4:A:363:PX4:H62	0.41	1.56	10	1
4:A:389:PX4:H68	4:A:390:PX4:H38	0.41	1.92	10	1
4:A:369:PX4:C19	4:A:416:PX4:H63	0.41	2.45	11	1
4:A:410:PX4:H57	4:A:417:PX4:H69	0.41	1.91	11	1
4:A:308:PX4:H41	4:A:410:PX4:H45	0.41	1.91	12	1
4:A:423:PX4:H40	4:A:430:PX4:H36	0.41	1.92	12	1
4:A:322:PX4:H37	4:A:361:PX4:H25	0.41	1.91	13	1
4:A:346:PX4:H24	4:A:360:PX4:H55	0.41	1.92	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:403:PX4:H48	4:A:419:PX4:H9	0.41	1.91	14	1
4:A:309:PX4:H23	4:A:320:PX4:H49	0.41	1.92	1	1
4:A:410:PX4:H14	4:A:418:PX4:H40	0.41	1.92	1	1
4:A:349:PX4:H27	4:A:356:PX4:H30	0.41	1.92	3	1
4:A:308:PX4:H32	4:A:364:PX4:H52	0.41	1.91	4	1
4:A:345:PX4:H68	4:A:345:PX4:H45	0.41	1.91	4	1
4:A:403:PX4:H49	4:A:404:PX4:H28	0.41	1.90	5	1
4:A:347:PX4:H20	4:A:348:PX4:O3	0.41	2.14	6	1
4:A:416:PX4:H22	4:A:425:PX4:H50	0.41	1.92	6	1
4:A:421:PX4:H35	4:A:430:PX4:H48	0.41	1.92	6	1
4:A:378:PX4:H47	4:A:410:PX4:H19	0.41	1.93	7	1
4:A:308:PX4:H68	4:A:308:PX4:H63	0.41	1.64	11	1
4:A:335:PX4:H39	4:A:344:PX4:H39	0.41	1.92	11	1
4:A:337:PX4:H5	4:A:337:PX4:H25	0.41	1.92	11	1
4:A:372:PX4:H39	4:A:420:PX4:H34	0.41	1.92	12	1
4:A:308:PX4:H67	4:A:359:PX4:H70	0.41	1.91	13	1
4:A:352:PX4:H38	4:A:352:PX4:H31	0.41	1.60	14	1
4:A:398:PX4:H63	4:A:398:PX4:H68	0.41	1.73	14	1
4:A:313:PX4:H62	4:A:329:PX4:H32	0.41	1.90	1	1
4:A:383:PX4:O6	4:A:392:PX4:H3	0.41	2.14	1	1
4:A:314:PX4:H34	4:A:356:PX4:H41	0.41	1.91	8	1
4:A:373:PX4:H66	4:A:381:PX4:H44	0.41	1.92	10	1
4:A:421:PX4:H34	4:A:423:PX4:H23	0.41	1.93	12	1
4:A:322:PX4:H17	4:A:361:PX4:H56	0.41	1.92	13	1
4:A:376:PX4:H65	4:A:392:PX4:H35	0.41	1.92	14	1
4:A:368:PX4:H46	4:A:429:PX4:H20	0.41	1.90	1	1
4:A:367:PX4:H20	4:A:424:PX4:H22	0.41	1.93	2	1
4:A:331:PX4:H8	4:A:340:PX4:O1	0.41	2.14	3	1
4:A:378:PX4:H35	4:A:378:PX4:H42	0.41	1.61	3	1
4:A:389:PX4:H60	4:A:398:PX4:H17	0.41	1.93	5	1
4:A:393:PX4:H16	4:A:401:PX4:H18	0.41	1.91	5	1
4:A:337:PX4:H24	4:A:346:PX4:H69	0.41	1.91	6	1
4:A:346:PX4:H27	4:A:353:PX4:H58	0.41	1.93	6	1
4:A:347:PX4:H68	4:A:390:PX4:H39	0.41	1.92	6	1
4:A:352:PX4:H13	4:A:352:PX4:H2	0.41	1.76	6	1
4:A:348:PX4:H37	4:A:357:PX4:H36	0.41	1.92	7	1
4:A:421:PX4:H41	4:A:423:PX4:H35	0.41	1.91	7	1
4:A:316:PX4:O2	4:A:364:PX4:H11	0.41	2.15	8	1
4:A:380:PX4:H25	4:A:380:PX4:H59	0.41	1.91	8	1
4:A:403:PX4:H26	4:A:404:PX4:H21	0.41	1.92	8	1
4:A:366:PX4:H55	4:A:366:PX4:H60	0.41	1.70	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:372:PX4:O2	4:A:420:PX4:H9	0.41	2.15	9	1
4:A:420:PX4:H50	4:A:420:PX4:H57	0.41	1.68	9	1
4:A:341:PX4:H29	4:A:341:PX4:H24	0.41	1.63	10	1
4:A:367:PX4:H63	4:A:367:PX4:H68	0.41	1.51	14	1
4:A:407:PX4:H29	4:A:408:PX4:H41	0.41	1.90	14	1
4:A:413:PX4:H9	4:A:430:PX4:O1	0.41	2.16	2	1
4:A:314:PX4:H41	4:A:314:PX4:H35	0.41	1.64	3	1
4:A:359:PX4:H53	4:A:359:PX4:H47	0.41	1.64	3	1
4:A:369:PX4:O1	4:A:425:PX4:H1	0.41	2.15	4	1
4:A:405:PX4:H48	4:A:406:PX4:H52	0.41	1.92	4	1
1:A:244:ASP:OD1	4:A:349:PX4:H3	0.41	2.15	5	1
4:A:325:PX4:H27	4:A:334:PX4:H21	0.41	1.93	5	1
4:A:406:PX4:H34	4:A:406:PX4:H39	0.41	1.55	7	1
1:A:214:LEU:HD22	1:A:243:VAL:CG2	0.41	2.45	8	1
4:A:347:PX4:O1	4:A:348:PX4:H3	0.41	2.15	8	1
4:A:362:PX4:H21	4:A:362:PX4:H28	0.41	1.65	8	1
4:A:337:PX4:H61	4:A:353:PX4:H48	0.41	1.93	9	1
4:A:340:PX4:H43	4:A:389:PX4:H27	0.41	1.93	12	1
4:A:423:PX4:H36	4:A:423:PX4:H42	0.41	1.54	12	1
4:A:306:PX4:H37	4:A:367:PX4:H72	0.41	1.92	14	1
4:A:332:PX4:H38	4:A:407:PX4:H61	0.41	1.93	14	1
4:A:392:PX4:H56	4:A:392:PX4:H63	0.41	1.65	14	1
4:A:321:PX4:H61	4:A:361:PX4:H57	0.41	1.93	1	1
4:A:308:PX4:H14	4:A:311:PX4:H16	0.41	1.92	2	1
4:A:408:PX4:H32	4:A:415:PX4:H42	0.41	1.92	2	1
4:A:345:PX4:O4	4:A:346:PX4:H10	0.41	2.15	3	1
4:A:308:PX4:H72	4:A:308:PX4:H65	0.41	1.59	4	1
4:A:369:PX4:O1	4:A:425:PX4:H13	0.41	2.16	4	1
1:A:138:PHE:CD1	1:A:149:PHE:CD1	0.41	3.08	6	2
4:A:385:PX4:H67	4:A:392:PX4:H26	0.41	1.90	5	1
4:A:383:PX4:H65	4:A:407:PX4:H27	0.41	1.92	6	1
4:A:367:PX4:H60	4:A:429:PX4:H41	0.41	1.91	8	1
4:A:420:PX4:H67	4:A:426:PX4:H38	0.41	1.92	8	1
4:A:360:PX4:H30	4:A:366:PX4:H61	0.41	1.91	9	1
4:A:398:PX4:H42	4:A:408:PX4:H26	0.41	1.92	9	1
4:A:355:PX4:H30	4:A:356:PX4:H51	0.41	1.91	10	1
4:A:350:PX4:H60	4:A:400:PX4:H44	0.41	1.93	11	1
4:A:418:PX4:H72	4:A:418:PX4:H64	0.41	1.59	12	1
4:A:388:PX4:H3	4:A:395:PX4:O1	0.41	2.15	13	1
4:A:337:PX4:H65	4:A:345:PX4:H71	0.41	1.92	14	1
4:A:338:PX4:H63	4:A:338:PX4:H68	0.41	1.58	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:344:PX4:H49	4:A:344:PX4:H54	0.41	1.71	14	1
4:A:308:PX4:H23	4:A:311:PX4:H54	0.41	1.92	1	1
4:A:311:PX4:H17	4:A:359:PX4:H50	0.41	1.93	2	1
4:A:382:PX4:H29	4:A:382:PX4:H36	0.41	1.73	2	1
4:A:409:PX4:H37	4:A:410:PX4:H53	0.41	1.93	3	1
4:A:323:PX4:H19	4:A:333:PX4:H47	0.41	1.92	4	1
4:A:363:PX4:H38	4:A:365:PX4:H30	0.41	1.92	4	1
4:A:391:PX4:H54	4:A:391:PX4:H48	0.41	1.60	4	1
4:A:416:PX4:H40	4:A:421:PX4:H70	0.41	1.92	5	1
4:A:377:PX4:H44	4:A:377:PX4:H38	0.41	1.75	6	1
4:A:395:PX4:H56	4:A:402:PX4:H50	0.41	1.91	6	1
4:A:319:PX4:H60	4:A:324:PX4:H59	0.41	1.92	7	1
4:A:380:PX4:H59	4:A:388:PX4:H40	0.41	1.91	7	1
4:A:381:PX4:H42	4:A:381:PX4:H60	0.41	1.92	8	1
4:A:338:PX4:H45	4:A:338:PX4:H38	0.41	1.58	11	1
4:A:392:PX4:H72	4:A:392:PX4:H65	0.41	1.73	14	1
4:A:415:PX4:H55	4:A:421:PX4:H56	0.41	1.93	2	1
4:A:307:PX4:H10	4:A:322:PX4:O8	0.41	2.16	4	1
4:A:428:PX4:H44	4:A:428:PX4:H38	0.41	1.78	4	1
4:A:395:PX4:H54	4:A:395:PX4:H61	0.41	1.72	5	1
4:A:388:PX4:H39	4:A:388:PX4:H34	0.41	1.63	6	1
4:A:421:PX4:H59	4:A:421:PX4:H52	0.41	1.65	6	1
4:A:332:PX4:H14	4:A:356:PX4:H9	0.41	1.92	7	1
4:A:352:PX4:H16	4:A:358:PX4:H47	0.41	1.93	8	1
4:A:407:PX4:H17	4:A:414:PX4:O8	0.41	2.16	10	1
4:A:309:PX4:O8	4:A:316:PX4:H46	0.41	2.16	11	1
4:A:367:PX4:H42	4:A:423:PX4:H36	0.41	1.90	11	1
4:A:307:PX4:H46	4:A:307:PX4:H16	0.41	1.69	12	1
4:A:349:PX4:H45	4:A:355:PX4:H45	0.41	1.93	13	1
4:A:378:PX4:H63	4:A:418:PX4:H62	0.41	1.93	13	1
4:A:398:PX4:H21	4:A:407:PX4:H22	0.41	1.93	13	1
4:A:400:PX4:H56	4:A:409:PX4:H34	0.41	1.93	13	1
4:A:328:PX4:H25	4:A:328:PX4:H20	0.41	1.67	14	1
4:A:306:PX4:H56	4:A:354:PX4:C13	0.41	2.46	1	1
4:A:330:PX4:H16	4:A:343:PX4:H2	0.41	1.93	1	1
4:A:345:PX4:H69	4:A:388:PX4:H35	0.41	1.92	1	1
4:A:348:PX4:H63	4:A:348:PX4:H68	0.41	1.63	1	1
4:A:314:PX4:H47	4:A:350:PX4:H37	0.41	1.91	2	1
4:A:337:PX4:H45	4:A:338:PX4:H56	0.41	1.93	2	1
4:A:375:PX4:H60	4:A:375:PX4:H67	0.41	1.66	2	1
4:A:376:PX4:H46	4:A:384:PX4:H3	0.41	1.93	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:404:PX4:H59	4:A:404:PX4:H52	0.41	1.53	2	1
4:A:312:PX4:H39	4:A:365:PX4:H37	0.41	1.93	3	1
4:A:358:PX4:H35	4:A:365:PX4:H31	0.41	1.91	3	1
4:A:363:PX4:H60	4:A:363:PX4:H55	0.41	1.65	3	1
4:A:375:PX4:H18	4:A:382:PX4:O6	0.41	2.16	3	1
4:A:306:PX4:O2	4:A:329:PX4:H12	0.41	2.15	4	1
4:A:314:PX4:H42	4:A:362:PX4:H21	0.41	1.91	4	1
4:A:316:PX4:H26	4:A:364:PX4:H47	0.41	1.92	5	1
4:A:326:PX4:H29	4:A:350:PX4:H51	0.41	1.92	5	1
4:A:345:PX4:H17	4:A:346:PX4:H6	0.41	1.93	5	1
4:A:415:PX4:H5	4:A:421:PX4:H14	0.41	1.92	5	1
4:A:375:PX4:H47	4:A:429:PX4:H40	0.41	1.92	6	1
4:A:404:PX4:H63	4:A:404:PX4:H68	0.41	1.65	7	1
4:A:372:PX4:H47	4:A:372:PX4:H52	0.41	1.71	8	1
4:A:423:PX4:H4	4:A:430:PX4:O8	0.41	2.16	8	1
4:A:315:PX4:H24	4:A:322:PX4:H36	0.41	1.92	9	1
4:A:363:PX4:H28	4:A:365:PX4:H21	0.41	1.92	9	1
4:A:391:PX4:H47	4:A:408:PX4:H16	0.41	1.93	9	1
4:A:416:PX4:H48	4:A:425:PX4:H53	0.41	1.92	9	1
4:A:429:PX4:H33	4:A:429:PX4:C27	0.41	2.46	9	1
4:A:366:PX4:H68	4:A:419:PX4:H38	0.41	1.93	10	1
4:A:335:PX4:H23	4:A:343:PX4:H53	0.41	1.91	12	1
4:A:383:PX4:H20	4:A:392:PX4:C14	0.41	2.46	12	1
4:A:390:PX4:H63	4:A:397:PX4:H40	0.41	1.92	12	1
4:A:307:PX4:H41	4:A:361:PX4:H42	0.41	1.92	13	1
4:A:325:PX4:H9	4:A:341:PX4:O6	0.41	2.15	13	1
4:A:338:PX4:H62	4:A:362:PX4:H62	0.41	1.93	13	1
4:A:331:PX4:H7	4:A:331:PX4:O6	0.41	2.16	14	1
4:A:424:PX4:H25	4:A:424:PX4:H32	0.41	1.37	14	1
4:A:326:PX4:H27	4:A:350:PX4:H21	0.41	1.92	3	1
4:A:325:PX4:H45	4:A:334:PX4:H40	0.41	1.93	4	1
4:A:341:PX4:H32	4:A:383:PX4:H70	0.41	1.93	6	1
4:A:330:PX4:C3	4:A:330:PX4:H19	0.41	2.46	7	1
4:A:332:PX4:O3	4:A:356:PX4:H4	0.41	2.16	7	1
4:A:354:PX4:H21	4:A:362:PX4:C5	0.41	2.46	7	1
4:A:309:PX4:H27	4:A:318:PX4:H28	0.41	1.93	8	1
4:A:382:PX4:H67	4:A:428:PX4:H20	0.41	1.93	9	1
4:A:388:PX4:H15	4:A:396:PX4:H18	0.41	1.92	9	1
4:A:424:PX4:H56	4:A:425:PX4:H31	0.41	1.93	9	1
4:A:349:PX4:H66	4:A:349:PX4:H60	0.41	1.58	10	1
4:A:388:PX4:H51	4:A:396:PX4:C25	0.41	2.45	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:353:PX4:H31	4:A:366:PX4:H25	0.41	1.93	11	1
4:A:311:PX4:H71	4:A:316:PX4:H38	0.41	1.93	12	1
4:A:369:PX4:H71	4:A:369:PX4:H65	0.41	1.47	12	1
4:A:319:PX4:H19	4:A:342:PX4:H50	0.41	1.92	14	1
4:A:326:PX4:H64	4:A:391:PX4:H43	0.41	1.92	14	1
4:A:345:PX4:H4	4:A:353:PX4:O4	0.41	2.16	14	1
4:A:405:PX4:H45	4:A:405:PX4:H37	0.41	1.61	14	1
4:A:387:PX4:H31	4:A:387:PX4:H38	0.40	1.72	1	1
4:A:403:PX4:O8	4:A:419:PX4:H8	0.40	2.15	1	1
4:A:316:PX4:O4	4:A:364:PX4:H5	0.40	2.16	2	1
4:A:314:PX4:H59	4:A:314:PX4:H64	0.40	1.39	4	1
4:A:334:PX4:H65	4:A:363:PX4:H69	0.40	1.93	4	1
4:A:350:PX4:H56	4:A:363:PX4:H52	0.40	1.92	4	1
4:A:371:PX4:H65	4:A:417:PX4:H65	0.40	1.92	4	1
1:A:214:LEU:HD23	1:A:214:LEU:H	0.40	1.75	6	1
4:A:358:PX4:H27	4:A:364:PX4:H42	0.40	1.92	6	1
4:A:366:PX4:H41	4:A:366:PX4:H36	0.40	1.64	7	1
4:A:416:PX4:H35	4:A:421:PX4:H66	0.40	1.92	8	1
4:A:313:PX4:H18	4:A:318:PX4:C24	0.40	2.36	9	1
4:A:389:PX4:H61	4:A:389:PX4:H66	0.40	1.60	10	1
4:A:384:PX4:H46	4:A:386:PX4:H49	0.40	1.93	11	1
4:A:326:PX4:H55	4:A:326:PX4:H60	0.40	1.78	12	1
4:A:380:PX4:H31	4:A:381:PX4:H60	0.40	1.92	12	1
4:A:427:PX4:H37	4:A:427:PX4:H32	0.40	1.63	12	1
4:A:322:PX4:H69	4:A:322:PX4:H62	0.40	1.62	13	1
4:A:378:PX4:H17	4:A:410:PX4:O6	0.40	2.15	13	1
4:A:384:PX4:H17	4:A:385:PX4:H20	0.40	1.93	13	1
4:A:313:PX4:H15	4:A:360:PX4:O6	0.40	2.16	14	1
4:A:404:PX4:H8	4:A:412:PX4:O6	0.40	2.17	14	1
4:A:315:PX4:H43	4:A:425:PX4:H32	0.40	1.92	2	1
4:A:308:PX4:H41	4:A:316:PX4:H39	0.40	1.92	3	1
4:A:419:PX4:H71	4:A:427:PX4:H64	0.40	1.93	3	1
4:A:323:PX4:H58	4:A:323:PX4:H65	0.40	1.68	5	1
4:A:377:PX4:H62	4:A:416:PX4:H55	0.40	1.92	6	1
4:A:330:PX4:H14	4:A:338:PX4:H19	0.40	1.91	7	1
4:A:334:PX4:H59	4:A:334:PX4:H64	0.40	1.36	8	1
4:A:308:PX4:H51	4:A:363:PX4:H19	0.40	1.92	10	1
4:A:308:PX4:H25	4:A:311:PX4:H23	0.40	1.93	10	1
4:A:368:PX4:H20	4:A:377:PX4:H57	0.40	1.92	11	1
4:A:428:PX4:H65	4:A:430:PX4:H48	0.40	1.93	11	1
4:A:327:PX4:H43	4:A:374:PX4:H66	0.40	1.93	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:332:PX4:H45	4:A:407:PX4:H53	0.40	1.93	13	1
4:A:389:PX4:H52	4:A:389:PX4:H59	0.40	1.59	13	1
4:A:391:PX4:H31	4:A:408:PX4:H23	0.40	1.91	13	1
4:A:352:PX4:H15	4:A:352:PX4:H7	0.40	1.93	14	1
4:A:321:PX4:H45	4:A:360:PX4:H69	0.40	1.93	1	1
4:A:323:PX4:H14	4:A:323:PX4:H9	0.40	1.92	4	1
4:A:372:PX4:H38	4:A:372:PX4:H32	0.40	1.63	5	1
4:A:401:PX4:H44	4:A:401:PX4:H38	0.40	1.72	6	1
4:A:319:PX4:O2	4:A:324:PX4:H4	0.40	2.16	7	1
4:A:317:PX4:O5	4:A:351:PX4:H23	0.40	2.17	8	1
4:A:405:PX4:H58	4:A:414:PX4:H30	0.40	1.93	8	1
1:A:109:TRP:CH2	1:A:158:ASP:HB3	0.40	2.51	11	1
4:A:348:PX4:H56	4:A:355:PX4:H72	0.40	1.93	11	1
4:A:383:PX4:H55	4:A:399:PX4:H17	0.40	1.92	13	1
4:A:404:PX4:H2	4:A:412:PX4:O1	0.40	2.16	13	1
4:A:417:PX4:H65	4:A:417:PX4:H58	0.40	1.62	14	1
4:A:410:PX4:H61	4:A:410:PX4:H40	0.40	1.92	2	1
4:A:326:PX4:H34	4:A:406:PX4:H36	0.40	1.93	3	1
4:A:345:PX4:H33	4:A:353:PX4:H61	0.40	1.94	5	1
4:A:416:PX4:H47	4:A:416:PX4:H52	0.40	1.75	5	1
4:A:410:PX4:O2	4:A:416:PX4:H4	0.40	2.17	8	1
4:A:388:PX4:H25	4:A:388:PX4:H32	0.40	1.65	9	1
4:A:375:PX4:H32	4:A:375:PX4:H37	0.40	1.68	10	1
4:A:412:PX4:H16	4:A:428:PX4:H16	0.40	1.93	10	1
4:A:307:PX4:C12	4:A:314:PX4:H16	0.40	2.47	11	1
4:A:362:PX4:H54	4:A:362:PX4:H60	0.40	1.39	11	1
4:A:381:PX4:H10	4:A:381:PX4:H14	0.40	1.93	11	1
4:A:321:PX4:H68	4:A:321:PX4:H63	0.40	1.68	12	1
4:A:402:PX4:H34	4:A:402:PX4:H39	0.40	1.45	12	1
4:A:336:PX4:H28	4:A:361:PX4:H63	0.40	1.93	13	1
4:A:378:PX4:H67	4:A:418:PX4:H66	0.40	1.93	13	1
4:A:378:PX4:H47	4:A:418:PX4:H46	0.40	1.92	13	1
4:A:380:PX4:H20	4:A:381:PX4:H6	0.40	1.93	13	1
4:A:395:PX4:H15	4:A:396:PX4:H15	0.40	1.93	13	1
4:A:394:PX4:H65	4:A:394:PX4:H71	0.40	1.66	14	1
4:A:364:PX4:H32	4:A:364:PX4:H25	0.40	1.68	1	1
4:A:380:PX4:H28	4:A:380:PX4:H33	0.40	1.75	1	1
4:A:345:PX4:H17	4:A:346:PX4:H10	0.40	1.91	2	1
4:A:374:PX4:H34	4:A:374:PX4:H27	0.40	1.72	3	1
4:A:320:PX4:H20	4:A:359:PX4:H58	0.40	1.94	4	1
4:A:316:PX4:H60	4:A:320:PX4:H36	0.40	1.93	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:344:PX4:H38	4:A:347:PX4:H38	0.40	1.93	5	1
4:A:429:PX4:H29	4:A:429:PX4:H53	0.40	1.93	5	1
4:A:319:PX4:H44	4:A:319:PX4:H38	0.40	1.70	6	1
4:A:353:PX4:H35	4:A:353:PX4:H30	0.40	1.62	7	1
4:A:385:PX4:O1	4:A:392:PX4:H8	0.40	2.17	8	1
4:A:319:PX4:H58	4:A:324:PX4:H30	0.40	1.94	11	1
4:A:332:PX4:H39	4:A:334:PX4:H57	0.40	1.92	11	1
4:A:398:PX4:H60	4:A:405:PX4:H29	0.40	1.94	13	1
4:A:355:PX4:C10	4:A:362:PX4:H51	0.40	2.47	14	1
4:A:374:PX4:H20	4:A:374:PX4:H25	0.40	1.49	14	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	158/164 (96%)	145±3 (92±2%)	12±3 (8±2%)	1±1 (1±0%)	29	74
All	All	2212/2296 (96%)	2030 (92%)	168 (8%)	14 (1%)	29	74

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

Mol	Chain	Res	Type	Models (Total)
1	A	171	PHE	5
1	A	175	ASP	3
1	A	107	PRO	2
1	A	183	HIS	1
1	A	146	PRO	1
1	A	179	GLY	1
1	A	213	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	129/131 (98%)	123±2 (95±2%)	6±2 (5±2%)	28 77
All	All	1806/1834 (98%)	1716 (95%)	90 (5%)	28 77

All 25 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	101	ARG	14
1	A	244	ASP	14
1	A	199	GLU	9
1	A	222	HIS	8
1	A	249	ARG	7
1	A	214	LEU	6
1	A	175	ASP	5
1	A	243	VAL	4
1	A	170	ASP	3
1	A	142	SER	3
1	A	129	ASP	2
1	A	198	ASP	2
1	A	134	ILE	1
1	A	205	THR	1
1	A	122	THR	1
1	A	146	PRO	1
1	A	139	GLN	1
1	A	140	VAL	1
1	A	168	HIS	1
1	A	108	VAL	1
1	A	200	ASP	1
1	A	115	THR	1
1	A	156	MET	1
1	A	162	VAL	1
1	A	103	MET	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

Of 130 ligands modelled in this entry, 5 are monoatomic - leaving 125 for Mogul analysis.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	PX4	A	418	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	328	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	367	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	381	-	45,45,45	0.63±0.03	0±0 (0±0%)
4	PX4	A	396	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	394	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	345	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	322	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	373	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	342	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	412	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	314	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	400	-	45,45,45	0.63±0.01	0±0 (0±0%)
4	PX4	A	415	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	419	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	356	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	365	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	410	-	45,45,45	0.63±0.01	0±0 (0±0%)
4	PX4	A	320	-	45,45,45	0.63±0.01	0±0 (0±0%)
4	PX4	A	424	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	399	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	420	-	45,45,45	0.63±0.02	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	PX4	A	414	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	327	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	335	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	374	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	323	-	45,45,45	0.63±0.01	0±0 (0±0%)
4	PX4	A	405	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	401	-	45,45,45	0.63±0.01	0±0 (0±0%)
4	PX4	A	366	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	354	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	411	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	316	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	350	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	339	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	404	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	372	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	426	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	425	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	387	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	336	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	312	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	361	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	311	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	308	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	403	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	348	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	331	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	325	-	45,45,45	0.63±0.01	0±0 (0±0%)
4	PX4	A	309	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	359	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	338	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	407	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	333	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	375	-	45,45,45	0.63±0.01	0±0 (0±0%)
4	PX4	A	391	-	45,45,45	0.63±0.01	0±0 (0±0%)
4	PX4	A	388	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	313	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	395	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	430	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	349	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	337	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	389	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	416	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	351	-	45,45,45	0.63±0.01	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	PX4	A	390	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	371	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	321	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	409	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	379	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	319	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	369	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	329	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	428	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	310	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	306	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	377	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	352	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	392	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	340	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	334	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	413	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	370	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	383	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	307	-	45,45,45	0.63±0.01	0±0 (0±0%)
4	PX4	A	397	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	317	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	398	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	386	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	315	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	429	-	45,45,45	0.63±0.01	0±0 (0±0%)
4	PX4	A	427	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	332	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	408	-	45,45,45	0.63±0.01	0±0 (0±0%)
4	PX4	A	357	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	417	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	393	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	318	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	385	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	341	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	343	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	402	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	360	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	364	-	45,45,45	0.63±0.01	0±0 (0±0%)
4	PX4	A	330	-	45,45,45	0.63±0.01	0±0 (0±0%)
4	PX4	A	346	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	363	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	368	-	45,45,45	0.63±0.02	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	PX4	A	422	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	384	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	380	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	362	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	355	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	406	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	423	-	45,45,45	0.63±0.01	0±0 (0±0%)
4	PX4	A	378	-	45,45,45	0.63±0.01	0±0 (0±0%)
4	PX4	A	358	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	326	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	382	-	45,45,45	0.63±0.01	0±0 (0±0%)
4	PX4	A	347	-	45,45,45	0.63±0.01	0±0 (0±0%)
4	PX4	A	344	-	45,45,45	0.63±0.01	0±0 (0±0%)
4	PX4	A	376	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	353	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	421	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	324	-	45,45,45	0.63±0.02	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
4	PX4	A	418	-	51,53,53	1.49±0.15	9±2 (16±3%)
4	PX4	A	328	-	51,53,53	1.50±0.14	9±2 (18±4%)
4	PX4	A	367	-	51,53,53	1.49±0.18	8±3 (15±6%)
4	PX4	A	381	-	51,53,53	1.57±0.13	10±2 (19±4%)
4	PX4	A	396	-	51,53,53	1.53±0.16	9±2 (17±3%)
4	PX4	A	394	-	51,53,53	1.49±0.15	9±2 (17±4%)
4	PX4	A	345	-	51,53,53	1.44±0.16	8±2 (16±4%)
4	PX4	A	322	-	51,53,53	1.50±0.16	10±3 (19±6%)
4	PX4	A	373	-	51,53,53	1.58±0.16	10±3 (20±5%)
4	PX4	A	342	-	51,53,53	1.51±0.13	9±3 (17±5%)
4	PX4	A	412	-	51,53,53	1.41±0.13	8±3 (15±5%)
4	PX4	A	314	-	51,53,53	1.46±0.16	8±3 (16±5%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	400	-	51,53,53	1.48±0.18	9±2 (17±4%)
4	PX4	A	415	-	51,53,53	1.55±0.16	10±2 (19±3%)
4	PX4	A	419	-	51,53,53	1.52±0.11	10±3 (18±5%)
4	PX4	A	356	-	51,53,53	1.48±0.19	8±3 (15±5%)
4	PX4	A	365	-	51,53,53	1.47±0.12	8±2 (16±3%)
4	PX4	A	410	-	51,53,53	1.49±0.17	9±2 (16±3%)
4	PX4	A	320	-	51,53,53	1.45±0.14	8±2 (16±3%)
4	PX4	A	424	-	51,53,53	1.42±0.17	8±2 (16±4%)
4	PX4	A	399	-	51,53,53	1.46±0.16	9±2 (18±4%)
4	PX4	A	420	-	51,53,53	1.49±0.12	9±2 (17±3%)
4	PX4	A	414	-	51,53,53	1.53±0.14	9±2 (17±4%)
4	PX4	A	327	-	51,53,53	1.54±0.11	9±2 (18±3%)
4	PX4	A	335	-	51,53,53	1.46±0.14	9±2 (16±4%)
4	PX4	A	374	-	51,53,53	1.46±0.15	9±3 (17±4%)
4	PX4	A	323	-	51,53,53	1.43±0.17	8±2 (16±3%)
4	PX4	A	405	-	51,53,53	1.51±0.14	10±2 (19±4%)
4	PX4	A	401	-	51,53,53	1.56±0.15	10±2 (19±3%)
4	PX4	A	366	-	51,53,53	1.52±0.12	10±2 (19±4%)
4	PX4	A	354	-	51,53,53	1.56±0.15	9±2 (18±4%)
4	PX4	A	411	-	51,53,53	1.47±0.08	9±2 (17±3%)
4	PX4	A	316	-	51,53,53	1.43±0.10	8±2 (14±4%)
4	PX4	A	350	-	51,53,53	1.41±0.10	8±1 (14±2%)
4	PX4	A	339	-	51,53,53	1.44±0.21	8±3 (15±5%)
4	PX4	A	404	-	51,53,53	1.53±0.14	9±2 (17±3%)
4	PX4	A	372	-	51,53,53	1.46±0.16	9±2 (16±3%)
4	PX4	A	426	-	51,53,53	1.45±0.14	8±2 (15±3%)
4	PX4	A	425	-	51,53,53	1.45±0.10	9±3 (16±5%)
4	PX4	A	387	-	51,53,53	1.52±0.16	10±3 (18±5%)
4	PX4	A	336	-	51,53,53	1.49±0.17	10±3 (19±5%)
4	PX4	A	312	-	51,53,53	1.47±0.16	8±2 (16±4%)
4	PX4	A	361	-	51,53,53	1.52±0.10	9±2 (17±3%)
4	PX4	A	311	-	51,53,53	1.53±0.20	9±3 (17±5%)
4	PX4	A	308	-	51,53,53	1.51±0.14	9±2 (18±4%)
4	PX4	A	403	-	51,53,53	1.49±0.14	9±2 (16±3%)
4	PX4	A	348	-	51,53,53	1.48±0.15	9±2 (16±4%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	331	-	51,53,53	1.51±0.11	9±2 (17±4%)
4	PX4	A	325	-	51,53,53	1.50±0.15	10±2 (19±3%)
4	PX4	A	309	-	51,53,53	1.50±0.14	9±2 (17±4%)
4	PX4	A	359	-	51,53,53	1.52±0.14	9±2 (17±3%)
4	PX4	A	338	-	51,53,53	1.54±0.14	10±2 (18±4%)
4	PX4	A	407	-	51,53,53	1.45±0.17	8±3 (15±5%)
4	PX4	A	333	-	51,53,53	1.49±0.15	8±2 (15±4%)
4	PX4	A	375	-	51,53,53	1.51±0.14	9±2 (17±3%)
4	PX4	A	391	-	51,53,53	1.51±0.16	9±2 (16±3%)
4	PX4	A	388	-	51,53,53	1.44±0.12	8±2 (15±3%)
4	PX4	A	313	-	51,53,53	1.50±0.14	9±2 (17±4%)
4	PX4	A	395	-	51,53,53	1.49±0.12	9±2 (17±4%)
4	PX4	A	430	-	51,53,53	1.55±0.13	10±1 (19±2%)
4	PX4	A	349	-	51,53,53	1.52±0.11	9±2 (17±3%)
4	PX4	A	337	-	51,53,53	1.45±0.18	8±2 (15±3%)
4	PX4	A	389	-	51,53,53	1.53±0.14	9±2 (17±4%)
4	PX4	A	416	-	51,53,53	1.48±0.16	9±3 (17±6%)
4	PX4	A	351	-	51,53,53	1.48±0.13	8±2 (16±4%)
4	PX4	A	390	-	51,53,53	1.47±0.13	9±2 (17±3%)
4	PX4	A	371	-	51,53,53	1.68±0.15	11±2 (22±3%)
4	PX4	A	321	-	51,53,53	1.43±0.14	9±2 (17±4%)
4	PX4	A	409	-	51,53,53	1.51±0.10	10±2 (19±3%)
4	PX4	A	379	-	51,53,53	1.54±0.13	10±3 (19±5%)
4	PX4	A	319	-	51,53,53	1.51±0.13	9±2 (17±4%)
4	PX4	A	369	-	51,53,53	1.40±0.13	8±2 (14±4%)
4	PX4	A	329	-	51,53,53	1.50±0.12	9±2 (18±4%)
4	PX4	A	428	-	51,53,53	1.53±0.10	9±2 (16±4%)
4	PX4	A	310	-	51,53,53	1.48±0.15	9±2 (16±3%)
4	PX4	A	306	-	51,53,53	1.47±0.07	9±2 (18±3%)
4	PX4	A	377	-	51,53,53	1.51±0.18	8±2 (14±3%)
4	PX4	A	352	-	51,53,53	1.48±0.13	9±3 (17±5%)
4	PX4	A	392	-	51,53,53	1.51±0.12	9±2 (16±4%)
4	PX4	A	340	-	51,53,53	1.55±0.09	11±1 (21±2%)
4	PX4	A	334	-	51,53,53	1.50±0.12	9±2 (17±4%)
4	PX4	A	413	-	51,53,53	1.49±0.11	9±2 (17±4%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	370	-	51,53,53	1.47±0.13	9±2 (16±3%)
4	PX4	A	383	-	51,53,53	1.41±0.10	8±2 (15±3%)
4	PX4	A	307	-	51,53,53	1.57±0.19	9±3 (18±5%)
4	PX4	A	397	-	51,53,53	1.52±0.18	9±3 (17±5%)
4	PX4	A	317	-	51,53,53	1.43±0.14	9±3 (16±5%)
4	PX4	A	398	-	51,53,53	1.47±0.15	9±2 (17±3%)
4	PX4	A	386	-	51,53,53	1.48±0.15	9±2 (17±4%)
4	PX4	A	315	-	51,53,53	1.42±0.12	8±2 (16±4%)
4	PX4	A	429	-	51,53,53	1.47±0.18	8±3 (16±5%)
4	PX4	A	427	-	51,53,53	1.61±0.19	10±3 (18±5%)
4	PX4	A	332	-	51,53,53	1.46±0.13	9±3 (16±5%)
4	PX4	A	408	-	51,53,53	1.50±0.14	9±2 (17±4%)
4	PX4	A	357	-	51,53,53	1.48±0.14	9±3 (17±5%)
4	PX4	A	417	-	51,53,53	1.52±0.16	9±2 (18±4%)
4	PX4	A	393	-	51,53,53	1.54±0.12	8±2 (16±4%)
4	PX4	A	318	-	51,53,53	1.45±0.15	8±2 (15±3%)
4	PX4	A	385	-	51,53,53	1.51±0.16	8±2 (15±4%)
4	PX4	A	341	-	51,53,53	1.49±0.13	10±2 (18±3%)
4	PX4	A	343	-	51,53,53	1.47±0.17	8±3 (16±5%)
4	PX4	A	402	-	51,53,53	1.43±0.13	8±2 (16±4%)
4	PX4	A	360	-	51,53,53	1.50±0.10	9±1 (17±2%)
4	PX4	A	364	-	51,53,53	1.53±0.19	9±3 (18±5%)
4	PX4	A	330	-	51,53,53	1.48±0.11	9±2 (16±3%)
4	PX4	A	346	-	51,53,53	1.47±0.15	8±2 (16±4%)
4	PX4	A	363	-	51,53,53	1.46±0.14	8±2 (15±3%)
4	PX4	A	368	-	51,53,53	1.48±0.13	8±2 (16±4%)
4	PX4	A	422	-	51,53,53	1.48±0.13	9±2 (16±3%)
4	PX4	A	384	-	51,53,53	1.49±0.20	8±2 (16±4%)
4	PX4	A	380	-	51,53,53	1.46±0.13	8±2 (15±3%)
4	PX4	A	362	-	51,53,53	1.48±0.07	9±2 (17±3%)
4	PX4	A	355	-	51,53,53	1.48±0.12	9±2 (17±3%)
4	PX4	A	406	-	51,53,53	1.45±0.13	8±2 (16±4%)
4	PX4	A	423	-	51,53,53	1.46±0.13	8±2 (15±3%)
4	PX4	A	378	-	51,53,53	1.44±0.16	8±2 (15±4%)
4	PX4	A	358	-	51,53,53	1.46±0.13	8±2 (16±3%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	326	-	51,53,53	1.46±0.17	8±3 (16±4%)
4	PX4	A	382	-	51,53,53	1.45±0.16	8±2 (16±4%)
4	PX4	A	347	-	51,53,53	1.48±0.19	9±3 (18±6%)
4	PX4	A	344	-	51,53,53	1.52±0.14	9±2 (18±4%)
4	PX4	A	376	-	51,53,53	1.49±0.17	9±3 (17±6%)
4	PX4	A	353	-	51,53,53	1.49±0.10	8±3 (15±5%)
4	PX4	A	421	-	51,53,53	1.46±0.13	8±1 (16±2%)
4	PX4	A	324	-	51,53,53	1.44±0.15	8±3 (15±4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PX4	A	418	-	-	0±0,49,49,49	-
4	PX4	A	328	-	-	0±0,49,49,49	-
4	PX4	A	365	-	-	0±0,49,49,49	-
4	PX4	A	354	-	-	0±0,49,49,49	-
4	PX4	A	404	-	-	0±0,49,49,49	-
4	PX4	A	333	-	-	0±0,49,49,49	-
4	PX4	A	310	-	-	0±0,49,49,49	-
4	PX4	A	397	-	-	0±0,49,49,49	-
4	PX4	A	349	-	-	0±0,49,49,49	-
4	PX4	A	348	-	-	0±0,49,49,49	-
4	PX4	A	341	-	-	0±0,49,49,49	-
4	PX4	A	364	-	-	0±0,49,49,49	-
4	PX4	A	424	-	-	0±0,49,49,49	-
4	PX4	A	383	-	-	0±0,49,49,49	-
4	PX4	A	380	-	-	0±0,49,49,49	-
4	PX4	A	338	-	-	0±0,49,49,49	-
4	PX4	A	355	-	-	0±0,49,49,49	-
4	PX4	A	306	-	-	0±0,49,49,49	-
4	PX4	A	368	-	-	0±0,49,49,49	-
4	PX4	A	323	-	-	0±0,49,49,49	-
4	PX4	A	339	-	-	0±0,49,49,49	-
4	PX4	A	369	-	-	0±0,49,49,49	-
4	PX4	A	307	-	-	0±0,49,49,49	-
4	PX4	A	390	-	-	0±0,49,49,49	-
4	PX4	A	378	-	-	0±0,49,49,49	-
4	PX4	A	414	-	-	0±0,49,49,49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PX4	A	315	-	-	0±0,49,49,49	-
4	PX4	A	366	-	-	0±0,49,49,49	-
4	PX4	A	325	-	-	0±0,49,49,49	-
4	PX4	A	346	-	-	0±0,49,49,49	-
4	PX4	A	363	-	-	0±0,49,49,49	-
4	PX4	A	362	-	-	0±0,49,49,49	-
4	PX4	A	408	-	-	0±0,49,49,49	-
4	PX4	A	430	-	-	0±0,49,49,49	-
4	PX4	A	316	-	-	0±0,49,49,49	-
4	PX4	A	400	-	-	0±0,49,49,49	-
4	PX4	A	359	-	-	0±0,49,49,49	-
4	PX4	A	379	-	-	0±0,49,49,49	-
4	PX4	A	372	-	-	0±0,49,49,49	-
4	PX4	A	386	-	-	0±0,49,49,49	-
4	PX4	A	427	-	-	0±0,49,49,49	-
4	PX4	A	356	-	-	0±0,49,49,49	-
4	PX4	A	389	-	-	0±0,49,49,49	-
4	PX4	A	324	-	-	0±0,49,49,49	-
4	PX4	A	335	-	-	0±0,49,49,49	-
4	PX4	A	412	-	-	0±0,49,49,49	-
4	PX4	A	321	-	-	0±0,49,49,49	-
4	PX4	A	357	-	-	0±0,49,49,49	-
4	PX4	A	422	-	-	0±0,49,49,49	-
4	PX4	A	371	-	-	1±0,49,49,49	-
4	PX4	A	327	-	-	0±0,49,49,49	-
4	PX4	A	337	-	-	0±0,49,49,49	-
4	PX4	A	376	-	-	0±0,49,49,49	-
4	PX4	A	342	-	-	0±0,49,49,49	-
4	PX4	A	420	-	-	0±0,49,49,49	-
4	PX4	A	411	-	-	0±0,49,49,49	-
4	PX4	A	317	-	-	0±0,49,49,49	-
4	PX4	A	367	-	-	0±0,49,49,49	-
4	PX4	A	370	-	-	0±0,49,49,49	-
4	PX4	A	336	-	-	0±0,49,49,49	-
4	PX4	A	332	-	-	0±0,49,49,49	-
4	PX4	A	398	-	-	0±0,49,49,49	-
4	PX4	A	382	-	-	0±0,49,49,49	-
4	PX4	A	314	-	-	0±0,49,49,49	-
4	PX4	A	419	-	-	0±0,49,49,49	-
4	PX4	A	421	-	-	0±0,49,49,49	-
4	PX4	A	391	-	-	0±0,49,49,49	-
4	PX4	A	417	-	-	0±0,49,49,49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PX4	A	375	-	-	0±0,49,49,49	-
4	PX4	A	394	-	-	0±0,49,49,49	-
4	PX4	A	423	-	-	0±0,49,49,49	-
4	PX4	A	329	-	-	0±0,49,49,49	-
4	PX4	A	385	-	-	0±0,49,49,49	-
4	PX4	A	406	-	-	0±0,49,49,49	-
4	PX4	A	384	-	-	0±0,49,49,49	-
4	PX4	A	426	-	-	0±0,49,49,49	-
4	PX4	A	352	-	-	0±0,49,49,49	-
4	PX4	A	403	-	-	0±0,49,49,49	-
4	PX4	A	361	-	-	0±0,49,49,49	-
4	PX4	A	429	-	-	0±0,49,49,49	-
4	PX4	A	392	-	-	0±0,49,49,49	-
4	PX4	A	410	-	-	0±0,49,49,49	-
4	PX4	A	330	-	-	0±0,49,49,49	-
4	PX4	A	405	-	-	0±0,49,49,49	-
4	PX4	A	425	-	-	0±0,49,49,49	-
4	PX4	A	350	-	-	0±0,49,49,49	-
4	PX4	A	381	-	-	0±0,49,49,49	-
4	PX4	A	322	-	-	0±0,49,49,49	-
4	PX4	A	415	-	-	0±0,49,49,49	-
4	PX4	A	351	-	-	0±0,49,49,49	-
4	PX4	A	393	-	-	0±0,49,49,49	-
4	PX4	A	334	-	-	0±0,49,49,49	-
4	PX4	A	407	-	-	0±0,49,49,49	-
4	PX4	A	416	-	-	0±0,49,49,49	-
4	PX4	A	402	-	-	0±0,49,49,49	-
4	PX4	A	343	-	-	0±0,49,49,49	-
4	PX4	A	309	-	-	0±0,49,49,49	-
4	PX4	A	428	-	-	0±0,49,49,49	-
4	PX4	A	399	-	-	0±0,49,49,49	-
4	PX4	A	413	-	-	0±0,49,49,49	-
4	PX4	A	409	-	-	0±0,49,49,49	-
4	PX4	A	373	-	-	0±0,49,49,49	-
4	PX4	A	312	-	-	0±0,49,49,49	-
4	PX4	A	313	-	-	0±0,49,49,49	-
4	PX4	A	319	-	-	0±0,49,49,49	-
4	PX4	A	331	-	-	0±0,49,49,49	-
4	PX4	A	353	-	-	0±0,49,49,49	-
4	PX4	A	318	-	-	0±0,49,49,49	-
4	PX4	A	395	-	-	0±0,49,49,49	-
4	PX4	A	374	-	-	0±0,49,49,49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PX4	A	340	-	-	0±0,49,49,49	-
4	PX4	A	388	-	-	0±0,49,49,49	-
4	PX4	A	311	-	-	0±0,49,49,49	-
4	PX4	A	377	-	-	0±0,49,49,49	-
4	PX4	A	360	-	-	0±0,49,49,49	-
4	PX4	A	308	-	-	0±0,49,49,49	-
4	PX4	A	326	-	-	0±0,49,49,49	-
4	PX4	A	345	-	-	0±0,49,49,49	-
4	PX4	A	320	-	-	0±0,49,49,49	-
4	PX4	A	347	-	-	0±0,49,49,49	-
4	PX4	A	387	-	-	0±0,49,49,49	-
4	PX4	A	358	-	-	0±0,49,49,49	-
4	PX4	A	396	-	-	0±0,49,49,49	-
4	PX4	A	401	-	-	0±0,49,49,49	-
4	PX4	A	344	-	-	0±0,49,49,49	-

There are no bond-length outliers.

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
4	A	417	PX4	O7-C23-C24	7.55	127.78	111.50	6	10
4	A	413	PX4	C8-C7-C6	6.97	95.29	111.79	8	12
4	A	396	PX4	C8-C7-C6	6.91	95.44	111.79	3	11
4	A	426	PX4	O7-C23-C24	6.86	126.28	111.50	7	8
4	A	385	PX4	O7-C23-C24	6.85	126.27	111.50	6	5
4	A	427	PX4	C8-C7-C6	6.76	95.79	111.79	14	11
4	A	349	PX4	O7-C23-C24	6.68	125.89	111.50	8	6
4	A	424	PX4	O7-C23-C24	6.64	125.82	111.50	7	8
4	A	397	PX4	O7-C23-C24	6.64	125.81	111.50	13	9
4	A	353	PX4	C8-C7-C6	6.63	96.10	111.79	11	11
4	A	376	PX4	C8-C7-C6	6.61	96.16	111.79	2	9
4	A	371	PX4	O7-C23-C24	6.57	125.67	111.50	3	14
4	A	389	PX4	C8-C7-C6	6.57	96.24	111.79	10	6
4	A	367	PX4	O7-C23-C24	6.52	125.56	111.50	5	7
4	A	427	PX4	O5-C8-C7	6.47	127.26	108.43	6	11
4	A	310	PX4	C8-C7-C6	6.42	96.60	111.79	3	9
4	A	403	PX4	O3-P1-O2	6.38	84.12	109.07	2	6
4	A	428	PX4	C8-C7-C6	6.36	96.74	111.79	6	8
4	A	331	PX4	C8-C7-C6	6.33	96.81	111.79	12	12
4	A	401	PX4	C8-C7-C6	6.32	96.84	111.79	13	13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	337	PX4	C7-O7-C23	6.30	133.29	117.79	12	4
4	A	380	PX4	C8-C7-C6	6.29	96.92	111.79	14	6
4	A	397	PX4	C8-C7-C6	6.20	97.12	111.79	3	6
4	A	403	PX4	C5-N1-C3	6.12	93.24	108.97	7	4
4	A	370	PX4	O5-C8-C7	6.10	126.20	108.43	1	10
4	A	359	PX4	O7-C23-C24	6.10	124.65	111.50	7	8
4	A	361	PX4	C8-C7-C6	6.08	97.41	111.79	3	6
4	A	320	PX4	O5-C8-C7	6.07	126.09	108.43	7	11
4	A	388	PX4	O5-C8-C7	6.07	126.09	108.43	7	7
4	A	321	PX4	C8-C7-C6	6.05	97.48	111.79	13	9
4	A	399	PX4	O7-C23-C24	6.05	124.53	111.50	10	9
4	A	389	PX4	O7-C23-C24	6.04	124.53	111.50	11	6
4	A	317	PX4	C7-O7-C23	6.04	132.66	117.79	5	3
4	A	312	PX4	O5-C8-C7	6.03	126.00	108.43	5	8
4	A	339	PX4	O7-C23-C24	6.03	124.50	111.50	3	8
4	A	348	PX4	O7-C7-C8	6.02	130.20	108.40	6	7
4	A	427	PX4	O7-C23-C24	6.02	124.47	111.50	1	8
4	A	334	PX4	O5-C8-C7	6.01	125.92	108.43	4	10
4	A	382	PX4	C8-C7-C6	5.99	97.61	111.79	8	7
4	A	377	PX4	C8-C7-C6	5.99	97.62	111.79	14	8
4	A	345	PX4	C8-C7-C6	5.99	97.63	111.79	6	9
4	A	415	PX4	C4-N1-C3	5.99	93.59	108.97	14	4
4	A	401	PX4	C5-N1-C3	5.97	93.61	108.97	13	2
4	A	425	PX4	C8-C7-C6	5.89	97.86	111.79	14	8
4	A	414	PX4	C8-C7-C6	5.88	97.88	111.79	6	9
4	A	345	PX4	O5-C8-C7	5.87	125.52	108.43	7	5
4	A	387	PX4	P1-O3-C1	5.87	92.70	121.59	5	11
4	A	378	PX4	O3-P1-O2	5.86	86.18	109.07	4	3
4	A	380	PX4	O5-C8-C7	5.86	125.48	108.43	11	9
4	A	311	PX4	C5-N1-C3	5.83	93.99	108.97	10	4
4	A	318	PX4	C8-C7-C6	5.82	98.02	111.79	3	12
4	A	386	PX4	O7-C23-C24	5.82	124.04	111.50	8	8
4	A	341	PX4	O7-C23-C24	5.81	124.03	111.50	5	12
4	A	429	PX4	O5-C8-C7	5.78	125.26	108.43	5	6
4	A	418	PX4	O7-C23-C24	5.77	123.95	111.50	4	8
4	A	311	PX4	C8-C7-C6	5.76	98.17	111.79	8	7
4	A	390	PX4	O7-C23-C24	5.76	123.91	111.50	7	7
4	A	326	PX4	O5-C8-C7	5.75	125.18	108.43	6	7
4	A	327	PX4	O7-C23-C24	5.75	123.89	111.50	11	9
4	A	323	PX4	O7-C23-C24	5.74	123.88	111.50	8	8
4	A	430	PX4	C8-C7-C6	5.73	98.24	111.79	10	12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	405	PX4	O5-C8-C7	5.72	125.09	108.43	11	9
4	A	335	PX4	O5-C8-C7	5.72	125.09	108.43	8	12
4	A	356	PX4	O7-C23-C24	5.72	123.83	111.50	3	8
4	A	426	PX4	O7-C23-O8	5.72	109.89	123.70	7	3
4	A	377	PX4	C7-O7-C23	5.70	131.83	117.79	4	2
4	A	375	PX4	C8-C7-C6	5.69	98.33	111.79	1	9
4	A	423	PX4	O5-C9-O6	5.69	109.23	123.59	4	4
4	A	408	PX4	C4-N1-C3	5.66	123.53	108.97	14	4
4	A	333	PX4	O5-C8-C7	5.64	124.85	108.43	13	9
4	A	307	PX4	O7-C23-C24	5.63	123.64	111.50	9	8
4	A	331	PX4	O7-C23-O8	5.63	110.10	123.70	8	6
4	A	415	PX4	C8-C7-C6	5.63	98.48	111.79	3	10
4	A	365	PX4	O5-C8-C7	5.63	124.81	108.43	6	11
4	A	363	PX4	O5-C8-C7	5.62	124.80	108.43	9	10
4	A	379	PX4	C7-O7-C23	5.57	131.51	117.79	2	6
4	A	413	PX4	O5-C8-C7	5.57	124.65	108.43	10	10
4	A	339	PX4	O5-C8-C7	5.57	124.64	108.43	5	5
4	A	363	PX4	C8-C7-C6	5.57	98.63	111.79	11	9
4	A	390	PX4	O5-C8-C7	5.56	124.61	108.43	6	6
4	A	306	PX4	O7-C23-C24	5.55	123.46	111.50	5	6
4	A	331	PX4	O7-C23-C24	5.55	123.46	111.50	8	11
4	A	406	PX4	O7-C23-C24	5.54	123.44	111.50	6	7
4	A	342	PX4	O7-C23-C24	5.53	123.43	111.50	14	10
4	A	416	PX4	O7-C23-C24	5.51	123.38	111.50	13	5
4	A	348	PX4	O7-C23-O8	5.49	110.43	123.70	5	6
4	A	360	PX4	O5-C8-C7	5.49	124.41	108.43	12	9
4	A	402	PX4	P1-O3-C1	5.49	94.57	121.59	10	13
4	A	422	PX4	C4-N1-C3	5.49	94.87	108.97	9	5
4	A	370	PX4	C8-C7-C6	5.48	98.82	111.79	7	10
4	A	359	PX4	C8-C7-C6	5.48	98.83	111.79	5	8
4	A	327	PX4	C7-O7-C23	5.47	131.26	117.79	6	5
4	A	319	PX4	C8-C7-C6	5.47	98.85	111.79	6	11
4	A	350	PX4	C8-C7-C6	5.46	98.88	111.79	10	8
4	A	422	PX4	O7-C23-C24	5.46	123.27	111.50	10	9
4	A	327	PX4	C8-C7-C6	5.45	98.89	111.79	4	9
4	A	375	PX4	O7-C23-C24	5.44	123.23	111.50	3	8
4	A	401	PX4	O5-C8-C7	5.43	124.25	108.43	7	9
4	A	307	PX4	C7-O7-C23	5.43	131.16	117.79	3	10
4	A	394	PX4	P1-O3-C1	5.43	94.87	121.59	12	11
4	A	400	PX4	C8-C7-C6	5.43	98.95	111.79	8	10
4	A	351	PX4	C8-C7-C6	5.42	98.96	111.79	4	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	407	PX4	C8-C7-C6	5.42	98.97	111.79	11	8
4	A	312	PX4	C8-C7-C6	5.41	99.00	111.79	5	6
4	A	343	PX4	O7-C23-C24	5.41	123.15	111.50	14	8
4	A	389	PX4	P1-O3-C1	5.41	94.98	121.59	6	9
4	A	314	PX4	O5-C8-C7	5.40	124.16	108.43	11	10
4	A	353	PX4	O5-C8-C7	5.40	124.15	108.43	14	9
4	A	381	PX4	C7-O7-C23	5.40	104.49	117.79	8	3
4	A	377	PX4	O5-C8-C7	5.40	124.14	108.43	11	10
4	A	385	PX4	C8-C7-C6	5.40	99.03	111.79	8	10
4	A	330	PX4	C8-C7-C6	5.38	99.06	111.79	13	7
4	A	334	PX4	C8-C7-C6	5.38	99.06	111.79	9	11
4	A	367	PX4	C8-C7-C6	5.37	99.08	111.79	13	8
4	A	394	PX4	C8-C7-C6	5.35	99.13	111.79	10	8
4	A	371	PX4	C8-C7-C6	5.34	99.15	111.79	9	9
4	A	421	PX4	O5-C8-C7	5.34	123.98	108.43	9	5
4	A	346	PX4	O7-C23-C24	5.33	122.99	111.50	6	8
4	A	313	PX4	O3-P1-O2	5.33	88.25	109.07	13	5
4	A	429	PX4	C8-C7-C6	5.33	99.18	111.79	14	8
4	A	410	PX4	O3-P1-O2	5.32	88.28	109.07	13	4
4	A	320	PX4	C8-C7-C6	5.32	99.21	111.79	7	11
4	A	380	PX4	O7-C23-C24	5.31	122.95	111.50	6	6
4	A	362	PX4	C8-C7-C6	5.31	99.23	111.79	10	13
4	A	328	PX4	P1-O3-C1	5.31	95.47	121.59	10	12
4	A	428	PX4	O5-C8-C7	5.30	123.88	108.43	1	10
4	A	333	PX4	C8-C7-C6	5.30	99.25	111.79	7	9
4	A	381	PX4	P1-O3-C1	5.30	95.49	121.59	10	11
4	A	368	PX4	C8-C7-C6	5.29	99.28	111.79	11	10
4	A	388	PX4	C5-N1-C4	5.27	95.42	108.97	3	3
4	A	313	PX4	O7-C23-C24	5.26	122.83	111.50	7	6
4	A	346	PX4	C8-C7-C6	5.26	99.35	111.79	9	9
4	A	338	PX4	C8-C7-C6	5.25	99.36	111.79	14	7
4	A	430	PX4	O5-C8-C7	5.25	123.71	108.43	8	6
4	A	387	PX4	C8-C7-C6	5.25	99.38	111.79	4	11
4	A	324	PX4	C8-C7-C6	5.23	99.43	111.79	9	6
4	A	369	PX4	P1-O3-C1	5.23	95.87	121.59	5	10
4	A	398	PX4	O5-C8-C7	5.22	123.62	108.43	11	4
4	A	340	PX4	C8-C7-C6	5.21	99.47	111.79	11	9
4	A	328	PX4	O7-C23-C24	5.20	122.72	111.50	10	8
4	A	411	PX4	C4-N1-C3	5.20	122.35	108.97	1	7
4	A	339	PX4	C8-C7-C6	5.20	99.49	111.79	11	9
4	A	415	PX4	P1-O3-C1	5.19	96.02	121.59	3	13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	378	PX4	P1-O3-C1	5.18	96.07	121.59	7	11
4	A	390	PX4	O7-C23-O8	5.17	111.20	123.70	13	5
4	A	368	PX4	O5-C8-C7	5.17	123.49	108.43	13	8
4	A	374	PX4	O5-C8-C7	5.17	123.49	108.43	10	7
4	A	348	PX4	C8-C7-C6	5.17	99.57	111.79	6	8
4	A	381	PX4	O7-C23-C24	5.16	122.63	111.50	12	7
4	A	311	PX4	O5-C8-C7	5.16	123.44	108.43	8	8
4	A	317	PX4	C8-C7-C6	5.16	99.59	111.79	11	7
4	A	328	PX4	C5-N1-C4	5.16	95.72	108.97	5	8
4	A	341	PX4	O7-C7-C8	5.15	127.06	108.40	7	5
4	A	355	PX4	O5-C8-C7	5.15	123.44	108.43	7	6
4	A	344	PX4	C5-N1-C4	5.15	95.72	108.97	6	3
4	A	393	PX4	C8-C7-C6	5.14	99.64	111.79	2	7
4	A	309	PX4	O7-C23-C24	5.13	122.56	111.50	13	8
4	A	397	PX4	O5-C8-C7	5.13	123.35	108.43	11	10
4	A	373	PX4	O5-C8-C7	5.12	123.33	108.43	4	9
4	A	418	PX4	O5-C8-C7	5.12	123.33	108.43	13	8
4	A	360	PX4	C8-C7-C6	5.11	99.70	111.79	12	7
4	A	408	PX4	C8-C7-C6	5.11	99.70	111.79	11	11
4	A	422	PX4	O5-C8-C7	5.10	123.29	108.43	6	12
4	A	420	PX4	O7-C23-C24	5.09	122.46	111.50	13	8
4	A	329	PX4	O5-C8-C7	5.06	123.17	108.43	1	9
4	A	394	PX4	O5-C8-C7	5.06	123.17	108.43	6	11
4	A	364	PX4	C7-O7-C23	5.06	130.25	117.79	9	7
4	A	342	PX4	C8-C7-C6	5.05	99.84	111.79	6	9
4	A	391	PX4	O3-P1-O2	5.05	89.33	109.07	2	4
4	A	412	PX4	O7-C23-C24	5.05	122.39	111.50	7	7
4	A	372	PX4	O5-C9-O6	5.03	110.89	123.59	8	4
4	A	352	PX4	C8-C7-C6	5.03	99.89	111.79	6	9
4	A	335	PX4	C8-C7-C6	5.03	99.90	111.79	11	11
4	A	387	PX4	O7-C23-C24	5.03	122.33	111.50	12	6
4	A	417	PX4	O5-C8-C7	5.02	123.06	108.43	14	9
4	A	417	PX4	C8-C7-C6	5.02	99.91	111.79	1	9
4	A	392	PX4	C8-C7-C6	5.02	99.93	111.79	12	11
4	A	425	PX4	O7-C23-C24	5.02	122.31	111.50	13	7
4	A	377	PX4	C5-N1-C4	5.01	96.10	108.97	10	3
4	A	379	PX4	P1-O3-C1	5.01	96.94	121.59	13	12
4	A	412	PX4	P1-O3-C1	5.01	96.95	121.59	12	6
4	A	410	PX4	C8-C7-C6	5.00	99.95	111.79	8	10
4	A	308	PX4	O3-P1-O2	4.99	89.56	109.07	8	5
4	A	354	PX4	O5-C8-C7	4.99	122.96	108.43	1	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	330	PX4	O7-C23-O8	4.98	111.66	123.70	11	7
4	A	365	PX4	C8-C7-C6	4.98	100.00	111.79	5	8
4	A	392	PX4	O5-C8-C7	4.98	122.93	108.43	2	9
4	A	361	PX4	C7-O7-C23	4.97	130.04	117.79	1	13
4	A	344	PX4	C8-C7-C6	4.97	100.03	111.79	7	10
4	A	411	PX4	O5-C8-C7	4.97	122.89	108.43	12	8
4	A	396	PX4	O7-C7-C6	4.97	126.38	108.40	10	9
4	A	384	PX4	O7-C23-C24	4.96	122.19	111.50	3	7
4	A	371	PX4	C7-O7-C23	4.96	129.99	117.79	14	8
4	A	391	PX4	C8-C7-C6	4.96	100.07	111.79	14	9
4	A	349	PX4	C7-O7-C23	4.95	129.97	117.79	5	13
4	A	421	PX4	C8-C7-C6	4.95	100.09	111.79	8	6
4	A	421	PX4	O7-C23-C24	4.94	122.16	111.50	9	6
4	A	383	PX4	P1-O3-C1	4.94	97.27	121.59	9	7
4	A	428	PX4	P1-O3-C1	4.94	97.27	121.59	10	13
4	A	384	PX4	O5-C8-C7	4.94	122.81	108.43	13	9
4	A	385	PX4	O7-C23-O8	4.93	111.78	123.70	6	5
4	A	322	PX4	C7-O7-C23	4.93	129.92	117.79	6	5
4	A	400	PX4	O7-C23-C24	4.93	122.12	111.50	8	8
4	A	424	PX4	C7-O7-C23	4.92	129.91	117.79	13	4
4	A	310	PX4	O7-C23-C24	4.92	122.10	111.50	14	10
4	A	415	PX4	O5-C8-C7	4.92	122.75	108.43	14	11
4	A	311	PX4	O7-C23-C24	4.91	122.09	111.50	7	9
4	A	329	PX4	P1-O3-C1	4.91	97.43	121.59	13	11
4	A	322	PX4	O7-C23-C24	4.91	122.07	111.50	1	9
4	A	316	PX4	C8-C7-C6	4.90	100.21	111.79	9	9
4	A	334	PX4	C5-N1-C3	4.89	96.41	108.97	9	7
4	A	388	PX4	C8-C7-C6	4.89	100.23	111.79	1	9
4	A	410	PX4	C7-O7-C23	4.88	129.82	117.79	7	10
4	A	313	PX4	O5-C8-C7	4.87	122.62	108.43	14	11
4	A	364	PX4	O7-C23-O8	4.87	111.93	123.70	8	8
4	A	400	PX4	O5-C8-C7	4.87	122.61	108.43	7	4
4	A	403	PX4	O7-C23-C24	4.87	121.99	111.50	2	8
4	A	371	PX4	O7-C23-O8	4.86	111.95	123.70	3	10
4	A	386	PX4	O5-C8-C7	4.86	122.58	108.43	10	8
4	A	373	PX4	P1-O3-C1	4.86	97.67	121.59	8	11
4	A	423	PX4	O5-C8-C7	4.86	122.57	108.43	5	7
4	A	393	PX4	P1-O3-C1	4.85	97.69	121.59	12	10
4	A	356	PX4	C7-O7-C23	4.85	129.74	117.79	10	3
4	A	372	PX4	O3-P1-O2	4.85	90.12	109.07	8	4
4	A	316	PX4	O5-C8-C7	4.84	122.53	108.43	12	11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	378	PX4	O5-C8-C7	4.84	122.53	108.43	12	8
4	A	377	PX4	O5-C9-O6	4.84	111.37	123.59	14	2
4	A	427	PX4	O7-C23-O8	4.84	112.00	123.70	3	5
4	A	365	PX4	C7-O7-C23	4.84	129.71	117.79	7	4
4	A	309	PX4	O3-P1-O2	4.84	90.16	109.07	12	7
4	A	353	PX4	O7-C23-C24	4.83	121.92	111.50	7	5
4	A	395	PX4	C8-C7-C6	4.83	100.35	111.79	8	8
4	A	308	PX4	O7-C23-C24	4.83	121.91	111.50	3	8
4	A	381	PX4	C8-C7-C6	4.83	100.37	111.79	12	10
4	A	381	PX4	O3-P1-O2	4.83	90.21	109.07	8	3
4	A	404	PX4	C5-N1-C4	4.82	96.57	108.97	9	1
4	A	366	PX4	C7-O7-C23	4.82	129.66	117.79	13	5
4	A	402	PX4	O5-C9-O6	4.82	111.44	123.59	13	3
4	A	419	PX4	C7-O7-C23	4.81	129.64	117.79	1	5
4	A	347	PX4	O7-C23-C24	4.81	121.86	111.50	2	10
4	A	338	PX4	O5-C9-C10	4.80	126.98	111.91	12	3
4	A	353	PX4	O1-P1-O2	4.80	135.99	112.24	2	9
4	A	402	PX4	O7-C23-C24	4.80	121.86	111.50	7	3
4	A	404	PX4	C8-C7-C6	4.80	100.42	111.79	10	10
4	A	365	PX4	O7-C23-C24	4.80	121.85	111.50	14	7
4	A	419	PX4	C5-N1-C3	4.80	96.63	108.97	4	4
4	A	338	PX4	O7-C23-C24	4.79	121.83	111.50	12	10
4	A	307	PX4	C8-C7-C6	4.79	100.46	111.79	12	8
4	A	354	PX4	O7-C23-C24	4.79	121.82	111.50	10	5
4	A	347	PX4	P1-O3-C1	4.79	98.03	121.59	14	7
4	A	330	PX4	O7-C23-C24	4.77	121.79	111.50	10	8
4	A	423	PX4	O7-C7-C6	4.77	125.67	108.40	10	6
4	A	359	PX4	O5-C8-C7	4.77	122.30	108.43	5	11
4	A	314	PX4	C5-N1-C3	4.76	121.21	108.97	12	3
4	A	347	PX4	O5-C8-C7	4.76	122.28	108.43	1	9
4	A	395	PX4	O7-C23-C24	4.76	121.75	111.50	12	7
4	A	308	PX4	O5-C8-C7	4.75	122.26	108.43	10	9
4	A	414	PX4	C5-N1-C3	4.75	96.76	108.97	12	2
4	A	322	PX4	C8-C7-C6	4.75	100.56	111.79	10	11
4	A	391	PX4	O7-C23-O8	4.74	112.24	123.70	6	6
4	A	404	PX4	O5-C8-C7	4.74	122.24	108.43	13	7
4	A	413	PX4	P1-O3-C1	4.74	98.24	121.59	13	13
4	A	419	PX4	C5-N1-C4	4.74	96.79	108.97	9	3
4	A	427	PX4	P1-O3-C1	4.74	98.26	121.59	11	11
4	A	340	PX4	O7-C23-C24	4.73	121.70	111.50	10	8
4	A	410	PX4	P1-O3-C1	4.73	98.31	121.59	3	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	379	PX4	O5-C8-C7	4.72	122.19	108.43	12	9
4	A	429	PX4	O7-C23-C24	4.72	121.68	111.50	12	6
4	A	307	PX4	O7-C23-O8	4.72	112.30	123.70	8	4
4	A	404	PX4	O5-C9-C10	4.72	126.72	111.91	3	4
4	A	358	PX4	P1-O3-C1	4.71	98.39	121.59	14	12
4	A	408	PX4	O7-C23-C24	4.71	121.65	111.50	14	10
4	A	310	PX4	O7-C23-O8	4.71	112.33	123.70	14	6
4	A	375	PX4	O5-C8-C7	4.70	122.11	108.43	4	7
4	A	430	PX4	P1-O3-C1	4.70	98.47	121.59	1	10
4	A	405	PX4	O7-C23-O8	4.69	112.36	123.70	4	7
4	A	312	PX4	O7-C23-C24	4.69	121.62	111.50	11	7
4	A	351	PX4	O5-C8-C7	4.69	122.09	108.43	14	11
4	A	383	PX4	C8-C7-C6	4.69	100.69	111.79	3	11
4	A	337	PX4	C26-C25-C24	4.69	96.33	113.19	12	3
4	A	379	PX4	O7-C23-C24	4.69	121.61	111.50	14	8
4	A	415	PX4	C5-N1-C4	4.69	96.91	108.97	10	5
4	A	399	PX4	C4-N1-C3	4.68	96.93	108.97	10	7
4	A	413	PX4	O7-C7-C8	4.68	125.35	108.40	13	6
4	A	354	PX4	O3-P1-O2	4.68	90.79	109.07	7	4
4	A	394	PX4	O3-P1-O2	4.68	90.79	109.07	5	2
4	A	430	PX4	O7-C23-O8	4.68	112.40	123.70	9	4
4	A	396	PX4	C4-N1-C3	4.67	120.98	108.97	3	3
4	A	372	PX4	O7-C7-C8	4.67	125.30	108.40	10	5
4	A	411	PX4	C8-C7-C6	4.67	100.75	111.79	4	7
4	A	320	PX4	O7-C7-C8	4.66	125.27	108.40	13	3
4	A	395	PX4	C7-O7-C23	4.66	129.26	117.79	13	4
4	A	354	PX4	O5-C9-O6	4.66	111.84	123.59	11	4
4	A	386	PX4	O7-C7-C8	4.66	125.27	108.40	9	4
4	A	366	PX4	C8-C7-C6	4.65	100.78	111.79	2	11
4	A	425	PX4	C11-C10-C9	4.65	96.69	113.62	1	1
4	A	387	PX4	C5-N1-C3	4.65	97.01	108.97	14	5
4	A	323	PX4	C8-C7-C6	4.65	100.79	111.79	8	6
4	A	347	PX4	C5-N1-C4	4.65	120.92	108.97	10	3
4	A	360	PX4	P1-O3-C1	4.64	98.73	121.59	12	14
4	A	391	PX4	P1-O3-C1	4.64	98.74	121.59	14	9
4	A	329	PX4	C7-O7-C23	4.63	129.19	117.79	7	5
4	A	421	PX4	C4-N1-C3	4.63	120.88	108.97	12	4
4	A	409	PX4	O5-C8-C7	4.62	121.88	108.43	6	11
4	A	414	PX4	O5-C9-O6	4.62	111.93	123.59	8	4
4	A	411	PX4	C5-N1-C3	4.62	97.10	108.97	11	4
4	A	329	PX4	C8-C7-C6	4.61	100.89	111.79	4	12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	424	PX4	C8-C7-C6	4.61	100.88	111.79	14	8
4	A	326	PX4	C8-C7-C6	4.61	100.90	111.79	13	8
4	A	337	PX4	C8-C7-C6	4.61	100.89	111.79	12	9
4	A	416	PX4	O1-P1-O2	4.61	135.01	112.24	4	6
4	A	345	PX4	O7-C23-O8	4.60	112.58	123.70	2	6
4	A	403	PX4	O5-C8-C7	4.60	121.81	108.43	5	5
4	A	407	PX4	C7-O7-C23	4.60	129.11	117.79	11	5
4	A	382	PX4	O5-C8-C7	4.60	121.81	108.43	7	7
4	A	385	PX4	C7-O7-C23	4.59	106.48	117.79	14	3
4	A	362	PX4	P1-O3-C1	4.59	98.98	121.59	9	13
4	A	358	PX4	C8-C7-C6	4.59	100.93	111.79	8	6
4	A	341	PX4	O7-C23-O8	4.59	112.61	123.70	5	5
4	A	364	PX4	O7-C23-C24	4.59	121.39	111.50	14	9
4	A	311	PX4	C12-C11-C10	4.59	96.71	113.19	2	3
4	A	315	PX4	O5-C9-C10	4.58	126.29	111.91	3	3
4	A	312	PX4	O1-P1-O4	4.58	129.01	107.75	11	1
4	A	421	PX4	O7-C7-C8	4.58	124.98	108.40	13	9
4	A	384	PX4	C8-C7-C6	4.58	100.96	111.79	13	9
4	A	400	PX4	P1-O3-C1	4.57	99.07	121.59	5	13
4	A	408	PX4	O5-C8-C7	4.57	121.75	108.43	13	9
4	A	332	PX4	C7-O7-C23	4.57	129.05	117.79	14	6
4	A	352	PX4	O5-C8-C7	4.57	121.74	108.43	1	10
4	A	319	PX4	O5-C8-C7	4.56	121.70	108.43	2	10
4	A	393	PX4	O5-C8-C7	4.56	121.70	108.43	6	9
4	A	355	PX4	O7-C23-C24	4.56	121.32	111.50	4	5
4	A	367	PX4	O5-C8-C7	4.55	121.68	108.43	8	10
4	A	307	PX4	O3-P1-O2	4.55	91.30	109.07	2	6
4	A	373	PX4	O7-C23-C24	4.55	121.30	111.50	8	7
4	A	406	PX4	O5-C8-C7	4.55	121.67	108.43	9	7
4	A	306	PX4	O5-C8-C7	4.54	121.65	108.43	2	8
4	A	310	PX4	C5-N1-C4	4.54	97.30	108.97	5	3
4	A	404	PX4	P1-O3-C1	4.54	99.25	121.59	9	12
4	A	423	PX4	C5-N1-C3	4.54	97.31	108.97	9	5
4	A	348	PX4	O7-C23-C24	4.54	121.28	111.50	5	10
4	A	404	PX4	C7-O7-C23	4.53	128.95	117.79	4	4
4	A	344	PX4	C4-N1-C3	4.52	97.34	108.97	7	4
4	A	418	PX4	C8-C7-C6	4.53	101.08	111.79	13	8
4	A	428	PX4	C4-N1-C3	4.53	97.34	108.97	6	5
4	A	371	PX4	C5-N1-C4	4.52	120.60	108.97	8	3
4	A	372	PX4	C8-C7-C6	4.52	101.09	111.79	14	7
4	A	379	PX4	C5-N1-C3	4.52	97.35	108.97	10	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	313	PX4	C8-C7-C6	4.52	101.10	111.79	13	7
4	A	353	PX4	P1-O3-C1	4.52	99.34	121.59	9	11
4	A	325	PX4	C8-C7-C6	4.52	101.11	111.79	11	12
4	A	399	PX4	P1-O3-C1	4.51	99.38	121.59	10	11
4	A	384	PX4	O1-P1-O2	4.51	134.54	112.24	13	7
4	A	349	PX4	O5-C8-C7	4.51	121.56	108.43	1	6
4	A	359	PX4	O7-C7-C8	4.50	124.71	108.40	9	6
4	A	364	PX4	O5-C8-C7	4.50	121.55	108.43	12	7
4	A	385	PX4	O5-C8-C7	4.50	121.54	108.43	13	9
4	A	423	PX4	P1-O4-C6	4.50	95.29	121.68	9	8
4	A	367	PX4	C7-O7-C23	4.50	128.87	117.79	13	6
4	A	333	PX4	O7-C23-C24	4.50	121.19	111.50	9	6
4	A	399	PX4	O5-C8-C7	4.50	121.52	108.43	2	8
4	A	395	PX4	O5-C8-C7	4.50	121.52	108.43	6	10
4	A	336	PX4	C8-C7-C6	4.49	101.16	111.79	10	9
4	A	408	PX4	C7-O7-C23	4.49	128.85	117.79	9	6
4	A	356	PX4	O5-C9-O6	4.49	112.26	123.59	14	1
4	A	323	PX4	P1-O3-C1	4.49	99.49	121.59	12	12
4	A	356	PX4	C4-N1-C3	4.48	97.45	108.97	11	2
4	A	393	PX4	O3-P1-O2	4.48	91.55	109.07	9	4
4	A	357	PX4	O7-C23-C24	4.47	121.14	111.50	2	6
4	A	409	PX4	O7-C23-C24	4.47	121.14	111.50	12	8
4	A	346	PX4	O5-C8-C7	4.47	121.44	108.43	10	6
4	A	348	PX4	O5-C8-C7	4.47	121.44	108.43	3	9
4	A	396	PX4	P1-O3-C1	4.47	99.60	121.59	8	10
4	A	310	PX4	P1-O3-C1	4.47	99.60	121.59	6	8
4	A	319	PX4	P1-O3-C1	4.47	99.60	121.59	13	11
4	A	314	PX4	C7-O7-C23	4.46	128.77	117.79	14	2
4	A	371	PX4	C4-N1-C3	4.46	97.51	108.97	3	4
4	A	420	PX4	O5-C8-C7	4.46	121.41	108.43	13	7
4	A	393	PX4	O7-C23-C24	4.45	121.10	111.50	8	7
4	A	372	PX4	O7-C23-C24	4.45	121.09	111.50	10	5
4	A	387	PX4	O5-C8-C7	4.45	121.39	108.43	6	10
4	A	378	PX4	C8-C7-C6	4.45	101.27	111.79	8	5
4	A	401	PX4	P1-O3-C1	4.45	99.69	121.59	6	11
4	A	312	PX4	O7-C7-C8	4.44	124.49	108.40	7	11
4	A	428	PX4	O7-C23-O8	4.44	112.97	123.70	4	4
4	A	398	PX4	O3-P1-O2	4.44	91.72	109.07	3	6
4	A	306	PX4	O7-C7-C8	4.43	124.45	108.40	1	9
4	A	373	PX4	O3-P1-O2	4.43	91.75	109.07	9	6
4	A	373	PX4	C8-C7-C6	4.43	101.31	111.79	11	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	374	PX4	O7-C7-C8	4.43	124.44	108.40	8	4
4	A	401	PX4	O7-C23-C24	4.43	121.05	111.50	3	6
4	A	416	PX4	O3-P1-O2	4.42	91.78	109.07	4	3
4	A	397	PX4	O7-C23-O8	4.42	113.02	123.70	6	5
4	A	327	PX4	C5-N1-C3	4.42	97.62	108.97	8	3
4	A	416	PX4	C5-N1-C3	4.42	97.62	108.97	9	3
4	A	406	PX4	O3-P1-O2	4.42	91.81	109.07	1	5
4	A	416	PX4	C1-C2-N1	4.42	130.52	115.78	11	2
4	A	366	PX4	O5-C8-C7	4.41	121.28	108.43	7	10
4	A	324	PX4	O5-C8-C7	4.41	121.28	108.43	5	7
4	A	332	PX4	C8-C7-C6	4.41	101.36	111.79	6	11
4	A	310	PX4	P1-O4-C6	4.40	95.86	121.68	13	10
4	A	333	PX4	O7-C7-C6	4.40	124.34	108.40	4	8
4	A	344	PX4	C7-O7-C23	4.40	128.63	117.79	14	4
4	A	350	PX4	O7-C23-O8	4.40	113.06	123.70	2	5
4	A	336	PX4	O4-P1-O2	4.40	126.26	109.07	14	4
4	A	324	PX4	P1-O3-C1	4.40	99.95	121.59	10	11
4	A	410	PX4	O7-C7-C8	4.40	124.32	108.40	13	11
4	A	430	PX4	O7-C23-C24	4.40	120.98	111.50	1	6
4	A	331	PX4	O5-C8-C7	4.39	121.22	108.43	12	9
4	A	418	PX4	O7-C23-O8	4.39	113.09	123.70	5	7
4	A	372	PX4	C7-O7-C23	4.39	128.60	117.79	6	7
4	A	363	PX4	C4-N1-C3	4.39	97.69	108.97	9	2
4	A	384	PX4	O5-C9-O6	4.39	112.52	123.59	10	4
4	A	397	PX4	C7-O7-C23	4.39	128.59	117.79	10	3
4	A	383	PX4	O7-C23-C24	4.39	120.95	111.50	5	7
4	A	330	PX4	O5-C8-C7	4.38	121.19	108.43	5	9
4	A	412	PX4	O5-C8-C7	4.38	121.19	108.43	3	6
4	A	403	PX4	C8-C7-C6	4.38	101.42	111.79	2	9
4	A	370	PX4	O7-C23-C24	4.38	120.94	111.50	8	8
4	A	415	PX4	O7-C23-O8	4.37	113.13	123.70	13	3
4	A	358	PX4	O5-C8-C7	4.37	121.16	108.43	10	8
4	A	391	PX4	O7-C23-C24	4.37	120.92	111.50	2	7
4	A	417	PX4	O4-P1-O2	4.37	126.14	109.07	13	3
4	A	350	PX4	P1-O4-C6	4.37	96.06	121.68	12	4
4	A	409	PX4	O3-P1-O2	4.37	92.01	109.07	8	6
4	A	411	PX4	O7-C23-C24	4.37	120.91	111.50	7	6
4	A	390	PX4	O3-P1-O2	4.37	92.01	109.07	2	5
4	A	355	PX4	P1-O3-C1	4.36	100.12	121.59	12	12
4	A	367	PX4	P1-O3-C1	4.36	100.14	121.59	9	12
4	A	325	PX4	O7-C23-C24	4.36	120.89	111.50	12	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	354	PX4	C5-N1-C4	4.35	97.78	108.97	14	5
4	A	378	PX4	O7-C23-O8	4.35	113.18	123.70	12	3
4	A	381	PX4	O5-C8-C7	4.35	121.10	108.43	2	12
4	A	371	PX4	P1-O3-C1	4.35	100.19	121.59	6	13
4	A	411	PX4	O7-C23-O8	4.35	113.20	123.70	2	3
4	A	334	PX4	O5-C9-O6	4.34	112.63	123.59	5	2
4	A	365	PX4	P1-O3-C1	4.34	100.21	121.59	13	10
4	A	309	PX4	P1-O3-C1	4.34	100.22	121.59	14	11
4	A	345	PX4	O7-C23-C24	4.33	120.84	111.50	10	7
4	A	338	PX4	O5-C8-C7	4.33	121.04	108.43	12	5
4	A	428	PX4	P1-O4-C6	4.33	96.29	121.68	8	8
4	A	369	PX4	C8-C7-C6	4.33	101.55	111.79	8	7
4	A	429	PX4	P1-O3-C1	4.33	100.28	121.59	5	11
4	A	309	PX4	O5-C8-C7	4.33	121.03	108.43	5	8
4	A	342	PX4	O5-C8-C7	4.32	121.02	108.43	2	6
4	A	394	PX4	O7-C23-O8	4.32	113.25	123.70	13	3
4	A	364	PX4	C4-N1-C3	4.32	97.87	108.97	13	5
4	A	313	PX4	O7-C23-O8	4.31	113.28	123.70	7	6
4	A	342	PX4	C4-N1-C3	4.31	120.06	108.97	5	3
4	A	327	PX4	O5-C8-C7	4.31	120.98	108.43	11	7
4	A	318	PX4	P1-O3-C1	4.31	100.38	121.59	4	9
4	A	321	PX4	O5-C8-C7	4.31	120.98	108.43	13	7
4	A	400	PX4	C5-N1-C4	4.31	120.05	108.97	10	1
4	A	419	PX4	O7-C23-C24	4.31	120.78	111.50	11	6
4	A	360	PX4	O7-C23-C24	4.30	120.77	111.50	2	10
4	A	364	PX4	O1-P1-O2	4.30	133.49	112.24	8	4
4	A	366	PX4	O3-P1-O2	4.30	92.28	109.07	12	7
4	A	382	PX4	O7-C23-C24	4.30	120.76	111.50	8	6
4	A	388	PX4	O7-C23-C24	4.29	120.75	111.50	2	6
4	A	328	PX4	O5-C8-C7	4.29	120.92	108.43	6	8
4	A	355	PX4	C5-N1-C4	4.29	97.95	108.97	7	6
4	A	376	PX4	O7-C7-C8	4.28	123.91	108.40	1	7
4	A	336	PX4	O5-C8-C7	4.28	120.90	108.43	10	9
4	A	338	PX4	C12-C11-C10	4.28	97.80	113.19	8	2
4	A	392	PX4	O7-C23-C24	4.28	120.73	111.50	7	7
4	A	400	PX4	O7-C7-C8	4.28	123.90	108.40	7	7
4	A	326	PX4	C4-N1-C3	4.28	97.98	108.97	1	1
4	A	426	PX4	P1-O3-C1	4.28	100.54	121.59	13	10
4	A	372	PX4	P1-O3-C1	4.27	100.55	121.59	4	9
4	A	376	PX4	P1-O3-C1	4.27	100.56	121.59	9	13
4	A	393	PX4	O7-C7-C8	4.27	123.87	108.40	13	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	338	PX4	C5-N1-C3	4.27	97.99	108.97	9	5
4	A	315	PX4	C4-N1-C3	4.27	98.00	108.97	14	7
4	A	355	PX4	C8-C7-C6	4.27	101.69	111.79	6	8
4	A	355	PX4	P1-O4-C6	4.27	96.66	121.68	1	10
4	A	345	PX4	O5-C9-C10	4.26	125.29	111.91	2	4
4	A	347	PX4	O7-C7-C8	4.27	123.84	108.40	2	7
4	A	316	PX4	O7-C23-C24	4.26	120.69	111.50	1	8
4	A	333	PX4	C7-O7-C23	4.26	128.28	117.79	6	4
4	A	419	PX4	P1-O3-C1	4.26	100.61	121.59	6	9
4	A	355	PX4	C7-O7-C23	4.26	107.31	117.79	13	2
4	A	344	PX4	O5-C8-C7	4.25	120.81	108.43	5	8
4	A	366	PX4	P1-O3-C1	4.25	100.66	121.59	2	12
4	A	424	PX4	O5-C8-C7	4.25	120.80	108.43	5	7
4	A	371	PX4	O5-C8-C7	4.25	120.80	108.43	5	5
4	A	338	PX4	P1-O3-C1	4.24	100.69	121.59	3	13
4	A	364	PX4	C8-C7-C6	4.25	101.75	111.79	13	9
4	A	416	PX4	C8-C7-C6	4.24	101.75	111.79	3	7
4	A	343	PX4	O3-P1-O2	4.24	125.64	109.07	6	3
4	A	326	PX4	O7-C23-C24	4.24	120.64	111.50	5	5
4	A	422	PX4	P1-O3-C1	4.24	100.72	121.59	10	7
4	A	397	PX4	P1-O3-C1	4.24	100.72	121.59	14	10
4	A	327	PX4	C4-N1-C3	4.24	98.08	108.97	5	6
4	A	427	PX4	O7-C7-C8	4.24	123.74	108.40	12	8
4	A	420	PX4	P1-O3-C1	4.23	100.75	121.59	7	8
4	A	342	PX4	P1-O3-C1	4.23	100.76	121.59	10	14
4	A	361	PX4	O5-C9-C10	4.23	125.19	111.91	2	2
4	A	343	PX4	O5-C8-C7	4.23	120.74	108.43	7	6
4	A	326	PX4	P1-O3-C1	4.22	100.79	121.59	7	13
4	A	410	PX4	C4-N1-C3	4.23	119.84	108.97	13	2
4	A	308	PX4	O7-C23-O8	4.22	113.50	123.70	3	5
4	A	388	PX4	P1-O3-C1	4.22	100.82	121.59	6	8
4	A	309	PX4	O4-P1-O2	4.22	125.54	109.07	9	3
4	A	414	PX4	O7-C23-O8	4.22	113.51	123.70	1	5
4	A	407	PX4	P1-O4-C6	4.22	96.96	121.68	7	7
4	A	418	PX4	C4-N1-C3	4.22	98.13	108.97	9	4
4	A	426	PX4	C5-N1-C4	4.22	98.13	108.97	5	2
4	A	403	PX4	O4-P1-O2	4.21	125.52	109.07	4	2
4	A	416	PX4	P1-O4-C6	4.21	96.98	121.68	9	9
4	A	427	PX4	C4-N1-C3	4.21	98.15	108.97	12	2
4	A	407	PX4	O7-C23-C24	4.21	120.57	111.50	8	8
4	A	381	PX4	O7-C7-C8	4.21	123.63	108.40	10	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	363	PX4	P1-O3-C1	4.20	100.91	121.59	8	8
4	A	375	PX4	C5-N1-C3	4.20	98.17	108.97	3	2
4	A	376	PX4	O7-C23-C24	4.20	120.55	111.50	14	7
4	A	321	PX4	C7-O7-C23	4.20	128.13	117.79	8	6
4	A	340	PX4	C26-C25-C24	4.20	98.11	113.19	11	3
4	A	389	PX4	O5-C8-C7	4.20	120.65	108.43	13	10
4	A	308	PX4	P1-O3-C1	4.19	100.96	121.59	7	9
4	A	339	PX4	P1-O3-C1	4.19	100.97	121.59	8	11
4	A	390	PX4	C8-C7-C6	4.19	101.88	111.79	5	8
4	A	421	PX4	P1-O3-C1	4.19	100.97	121.59	7	8
4	A	421	PX4	C7-O7-C23	4.19	128.10	117.79	12	5
4	A	351	PX4	C4-N1-C3	4.18	98.21	108.97	2	2
4	A	341	PX4	O5-C8-C7	4.18	120.61	108.43	6	6
4	A	386	PX4	O1-P1-O2	4.18	132.92	112.24	5	6
4	A	358	PX4	O7-C23-O8	4.18	113.60	123.70	1	5
4	A	331	PX4	P1-O4-C6	4.18	97.17	121.68	14	8
4	A	341	PX4	P1-O3-C1	4.18	101.02	121.59	4	12
4	A	351	PX4	O7-C7-C6	4.18	123.53	108.40	3	7
4	A	307	PX4	P1-O3-C1	4.18	101.03	121.59	2	9
4	A	340	PX4	O5-C8-C7	4.18	120.59	108.43	3	12
4	A	344	PX4	P1-O3-C1	4.17	101.04	121.59	7	11
4	A	383	PX4	O5-C8-C7	4.17	120.59	108.43	3	10
4	A	326	PX4	O5-C9-C10	4.17	125.01	111.91	6	2
4	A	361	PX4	O7-C7-C6	4.17	123.51	108.40	8	3
4	A	353	PX4	P1-O4-C6	4.17	97.22	121.68	12	9
4	A	394	PX4	O7-C23-C24	4.17	120.49	111.50	6	8
4	A	354	PX4	C8-C7-C6	4.16	101.94	111.79	1	7
4	A	362	PX4	O5-C8-C7	4.16	120.56	108.43	7	11
4	A	340	PX4	C5-N1-C4	4.16	98.27	108.97	5	2
4	A	384	PX4	O7-C23-O8	4.16	113.64	123.70	9	4
4	A	421	PX4	O5-C9-O6	4.16	113.09	123.59	9	6
4	A	385	PX4	O7-C7-C6	4.16	123.46	108.40	2	4
4	A	385	PX4	C5-N1-C4	4.16	98.29	108.97	6	1
4	A	399	PX4	C8-C7-C6	4.15	101.96	111.79	11	11
4	A	414	PX4	C5-N1-C4	4.16	98.29	108.97	12	4
4	A	310	PX4	O3-P1-O2	4.15	92.85	109.07	14	3
4	A	315	PX4	O5-C8-C7	4.15	120.51	108.43	2	6
4	A	344	PX4	C5-N1-C3	4.15	98.30	108.97	2	5
4	A	392	PX4	P1-O3-C1	4.15	101.16	121.59	8	12
4	A	384	PX4	O7-C7-C8	4.15	123.42	108.40	3	5
4	A	413	PX4	O7-C23-C24	4.15	120.44	111.50	6	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	426	PX4	C8-C7-C6	4.15	101.98	111.79	6	4
4	A	403	PX4	C7-O7-C23	4.15	107.58	117.79	10	3
4	A	410	PX4	O7-C23-C24	4.15	120.44	111.50	7	4
4	A	417	PX4	C26-C25-C24	4.14	98.29	113.19	6	3
4	A	402	PX4	O5-C8-C7	4.14	120.48	108.43	6	6
4	A	380	PX4	C7-O7-C23	4.14	107.61	117.79	5	5
4	A	396	PX4	P1-O4-C6	4.14	97.42	121.68	4	8
4	A	407	PX4	O7-C7-C8	4.14	123.38	108.40	9	7
4	A	356	PX4	C8-C7-C6	4.13	102.02	111.79	3	10
4	A	417	PX4	C12-C11-C10	4.13	98.35	113.19	1	3
4	A	376	PX4	O5-C9-O6	4.12	113.18	123.59	4	4
4	A	383	PX4	O7-C7-C6	4.12	123.34	108.40	13	4
4	A	388	PX4	P1-O4-C6	4.12	97.50	121.68	13	8
4	A	396	PX4	O5-C8-C7	4.12	120.44	108.43	2	10
4	A	335	PX4	O7-C23-C24	4.12	120.38	111.50	3	7
4	A	329	PX4	O7-C23-O8	4.12	113.76	123.70	2	6
4	A	409	PX4	O5-C9-O6	4.12	113.20	123.59	3	3
4	A	307	PX4	O5-C8-C7	4.11	120.41	108.43	8	9
4	A	416	PX4	P1-O3-C1	4.11	101.34	121.59	12	10
4	A	329	PX4	O7-C23-C24	4.11	120.36	111.50	12	10
4	A	377	PX4	O7-C23-C24	4.11	120.36	111.50	7	9
4	A	338	PX4	C7-O7-C23	4.11	127.90	117.79	12	3
4	A	405	PX4	P1-O4-C6	4.11	97.61	121.68	13	13
4	A	409	PX4	C8-C7-C6	4.11	102.08	111.79	5	7
4	A	374	PX4	C8-C7-C6	4.10	102.08	111.79	8	6
4	A	340	PX4	C7-O7-C23	4.10	107.69	117.79	6	5
4	A	367	PX4	O5-C9-O6	4.10	113.24	123.59	8	5
4	A	403	PX4	O1-P1-O4	4.10	126.80	107.75	9	5
4	A	396	PX4	O7-C7-C8	4.10	123.25	108.40	13	6
4	A	402	PX4	C5-N1-C3	4.10	98.43	108.97	11	2
4	A	348	PX4	C5-N1-C4	4.10	98.44	108.97	7	3
4	A	374	PX4	O5-C9-O6	4.10	113.25	123.59	2	3
4	A	313	PX4	C12-C11-C10	4.09	98.47	113.19	2	4
4	A	343	PX4	C5-N1-C3	4.09	98.45	108.97	6	2
4	A	382	PX4	O7-C7-C8	4.09	123.23	108.40	4	5
4	A	392	PX4	C1-C2-N1	4.09	129.45	115.78	9	3
4	A	317	PX4	C1-C2-N1	4.09	129.44	115.78	7	5
4	A	319	PX4	O7-C23-C24	4.09	120.32	111.50	12	6
4	A	343	PX4	P1-O3-C1	4.09	101.44	121.59	2	11
4	A	357	PX4	O5-C8-C7	4.09	120.35	108.43	3	8
4	A	313	PX4	O5-C9-O6	4.09	113.27	123.59	2	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	315	PX4	C8-C7-C6	4.09	102.11	111.79	10	9
4	A	335	PX4	P1-O3-C1	4.09	101.45	121.59	4	8
4	A	418	PX4	C12-C11-C10	4.09	98.49	113.19	5	2
4	A	420	PX4	C4-N1-C3	4.09	98.46	108.97	5	4
4	A	330	PX4	O5-C9-O6	4.09	113.27	123.59	12	4
4	A	356	PX4	O7-C7-C8	4.09	123.20	108.40	14	7
4	A	389	PX4	O5-C9-C10	4.09	124.73	111.91	9	2
4	A	416	PX4	O1-P1-O4	4.09	126.72	107.75	3	4
4	A	325	PX4	C7-O7-C23	4.08	127.84	117.79	1	3
4	A	359	PX4	P1-O3-C1	4.08	101.50	121.59	10	10
4	A	313	PX4	C7-O7-C23	4.08	127.83	117.79	7	4
4	A	349	PX4	C8-C7-C6	4.08	102.14	111.79	4	5
4	A	414	PX4	P1-O3-C1	4.08	101.53	121.59	3	11
4	A	344	PX4	O5-C9-C10	4.07	124.69	111.91	7	5
4	A	392	PX4	O7-C7-C8	4.07	123.15	108.40	8	5
4	A	337	PX4	O7-C7-C6	4.07	123.14	108.40	13	3
4	A	408	PX4	C12-C11-C10	4.07	98.57	113.19	10	1
4	A	398	PX4	O1-P1-O2	4.07	132.34	112.24	3	7
4	A	421	PX4	O7-C23-O8	4.07	113.88	123.70	9	3
4	A	315	PX4	O7-C23-C24	4.06	120.26	111.50	12	10
4	A	394	PX4	C4-N1-C3	4.06	98.53	108.97	1	2
4	A	424	PX4	O7-C23-O8	4.06	113.89	123.70	7	5
4	A	332	PX4	O5-C9-O6	4.06	113.35	123.59	13	4
4	A	393	PX4	O1-P1-O2	4.06	132.30	112.24	9	9
4	A	386	PX4	P1-O4-C6	4.06	97.90	121.68	10	11
4	A	352	PX4	O5-C9-O6	4.05	113.36	123.59	1	5
4	A	318	PX4	O5-C8-C7	4.05	120.22	108.43	13	8
4	A	325	PX4	O5-C8-C7	4.05	120.22	108.43	7	10
4	A	331	PX4	P1-O3-C1	4.05	101.67	121.59	14	12
4	A	354	PX4	O1-P1-O2	4.05	132.25	112.24	7	11
4	A	373	PX4	O7-C7-C8	4.05	123.06	108.40	3	8
4	A	406	PX4	O7-C7-C8	4.05	123.06	108.40	13	3
4	A	319	PX4	O1-P1-O3	4.04	88.96	107.75	6	4
4	A	341	PX4	C8-C7-C6	4.04	102.23	111.79	5	9
4	A	346	PX4	O1-P1-O3	4.04	88.97	107.75	14	2
4	A	398	PX4	P1-O3-C1	4.04	101.70	121.59	1	11
4	A	354	PX4	P1-O3-C1	4.04	101.71	121.59	12	13
4	A	377	PX4	P1-O4-C6	4.04	98.02	121.68	13	4
4	A	406	PX4	C8-C7-C6	4.04	102.24	111.79	6	9
4	A	318	PX4	P1-O4-C6	4.03	98.03	121.68	14	9
4	A	414	PX4	O7-C23-C24	4.03	120.19	111.50	14	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	311	PX4	O7-C23-O8	4.03	113.96	123.70	2	4
4	A	314	PX4	C8-C7-C6	4.03	102.26	111.79	2	12
4	A	350	PX4	O1-P1-O2	4.03	132.17	112.24	9	6
4	A	336	PX4	O1-P1-O2	4.03	132.16	112.24	7	8
4	A	309	PX4	O7-C23-O8	4.03	113.97	123.70	14	9
4	A	316	PX4	O1-P1-O3	4.03	89.04	107.75	5	3
4	A	338	PX4	P1-O4-C6	4.03	98.06	121.68	10	13
4	A	400	PX4	O7-C7-C6	4.03	122.98	108.40	1	5
4	A	373	PX4	C5-N1-C4	4.03	98.62	108.97	12	3
4	A	376	PX4	O3-P1-O2	4.03	93.34	109.07	10	3
4	A	404	PX4	O7-C7-C8	4.03	122.98	108.40	13	6
4	A	411	PX4	C5-N1-C4	4.03	98.62	108.97	1	6
4	A	335	PX4	C7-O7-C23	4.02	107.88	117.79	9	4
4	A	398	PX4	O7-C23-C24	4.02	120.17	111.50	9	9
4	A	346	PX4	P1-O3-C1	4.02	101.79	121.59	10	13
4	A	363	PX4	C5-N1-C3	4.02	119.31	108.97	9	3
4	A	343	PX4	O7-C7-C6	4.02	122.95	108.40	9	6
4	A	310	PX4	O5-C8-C7	4.02	120.13	108.43	8	4
4	A	402	PX4	C1-C2-N1	4.02	129.19	115.78	8	4
4	A	373	PX4	O1-P1-O2	4.01	132.09	112.24	5	9
4	A	347	PX4	C8-C7-C6	4.01	102.30	111.79	1	7
4	A	401	PX4	O7-C7-C8	4.01	122.93	108.40	5	6
4	A	361	PX4	O7-C23-C24	4.01	120.14	111.50	4	6
4	A	425	PX4	P1-O3-C1	4.01	101.86	121.59	5	12
4	A	412	PX4	C4-N1-C3	4.01	119.27	108.97	9	3
4	A	371	PX4	O1-P1-O4	4.00	126.34	107.75	12	3
4	A	387	PX4	C5-N1-C4	4.00	98.68	108.97	13	4
4	A	328	PX4	C8-C7-C6	4.00	102.32	111.79	2	11
4	A	332	PX4	O7-C23-C24	4.00	120.13	111.50	9	4
4	A	350	PX4	O5-C8-C7	4.00	120.08	108.43	9	6
4	A	407	PX4	C4-N1-C3	4.00	98.70	108.97	8	3
4	A	349	PX4	O7-C7-C8	4.00	122.87	108.40	9	9
4	A	400	PX4	O7-C23-O8	3.99	114.05	123.70	7	8
4	A	318	PX4	O1-P1-O2	3.99	131.97	112.24	10	5
4	A	369	PX4	C5-N1-C4	3.99	98.71	108.97	4	7
4	A	396	PX4	O7-C23-C24	3.99	120.10	111.50	10	5
4	A	403	PX4	O7-C7-C6	3.99	122.84	108.40	6	5
4	A	422	PX4	C8-C7-C6	3.99	102.35	111.79	11	8
4	A	398	PX4	O4-P1-O2	3.99	124.64	109.07	5	2
4	A	386	PX4	P1-O3-C1	3.98	101.98	121.59	6	11
4	A	346	PX4	P1-O4-C6	3.98	98.33	121.68	14	11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	415	PX4	O1-P1-O2	3.98	131.93	112.24	8	6
4	A	420	PX4	C8-C7-C6	3.98	102.37	111.79	7	10
4	A	314	PX4	C5-N1-C4	3.98	98.75	108.97	11	5
4	A	410	PX4	C26-C25-C24	3.98	98.89	113.19	5	2
4	A	408	PX4	C5-N1-C4	3.97	98.77	108.97	5	4
4	A	309	PX4	C4-N1-C3	3.97	98.77	108.97	9	3
4	A	402	PX4	C5-N1-C4	3.97	98.77	108.97	14	4
4	A	374	PX4	P1-O3-C1	3.97	102.06	121.59	9	11
4	A	327	PX4	O7-C23-O8	3.96	114.12	123.70	4	6
4	A	401	PX4	O7-C7-C6	3.96	122.75	108.40	9	9
4	A	325	PX4	O7-C23-O8	3.96	114.14	123.70	3	6
4	A	363	PX4	O1-P1-O4	3.95	126.11	107.75	10	3
4	A	375	PX4	P1-O3-C1	3.95	102.12	121.59	1	11
4	A	384	PX4	P1-O4-C6	3.95	98.49	121.68	5	9
4	A	405	PX4	C8-C7-C6	3.95	102.43	111.79	14	9
4	A	369	PX4	C25-C24-C23	3.95	99.24	113.62	1	3
4	A	399	PX4	C7-O7-C23	3.95	127.52	117.79	9	5
4	A	357	PX4	O7-C23-O8	3.95	114.17	123.70	1	5
4	A	397	PX4	O7-C7-C8	3.94	122.66	108.40	3	8
4	A	410	PX4	O1-P1-O2	3.94	131.72	112.24	5	4
4	A	315	PX4	C12-C11-C10	3.94	99.03	113.19	11	2
4	A	332	PX4	O7-C7-C8	3.94	122.66	108.40	4	6
4	A	344	PX4	O7-C23-C24	3.94	119.99	111.50	14	6
4	A	356	PX4	O5-C8-C7	3.94	119.89	108.43	1	11
4	A	372	PX4	C5-N1-C3	3.94	98.85	108.97	3	3
4	A	419	PX4	C8-C7-C6	3.94	102.48	111.79	6	12
4	A	378	PX4	O7-C23-C24	3.94	119.98	111.50	11	5
4	A	398	PX4	O7-C7-C8	3.94	122.65	108.40	13	5
4	A	319	PX4	O7-C7-C6	3.93	122.64	108.40	14	4
4	A	326	PX4	C11-C10-C9	3.93	99.32	113.62	4	2
4	A	411	PX4	O7-C7-C8	3.93	122.63	108.40	12	6
4	A	342	PX4	C5-N1-C3	3.93	98.88	108.97	12	3
4	A	365	PX4	O5-C9-C10	3.93	124.24	111.91	1	5
4	A	337	PX4	O5-C8-C7	3.93	119.86	108.43	5	9
4	A	375	PX4	P1-O4-C6	3.93	98.66	121.68	10	9
4	A	416	PX4	C5-N1-C4	3.93	119.07	108.97	8	5
4	A	419	PX4	P1-O4-C6	3.93	98.66	121.68	3	9
4	A	361	PX4	O5-C8-C7	3.92	119.86	108.43	1	6
4	A	306	PX4	C8-C7-C6	3.92	102.51	111.79	14	7
4	A	384	PX4	P1-O3-C1	3.92	102.28	121.59	2	11
4	A	336	PX4	O1-P1-O3	3.92	89.54	107.75	14	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	377	PX4	P1-O3-C1	3.92	102.30	121.59	13	9
4	A	322	PX4	P1-O3-C1	3.92	102.30	121.59	14	12
4	A	338	PX4	O5-C9-O6	3.92	113.70	123.59	11	5
4	A	399	PX4	C5-N1-C4	3.92	119.05	108.97	10	4
4	A	402	PX4	C8-C7-C6	3.92	102.52	111.79	3	9
4	A	339	PX4	C7-O7-C23	3.92	127.43	117.79	12	3
4	A	405	PX4	P1-O3-C1	3.91	102.32	121.59	9	12
4	A	419	PX4	O5-C9-O6	3.92	113.71	123.59	5	1
4	A	314	PX4	P1-O3-C1	3.91	102.33	121.59	10	10
4	A	352	PX4	C7-O7-C23	3.91	127.41	117.79	11	5
4	A	358	PX4	O7-C23-C24	3.91	119.92	111.50	13	8
4	A	384	PX4	O5-C9-C10	3.91	124.17	111.91	10	4
4	A	399	PX4	O5-C9-O6	3.91	113.73	123.59	3	4
4	A	404	PX4	P1-O4-C6	3.91	98.77	121.68	5	7
4	A	414	PX4	O5-C9-C10	3.91	124.16	111.91	14	6
4	A	371	PX4	C1-C2-N1	3.90	128.81	115.78	4	4
4	A	404	PX4	O7-C23-O8	3.90	114.27	123.70	4	8
4	A	406	PX4	P1-O3-C1	3.90	102.39	121.59	3	9
4	A	380	PX4	P1-O3-C1	3.90	102.40	121.59	4	12
4	A	380	PX4	O7-C23-O8	3.90	114.28	123.70	6	5
4	A	377	PX4	O7-C7-C8	3.90	122.51	108.40	8	4
4	A	409	PX4	P1-O3-C1	3.90	102.40	121.59	1	11
4	A	315	PX4	P1-O4-C6	3.89	98.86	121.68	5	8
4	A	364	PX4	P1-O3-C1	3.89	102.43	121.59	9	12
4	A	423	PX4	P1-O3-C1	3.89	102.44	121.59	14	10
4	A	429	PX4	O4-P1-O2	3.89	124.27	109.07	2	2
4	A	314	PX4	C12-C11-C10	3.89	99.21	113.19	10	3
4	A	418	PX4	C5-N1-C3	3.89	98.98	108.97	2	2
4	A	392	PX4	O1-P1-O2	3.89	131.46	112.24	7	4
4	A	430	PX4	C5-N1-C3	3.89	98.98	108.97	3	3
4	A	317	PX4	O5-C8-C7	3.89	119.74	108.43	14	8
4	A	382	PX4	O3-P1-O2	3.89	93.89	109.07	13	3
4	A	322	PX4	O5-C9-O6	3.88	113.79	123.59	10	3
4	A	412	PX4	C1-C2-N1	3.88	128.74	115.78	4	5
4	A	419	PX4	O1-P1-O3	3.88	89.71	107.75	2	3
4	A	356	PX4	C26-C25-C24	3.88	99.24	113.19	8	3
4	A	357	PX4	O5-C9-O6	3.88	113.80	123.59	12	9
4	A	369	PX4	O7-C23-C24	3.88	119.87	111.50	7	4
4	A	425	PX4	O7-C7-C8	3.88	122.45	108.40	1	7
4	A	311	PX4	O5-C9-O6	3.88	113.80	123.59	10	5
4	A	408	PX4	O7-C7-C8	3.88	122.45	108.40	5	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	418	PX4	P1-O4-C6	3.88	98.93	121.68	4	10
4	A	422	PX4	O5-C9-C10	3.88	124.08	111.91	8	4
4	A	324	PX4	O7-C7-C6	3.88	122.44	108.40	6	8
4	A	341	PX4	O5-C9-O6	3.88	113.81	123.59	14	4
4	A	397	PX4	C4-N1-C3	3.87	99.01	108.97	8	4
4	A	354	PX4	C4-N1-C3	3.87	99.03	108.97	2	1
4	A	429	PX4	C5-N1-C4	3.87	118.92	108.97	1	2
4	A	343	PX4	P1-O4-C6	3.87	99.01	121.68	8	8
4	A	324	PX4	P1-O4-C6	3.86	99.02	121.68	1	10
4	A	420	PX4	C1-C2-N1	3.87	128.69	115.78	6	3
4	A	323	PX4	P1-O4-C6	3.86	99.03	121.68	14	12
4	A	380	PX4	O3-P1-O2	3.86	93.98	109.07	9	4
4	A	424	PX4	P1-O4-C6	3.86	99.03	121.68	14	9
4	A	331	PX4	O3-P1-O2	3.86	93.99	109.07	4	3
4	A	372	PX4	O5-C8-C7	3.86	119.67	108.43	8	8
4	A	391	PX4	C5-N1-C4	3.86	99.05	108.97	3	3
4	A	398	PX4	C5-N1-C3	3.86	99.05	108.97	10	3
4	A	309	PX4	O5-C9-O6	3.86	113.86	123.59	14	5
4	A	391	PX4	P1-O4-C6	3.86	99.07	121.68	9	9
4	A	327	PX4	P1-O3-C1	3.85	102.62	121.59	13	12
4	A	317	PX4	P1-O3-C1	3.85	102.64	121.59	5	9
4	A	349	PX4	P1-O3-C1	3.85	102.64	121.59	9	12
4	A	400	PX4	P1-O4-C6	3.85	99.12	121.68	8	9
4	A	397	PX4	O3-P1-O2	3.84	94.05	109.07	4	4
4	A	313	PX4	P1-O3-C1	3.84	102.68	121.59	8	11
4	A	346	PX4	C4-N1-C3	3.84	99.10	108.97	7	4
4	A	357	PX4	C7-O7-C23	3.84	127.25	117.79	6	5
4	A	402	PX4	C7-O7-C23	3.84	127.25	117.79	5	4
4	A	330	PX4	O1-P1-O2	3.84	131.22	112.24	3	8
4	A	375	PX4	O7-C23-O8	3.84	114.42	123.70	8	5
4	A	408	PX4	P1-O3-C1	3.84	102.69	121.59	8	12
4	A	325	PX4	C4-N1-C3	3.84	99.11	108.97	11	4
4	A	320	PX4	P1-O3-C1	3.83	102.71	121.59	6	8
4	A	373	PX4	C11-C10-C9	3.84	99.67	113.62	10	3
4	A	338	PX4	O3-P1-O2	3.83	94.09	109.07	4	2
4	A	409	PX4	C7-O7-C23	3.83	108.35	117.79	14	6
4	A	356	PX4	O5-C9-C10	3.83	123.94	111.91	14	7
4	A	370	PX4	O7-C23-O8	3.83	114.44	123.70	9	7
4	A	417	PX4	O7-C23-O8	3.83	114.44	123.70	6	4
4	A	354	PX4	P1-O4-C6	3.83	99.22	121.68	13	8
4	A	368	PX4	O7-C7-C8	3.83	122.27	108.40	3	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	353	PX4	O7-C7-C8	3.83	122.26	108.40	6	8
4	A	363	PX4	O7-C23-C24	3.83	119.75	111.50	3	3
4	A	309	PX4	O7-C7-C6	3.83	122.25	108.40	7	4
4	A	359	PX4	O3-P1-O2	3.83	94.12	109.07	11	4
4	A	376	PX4	O5-C9-C10	3.83	123.91	111.91	8	3
4	A	369	PX4	O7-C7-C8	3.82	122.25	108.40	10	6
4	A	369	PX4	O5-C8-C7	3.82	119.56	108.43	8	4
4	A	407	PX4	O5-C9-O6	3.82	113.94	123.59	12	4
4	A	410	PX4	P1-O4-C6	3.82	99.26	121.68	7	10
4	A	428	PX4	O5-C9-O6	3.82	113.94	123.59	2	4
4	A	356	PX4	P1-O3-C1	3.82	102.77	121.59	9	8
4	A	347	PX4	O1-P1-O3	3.82	90.00	107.75	2	1
4	A	312	PX4	C12-C11-C10	3.82	99.46	113.19	2	1
4	A	315	PX4	O7-C7-C8	3.82	122.23	108.40	1	6
4	A	347	PX4	O5-C9-O6	3.82	113.96	123.59	8	3
4	A	345	PX4	O3-P1-O2	3.82	94.16	109.07	1	4
4	A	308	PX4	C25-C24-C23	3.81	99.75	113.62	13	1
4	A	314	PX4	C4-N1-C3	3.81	99.17	108.97	7	6
4	A	425	PX4	O3-P1-O2	3.81	94.19	109.07	6	3
4	A	320	PX4	O7-C23-C24	3.81	119.70	111.50	1	6
4	A	385	PX4	P1-O3-C1	3.81	102.85	121.59	9	9
4	A	380	PX4	O5-C9-C10	3.80	123.84	111.91	1	6
4	A	427	PX4	O5-C9-C10	3.80	123.85	111.91	3	3
4	A	334	PX4	P1-O3-C1	3.80	102.87	121.59	8	7
4	A	344	PX4	P1-O4-C6	3.80	99.38	121.68	9	7
4	A	403	PX4	C1-C2-N1	3.80	128.47	115.78	12	5
4	A	424	PX4	P1-O3-C1	3.80	102.88	121.59	1	10
4	A	317	PX4	O7-C23-C24	3.80	119.69	111.50	1	7
4	A	321	PX4	O7-C7-C8	3.80	122.15	108.40	3	7
4	A	330	PX4	P1-O4-C6	3.79	99.43	121.68	14	12
4	A	416	PX4	O7-C7-C6	3.80	122.14	108.40	3	7
4	A	318	PX4	C5-N1-C3	3.79	99.22	108.97	9	4
4	A	414	PX4	C1-C2-N1	3.79	128.44	115.78	11	2
4	A	423	PX4	O5-C9-C10	3.79	123.81	111.91	4	1
4	A	336	PX4	O7-C23-C24	3.79	119.67	111.50	11	5
4	A	308	PX4	C8-C7-C6	3.79	102.83	111.79	4	10
4	A	389	PX4	O7-C7-C8	3.79	122.12	108.40	10	8
4	A	337	PX4	O5-C9-O6	3.79	114.04	123.59	14	4
4	A	379	PX4	O5-C9-C10	3.78	123.79	111.91	4	4
4	A	391	PX4	O7-C7-C8	3.79	122.11	108.40	12	5
4	A	415	PX4	C7-O7-C23	3.79	127.11	117.79	14	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	416	PX4	C7-O7-C23	3.79	127.11	117.79	3	3
4	A	418	PX4	O7-C7-C8	3.79	122.11	108.40	10	6
4	A	383	PX4	O7-C7-C8	3.78	122.10	108.40	8	5
4	A	352	PX4	O7-C23-C24	3.78	119.65	111.50	13	8
4	A	306	PX4	C7-O7-C23	3.78	127.10	117.79	13	4
4	A	351	PX4	P1-O3-C1	3.78	102.97	121.59	5	8
4	A	357	PX4	P1-O3-C1	3.78	102.97	121.59	8	8
4	A	353	PX4	O7-C23-O8	3.78	114.58	123.70	4	3
4	A	334	PX4	O7-C23-C24	3.78	119.64	111.50	11	7
4	A	390	PX4	O5-C9-O6	3.77	114.07	123.59	12	2
4	A	317	PX4	C5-N1-C3	3.77	118.68	108.97	14	5
4	A	395	PX4	C5-N1-C4	3.77	99.29	108.97	6	2
4	A	386	PX4	O3-P1-O2	3.77	94.35	109.07	10	3
4	A	326	PX4	P1-O4-C6	3.76	99.61	121.68	9	10
4	A	331	PX4	C4-N1-C3	3.76	99.30	108.97	11	3
4	A	314	PX4	O7-C23-C24	3.76	103.39	111.50	10	7
4	A	336	PX4	P1-O3-C1	3.76	103.07	121.59	6	9
4	A	364	PX4	P1-O4-C6	3.76	99.63	121.68	12	7
4	A	369	PX4	C7-O7-C23	3.76	108.53	117.79	1	3
4	A	347	PX4	O1-P1-O2	3.76	130.82	112.24	2	9
4	A	309	PX4	O1-P1-O2	3.76	130.81	112.24	11	7
4	A	310	PX4	C7-O7-C23	3.76	127.04	117.79	4	4
4	A	359	PX4	P1-O4-C6	3.76	99.66	121.68	9	8
4	A	373	PX4	O1-P1-O3	3.76	90.30	107.75	3	3
4	A	368	PX4	O1-P1-O4	3.75	125.18	107.75	11	1
4	A	329	PX4	P1-O4-C6	3.75	99.69	121.68	6	8
4	A	378	PX4	O5-C9-C10	3.75	123.68	111.91	6	1
4	A	347	PX4	O3-P1-O2	3.75	94.42	109.07	2	5
4	A	385	PX4	C8-O5-C9	3.75	103.24	117.12	7	1
4	A	321	PX4	C11-C10-C9	3.74	100.00	113.62	12	1
4	A	327	PX4	O7-C7-C6	3.75	121.96	108.40	14	4
4	A	337	PX4	P1-O3-C1	3.74	103.18	121.59	10	11
4	A	346	PX4	C7-O7-C23	3.74	127.00	117.79	9	4
4	A	401	PX4	C1-C2-N1	3.74	128.27	115.78	4	3
4	A	317	PX4	C4-N1-C3	3.74	99.37	108.97	4	6
4	A	338	PX4	O7-C7-C8	3.74	121.93	108.40	4	7
4	A	343	PX4	C8-C7-C6	3.74	102.95	111.79	9	9
4	A	393	PX4	C5-N1-C3	3.74	118.58	108.97	2	8
4	A	306	PX4	O5-C9-O6	3.73	114.17	123.59	7	5
4	A	370	PX4	O5-C9-C10	3.73	123.62	111.91	3	3
4	A	393	PX4	O7-C23-O8	3.73	114.69	123.70	2	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	310	PX4	C5-N1-C3	3.73	99.39	108.97	13	5
4	A	331	PX4	O7-C7-C8	3.73	121.89	108.40	13	7
4	A	368	PX4	P1-O3-C1	3.73	103.24	121.59	4	9
4	A	351	PX4	O1-P1-O2	3.72	130.65	112.24	10	9
4	A	359	PX4	O7-C7-C6	3.72	121.89	108.40	4	8
4	A	418	PX4	P1-O3-C1	3.73	103.25	121.59	3	9
4	A	407	PX4	O5-C8-C7	3.72	119.27	108.43	1	9
4	A	369	PX4	C26-C25-C24	3.72	99.81	113.19	5	4
4	A	404	PX4	O1-P1-O3	3.72	90.46	107.75	13	1
4	A	391	PX4	O5-C8-C7	3.72	119.26	108.43	1	10
4	A	341	PX4	C5-N1-C4	3.72	99.42	108.97	1	3
4	A	394	PX4	O5-C9-C10	3.72	123.58	111.91	3	6
4	A	332	PX4	O7-C23-O8	3.72	114.72	123.70	1	5
4	A	344	PX4	C13-C12-C11	3.72	95.56	114.42	7	3
4	A	423	PX4	O7-C23-O8	3.72	114.72	123.70	9	4
4	A	330	PX4	O7-C7-C8	3.72	121.85	108.40	9	8
4	A	365	PX4	C5-N1-C4	3.71	99.42	108.97	3	4
4	A	370	PX4	C5-N1-C4	3.71	118.52	108.97	11	2
4	A	388	PX4	O3-P1-O2	3.71	94.58	109.07	5	2
4	A	394	PX4	O1-P1-O2	3.71	130.58	112.24	5	12
4	A	415	PX4	O7-C7-C8	3.71	121.83	108.40	4	5
4	A	321	PX4	O7-C23-C24	3.71	119.49	111.50	4	10
4	A	395	PX4	O5-C9-O6	3.71	114.23	123.59	1	3
4	A	426	PX4	C7-O7-C23	3.71	126.92	117.79	5	11
4	A	357	PX4	C25-C24-C23	3.71	127.10	113.62	8	3
4	A	359	PX4	O7-C23-O8	3.71	114.75	123.70	7	7
4	A	315	PX4	P1-O3-C1	3.70	103.35	121.59	2	10
4	A	379	PX4	C1-C2-N1	3.70	128.14	115.78	4	2
4	A	383	PX4	O1-P1-O2	3.70	130.55	112.24	3	8
4	A	349	PX4	P1-O4-C6	3.70	99.97	121.68	11	10
4	A	321	PX4	P1-O3-C1	3.70	103.38	121.59	14	12
4	A	367	PX4	C5-N1-C2	3.70	94.78	109.92	10	2
4	A	392	PX4	C4-N1-C3	3.70	99.47	108.97	10	5
4	A	339	PX4	C27-C26-C25	3.70	95.66	114.42	5	2
4	A	429	PX4	O1-P1-O4	3.70	124.91	107.75	13	4
4	A	393	PX4	O7-C7-C6	3.70	121.78	108.40	9	7
4	A	325	PX4	O5-C9-C10	3.69	123.50	111.91	9	4
4	A	336	PX4	C26-C25-C24	3.69	99.91	113.19	10	4
4	A	371	PX4	O7-C7-C8	3.69	121.77	108.40	9	9
4	A	330	PX4	O7-C7-C6	3.69	121.76	108.40	13	3
4	A	362	PX4	C5-N1-C4	3.69	99.49	108.97	14	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	396	PX4	O5-C9-C10	3.69	123.48	111.91	7	1
4	A	391	PX4	O5-C9-O6	3.69	114.29	123.59	10	3
4	A	407	PX4	P1-O3-C1	3.69	103.44	121.59	10	10
4	A	425	PX4	O1-P1-O2	3.69	130.47	112.24	1	10
4	A	330	PX4	C15-C14-C13	3.68	95.72	114.42	13	1
4	A	386	PX4	C8-C7-C6	3.68	103.08	111.79	9	8
4	A	389	PX4	O7-C23-O8	3.68	114.80	123.70	11	7
4	A	405	PX4	O1-P1-O3	3.68	90.63	107.75	9	2
4	A	409	PX4	P1-O4-C6	3.68	100.09	121.68	14	11
4	A	409	PX4	C5-N1-C3	3.68	99.51	108.97	6	4
4	A	372	PX4	C19-C18-C17	3.68	95.74	114.42	5	1
4	A	379	PX4	O7-C7-C8	3.68	121.72	108.40	7	6
4	A	349	PX4	O1-P1-O2	3.68	130.41	112.24	11	8
4	A	367	PX4	O7-C7-C6	3.68	121.71	108.40	9	5
4	A	385	PX4	O1-P1-O2	3.68	130.41	112.24	10	7
4	A	389	PX4	O5-C9-O6	3.68	114.31	123.59	7	5
4	A	314	PX4	O5-C9-O6	3.67	114.32	123.59	6	3
4	A	358	PX4	O1-P1-O2	3.67	130.41	112.24	8	9
4	A	392	PX4	C5-N1-C3	3.68	118.42	108.97	9	4
4	A	382	PX4	O7-C23-O8	3.67	114.82	123.70	13	6
4	A	422	PX4	O7-C7-C8	3.67	121.70	108.40	14	4
4	A	423	PX4	O7-C7-C8	3.67	121.70	108.40	3	5
4	A	354	PX4	O7-C23-O8	3.67	114.83	123.70	6	6
4	A	332	PX4	P1-O3-C1	3.67	103.52	121.59	7	11
4	A	314	PX4	O7-C7-C6	3.67	121.69	108.40	12	5
4	A	349	PX4	O7-C23-O8	3.67	114.83	123.70	8	4
4	A	322	PX4	O7-C23-O8	3.67	114.84	123.70	1	4
4	A	395	PX4	O7-C7-C8	3.67	121.68	108.40	7	8
4	A	348	PX4	O5-C9-O6	3.66	114.34	123.59	14	7
4	A	361	PX4	C5-N1-C3	3.66	99.55	108.97	11	4
4	A	327	PX4	O3-P1-O2	3.66	94.76	109.07	12	7
4	A	340	PX4	P1-O3-C1	3.66	103.56	121.59	9	12
4	A	323	PX4	C7-O7-C23	3.66	126.80	117.79	10	5
4	A	398	PX4	C8-C7-C6	3.66	103.13	111.79	13	6
4	A	417	PX4	O1-P1-O2	3.66	130.34	112.24	9	6
4	A	345	PX4	O5-C9-O6	3.66	114.36	123.59	7	2
4	A	352	PX4	P1-O3-C1	3.66	103.59	121.59	10	7
4	A	357	PX4	C5-N1-C3	3.66	99.57	108.97	4	4
4	A	321	PX4	C8-O5-C9	3.66	103.58	117.12	12	1
4	A	336	PX4	C5-N1-C3	3.66	99.58	108.97	11	5
4	A	382	PX4	P1-O3-C1	3.65	103.60	121.59	6	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	392	PX4	O7-C7-C6	3.65	121.64	108.40	1	7
4	A	423	PX4	C8-C7-C6	3.66	103.14	111.79	8	8
4	A	390	PX4	P1-O3-C1	3.65	103.60	121.59	11	10
4	A	345	PX4	P1-O3-C1	3.65	103.62	121.59	8	11
4	A	371	PX4	C5-N1-C3	3.65	99.59	108.97	12	4
4	A	306	PX4	C5-N1-C4	3.65	118.35	108.97	3	3
4	A	327	PX4	O5-C9-O6	3.65	114.38	123.59	10	5
4	A	323	PX4	C4-N1-C2	3.64	95.00	109.92	8	3
4	A	345	PX4	P1-O4-C6	3.64	100.31	121.68	14	8
4	A	419	PX4	O5-C8-C7	3.64	119.04	108.43	13	7
4	A	419	PX4	O5-C9-C10	3.64	123.34	111.91	5	4
4	A	358	PX4	P1-O4-C6	3.64	100.33	121.68	7	11
4	A	314	PX4	C32-C31-C30	3.64	95.95	114.42	10	2
4	A	320	PX4	C1-C2-N1	3.64	127.93	115.78	2	2
4	A	340	PX4	C25-C24-C23	3.64	100.39	113.62	7	4
4	A	348	PX4	P1-O3-C1	3.64	103.68	121.59	11	11
4	A	367	PX4	P1-O4-C6	3.64	100.34	121.68	7	6
4	A	342	PX4	O7-C23-O8	3.64	114.91	123.70	7	7
4	A	390	PX4	C5-N1-C3	3.64	99.63	108.97	2	5
4	A	369	PX4	O7-C23-O8	3.63	114.92	123.70	7	3
4	A	380	PX4	C17-C16-C15	3.63	95.99	114.42	2	2
4	A	374	PX4	P1-O4-C6	3.63	100.39	121.68	13	11
4	A	430	PX4	O7-C7-C8	3.63	121.53	108.40	8	6
4	A	335	PX4	O4-P1-O2	3.62	123.23	109.07	9	3
4	A	348	PX4	O3-P1-O2	3.62	94.91	109.07	12	2
4	A	354	PX4	C1-C2-N1	3.62	127.88	115.78	9	1
4	A	346	PX4	O1-P1-O2	3.62	130.14	112.24	12	5
4	A	335	PX4	P1-O4-C6	3.62	100.45	121.68	6	5
4	A	374	PX4	O7-C23-C24	3.62	119.30	111.50	6	6
4	A	422	PX4	O5-C9-O6	3.62	114.46	123.59	5	6
4	A	334	PX4	O3-P1-O2	3.62	94.94	109.07	8	5
4	A	427	PX4	C5-N1-C3	3.62	99.68	108.97	2	3
4	A	428	PX4	O7-C23-C24	3.62	119.30	111.50	12	8
4	A	329	PX4	O5-C9-C10	3.61	123.25	111.91	8	2
4	A	360	PX4	O7-C7-C6	3.61	121.49	108.40	10	4
4	A	362	PX4	O7-C23-C24	3.61	119.28	111.50	13	7
4	A	401	PX4	P1-O4-C6	3.61	100.50	121.68	13	11
4	A	356	PX4	C5-N1-C3	3.61	99.69	108.97	13	4
4	A	361	PX4	O7-C7-C8	3.61	121.47	108.40	4	6
4	A	362	PX4	C4-N1-C3	3.61	118.25	108.97	11	3
4	A	410	PX4	C5-N1-C3	3.61	99.70	108.97	10	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	423	PX4	O7-C23-C24	3.61	119.28	111.50	2	5
4	A	357	PX4	P1-O4-C6	3.61	100.53	121.68	14	9
4	A	409	PX4	O7-C23-O8	3.61	114.98	123.70	8	4
4	A	429	PX4	C25-C24-C23	3.61	100.50	113.62	11	1
4	A	336	PX4	O7-C23-O8	3.61	114.99	123.70	3	4
4	A	351	PX4	C26-C25-C24	3.61	100.23	113.19	11	2
4	A	374	PX4	C1-C2-N1	3.61	127.82	115.78	13	6
4	A	376	PX4	C13-C12-C11	3.60	96.12	114.42	11	3
4	A	403	PX4	P1-O3-C1	3.60	103.86	121.59	14	9
4	A	363	PX4	P1-O4-C6	3.60	100.56	121.68	11	9
4	A	346	PX4	C8-O5-C9	3.60	130.45	117.12	2	2
4	A	396	PX4	O1-P1-O2	3.60	130.03	112.24	3	6
4	A	427	PX4	O3-P1-O2	3.60	95.00	109.07	9	5
4	A	400	PX4	C8-O5-C9	3.60	103.80	117.12	9	3
4	A	408	PX4	O1-P1-O2	3.59	130.01	112.24	3	8
4	A	390	PX4	O4-P1-O2	3.59	123.11	109.07	5	4
4	A	416	PX4	C4-N1-C3	3.59	99.73	108.97	10	5
4	A	307	PX4	O1-P1-O2	3.59	130.00	112.24	10	7
4	A	325	PX4	P1-O4-C6	3.59	100.62	121.68	12	10
4	A	356	PX4	C5-N1-C4	3.59	99.74	108.97	10	5
4	A	331	PX4	O1-P1-O2	3.59	129.98	112.24	1	6
4	A	357	PX4	C5-N1-C4	3.59	99.75	108.97	5	5
4	A	393	PX4	P1-O4-C6	3.59	100.63	121.68	3	9
4	A	325	PX4	O1-P1-O4	3.59	124.41	107.75	5	4
4	A	415	PX4	C5-N1-C2	3.59	95.24	109.92	3	2
4	A	381	PX4	C25-C24-C23	3.59	100.58	113.62	1	2
4	A	326	PX4	C5-N1-C4	3.59	118.19	108.97	11	2
4	A	391	PX4	C4-N1-C3	3.58	99.76	108.97	9	3
4	A	326	PX4	O1-P1-O2	3.58	129.95	112.24	2	11
4	A	369	PX4	O1-P1-O2	3.58	129.96	112.24	7	7
4	A	402	PX4	O7-C23-O8	3.58	115.04	123.70	9	4
4	A	357	PX4	O1-P1-O3	3.58	91.12	107.75	2	2
4	A	405	PX4	O5-C9-O6	3.58	114.56	123.59	12	6
4	A	429	PX4	O1-P1-O3	3.58	91.12	107.75	2	5
4	A	324	PX4	O7-C23-C24	3.58	119.21	111.50	9	5
4	A	343	PX4	O5-C9-C10	3.58	123.14	111.91	5	3
4	A	395	PX4	O7-C7-C6	3.58	121.36	108.40	2	5
4	A	307	PX4	O7-C7-C8	3.58	121.35	108.40	9	3
4	A	331	PX4	C26-C25-C24	3.58	100.33	113.19	2	3
4	A	366	PX4	O5-C9-C10	3.58	123.13	111.91	1	3
4	A	387	PX4	C7-O7-C23	3.58	126.60	117.79	5	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	418	PX4	O1-P1-O2	3.58	129.93	112.24	14	6
4	A	325	PX4	O5-C9-O6	3.58	114.57	123.59	4	3
4	A	324	PX4	O7-C7-C8	3.57	121.34	108.40	9	5
4	A	382	PX4	P1-O4-C6	3.57	100.74	121.68	13	10
4	A	372	PX4	P1-O4-C6	3.57	100.75	121.68	7	10
4	A	419	PX4	O7-C7-C8	3.57	95.48	108.40	3	6
4	A	329	PX4	C5-N1-C4	3.57	118.15	108.97	2	2
4	A	393	PX4	C7-O7-C23	3.57	126.57	117.79	5	2
4	A	323	PX4	O7-C23-O8	3.56	115.09	123.70	8	4
4	A	328	PX4	P1-O4-C6	3.56	100.78	121.68	14	11
4	A	376	PX4	O1-P1-O2	3.57	129.87	112.24	11	9
4	A	386	PX4	O5-C9-C10	3.56	123.09	111.91	5	6
4	A	410	PX4	O5-C9-C10	3.56	123.09	111.91	7	3
4	A	318	PX4	O7-C7-C6	3.56	121.30	108.40	4	7
4	A	349	PX4	O5-C9-O6	3.56	114.60	123.59	12	5
4	A	315	PX4	C5-N1-C4	3.56	99.82	108.97	6	4
4	A	321	PX4	C1-C2-N1	3.56	127.66	115.78	4	3
4	A	349	PX4	O5-C9-C10	3.56	123.08	111.91	8	2
4	A	330	PX4	C33-C32-C31	3.56	96.37	114.42	3	3
4	A	396	PX4	C7-O7-C23	3.56	126.55	117.79	10	4
4	A	312	PX4	O4-P1-O2	3.55	122.95	109.07	14	2
4	A	361	PX4	P1-O3-C1	3.55	104.09	121.59	4	12
4	A	427	PX4	P1-O4-C6	3.56	100.83	121.68	1	9
4	A	380	PX4	O7-C7-C8	3.55	121.27	108.40	13	9
4	A	338	PX4	C26-C25-C24	3.55	100.42	113.19	4	6
4	A	360	PX4	C5-N1-C4	3.55	99.84	108.97	11	3
4	A	360	PX4	C26-C25-C24	3.55	100.43	113.19	12	2
4	A	325	PX4	C13-C12-C11	3.55	96.41	114.42	12	2
4	A	336	PX4	P1-O4-C6	3.55	100.87	121.68	8	9
4	A	318	PX4	O7-C23-C24	3.55	119.14	111.50	2	6
4	A	372	PX4	C4-N1-C3	3.55	99.86	108.97	2	3
4	A	404	PX4	C5-N1-C3	3.55	99.86	108.97	14	5
4	A	419	PX4	O3-P1-O2	3.55	95.21	109.07	1	7
4	A	309	PX4	C8-C7-C6	3.54	103.41	111.79	2	6
4	A	374	PX4	O7-C7-C6	3.54	121.23	108.40	6	5
4	A	395	PX4	C4-N1-C3	3.54	99.87	108.97	7	1
4	A	311	PX4	P1-O3-C1	3.54	104.16	121.59	11	9
4	A	323	PX4	O5-C9-O6	3.54	114.66	123.59	9	3
4	A	340	PX4	C5-N1-C3	3.54	99.88	108.97	4	2
4	A	415	PX4	P1-O4-C6	3.54	100.93	121.68	9	10
4	A	343	PX4	O1-P1-O3	3.54	91.32	107.75	14	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	399	PX4	C5-N1-C3	3.54	118.06	108.97	3	2
4	A	308	PX4	O7-C7-C6	3.53	121.18	108.40	3	6
4	A	333	PX4	C5-N1-C3	3.53	99.90	108.97	13	5
4	A	414	PX4	C7-O7-C23	3.53	126.48	117.79	6	4
4	A	415	PX4	O3-P1-O2	3.53	95.27	109.07	9	4
4	A	427	PX4	C4-N1-C2	3.53	95.47	109.92	5	3
4	A	336	PX4	C5-N1-C4	3.53	99.90	108.97	7	8
4	A	407	PX4	O7-C7-C6	3.53	121.17	108.40	11	3
4	A	380	PX4	O7-C7-C6	3.52	121.16	108.40	7	3
4	A	334	PX4	O7-C7-C6	3.52	121.16	108.40	10	8
4	A	307	PX4	C12-C11-C10	3.52	100.53	113.19	9	3
4	A	378	PX4	C31-C30-C29	3.52	96.54	114.42	9	1
4	A	352	PX4	O1-P1-O2	3.52	129.65	112.24	3	10
4	A	379	PX4	O5-C9-O6	3.52	114.70	123.59	1	5
4	A	365	PX4	O3-P1-O2	3.52	95.32	109.07	9	2
4	A	403	PX4	O5-C9-C10	3.52	122.94	111.91	10	4
4	A	415	PX4	O1-P1-O3	3.52	91.41	107.75	1	2
4	A	429	PX4	O5-C9-C10	3.52	122.95	111.91	13	3
4	A	340	PX4	O7-C7-C6	3.51	121.13	108.40	5	10
4	A	322	PX4	O7-C7-C8	3.51	121.12	108.40	8	5
4	A	324	PX4	O5-C9-C10	3.51	122.92	111.91	13	3
4	A	377	PX4	C5-N1-C3	3.51	99.95	108.97	11	5
4	A	332	PX4	C13-C12-C11	3.51	96.61	114.42	6	1
4	A	368	PX4	C1-C2-N1	3.51	127.50	115.78	5	5
4	A	321	PX4	O1-P1-O2	3.51	129.58	112.24	10	6
4	A	342	PX4	O1-P1-O2	3.51	129.57	112.24	4	9
4	A	312	PX4	C4-N1-C3	3.50	117.98	108.97	4	2
4	A	395	PX4	P1-O3-C1	3.50	104.34	121.59	12	13
4	A	422	PX4	P1-O4-C6	3.50	101.14	121.68	10	7
4	A	429	PX4	P1-O4-C6	3.50	101.14	121.68	8	9
4	A	319	PX4	O7-C7-C8	3.50	121.08	108.40	6	6
4	A	325	PX4	P1-O3-C1	3.50	104.35	121.59	11	6
4	A	379	PX4	C8-C7-C6	3.50	103.51	111.79	1	7
4	A	369	PX4	C4-N1-C3	3.50	117.97	108.97	5	2
4	A	415	PX4	C12-C11-C10	3.50	100.61	113.19	6	5
4	A	396	PX4	O1-P1-O3	3.50	124.00	107.75	12	4
4	A	430	PX4	O3-P1-O2	3.50	95.39	109.07	7	6
4	A	412	PX4	O5-C9-O6	3.50	114.76	123.59	3	5
4	A	336	PX4	C12-C11-C10	3.50	100.62	113.19	10	1
4	A	340	PX4	C11-C10-C9	3.50	100.91	113.62	6	2
4	A	344	PX4	O3-P1-O2	3.50	95.40	109.07	12	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	343	PX4	C4-N1-C3	3.50	117.96	108.97	7	4
4	A	343	PX4	C7-O7-C23	3.50	109.18	117.79	8	6
4	A	424	PX4	O7-C7-C8	3.50	121.06	108.40	1	3
4	A	413	PX4	C5-N1-C4	3.49	99.99	108.97	4	4
4	A	391	PX4	O1-P1-O2	3.49	129.51	112.24	4	8
4	A	409	PX4	C25-C24-C23	3.49	100.92	113.62	8	3
4	A	383	PX4	C11-C10-C9	3.49	100.93	113.62	5	3
4	A	371	PX4	O1-P1-O2	3.49	129.48	112.24	4	10
4	A	415	PX4	C19-C18-C17	3.49	96.73	114.42	6	1
4	A	343	PX4	C1-C2-N1	3.48	127.41	115.78	4	6
4	A	366	PX4	C4-N1-C3	3.48	100.02	108.97	11	2
4	A	349	PX4	O1-P1-O3	3.48	91.58	107.75	14	2
4	A	366	PX4	P1-O4-C6	3.48	101.27	121.68	3	12
4	A	404	PX4	O7-C23-C24	3.48	119.00	111.50	13	9
4	A	426	PX4	O7-C7-C8	3.48	121.00	108.40	6	8
4	A	376	PX4	C5-N1-C3	3.48	100.03	108.97	1	3
4	A	402	PX4	P1-O4-C6	3.48	101.29	121.68	4	7
4	A	397	PX4	P1-O4-C6	3.48	101.30	121.68	13	8
4	A	322	PX4	O3-P1-O2	3.47	95.49	109.07	2	4
4	A	406	PX4	O1-P1-O2	3.47	129.41	112.24	3	7
4	A	426	PX4	O4-P1-O2	3.47	122.64	109.07	11	1
4	A	325	PX4	O7-C7-C6	3.47	120.98	108.40	13	5
4	A	346	PX4	C5-N1-C4	3.47	100.05	108.97	5	4
4	A	360	PX4	O7-C23-O8	3.47	115.31	123.70	14	4
4	A	329	PX4	O3-P1-O2	3.47	95.51	109.07	9	3
4	A	360	PX4	C1-C2-N1	3.47	127.37	115.78	7	4
4	A	411	PX4	C12-C11-C10	3.47	100.71	113.19	10	1
4	A	344	PX4	O5-C9-O6	3.47	114.83	123.59	5	3
4	A	342	PX4	P1-O4-C6	3.47	101.35	121.68	11	9
4	A	343	PX4	O1-P1-O2	3.47	129.38	112.24	6	7
4	A	381	PX4	O5-C9-O6	3.47	114.84	123.59	3	7
4	A	342	PX4	O7-C7-C6	3.47	120.95	108.40	7	6
4	A	395	PX4	O4-P1-O2	3.47	122.61	109.07	7	2
4	A	425	PX4	C5-N1-C3	3.47	100.06	108.97	4	3
4	A	342	PX4	C26-C25-C24	3.46	100.73	113.19	8	1
4	A	332	PX4	C1-C2-N1	3.46	127.34	115.78	8	5
4	A	370	PX4	P1-O4-C6	3.46	101.38	121.68	12	8
4	A	344	PX4	O7-C7-C6	3.46	120.93	108.40	5	4
4	A	374	PX4	C7-O7-C23	3.46	126.31	117.79	3	7
4	A	406	PX4	O7-C7-C6	3.46	120.93	108.40	8	5
4	A	381	PX4	O7-C23-O8	3.46	115.34	123.70	13	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	418	PX4	O3-P1-O2	3.46	95.56	109.07	10	5
4	A	357	PX4	C8-C7-C6	3.46	103.61	111.79	13	7
4	A	398	PX4	O5-C9-C10	3.46	122.75	111.91	7	3
4	A	337	PX4	P1-O4-C6	3.45	101.44	121.68	2	6
4	A	373	PX4	C7-O7-C23	3.45	126.29	117.79	6	2
4	A	312	PX4	O7-C23-O8	3.45	115.36	123.70	13	1
4	A	334	PX4	C4-N1-C3	3.45	100.11	108.97	2	4
4	A	341	PX4	C25-C24-C23	3.45	126.16	113.62	12	3
4	A	308	PX4	C5-N1-C3	3.45	100.11	108.97	3	6
4	A	343	PX4	O7-C7-C8	3.45	120.88	108.40	2	2
4	A	348	PX4	C30-C29-C28	3.45	96.93	114.42	11	1
4	A	385	PX4	C4-N1-C3	3.45	100.11	108.97	4	4
4	A	389	PX4	P1-O4-C6	3.45	101.47	121.68	7	9
4	A	411	PX4	P1-O4-C6	3.45	101.47	121.68	9	12
4	A	401	PX4	C7-O7-C23	3.45	109.31	117.79	8	1
4	A	405	PX4	O7-C7-C6	3.45	120.88	108.40	7	5
4	A	405	PX4	C7-O7-C23	3.45	126.28	117.79	14	4
4	A	332	PX4	O1-P1-O2	3.44	129.27	112.24	14	6
4	A	429	PX4	C27-C26-C25	3.45	96.94	114.42	1	3
4	A	373	PX4	O5-C9-C10	3.44	122.71	111.91	13	4
4	A	386	PX4	O5-C9-O6	3.44	114.90	123.59	5	3
4	A	393	PX4	O5-C9-O6	3.44	114.90	123.59	1	5
4	A	405	PX4	O7-C23-C24	3.44	118.92	111.50	5	11
4	A	413	PX4	C5-N1-C3	3.44	100.12	108.97	6	3
4	A	392	PX4	C5-N1-C4	3.44	117.82	108.97	5	6
4	A	429	PX4	O3-P1-O2	3.44	95.61	109.07	8	6
4	A	309	PX4	C1-C2-N1	3.44	127.27	115.78	11	1
4	A	314	PX4	P1-O4-C6	3.44	101.50	121.68	3	10
4	A	355	PX4	O7-C7-C8	3.44	120.86	108.40	3	7
4	A	340	PX4	O7-C23-O8	3.44	115.39	123.70	12	4
4	A	361	PX4	C4-N1-C3	3.44	100.13	108.97	4	3
4	A	323	PX4	O7-C7-C8	3.44	120.85	108.40	10	3
4	A	321	PX4	O3-P1-O2	3.44	95.64	109.07	6	4
4	A	340	PX4	C15-C14-C13	3.44	96.98	114.42	13	1
4	A	414	PX4	P1-O4-C6	3.44	101.53	121.68	3	11
4	A	330	PX4	C7-O7-C23	3.43	126.25	117.79	11	5
4	A	355	PX4	C5-N1-C3	3.43	100.14	108.97	14	3
4	A	335	PX4	C12-C11-C10	3.43	100.86	113.19	6	4
4	A	339	PX4	O1-P1-O2	3.43	129.21	112.24	12	7
4	A	313	PX4	O7-C7-C6	3.43	120.82	108.40	7	5
4	A	348	PX4	P1-O4-C6	3.43	101.57	121.68	10	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	371	PX4	O5-C9-C10	3.43	122.67	111.91	12	5
4	A	379	PX4	P1-O4-C6	3.43	101.57	121.68	12	11
4	A	339	PX4	O7-C7-C6	3.43	120.81	108.40	9	6
4	A	360	PX4	P1-O4-C6	3.43	101.58	121.68	6	8
4	A	313	PX4	P1-O4-C6	3.43	101.59	121.68	12	6
4	A	350	PX4	C20-C19-C18	3.43	97.03	114.42	14	3
4	A	322	PX4	O1-P1-O3	3.42	91.84	107.75	2	3
4	A	332	PX4	O5-C8-C7	3.42	118.40	108.43	4	6
4	A	367	PX4	C26-C25-C24	3.43	100.88	113.19	10	2
4	A	340	PX4	O5-C9-O6	3.42	114.95	123.59	3	3
4	A	396	PX4	C1-C2-N1	3.42	127.21	115.78	7	3
4	A	409	PX4	O1-P1-O4	3.42	123.63	107.75	3	2
4	A	319	PX4	O7-C23-O8	3.42	115.44	123.70	1	4
4	A	329	PX4	C5-N1-C3	3.42	100.19	108.97	6	4
4	A	348	PX4	C5-N1-C3	3.42	100.19	108.97	5	3
4	A	369	PX4	C3-N1-C2	3.42	123.90	109.92	11	4
4	A	427	PX4	C1-C2-N1	3.42	127.19	115.78	8	7
4	A	342	PX4	O3-P1-O2	3.42	95.72	109.07	4	3
4	A	352	PX4	O5-C9-C10	3.42	122.63	111.91	12	5
4	A	313	PX4	C4-N1-C3	3.42	100.19	108.97	3	3
4	A	361	PX4	P1-O4-C6	3.42	101.65	121.68	9	6
4	A	363	PX4	O7-C7-C6	3.41	120.77	108.40	9	5
4	A	326	PX4	O3-P1-O2	3.41	95.73	109.07	12	2
4	A	363	PX4	C12-C11-C10	3.41	100.92	113.19	3	5
4	A	422	PX4	O3-P1-O2	3.41	95.73	109.07	10	3
4	A	333	PX4	O3-P1-O2	3.41	95.74	109.07	8	4
4	A	312	PX4	C5-N1-C3	3.41	100.21	108.97	11	2
4	A	326	PX4	C12-C11-C10	3.41	100.93	113.19	8	2
4	A	355	PX4	O5-C9-O6	3.41	114.98	123.59	5	4
4	A	377	PX4	O5-C9-C10	3.41	122.61	111.91	14	2
4	A	425	PX4	O5-C9-C10	3.41	122.61	111.91	9	2
4	A	352	PX4	C4-N1-C3	3.41	100.21	108.97	3	2
4	A	368	PX4	O5-C9-O6	3.41	114.99	123.59	13	3
4	A	370	PX4	P1-O3-C1	3.41	104.80	121.59	11	10
4	A	385	PX4	O5-C9-C10	3.41	122.61	111.91	10	2
4	A	354	PX4	O7-C7-C6	3.41	120.74	108.40	12	7
4	A	362	PX4	O7-C7-C8	3.41	120.74	108.40	11	9
4	A	351	PX4	O7-C23-C24	3.41	118.84	111.50	12	9
4	A	352	PX4	O7-C23-O8	3.40	115.47	123.70	5	4
4	A	394	PX4	C5-N1-C3	3.40	117.72	108.97	1	2
4	A	401	PX4	O5-C9-C10	3.40	122.59	111.91	14	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	319	PX4	O5-C9-C10	3.40	122.58	111.91	12	4
4	A	349	PX4	C5-N1-C4	3.40	117.72	108.97	6	4
4	A	345	PX4	O4-P1-O2	3.40	122.35	109.07	8	1
4	A	375	PX4	C26-C25-C24	3.40	100.97	113.19	9	3
4	A	376	PX4	C5-N1-C4	3.40	100.23	108.97	3	4
4	A	409	PX4	O1-P1-O2	3.40	129.05	112.24	13	9
4	A	307	PX4	C5-N1-C4	3.40	117.71	108.97	9	4
4	A	337	PX4	C25-C24-C23	3.40	101.27	113.62	14	2
4	A	341	PX4	P1-O4-C6	3.40	101.76	121.68	6	10
4	A	349	PX4	O7-C7-C6	3.40	120.70	108.40	7	4
4	A	375	PX4	O7-C7-C8	3.40	120.70	108.40	10	9
4	A	310	PX4	O7-C7-C6	3.39	120.69	108.40	12	6
4	A	339	PX4	O4-P1-O2	3.40	122.33	109.07	1	3
4	A	381	PX4	C19-C18-C17	3.40	97.18	114.42	5	1
4	A	364	PX4	C5-N1-C3	3.39	100.25	108.97	2	5
4	A	401	PX4	C26-C25-C24	3.39	100.99	113.19	12	2
4	A	403	PX4	O7-C7-C8	3.39	120.69	108.40	12	5
4	A	367	PX4	C14-C13-C12	3.39	97.21	114.42	11	2
4	A	394	PX4	P1-O4-C6	3.39	101.79	121.68	10	7
4	A	401	PX4	O7-C23-O8	3.39	115.50	123.70	7	3
4	A	335	PX4	C5-N1-C3	3.39	117.69	108.97	13	1
4	A	340	PX4	C1-C2-N1	3.39	127.10	115.78	5	3
4	A	341	PX4	C26-C25-C24	3.39	101.01	113.19	6	3
4	A	356	PX4	P1-O4-C6	3.39	101.80	121.68	1	2
4	A	389	PX4	C28-C27-C26	3.39	97.22	114.42	9	1
4	A	379	PX4	O7-C7-C6	3.39	120.67	108.40	13	5
4	A	383	PX4	C13-C12-C11	3.39	97.24	114.42	12	2
4	A	418	PX4	O1-P1-O4	3.39	123.47	107.75	11	1
4	A	382	PX4	O5-C9-C10	3.38	122.53	111.91	9	3
4	A	311	PX4	O1-P1-O2	3.38	128.96	112.24	13	10
4	A	319	PX4	P1-O4-C6	3.38	101.86	121.68	10	8
4	A	381	PX4	C5-N1-C3	3.38	100.28	108.97	7	5
4	A	385	PX4	O3-C1-C2	3.38	126.94	109.16	9	1
4	A	372	PX4	C4-N1-C2	3.38	96.09	109.92	10	1
4	A	428	PX4	C5-N1-C3	3.38	100.29	108.97	1	1
4	A	428	PX4	O7-C7-C6	3.38	120.63	108.40	8	2
4	A	352	PX4	O7-C7-C6	3.38	120.62	108.40	5	8
4	A	367	PX4	C1-C2-N1	3.37	127.05	115.78	8	1
4	A	378	PX4	O1-P1-O2	3.37	128.92	112.24	4	7
4	A	425	PX4	P1-O4-C6	3.37	101.89	121.68	10	10
4	A	354	PX4	O1-P1-O3	3.37	92.09	107.75	4	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	354	PX4	O7-C7-C8	3.37	120.61	108.40	4	7
4	A	361	PX4	O3-P1-O2	3.37	95.89	109.07	9	6
4	A	375	PX4	O3-P1-O2	3.37	95.89	109.07	8	3
4	A	382	PX4	O1-P1-O2	3.37	128.91	112.24	11	10
4	A	388	PX4	O1-P1-O2	3.37	128.91	112.24	11	6
4	A	415	PX4	O7-C23-C24	3.37	118.77	111.50	7	8
4	A	318	PX4	O7-C7-C8	3.37	120.60	108.40	9	3
4	A	355	PX4	O3-P1-O2	3.37	95.90	109.07	1	4
4	A	350	PX4	O7-C7-C6	3.37	120.59	108.40	12	4
4	A	363	PX4	O1-P1-O2	3.37	128.88	112.24	12	4
4	A	319	PX4	C13-C12-C11	3.36	97.35	114.42	8	1
4	A	309	PX4	C7-O7-C23	3.36	109.52	117.79	13	3
4	A	387	PX4	P1-O4-C6	3.36	101.97	121.68	12	11
4	A	424	PX4	O1-P1-O2	3.36	128.86	112.24	11	11
4	A	324	PX4	C5-N1-C4	3.36	100.33	108.97	6	2
4	A	330	PX4	P1-O3-C1	3.36	105.05	121.59	6	9
4	A	331	PX4	O5-C9-C10	3.36	122.45	111.91	12	1
4	A	335	PX4	O5-C9-O6	3.36	115.11	123.59	11	5
4	A	353	PX4	C5-N1-C4	3.36	117.61	108.97	8	1
4	A	381	PX4	O1-P1-O2	3.36	128.85	112.24	8	10
4	A	317	PX4	C18-C17-C16	3.36	97.38	114.42	10	3
4	A	332	PX4	C12-C11-C10	3.36	101.12	113.19	14	1
4	A	373	PX4	C5-N1-C3	3.36	100.34	108.97	1	2
4	A	383	PX4	O7-C23-O8	3.36	115.59	123.70	2	3
4	A	401	PX4	C5-N1-C4	3.36	100.34	108.97	5	4
4	A	306	PX4	O7-C7-C6	3.36	120.55	108.40	4	6
4	A	312	PX4	P1-O3-C1	3.36	105.07	121.59	11	5
4	A	326	PX4	C1-C2-N1	3.36	126.98	115.78	2	5
4	A	332	PX4	O5-C9-C10	3.36	122.44	111.91	13	2
4	A	389	PX4	C4-N1-C3	3.36	100.34	108.97	7	5
4	A	375	PX4	C4-N1-C3	3.35	100.35	108.97	3	3
4	A	381	PX4	P1-O4-C6	3.35	102.02	121.68	6	10
4	A	393	PX4	C12-C11-C10	3.35	101.14	113.19	7	1
4	A	309	PX4	P1-O4-C6	3.35	102.03	121.68	12	10
4	A	350	PX4	O7-C23-C24	3.35	118.71	111.50	8	6
4	A	362	PX4	C5-N1-C3	3.35	100.37	108.97	1	2
4	A	363	PX4	O7-C7-C8	3.35	120.52	108.40	7	9
4	A	369	PX4	P1-O4-C6	3.35	102.05	121.68	12	10
4	A	401	PX4	O3-P1-O2	3.35	95.98	109.07	13	4
4	A	404	PX4	C1-C2-N1	3.35	126.96	115.78	2	4
4	A	411	PX4	O1-P1-O2	3.35	128.79	112.24	14	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	311	PX4	O3-P1-O2	3.34	96.00	109.07	1	8
4	A	311	PX4	C4-N1-C2	3.35	123.60	109.92	14	2
4	A	363	PX4	C5-N1-C4	3.35	100.37	108.97	12	4
4	A	399	PX4	P1-O4-C6	3.35	102.06	121.68	12	7
4	A	328	PX4	O1-P1-O2	3.34	128.77	112.24	3	7
4	A	369	PX4	C18-C17-C16	3.34	97.45	114.42	5	2
4	A	374	PX4	O1-P1-O2	3.34	128.77	112.24	4	8
4	A	366	PX4	O7-C23-C24	3.34	118.71	111.50	6	9
4	A	430	PX4	O7-C7-C6	3.34	120.50	108.40	7	8
4	A	382	PX4	C1-C2-N1	3.34	126.93	115.78	9	3
4	A	331	PX4	O5-C9-O6	3.34	115.17	123.59	7	5
4	A	384	PX4	C5-N1-C4	3.34	117.56	108.97	10	1
4	A	391	PX4	C7-O7-C23	3.34	126.01	117.79	9	3
4	A	326	PX4	O7-C7-C6	3.34	120.48	108.40	12	3
4	A	338	PX4	O4-P1-O2	3.33	122.10	109.07	4	4
4	A	375	PX4	O1-P1-O2	3.33	128.72	112.24	2	6
4	A	391	PX4	C1-C2-N1	3.33	126.91	115.78	13	3
4	A	372	PX4	O1-P1-O2	3.33	128.71	112.24	8	7
4	A	392	PX4	O7-C23-O8	3.33	115.65	123.70	7	3
4	A	419	PX4	C4-N1-C3	3.33	100.41	108.97	13	4
4	A	417	PX4	C7-O7-C23	3.33	109.59	117.79	11	3
4	A	426	PX4	C1-C2-N1	3.33	126.90	115.78	10	3
4	A	313	PX4	O1-P1-O2	3.33	128.70	112.24	1	10
4	A	321	PX4	C26-C25-C24	3.33	101.23	113.19	10	4
4	A	430	PX4	C27-C26-C25	3.33	97.53	114.42	14	3
4	A	339	PX4	C26-C25-C24	3.33	101.24	113.19	5	4
4	A	332	PX4	C8-O5-C9	3.32	104.81	117.12	7	4
4	A	379	PX4	C29-C28-C27	3.32	97.55	114.42	13	1
4	A	408	PX4	P1-O4-C6	3.32	102.19	121.68	4	10
4	A	382	PX4	C7-O7-C23	3.32	125.97	117.79	10	4
4	A	350	PX4	O5-C9-C10	3.32	122.32	111.91	4	6
4	A	372	PX4	O1-P1-O3	3.32	92.33	107.75	8	2
4	A	323	PX4	C4-N1-C3	3.32	117.50	108.97	10	3
4	A	334	PX4	O1-P1-O2	3.32	128.63	112.24	4	10
4	A	319	PX4	O1-P1-O2	3.31	128.63	112.24	11	9
4	A	425	PX4	O5-C8-C7	3.31	118.08	108.43	11	10
4	A	361	PX4	O7-C23-O8	3.31	115.69	123.70	6	3
4	A	394	PX4	C11-C10-C9	3.31	101.57	113.62	1	2
4	A	420	PX4	C5-N1-C3	3.31	117.49	108.97	5	1
4	A	331	PX4	C5-N1-C3	3.31	100.46	108.97	13	6
4	A	312	PX4	O3-P1-O2	3.31	122.00	109.07	5	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	360	PX4	C4-N1-C3	3.31	100.46	108.97	14	5
4	A	361	PX4	C25-C24-C23	3.31	101.58	113.62	4	3
4	A	329	PX4	O1-P1-O2	3.31	128.60	112.24	2	8
4	A	375	PX4	O5-C9-C10	3.31	122.30	111.91	7	4
4	A	401	PX4	O1-P1-O3	3.31	92.37	107.75	5	3
4	A	320	PX4	C5-N1-C3	3.31	117.48	108.97	14	6
4	A	406	PX4	P1-O4-C6	3.31	102.28	121.68	7	11
4	A	420	PX4	O7-C7-C8	3.31	120.38	108.40	2	5
4	A	381	PX4	O7-C7-C6	3.31	120.37	108.40	13	4
4	A	403	PX4	P1-O4-C6	3.31	102.30	121.68	12	6
4	A	342	PX4	O7-C7-C8	3.30	120.36	108.40	8	5
4	A	371	PX4	P1-O4-C6	3.30	102.31	121.68	8	10
4	A	373	PX4	C15-C14-C13	3.30	97.66	114.42	13	1
4	A	410	PX4	O4-P1-O2	3.30	121.97	109.07	13	3
4	A	320	PX4	C5-N1-C4	3.30	100.49	108.97	7	2
4	A	352	PX4	O7-C7-C8	3.30	120.36	108.40	12	7
4	A	422	PX4	O7-C7-C6	3.30	120.36	108.40	11	3
4	A	331	PX4	C7-O7-C23	3.30	125.92	117.79	8	2
4	A	371	PX4	C19-C18-C17	3.30	97.67	114.42	4	3
4	A	423	PX4	O3-P1-O2	3.30	96.17	109.07	1	3
4	A	423	PX4	O4-P1-O2	3.30	121.96	109.07	9	1
4	A	343	PX4	O4-P1-O2	3.30	96.18	109.07	6	1
4	A	311	PX4	O7-C7-C6	3.29	120.33	108.40	2	5
4	A	339	PX4	O7-C23-O8	3.29	115.74	123.70	12	3
4	A	374	PX4	O7-C23-O8	3.30	115.74	123.70	11	3
4	A	352	PX4	C26-C25-C24	3.29	101.36	113.19	8	2
4	A	414	PX4	O5-C8-C7	3.29	118.02	108.43	3	8
4	A	347	PX4	O7-C23-O8	3.29	115.75	123.70	4	5
4	A	382	PX4	O1-P1-O4	3.29	123.03	107.75	13	1
4	A	340	PX4	P1-O4-C6	3.29	102.39	121.68	2	8
4	A	355	PX4	C4-N1-C3	3.29	117.43	108.97	5	7
4	A	387	PX4	O7-C23-O8	3.29	115.75	123.70	12	5
4	A	359	PX4	C5-N1-C4	3.29	117.43	108.97	2	4
4	A	321	PX4	O7-C23-O8	3.29	115.76	123.70	4	4
4	A	350	PX4	C7-O7-C23	3.29	125.88	117.79	1	4
4	A	368	PX4	C28-C27-C26	3.29	97.75	114.42	13	1
4	A	411	PX4	O5-C9-O6	3.29	115.30	123.59	2	3
4	A	318	PX4	C7-O7-C23	3.28	125.88	117.79	13	5
4	A	313	PX4	C5-N1-C4	3.28	100.54	108.97	7	2
4	A	322	PX4	O7-C7-C6	3.28	120.28	108.40	2	6
4	A	328	PX4	O3-P1-O2	3.28	96.24	109.07	3	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	369	PX4	O1-P1-O4	3.28	122.97	107.75	14	1
4	A	415	PX4	C32-C31-C30	3.28	97.79	114.42	7	3
4	A	427	PX4	O1-P1-O2	3.28	128.44	112.24	7	5
4	A	410	PX4	O7-C7-C6	3.28	120.26	108.40	7	4
4	A	321	PX4	O5-C9-C10	3.27	122.18	111.91	14	3
4	A	416	PX4	O7-C7-C8	3.28	120.26	108.40	9	5
4	A	420	PX4	C7-O7-C23	3.28	125.86	117.79	6	3
4	A	385	PX4	O5-C9-O6	3.27	115.33	123.59	14	5
4	A	354	PX4	C18-C17-C16	3.27	97.82	114.42	2	1
4	A	400	PX4	O5-C9-C10	3.27	122.17	111.91	12	3
4	A	427	PX4	O4-P1-O2	3.27	121.85	109.07	14	2
4	A	358	PX4	C5-N1-C3	3.27	100.57	108.97	14	3
4	A	366	PX4	O4-P1-O2	3.27	121.83	109.07	12	4
4	A	398	PX4	O5-C9-O6	3.27	115.35	123.59	10	3
4	A	420	PX4	O5-C9-C10	3.26	122.15	111.91	8	2
4	A	426	PX4	P1-O4-C6	3.27	102.53	121.68	5	7
4	A	427	PX4	O7-C7-C6	3.27	120.22	108.40	12	6
4	A	324	PX4	O3-P1-O2	3.26	96.32	109.07	12	1
4	A	358	PX4	O3-P1-O2	3.26	96.33	109.07	8	3
4	A	418	PX4	O5-C9-O6	3.26	115.36	123.59	13	5
4	A	422	PX4	C5-N1-C2	3.26	96.57	109.92	3	1
4	A	357	PX4	O5-C9-C10	3.26	122.13	111.91	3	4
4	A	411	PX4	P1-O3-C1	3.26	105.56	121.59	5	12
4	A	373	PX4	C4-N1-C3	3.25	100.61	108.97	10	4
4	A	380	PX4	O1-P1-O2	3.25	128.32	112.24	10	7
4	A	398	PX4	P1-O4-C6	3.25	102.62	121.68	3	12
4	A	403	PX4	C5-N1-C4	3.25	100.62	108.97	12	3
4	A	415	PX4	C5-N1-C3	3.25	117.33	108.97	1	4
4	A	430	PX4	O5-C9-O6	3.25	115.39	123.59	13	3
4	A	408	PX4	O5-C9-C10	3.25	122.11	111.91	3	3
4	A	307	PX4	C4-N1-C3	3.25	117.33	108.97	5	5
4	A	357	PX4	O1-P1-O2	3.25	128.30	112.24	2	8
4	A	377	PX4	O3-P1-O2	3.25	96.38	109.07	11	2
4	A	412	PX4	C30-C29-C28	3.25	97.94	114.42	14	3
4	A	376	PX4	O5-C8-C7	3.24	117.88	108.43	3	7
4	A	317	PX4	C26-C25-C24	3.24	101.54	113.19	13	3
4	A	324	PX4	O1-P1-O2	3.24	128.27	112.24	12	10
4	A	362	PX4	O7-C23-O8	3.24	115.86	123.70	4	7
4	A	329	PX4	C25-C24-C23	3.24	101.83	113.62	6	1
4	A	326	PX4	C7-O7-C23	3.24	125.76	117.79	3	3
4	A	349	PX4	C4-N1-C3	3.24	100.64	108.97	5	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	306	PX4	O1-P1-O2	3.24	128.24	112.24	3	10
4	A	420	PX4	C5-N1-C2	3.24	123.16	109.92	12	2
4	A	319	PX4	O4-P1-O2	3.24	121.71	109.07	6	3
4	A	328	PX4	O7-C23-O8	3.23	115.88	123.70	8	6
4	A	360	PX4	C8-O5-C9	3.24	105.14	117.12	8	2
4	A	368	PX4	C12-C11-C10	3.24	101.56	113.19	6	3
4	A	390	PX4	C7-O7-C23	3.24	125.76	117.79	11	4
4	A	430	PX4	C5-N1-C4	3.24	100.65	108.97	12	3
4	A	332	PX4	C5-N1-C3	3.23	117.29	108.97	3	2
4	A	307	PX4	O5-C9-O6	3.23	115.43	123.59	13	3
4	A	360	PX4	O1-P1-O2	3.23	128.23	112.24	13	6
4	A	317	PX4	P1-O4-C6	3.23	102.73	121.68	1	11
4	A	388	PX4	C28-C27-C26	3.23	98.02	114.42	7	1
4	A	401	PX4	C18-C17-C16	3.23	98.01	114.42	10	1
4	A	405	PX4	O4-P1-O2	3.23	121.70	109.07	9	3
4	A	336	PX4	C4-N1-C3	3.23	100.67	108.97	5	4
4	A	351	PX4	P1-O4-C6	3.23	102.73	121.68	1	8
4	A	404	PX4	C8-O5-C9	3.23	105.16	117.12	9	2
4	A	413	PX4	O1-P1-O2	3.23	128.22	112.24	4	7
4	A	307	PX4	C3-N1-C2	3.23	123.13	109.92	6	2
4	A	344	PX4	O4-P1-O2	3.23	121.68	109.07	10	3
4	A	365	PX4	O1-P1-O2	3.23	128.20	112.24	8	6
4	A	378	PX4	O7-C7-C8	3.23	120.09	108.40	11	4
4	A	398	PX4	O7-C7-C6	3.23	120.09	108.40	7	4
4	A	308	PX4	O1-P1-O2	3.23	128.19	112.24	8	9
4	A	336	PX4	O7-C7-C6	3.23	120.08	108.40	11	6
4	A	356	PX4	C1-C2-N1	3.23	126.55	115.78	1	5
4	A	368	PX4	O1-P1-O2	3.23	128.19	112.24	1	9
4	A	383	PX4	O1-P1-O4	3.23	122.73	107.75	11	3
4	A	392	PX4	C12-C11-C10	3.23	101.59	113.19	14	3
4	A	430	PX4	C4-N1-C3	3.23	117.27	108.97	6	4
4	A	406	PX4	O1-P1-O4	3.22	122.72	107.75	1	3
4	A	412	PX4	O7-C7-C6	3.22	120.08	108.40	1	4
4	A	308	PX4	C1-C2-N1	3.22	126.54	115.78	5	4
4	A	401	PX4	O1-P1-O2	3.22	128.17	112.24	3	9
4	A	379	PX4	C26-C25-C24	3.22	101.61	113.19	11	2
4	A	345	PX4	O7-C7-C8	3.22	120.05	108.40	7	3
4	A	363	PX4	O5-C9-O6	3.22	115.47	123.59	3	3
4	A	379	PX4	O1-P1-O2	3.22	128.15	112.24	4	8
4	A	376	PX4	C1-C2-N1	3.22	126.52	115.78	13	4
4	A	399	PX4	O7-C7-C6	3.22	120.05	108.40	4	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	403	PX4	C8-O5-C9	3.22	105.21	117.12	3	2
4	A	333	PX4	O5-C9-C10	3.22	122.00	111.91	6	6
4	A	331	PX4	O7-C7-C6	3.21	120.04	108.40	11	6
4	A	352	PX4	C5-N1-C3	3.21	100.71	108.97	12	1
4	A	412	PX4	C12-C11-C10	3.21	101.63	113.19	11	4
4	A	359	PX4	C14-C13-C12	3.21	98.11	114.42	9	1
4	A	351	PX4	O7-C7-C8	3.21	120.03	108.40	2	7
4	A	376	PX4	P1-O4-C6	3.21	102.85	121.68	14	9
4	A	306	PX4	P1-O3-C1	3.21	105.79	121.59	14	11
4	A	364	PX4	C5-N1-C4	3.21	100.72	108.97	8	3
4	A	378	PX4	C25-C24-C23	3.21	101.95	113.62	1	2
4	A	324	PX4	C14-C13-C12	3.21	98.14	114.42	5	2
4	A	412	PX4	C5-N1-C4	3.21	100.73	108.97	13	2
4	A	418	PX4	C26-C25-C24	3.21	101.66	113.19	4	3
4	A	422	PX4	O7-C23-O8	3.21	115.95	123.70	1	5
4	A	330	PX4	C27-C26-C25	3.20	98.16	114.42	9	2
4	A	362	PX4	C26-C25-C24	3.20	101.67	113.19	2	5
4	A	420	PX4	O1-P1-O4	3.20	92.87	107.75	14	1
4	A	371	PX4	O1-P1-O3	3.20	92.88	107.75	10	4
4	A	375	PX4	C28-C27-C26	3.20	98.17	114.42	11	1
4	A	430	PX4	P1-O4-C6	3.20	102.90	121.68	4	8
4	A	349	PX4	C20-C19-C18	3.20	98.17	114.42	11	1
4	A	362	PX4	P1-O4-C6	3.20	102.91	121.68	9	6
4	A	345	PX4	C5-N1-C3	3.20	100.75	108.97	10	3
4	A	352	PX4	P1-O4-C6	3.20	102.92	121.68	6	6
4	A	372	PX4	O5-C9-C10	3.20	121.95	111.91	5	7
4	A	417	PX4	P1-O3-C1	3.20	105.84	121.59	3	9
4	A	421	PX4	C1-C2-N1	3.20	126.46	115.78	12	3
4	A	335	PX4	O7-C7-C8	3.20	119.98	108.40	11	5
4	A	419	PX4	O1-P1-O2	3.20	128.05	112.24	4	11
4	A	365	PX4	P1-O4-C6	3.20	102.94	121.68	11	8
4	A	370	PX4	O7-C7-C8	3.19	119.97	108.40	2	7
4	A	381	PX4	O1-P1-O3	3.19	92.91	107.75	6	4
4	A	352	PX4	C32-C31-C30	3.19	98.21	114.42	12	1
4	A	378	PX4	O7-C7-C6	3.19	119.96	108.40	8	9
4	A	423	PX4	C26-C25-C24	3.19	101.71	113.19	3	1
4	A	308	PX4	P1-O4-C6	3.19	102.97	121.68	9	9
4	A	344	PX4	O7-C7-C8	3.19	119.96	108.40	8	6
4	A	345	PX4	C4-N1-C3	3.19	100.77	108.97	6	1
4	A	347	PX4	P1-O4-C6	3.19	102.96	121.68	4	10
4	A	387	PX4	C27-C26-C25	3.19	98.22	114.42	7	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	322	PX4	C26-C25-C24	3.19	101.72	113.19	3	7
4	A	342	PX4	O5-C9-C10	3.19	121.92	111.91	8	2
4	A	368	PX4	O7-C23-C24	3.19	118.38	111.50	7	5
4	A	391	PX4	O7-C7-C6	3.19	119.95	108.40	14	4
4	A	418	PX4	C34-C33-C32	3.19	98.23	114.42	6	2
4	A	333	PX4	C5-N1-C4	3.19	117.17	108.97	9	2
4	A	396	PX4	C5-N1-C2	3.19	96.87	109.92	3	4
4	A	398	PX4	O7-C23-O8	3.19	116.00	123.70	3	2
4	A	426	PX4	O7-C7-C6	3.19	119.94	108.40	13	6
4	A	335	PX4	C19-C18-C17	3.19	98.25	114.42	4	2
4	A	350	PX4	O7-C7-C8	3.19	119.94	108.40	8	4
4	A	312	PX4	C16-C15-C14	3.18	98.26	114.42	9	2
4	A	338	PX4	O1-P1-O2	3.18	127.97	112.24	7	8
4	A	386	PX4	C5-N1-C3	3.18	100.79	108.97	9	4
4	A	388	PX4	O7-C23-O8	3.18	116.01	123.70	12	7
4	A	368	PX4	O7-C7-C6	3.18	119.92	108.40	5	4
4	A	353	PX4	C4-N1-C3	3.18	100.80	108.97	4	5
4	A	414	PX4	C12-C11-C10	3.18	124.63	113.19	4	3
4	A	384	PX4	C4-N1-C3	3.18	100.80	108.97	10	3
4	A	418	PX4	O7-C7-C6	3.18	119.92	108.40	5	2
4	A	420	PX4	C5-N1-C4	3.18	100.80	108.97	3	5
4	A	325	PX4	C3-N1-C2	3.18	122.92	109.92	11	2
4	A	332	PX4	O1-P1-O3	3.18	92.99	107.75	13	3
4	A	367	PX4	O7-C23-O8	3.18	116.02	123.70	5	4
4	A	404	PX4	C4-N1-C3	3.18	100.81	108.97	1	6
4	A	319	PX4	C5-N1-C4	3.18	100.81	108.97	14	2
4	A	320	PX4	C7-O7-C23	3.17	125.61	117.79	11	3
4	A	358	PX4	O4-P1-O2	3.18	121.47	109.07	1	3
4	A	378	PX4	C27-C26-C25	3.17	98.31	114.42	8	1
4	A	319	PX4	O5-C9-O6	3.17	115.59	123.59	7	3
4	A	324	PX4	O7-C23-O8	3.17	116.04	123.70	7	3
4	A	333	PX4	P1-O3-C1	3.17	105.98	121.59	4	5
4	A	314	PX4	C3-N1-C2	3.17	96.95	109.92	8	2
4	A	408	PX4	O5-C9-O6	3.17	115.59	123.59	4	3
4	A	386	PX4	O7-C7-C6	3.17	119.87	108.40	5	3
4	A	417	PX4	C20-C19-C18	3.17	98.35	114.42	4	1
4	A	325	PX4	C5-N1-C3	3.17	100.83	108.97	3	2
4	A	362	PX4	C12-C11-C10	3.17	101.81	113.19	6	1
4	A	329	PX4	O5-C9-O6	3.16	115.61	123.59	10	6
4	A	331	PX4	C8-O5-C9	3.16	105.41	117.12	6	3
4	A	341	PX4	C7-O7-C23	3.16	125.58	117.79	11	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	358	PX4	C17-C16-C15	3.16	98.36	114.42	2	2
4	A	359	PX4	C29-C28-C27	3.16	98.36	114.42	8	1
4	A	313	PX4	C26-C25-C24	3.16	101.83	113.19	14	3
4	A	316	PX4	O3-P1-O2	3.16	96.71	109.07	5	4
4	A	377	PX4	O7-C23-O8	3.16	116.06	123.70	11	4
4	A	405	PX4	C5-N1-C3	3.16	117.10	108.97	8	4
4	A	413	PX4	O7-C23-O8	3.16	116.06	123.70	12	3
4	A	370	PX4	C25-C24-C23	3.16	102.14	113.62	1	2
4	A	385	PX4	O6-C9-C10	3.16	111.41	123.73	4	1
4	A	405	PX4	C5-N1-C4	3.16	117.10	108.97	3	3
4	A	315	PX4	C7-O7-C23	3.16	125.56	117.79	5	6
4	A	411	PX4	C26-C25-C24	3.16	101.84	113.19	7	3
4	A	339	PX4	C20-C19-C18	3.16	98.40	114.42	6	1
4	A	345	PX4	O1-P1-O2	3.16	127.84	112.24	13	6
4	A	346	PX4	O7-C7-C6	3.15	119.82	108.40	14	3
4	A	421	PX4	O4-P1-O2	3.15	96.74	109.07	13	2
4	A	312	PX4	P1-O4-C6	3.15	103.19	121.68	9	6
4	A	424	PX4	O5-C9-O6	3.15	115.63	123.59	1	5
4	A	402	PX4	O5-C9-C10	3.15	121.80	111.91	2	3
4	A	429	PX4	O1-P1-O2	3.15	127.82	112.24	7	8
4	A	389	PX4	O1-P1-O2	3.15	127.82	112.24	8	7
4	A	399	PX4	O7-C23-O8	3.15	116.09	123.70	10	4
4	A	383	PX4	O5-C9-O6	3.15	115.64	123.59	14	3
4	A	307	PX4	P1-O4-C6	3.15	103.23	121.68	7	7
4	A	311	PX4	O4-P1-O2	3.15	121.37	109.07	5	1
4	A	362	PX4	O5-C9-O6	3.15	115.65	123.59	5	3
4	A	415	PX4	O7-C7-C6	3.15	119.80	108.40	3	5
4	A	427	PX4	O5-C9-O6	3.15	115.65	123.59	3	8
4	A	312	PX4	C1-C2-N1	3.14	126.27	115.78	11	3
4	A	323	PX4	C8-O5-C9	3.14	105.48	117.12	3	3
4	A	360	PX4	O3-P1-O2	3.14	96.78	109.07	2	4
4	A	364	PX4	C1-C2-N1	3.14	126.27	115.78	12	4
4	A	379	PX4	O7-C23-O8	3.14	116.11	123.70	4	4
4	A	391	PX4	C31-C30-C29	3.14	98.47	114.42	9	1
4	A	320	PX4	O7-C7-C6	3.14	119.77	108.40	4	7
4	A	322	PX4	O1-P1-O2	3.14	127.76	112.24	4	8
4	A	342	PX4	C15-C14-C13	3.14	98.48	114.42	5	1
4	A	378	PX4	P1-O4-C6	3.14	103.27	121.68	3	8
4	A	381	PX4	C26-C25-C24	3.14	101.90	113.19	14	4
4	A	390	PX4	O1-P1-O3	3.14	93.16	107.75	11	3
4	A	394	PX4	C5-N1-C4	3.14	117.05	108.97	4	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	346	PX4	O7-C7-C8	3.14	119.77	108.40	10	10
4	A	414	PX4	O1-P1-O2	3.14	127.76	112.24	13	7
4	A	393	PX4	C1-C2-N1	3.14	126.26	115.78	11	3
4	A	426	PX4	C5-N1-C3	3.14	100.90	108.97	14	5
4	A	336	PX4	O5-C9-O6	3.14	115.67	123.59	5	5
4	A	351	PX4	O7-C23-O8	3.14	116.12	123.70	8	2
4	A	377	PX4	O1-P1-O2	3.14	127.75	112.24	2	4
4	A	323	PX4	C5-N1-C3	3.13	117.03	108.97	9	4
4	A	324	PX4	C5-N1-C2	3.13	97.09	109.92	5	1
4	A	328	PX4	C4-N1-C3	3.13	100.92	108.97	2	4
4	A	341	PX4	C5-N1-C3	3.13	100.91	108.97	3	3
4	A	365	PX4	C8-O5-C9	3.13	105.51	117.12	10	4
4	A	409	PX4	C26-C25-C24	3.13	101.92	113.19	11	2
4	A	329	PX4	C1-C2-N1	3.13	126.24	115.78	2	4
4	A	329	PX4	O7-C7-C8	3.13	119.75	108.40	5	5
4	A	357	PX4	O7-C7-C8	3.13	119.75	108.40	11	4
4	A	384	PX4	O4-P1-O2	3.13	96.82	109.07	4	3
4	A	385	PX4	P1-O4-C6	3.13	103.32	121.68	2	9
4	A	398	PX4	C32-C31-C30	3.13	98.53	114.42	12	2
4	A	344	PX4	O7-C23-O8	3.13	116.14	123.70	10	4
4	A	309	PX4	O7-C7-C8	3.13	119.73	108.40	8	3
4	A	411	PX4	C3-N1-C2	3.13	122.72	109.92	3	1
4	A	380	PX4	O5-C9-O6	3.13	115.70	123.59	7	2
4	A	309	PX4	C5-N1-C4	3.13	100.94	108.97	7	4
4	A	323	PX4	O5-C8-C7	3.13	117.54	108.43	12	6
4	A	367	PX4	C5-N1-C4	3.13	100.93	108.97	12	3
4	A	420	PX4	O7-C23-O8	3.13	116.14	123.70	2	3
4	A	367	PX4	O1-P1-O3	3.13	93.23	107.75	8	1
4	A	421	PX4	O1-P1-O2	3.13	127.69	112.24	14	7
4	A	360	PX4	O5-C9-C10	3.12	121.71	111.91	9	4
4	A	371	PX4	C16-C15-C14	3.12	98.57	114.42	11	1
4	A	422	PX4	C5-N1-C4	3.12	117.01	108.97	9	1
4	A	310	PX4	C1-C2-N1	3.12	126.20	115.78	1	3
4	A	354	PX4	C26-C25-C24	3.12	101.98	113.19	10	1
4	A	408	PX4	C1-C2-N1	3.12	126.20	115.78	6	4
4	A	313	PX4	O7-C7-C8	3.12	119.69	108.40	11	5
4	A	368	PX4	O5-C9-C10	3.12	121.69	111.91	6	4
4	A	420	PX4	P1-O4-C6	3.12	103.40	121.68	11	11
4	A	374	PX4	C18-C17-C16	3.12	98.60	114.42	13	3
4	A	372	PX4	C27-C26-C25	3.12	98.61	114.42	7	4
4	A	419	PX4	O4-P1-O2	3.12	121.24	109.07	3	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	425	PX4	C5-N1-C4	3.12	100.96	108.97	13	1
4	A	366	PX4	C29-C28-C27	3.11	98.62	114.42	1	5
4	A	375	PX4	C5-N1-C4	3.11	100.97	108.97	1	4
4	A	313	PX4	O8-C23-C24	3.11	111.59	123.73	6	2
4	A	334	PX4	O7-C23-O8	3.11	116.18	123.70	9	3
4	A	379	PX4	C8-O5-C9	3.11	105.59	117.12	5	3
4	A	330	PX4	C29-C28-C27	3.11	98.63	114.42	13	3
4	A	333	PX4	C1-C2-N1	3.11	126.17	115.78	1	3
4	A	354	PX4	C12-C11-C10	3.11	102.01	113.19	9	2
4	A	381	PX4	C4-N1-C2	3.11	97.19	109.92	13	5
4	A	424	PX4	C8-O5-C9	3.11	105.60	117.12	13	1
4	A	373	PX4	O5-C9-O6	3.11	115.75	123.59	6	5
4	A	339	PX4	P1-O4-C6	3.11	103.45	121.68	1	7
4	A	406	PX4	C5-N1-C2	3.11	122.64	109.92	12	2
4	A	341	PX4	O1-P1-O4	3.11	122.17	107.75	14	2
4	A	342	PX4	C20-C19-C18	3.11	98.65	114.42	4	2
4	A	412	PX4	C8-C7-C6	3.11	104.44	111.79	8	6
4	A	384	PX4	C12-C11-C10	3.11	102.03	113.19	3	1
4	A	397	PX4	C1-C2-N1	3.10	126.15	115.78	6	2
4	A	412	PX4	C7-O7-C23	3.10	125.43	117.79	1	3
4	A	413	PX4	O7-C7-C6	3.10	119.64	108.40	7	5
4	A	361	PX4	C8-O5-C9	3.10	105.64	117.12	10	1
4	A	363	PX4	O7-C23-O8	3.10	116.21	123.70	7	5
4	A	386	PX4	O3-C1-C2	3.10	125.47	109.16	8	1
4	A	398	PX4	C4-N1-C3	3.10	101.00	108.97	7	3
4	A	357	PX4	C31-C30-C29	3.10	98.70	114.42	7	1
4	A	375	PX4	O7-C7-C6	3.10	119.62	108.40	5	4
4	A	394	PX4	O7-C7-C6	3.10	119.62	108.40	14	5
4	A	307	PX4	C17-C16-C15	3.10	98.71	114.42	12	2
4	A	335	PX4	C26-C25-C24	3.10	102.06	113.19	11	2
4	A	337	PX4	C5-N1-C4	3.10	101.02	108.97	14	3
4	A	383	PX4	C5-N1-C4	3.10	101.02	108.97	13	5
4	A	409	PX4	C5-N1-C4	3.10	101.01	108.97	14	5
4	A	364	PX4	C34-C33-C32	3.09	98.72	114.42	5	1
4	A	336	PX4	C7-O7-C23	3.09	125.40	117.79	14	4
4	A	399	PX4	C34-C33-C32	3.09	98.72	114.42	3	2
4	A	325	PX4	O4-P1-O2	3.09	121.14	109.07	8	2
4	A	423	PX4	C1-C2-N1	3.09	126.10	115.78	12	3
4	A	306	PX4	O7-C23-O8	3.09	116.24	123.70	4	5
4	A	329	PX4	C4-N1-C3	3.09	101.03	108.97	13	2
4	A	385	PX4	C5-N1-C3	3.09	101.03	108.97	14	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	320	PX4	O5-C9-O6	3.09	115.80	123.59	10	5
4	A	306	PX4	O1-P1-O4	3.09	122.08	107.75	1	2
4	A	412	PX4	C5-N1-C3	3.09	116.91	108.97	10	2
4	A	413	PX4	P1-O4-C6	3.09	103.58	121.68	7	10
4	A	316	PX4	C4-N1-C3	3.08	101.04	108.97	1	2
4	A	390	PX4	C5-N1-C4	3.08	116.91	108.97	8	4
4	A	402	PX4	O3-P1-O2	3.08	97.02	109.07	6	3
4	A	318	PX4	C26-C25-C24	3.08	102.11	113.19	1	2
4	A	326	PX4	C5-N1-C3	3.08	101.05	108.97	12	3
4	A	332	PX4	C5-N1-C4	3.08	101.05	108.97	14	3
4	A	380	PX4	C33-C32-C31	3.08	98.78	114.42	5	1
4	A	340	PX4	C12-C11-C10	3.08	102.12	113.19	8	2
4	A	323	PX4	O1-P1-O2	3.08	127.45	112.24	10	5
4	A	412	PX4	O5-C9-C10	3.08	121.57	111.91	3	6
4	A	424	PX4	C5-N1-C3	3.08	101.06	108.97	6	4
4	A	326	PX4	O7-C7-C8	3.07	119.53	108.40	2	5
4	A	324	PX4	C4-N1-C3	3.07	116.87	108.97	5	3
4	A	368	PX4	C25-C24-C23	3.07	102.44	113.62	4	2
4	A	382	PX4	C19-C18-C17	3.07	98.82	114.42	3	2
4	A	424	PX4	C4-N1-C2	3.07	122.49	109.92	12	3
4	A	336	PX4	O5-C9-C10	3.07	121.54	111.91	4	2
4	A	406	PX4	C33-C32-C31	3.07	98.85	114.42	3	2
4	A	310	PX4	O1-P1-O2	3.07	127.40	112.24	2	8
4	A	316	PX4	P1-O4-C6	3.07	103.70	121.68	10	7
4	A	323	PX4	O4-P1-O2	3.07	121.05	109.07	8	1
4	A	335	PX4	C3-N1-C2	3.07	97.36	109.92	13	2
4	A	316	PX4	O4-P1-O2	3.07	121.05	109.07	4	2
4	A	378	PX4	C26-C25-C24	3.07	124.21	113.19	6	3
4	A	386	PX4	C4-N1-C3	3.07	101.09	108.97	7	2
4	A	425	PX4	O7-C23-O8	3.07	116.29	123.70	2	3
4	A	316	PX4	C7-O7-C23	3.06	125.34	117.79	14	2
4	A	351	PX4	O1-P1-O3	3.06	93.51	107.75	8	1
4	A	327	PX4	O7-C7-C8	3.06	119.49	108.40	7	5
4	A	383	PX4	O5-C9-C10	3.06	121.52	111.91	11	3
4	A	375	PX4	C25-C24-C23	3.06	102.48	113.62	6	2
4	A	386	PX4	C26-C25-C24	3.06	102.18	113.19	12	1
4	A	403	PX4	O7-C23-O8	3.06	116.30	123.70	2	4
4	A	357	PX4	O7-C7-C6	3.06	119.48	108.40	8	7
4	A	402	PX4	O7-C7-C8	3.06	119.48	108.40	2	7
4	A	417	PX4	O5-C9-C10	3.06	121.51	111.91	1	5
4	A	378	PX4	C4-N1-C3	3.06	116.84	108.97	13	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	401	PX4	O5-C9-O6	3.06	115.87	123.59	8	5
4	A	345	PX4	O1-P1-O4	3.06	121.94	107.75	10	2
4	A	382	PX4	C8-O5-C9	3.06	128.44	117.12	7	3
4	A	388	PX4	C1-C2-N1	3.06	125.99	115.78	7	2
4	A	377	PX4	C1-C2-N1	3.06	125.98	115.78	1	3
4	A	398	PX4	C1-C2-N1	3.06	125.98	115.78	11	5
4	A	412	PX4	P1-O4-C6	3.06	103.76	121.68	10	5
4	A	416	PX4	C8-O5-C9	3.06	105.80	117.12	13	3
4	A	417	PX4	C33-C32-C31	3.06	98.91	114.42	1	3
4	A	313	PX4	O4-P1-O2	3.05	121.00	109.07	13	2
4	A	322	PX4	P1-O4-C6	3.05	103.78	121.68	6	8
4	A	366	PX4	C30-C29-C28	3.05	98.92	114.42	10	2
4	A	353	PX4	C28-C27-C26	3.05	98.93	114.42	1	1
4	A	403	PX4	C26-C25-C24	3.05	102.22	113.19	11	2
4	A	424	PX4	C5-N1-C2	3.05	97.43	109.92	5	2
4	A	426	PX4	O5-C9-C10	3.05	121.49	111.91	6	4
4	A	382	PX4	O5-C9-O6	3.05	115.89	123.59	6	5
4	A	330	PX4	C5-N1-C2	3.05	122.40	109.92	1	1
4	A	346	PX4	C12-C11-C10	3.05	124.15	113.19	7	3
4	A	331	PX4	C11-C10-C9	3.05	102.54	113.62	6	1
4	A	351	PX4	O5-C9-O6	3.05	115.90	123.59	8	3
4	A	429	PX4	O7-C7-C8	3.05	119.43	108.40	2	5
4	A	382	PX4	O7-C7-C6	3.04	119.43	108.40	8	4
4	A	410	PX4	O7-C23-O8	3.05	116.34	123.70	14	4
4	A	333	PX4	C29-C28-C27	3.04	98.97	114.42	1	2
4	A	334	PX4	C8-O5-C9	3.04	105.85	117.12	4	3
4	A	343	PX4	C11-C10-C9	3.04	102.55	113.62	3	2
4	A	360	PX4	O7-C7-C8	3.04	119.42	108.40	7	3
4	A	314	PX4	O1-P1-O3	3.04	93.62	107.75	13	1
4	A	338	PX4	O7-C23-O8	3.04	116.35	123.70	13	5
4	A	408	PX4	O7-C7-C6	3.04	119.42	108.40	5	4
4	A	344	PX4	C26-C25-C24	3.04	102.26	113.19	12	1
4	A	350	PX4	C4-N1-C3	3.04	101.16	108.97	3	2
4	A	395	PX4	O1-P1-O4	3.04	121.87	107.75	4	3
4	A	420	PX4	C12-C11-C10	3.04	102.26	113.19	4	6
4	A	314	PX4	O1-P1-O2	3.04	127.26	112.24	3	4
4	A	339	PX4	C32-C31-C30	3.04	99.01	114.42	12	2
4	A	388	PX4	C8-O5-C9	3.04	105.88	117.12	5	2
4	A	389	PX4	C5-N1-C3	3.04	101.17	108.97	1	4
4	A	333	PX4	P1-O4-C6	3.03	103.89	121.68	9	8
4	A	335	PX4	O7-C23-O8	3.03	116.37	123.70	3	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	308	PX4	C4-N1-C3	3.03	101.18	108.97	13	4
4	A	360	PX4	C7-O7-C23	3.03	125.26	117.79	2	4
4	A	397	PX4	C15-C14-C13	3.03	99.03	114.42	13	1
4	A	407	PX4	O5-C9-C10	3.03	121.43	111.91	10	3
4	A	342	PX4	C5-N1-C4	3.03	101.18	108.97	12	5
4	A	420	PX4	C4-N1-C2	3.03	122.32	109.92	3	2
4	A	337	PX4	O1-P1-O2	3.03	127.22	112.24	12	9
4	A	369	PX4	C1-C2-N1	3.03	125.90	115.78	14	4
4	A	338	PX4	C4-N1-C3	3.03	116.76	108.97	5	1
4	A	417	PX4	O3-P1-O2	3.03	97.23	109.07	7	5
4	A	373	PX4	C16-C15-C14	3.03	99.05	114.42	3	4
4	A	338	PX4	C25-C24-C23	3.03	102.61	113.62	5	2
4	A	312	PX4	C26-C25-C24	3.03	124.07	113.19	6	3
4	A	340	PX4	C19-C18-C17	3.03	99.07	114.42	10	2
4	A	415	PX4	O4-P1-O2	3.03	120.89	109.07	9	1
4	A	333	PX4	O5-C9-O6	3.02	115.96	123.59	7	6
4	A	354	PX4	O1-P1-O4	3.02	121.79	107.75	4	2
4	A	412	PX4	O7-C7-C8	3.02	119.35	108.40	14	5
4	A	311	PX4	P1-O4-C6	3.02	103.96	121.68	1	4
4	A	397	PX4	O5-C9-C10	3.02	121.39	111.91	12	2
4	A	348	PX4	C12-C11-C10	3.02	124.05	113.19	8	1
4	A	308	PX4	C26-C25-C24	3.02	102.33	113.19	6	2
4	A	404	PX4	O7-C7-C6	3.02	119.34	108.40	2	6
4	A	417	PX4	C4-N1-C3	3.02	101.20	108.97	5	3
4	A	316	PX4	O7-C23-O8	3.02	116.41	123.70	10	6
4	A	347	PX4	O7-C7-C6	3.02	119.33	108.40	12	4
4	A	384	PX4	C5-N1-C3	3.02	101.21	108.97	13	1
4	A	321	PX4	O5-C9-O6	3.02	115.98	123.59	1	3
4	A	341	PX4	C11-C10-C9	3.02	102.65	113.62	1	2
4	A	354	PX4	C33-C32-C31	3.02	99.11	114.42	2	1
4	A	365	PX4	C5-N1-C2	3.02	122.26	109.92	1	1
4	A	376	PX4	O7-C23-O8	3.02	116.41	123.70	3	4
4	A	387	PX4	O1-P1-O3	3.02	93.73	107.75	12	1
4	A	388	PX4	C12-C11-C10	3.02	102.34	113.19	4	5
4	A	398	PX4	C7-O7-C23	3.02	110.36	117.79	1	1
4	A	405	PX4	O7-C7-C8	3.02	119.32	108.40	14	3
4	A	340	PX4	O1-P1-O2	3.02	127.15	112.24	6	9
4	A	342	PX4	C12-C11-C10	3.01	102.36	113.19	5	3
4	A	350	PX4	C5-N1-C3	3.01	101.23	108.97	10	4
4	A	365	PX4	C1-C2-N1	3.01	125.84	115.78	4	5
4	A	335	PX4	O7-C7-C6	3.01	119.31	108.40	3	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	354	PX4	C5-N1-C3	3.01	101.23	108.97	10	1
4	A	428	PX4	C26-C25-C24	3.01	102.36	113.19	1	4
4	A	428	PX4	O1-P1-O2	3.01	127.13	112.24	11	7
4	A	391	PX4	C14-C13-C12	3.01	99.15	114.42	14	1
4	A	308	PX4	C7-O7-C23	3.01	110.39	117.79	9	2
4	A	327	PX4	P1-O4-C6	3.01	104.05	121.68	7	5
4	A	353	PX4	O5-C9-C10	3.01	121.34	111.91	2	5
4	A	339	PX4	C15-C14-C13	3.00	99.17	114.42	4	2
4	A	365	PX4	O7-C7-C8	3.01	119.28	108.40	7	3
4	A	422	PX4	C19-C18-C17	3.01	99.16	114.42	3	1
4	A	319	PX4	C5-N1-C3	3.00	101.25	108.97	1	4
4	A	364	PX4	O5-C9-C10	3.00	121.34	111.91	13	4
4	A	424	PX4	O1-P1-O3	3.00	93.80	107.75	1	4
4	A	322	PX4	O5-C8-C7	3.00	117.17	108.43	6	6
4	A	359	PX4	C7-O7-C23	3.00	110.40	117.79	11	3
4	A	332	PX4	O4-P1-O2	3.00	120.78	109.07	13	2
4	A	355	PX4	O5-C9-C10	3.00	121.32	111.91	2	2
4	A	397	PX4	C25-C24-C23	3.00	102.72	113.62	1	2
4	A	401	PX4	C12-C11-C10	3.00	102.41	113.19	10	3
4	A	319	PX4	C26-C25-C24	3.00	102.42	113.19	5	2
4	A	361	PX4	O1-P1-O4	3.00	121.67	107.75	4	3
4	A	366	PX4	C28-C27-C26	3.00	99.21	114.42	2	1
4	A	408	PX4	O7-C23-O8	3.00	116.45	123.70	1	4
4	A	308	PX4	O1-P1-O3	3.00	93.83	107.75	8	1
4	A	328	PX4	C12-C11-C10	3.00	102.42	113.19	9	2
4	A	338	PX4	C18-C17-C16	3.00	99.22	114.42	5	3
4	A	396	PX4	C5-N1-C3	3.00	101.27	108.97	1	4
4	A	358	PX4	C15-C14-C13	2.99	99.22	114.42	3	2
4	A	361	PX4	C20-C19-C18	2.99	99.22	114.42	14	1
4	A	371	PX4	C17-C16-C15	2.99	99.22	114.42	2	1
4	A	410	PX4	O5-C8-C7	2.99	117.15	108.43	12	3
4	A	419	PX4	C1-C2-N1	3.00	125.78	115.78	3	5
4	A	430	PX4	O1-P1-O2	2.99	127.05	112.24	11	6
4	A	366	PX4	O1-P1-O4	2.99	121.65	107.75	5	4
4	A	370	PX4	O3-P1-O2	2.99	97.37	109.07	3	3
4	A	337	PX4	O7-C23-O8	2.99	116.48	123.70	7	3
4	A	428	PX4	C5-N1-C4	2.99	101.29	108.97	5	5
4	A	324	PX4	C17-C16-C15	2.99	99.26	114.42	2	2
4	A	394	PX4	C30-C29-C28	2.99	99.25	114.42	11	1
4	A	413	PX4	C8-O5-C9	2.99	106.05	117.12	2	5
4	A	426	PX4	O1-P1-O2	2.99	127.01	112.24	13	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	330	PX4	C8-O5-C9	2.99	106.06	117.12	5	1
4	A	333	PX4	O1-P1-O2	2.99	127.00	112.24	3	7
4	A	364	PX4	C16-C15-C14	2.99	99.27	114.42	12	2
4	A	387	PX4	C26-C25-C24	2.99	102.46	113.19	11	3
4	A	388	PX4	O7-C7-C8	2.99	119.21	108.40	12	3
4	A	430	PX4	C8-O5-C9	2.99	106.06	117.12	7	6
4	A	350	PX4	O4-P1-O2	2.98	120.73	109.07	1	3
4	A	357	PX4	C1-C2-N1	2.98	125.74	115.78	14	2
4	A	307	PX4	C4-N1-C2	2.98	97.72	109.92	6	4
4	A	342	PX4	C7-O7-C23	2.98	125.13	117.79	3	2
4	A	359	PX4	C32-C31-C30	2.98	99.29	114.42	6	1
4	A	421	PX4	C30-C29-C28	2.98	99.28	114.42	9	3
4	A	315	PX4	C5-N1-C3	2.98	101.31	108.97	12	3
4	A	318	PX4	C1-C2-N1	2.98	125.73	115.78	11	6
4	A	341	PX4	O1-P1-O2	2.98	126.97	112.24	7	8
4	A	345	PX4	C5-N1-C4	2.98	101.31	108.97	14	4
4	A	348	PX4	O7-C7-C6	2.98	119.19	108.40	8	5
4	A	384	PX4	C7-O7-C23	2.98	110.45	117.79	12	1
4	A	388	PX4	C11-C10-C9	2.98	102.78	113.62	12	2
4	A	399	PX4	O7-C7-C8	2.98	119.19	108.40	7	3
4	A	376	PX4	C29-C28-C27	2.98	99.30	114.42	10	2
4	A	401	PX4	C32-C31-C30	2.98	99.30	114.42	4	1
4	A	406	PX4	O7-C23-O8	2.98	116.50	123.70	4	4
4	A	414	PX4	O7-C7-C8	2.98	119.19	108.40	12	6
4	A	414	PX4	O7-C7-C6	2.98	119.19	108.40	4	3
4	A	386	PX4	C19-C18-C17	2.98	99.31	114.42	9	1
4	A	371	PX4	O3-C1-C2	2.98	124.81	109.16	3	2
4	A	410	PX4	C15-C14-C13	2.98	99.31	114.42	14	2
4	A	318	PX4	C4-N1-C3	2.97	116.62	108.97	13	3
4	A	373	PX4	C1-C2-N1	2.98	125.71	115.78	2	7
4	A	426	PX4	C8-O5-C9	2.98	128.14	117.12	6	3
4	A	321	PX4	C12-C11-C10	2.97	102.50	113.19	2	1
4	A	322	PX4	O4-P1-O2	2.97	120.69	109.07	6	3
4	A	337	PX4	O4-P1-O2	2.97	120.69	109.07	1	1
4	A	349	PX4	C5-N1-C3	2.97	116.62	108.97	13	3
4	A	367	PX4	O3-P1-O2	2.97	97.45	109.07	7	3
4	A	379	PX4	C14-C13-C12	2.97	99.33	114.42	6	2
4	A	344	PX4	O1-P1-O4	2.97	121.55	107.75	3	4
4	A	362	PX4	C29-C28-C27	2.97	99.35	114.42	5	2
4	A	366	PX4	O7-C7-C8	2.97	119.15	108.40	13	5
4	A	388	PX4	O5-C9-C10	2.97	121.22	111.91	5	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	394	PX4	C25-C24-C23	2.97	102.82	113.62	6	2
4	A	397	PX4	O1-P1-O3	2.97	93.95	107.75	11	1
4	A	307	PX4	C27-C26-C25	2.97	99.36	114.42	4	3
4	A	316	PX4	P1-O3-C1	2.97	106.99	121.59	14	9
4	A	374	PX4	C4-N1-C3	2.97	101.35	108.97	10	4
4	A	356	PX4	O1-P1-O2	2.96	126.89	112.24	14	9
4	A	358	PX4	C3-N1-C2	2.96	122.04	109.92	3	2
4	A	380	PX4	C5-N1-C2	2.96	122.04	109.92	6	1
4	A	409	PX4	C34-C33-C32	2.96	99.38	114.42	14	2
4	A	388	PX4	O1-P1-O3	2.96	93.99	107.75	10	2
4	A	316	PX4	O7-C7-C6	2.96	119.12	108.40	1	5
4	A	418	PX4	O5-C9-C10	2.96	121.20	111.91	8	5
4	A	320	PX4	O1-P1-O2	2.96	126.87	112.24	13	5
4	A	311	PX4	O1-P1-O4	2.96	121.49	107.75	12	4
4	A	377	PX4	C4-N1-C3	2.96	101.36	108.97	4	3
4	A	405	PX4	C29-C28-C27	2.96	99.40	114.42	13	1
4	A	391	PX4	O1-P1-O4	2.96	121.48	107.75	9	3
4	A	386	PX4	C8-O5-C9	2.96	106.17	117.12	5	4
4	A	388	PX4	C7-O7-C23	2.96	110.51	117.79	13	5
4	A	396	PX4	C5-N1-C4	2.96	116.58	108.97	6	3
4	A	308	PX4	O5-C9-C10	2.96	121.19	111.91	11	4
4	A	325	PX4	O3-P1-O2	2.95	97.52	109.07	4	4
4	A	336	PX4	O7-C7-C8	2.96	119.10	108.40	10	6
4	A	380	PX4	P1-O4-C6	2.96	104.35	121.68	12	9
4	A	310	PX4	O5-C9-O6	2.95	116.14	123.59	12	4
4	A	422	PX4	O1-P1-O3	2.95	94.02	107.75	6	1
4	A	315	PX4	O7-C7-C6	2.95	119.09	108.40	8	3
4	A	307	PX4	C5-N1-C3	2.95	116.56	108.97	12	3
4	A	323	PX4	O7-C7-C6	2.95	119.08	108.40	14	2
4	A	345	PX4	C8-O5-C9	2.95	106.19	117.12	10	2
4	A	413	PX4	C4-N1-C3	2.95	101.38	108.97	2	4
4	A	346	PX4	C25-C24-C23	2.95	102.89	113.62	2	1
4	A	352	PX4	O1-P1-O4	2.95	121.45	107.75	5	1
4	A	417	PX4	P1-O4-C6	2.95	104.38	121.68	12	9
4	A	429	PX4	C12-C11-C10	2.95	123.80	113.19	8	2
4	A	374	PX4	C11-C10-C9	2.95	102.90	113.62	10	3
4	A	354	PX4	C20-C19-C18	2.95	99.47	114.42	3	3
4	A	382	PX4	C5-N1-C4	2.95	101.40	108.97	8	3
4	A	337	PX4	C31-C30-C29	2.94	99.48	114.42	12	1
4	A	347	PX4	O4-P1-O2	2.94	120.57	109.07	4	3
4	A	383	PX4	C26-C25-C24	2.94	102.61	113.19	14	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	413	PX4	C11-C10-C9	2.95	102.91	113.62	1	2
4	A	340	PX4	C4-N1-C3	2.94	101.41	108.97	14	4
4	A	346	PX4	O4-P1-O2	2.94	120.57	109.07	8	4
4	A	333	PX4	O7-C7-C8	2.94	119.06	108.40	6	2
4	A	410	PX4	C11-C10-C9	2.94	102.92	113.62	9	3
4	A	422	PX4	O1-P1-O2	2.94	126.79	112.24	1	7
4	A	310	PX4	C12-C11-C10	2.94	102.63	113.19	4	2
4	A	328	PX4	O4-P1-O2	2.94	120.55	109.07	12	2
4	A	365	PX4	C5-N1-C3	2.94	101.42	108.97	10	2
4	A	395	PX4	O3-P1-O2	2.94	97.58	109.07	13	4
4	A	318	PX4	C13-C12-C11	2.94	99.51	114.42	9	1
4	A	374	PX4	C5-N1-C3	2.94	101.42	108.97	11	3
4	A	411	PX4	C5-N1-C2	2.94	121.94	109.92	6	2
4	A	339	PX4	O3-C1-C2	2.94	124.60	109.16	8	1
4	A	423	PX4	O1-P1-O3	2.94	94.11	107.75	12	2
4	A	421	PX4	C26-C25-C24	2.93	102.64	113.19	8	4
4	A	428	PX4	C3-N1-C2	2.94	97.91	109.92	9	1
4	A	336	PX4	C11-C10-C9	2.93	102.96	113.62	10	3
4	A	384	PX4	C1-C2-N1	2.93	125.57	115.78	4	3
4	A	394	PX4	C7-O7-C23	2.93	125.01	117.79	1	3
4	A	430	PX4	O4-P1-O2	2.93	120.53	109.07	4	5
4	A	335	PX4	O3-P1-O2	2.93	97.62	109.07	12	2
4	A	373	PX4	C26-C25-C24	2.93	102.65	113.19	14	3
4	A	334	PX4	C5-N1-C4	2.93	101.44	108.97	1	3
4	A	361	PX4	O5-C9-O6	2.93	116.20	123.59	12	3
4	A	340	PX4	O4-P1-O2	2.93	120.51	109.07	4	4
4	A	368	PX4	C5-N1-C3	2.93	101.44	108.97	4	3
4	A	387	PX4	O5-C9-C10	2.93	121.10	111.91	14	3
4	A	397	PX4	O7-C7-C6	2.93	119.01	108.40	2	1
4	A	419	PX4	O7-C7-C6	2.93	119.01	108.40	6	4
4	A	331	PX4	C14-C13-C12	2.93	99.56	114.42	5	3
4	A	355	PX4	O7-C23-O8	2.93	116.63	123.70	2	4
4	A	315	PX4	O7-C23-O8	2.93	116.63	123.70	3	3
4	A	352	PX4	C13-C12-C11	2.93	99.57	114.42	5	1
4	A	392	PX4	O3-P1-O2	2.93	97.64	109.07	7	2
4	A	430	PX4	C7-O7-C23	2.93	110.59	117.79	7	3
4	A	325	PX4	O7-C7-C8	2.92	118.98	108.40	4	4
4	A	345	PX4	O3-C1-C2	2.92	124.53	109.16	7	1
4	A	359	PX4	O5-C9-O6	2.92	130.97	123.59	10	1
4	A	342	PX4	O5-C9-O6	2.92	116.22	123.59	8	4
4	A	352	PX4	C1-C2-N1	2.92	125.53	115.78	11	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	367	PX4	C11-C10-C9	2.92	102.99	113.62	2	1
4	A	386	PX4	C7-O7-C23	2.92	124.98	117.79	6	2
4	A	390	PX4	P1-O4-C6	2.92	104.54	121.68	3	8
4	A	400	PX4	C33-C32-C31	2.92	99.59	114.42	9	1
4	A	412	PX4	O1-P1-O2	2.92	126.69	112.24	14	4
4	A	328	PX4	C7-O7-C23	2.92	124.98	117.79	13	2
4	A	372	PX4	C29-C28-C27	2.92	99.60	114.42	1	2
4	A	340	PX4	O1-P1-O3	2.92	94.18	107.75	14	3
4	A	347	PX4	C11-C10-C9	2.92	103.00	113.62	10	1
4	A	372	PX4	O7-C23-O8	2.92	116.65	123.70	7	2
4	A	395	PX4	P1-O4-C6	2.92	104.56	121.68	14	10
4	A	406	PX4	O5-C9-O6	2.92	116.22	123.59	5	2
4	A	320	PX4	O5-C9-C10	2.92	121.06	111.91	11	4
4	A	329	PX4	O7-C7-C6	2.92	118.96	108.40	2	6
4	A	368	PX4	O7-C23-O8	2.92	116.65	123.70	14	3
4	A	400	PX4	C32-C31-C30	2.92	99.62	114.42	9	1
4	A	423	PX4	O1-P1-O2	2.92	126.66	112.24	9	5
4	A	350	PX4	P1-O3-C1	2.91	107.25	121.59	7	8
4	A	354	PX4	C25-C24-C23	2.91	103.02	113.62	5	5
4	A	372	PX4	C12-C11-C10	2.91	102.71	113.19	12	2
4	A	361	PX4	C5-N1-C4	2.91	116.47	108.97	2	3
4	A	385	PX4	C26-C25-C24	2.91	102.72	113.19	3	2
4	A	397	PX4	C20-C19-C18	2.91	99.64	114.42	2	1
4	A	404	PX4	O3-P1-O2	2.91	120.44	109.07	3	2
4	A	318	PX4	C33-C32-C31	2.91	99.65	114.42	2	1
4	A	379	PX4	O3-P1-O2	2.91	97.70	109.07	1	6
4	A	389	PX4	C12-C11-C10	2.91	102.73	113.19	12	2
4	A	407	PX4	C5-N1-C4	2.91	101.49	108.97	12	3
4	A	397	PX4	C5-N1-C4	2.91	101.50	108.97	5	3
4	A	405	PX4	C4-N1-C3	2.91	101.49	108.97	14	3
4	A	333	PX4	C4-N1-C3	2.91	101.50	108.97	4	2
4	A	355	PX4	O4-P1-O2	2.91	97.70	109.07	11	3
4	A	307	PX4	C26-C25-C24	2.91	102.74	113.19	12	2
4	A	328	PX4	C5-N1-C3	2.91	116.45	108.97	10	1
4	A	395	PX4	O1-P1-O3	2.91	94.24	107.75	12	2
4	A	408	PX4	O8-C23-C24	2.91	112.39	123.73	3	1
4	A	318	PX4	C8-O5-C9	2.91	106.36	117.12	4	1
4	A	320	PX4	C4-N1-C3	2.90	116.44	108.97	3	2
4	A	323	PX4	C3-N1-C2	2.90	121.80	109.92	12	2
4	A	337	PX4	O7-C23-C24	2.91	117.76	111.50	1	4
4	A	335	PX4	C4-N1-C3	2.90	101.51	108.97	7	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	338	PX4	C32-C31-C30	2.90	99.69	114.42	6	3
4	A	339	PX4	C4-N1-C3	2.90	101.51	108.97	4	4
4	A	340	PX4	C5-N1-C2	2.90	121.80	109.92	4	2
4	A	344	PX4	C12-C11-C10	2.90	102.75	113.19	9	2
4	A	327	PX4	C33-C32-C31	2.90	99.69	114.42	3	1
4	A	350	PX4	C1-C2-N1	2.90	125.47	115.78	4	2
4	A	379	PX4	C4-N1-C3	2.90	101.51	108.97	11	1
4	A	374	PX4	O4-P1-O2	2.90	97.74	109.07	6	2
4	A	380	PX4	O6-C9-C10	2.90	112.42	123.73	5	1
4	A	399	PX4	O1-P1-O2	2.90	126.58	112.24	11	6
4	A	400	PX4	C4-N1-C3	2.90	101.52	108.97	4	5
4	A	405	PX4	O1-P1-O2	2.90	126.58	112.24	6	8
4	A	425	PX4	C34-C33-C32	2.90	99.70	114.42	10	2
4	A	427	PX4	C5-N1-C4	2.90	101.52	108.97	7	1
4	A	376	PX4	O1-P1-O3	2.90	121.21	107.75	7	1
4	A	395	PX4	C1-C2-N1	2.90	125.46	115.78	11	4
4	A	320	PX4	O4-P1-O2	2.90	97.75	109.07	11	1
4	A	324	PX4	C12-C11-C10	2.90	102.78	113.19	2	2
4	A	331	PX4	C18-C17-C16	2.90	99.72	114.42	4	2
4	A	337	PX4	C17-C16-C15	2.90	99.72	114.42	1	3
4	A	383	PX4	C5-N1-C3	2.90	101.53	108.97	2	2
4	A	332	PX4	C19-C18-C17	2.90	99.73	114.42	2	1
4	A	417	PX4	C8-O5-C9	2.90	106.40	117.12	9	3
4	A	340	PX4	C30-C29-C28	2.89	99.73	114.42	12	1
4	A	351	PX4	C12-C11-C10	2.89	102.79	113.19	3	2
4	A	346	PX4	C26-C25-C24	2.89	102.79	113.19	14	3
4	A	348	PX4	O5-C9-C10	2.89	120.98	111.91	7	5
4	A	387	PX4	O1-P1-O2	2.89	126.54	112.24	4	10
4	A	404	PX4	C19-C18-C17	2.89	99.74	114.42	11	1
4	A	421	PX4	O5-C9-C10	2.89	120.98	111.91	5	5
4	A	423	PX4	C16-C15-C14	2.89	99.75	114.42	4	2
4	A	312	PX4	O5-C9-O6	2.89	116.30	123.59	1	5
4	A	398	PX4	C5-N1-C4	2.89	101.55	108.97	14	3
4	A	308	PX4	O7-C7-C8	2.89	118.85	108.40	1	5
4	A	324	PX4	C19-C18-C17	2.88	99.78	114.42	12	2
4	A	330	PX4	C26-C25-C24	2.89	102.82	113.19	12	3
4	A	361	PX4	C32-C31-C30	2.89	99.77	114.42	13	2
4	A	352	PX4	C11-C10-C9	2.88	103.13	113.62	6	1
4	A	367	PX4	C4-N1-C3	2.88	101.56	108.97	6	2
4	A	400	PX4	O1-P1-O4	2.88	121.14	107.75	4	1
4	A	408	PX4	C8-O5-C9	2.88	106.44	117.12	7	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	311	PX4	C32-C31-C30	2.88	99.79	114.42	2	1
4	A	323	PX4	C27-C26-C25	2.88	99.79	114.42	1	1
4	A	328	PX4	C1-C2-N1	2.88	125.40	115.78	3	3
4	A	356	PX4	O7-C23-O8	2.88	116.74	123.70	12	3
4	A	359	PX4	O1-P1-O2	2.88	126.48	112.24	1	7
4	A	373	PX4	C8-O5-C9	2.88	106.45	117.12	6	2
4	A	375	PX4	C19-C18-C17	2.88	99.80	114.42	11	1
4	A	378	PX4	C5-N1-C4	2.88	116.38	108.97	5	4
4	A	380	PX4	O1-P1-O3	2.88	94.36	107.75	1	3
4	A	407	PX4	O3-C1-C2	2.88	124.31	109.16	4	1
4	A	408	PX4	C32-C31-C30	2.88	99.80	114.42	5	1
4	A	417	PX4	O1-P1-O3	2.88	94.36	107.75	5	1
4	A	350	PX4	C30-C29-C28	2.88	99.81	114.42	2	2
4	A	319	PX4	C18-C17-C16	2.88	99.82	114.42	1	1
4	A	361	PX4	O6-C9-C10	2.88	112.50	123.73	2	2
4	A	342	PX4	C13-C12-C11	2.88	99.82	114.42	11	1
4	A	350	PX4	C27-C26-C25	2.88	99.82	114.42	5	3
4	A	315	PX4	C26-C25-C24	2.88	102.85	113.19	2	1
4	A	372	PX4	O4-P1-O2	2.88	120.30	109.07	8	2
4	A	325	PX4	C12-C11-C10	2.87	102.86	113.19	1	2
4	A	355	PX4	O1-P1-O2	2.87	126.45	112.24	7	7
4	A	309	PX4	C5-N1-C3	2.87	101.59	108.97	2	4
4	A	312	PX4	C7-O7-C23	2.87	124.86	117.79	2	2
4	A	369	PX4	C30-C29-C28	2.87	99.84	114.42	2	3
4	A	381	PX4	C1-C2-N1	2.87	125.37	115.78	14	2
4	A	314	PX4	C18-C17-C16	2.87	99.85	114.42	14	1
4	A	344	PX4	C31-C30-C29	2.87	99.85	114.42	2	1
4	A	351	PX4	C16-C15-C14	2.87	99.86	114.42	11	2
4	A	352	PX4	O1-P1-O3	2.87	94.41	107.75	5	1
4	A	362	PX4	O5-C9-C10	2.87	120.92	111.91	3	3
4	A	399	PX4	O1-P1-O3	2.87	94.41	107.75	4	2
4	A	395	PX4	O1-P1-O2	2.87	126.42	112.24	13	6
4	A	413	PX4	O1-P1-O3	2.87	94.42	107.75	14	2
4	A	316	PX4	O1-P1-O2	2.87	126.41	112.24	9	8
4	A	317	PX4	C29-C28-C27	2.87	99.87	114.42	5	3
4	A	339	PX4	C4-N1-C2	2.87	121.65	109.92	5	1
4	A	428	PX4	C11-C10-C9	2.87	103.19	113.62	8	1
4	A	429	PX4	O5-C9-O6	2.87	116.35	123.59	8	4
4	A	329	PX4	C20-C19-C18	2.87	99.87	114.42	8	1
4	A	306	PX4	C5-N1-C3	2.86	116.34	108.97	10	2
4	A	307	PX4	O1-P1-O4	2.86	121.05	107.75	3	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	328	PX4	O7-C7-C6	2.87	118.78	108.40	14	2
4	A	347	PX4	C18-C17-C16	2.87	99.88	114.42	10	1
4	A	362	PX4	C19-C18-C17	2.87	99.87	114.42	12	1
4	A	367	PX4	C5-N1-C3	2.87	101.60	108.97	6	2
4	A	376	PX4	C4-N1-C3	2.87	101.60	108.97	13	2
4	A	373	PX4	C31-C30-C29	2.87	99.88	114.42	4	3
4	A	392	PX4	O5-C9-O6	2.87	116.36	123.59	6	4
4	A	307	PX4	C1-C2-N1	2.86	125.34	115.78	1	3
4	A	334	PX4	O5-C9-C10	2.86	120.90	111.91	5	5
4	A	376	PX4	C7-O7-C23	2.86	110.74	117.79	7	3
4	A	343	PX4	O7-C23-O8	2.86	116.78	123.70	13	6
4	A	394	PX4	O5-C9-O6	2.86	116.36	123.59	3	4
4	A	416	PX4	C26-C25-C24	2.86	102.90	113.19	10	1
4	A	337	PX4	C30-C29-C28	2.86	99.89	114.42	9	3
4	A	368	PX4	C5-N1-C4	2.86	101.61	108.97	5	4
4	A	390	PX4	C14-C13-C12	2.86	99.90	114.42	6	1
4	A	324	PX4	C7-O7-C23	2.86	110.75	117.79	6	2
4	A	423	PX4	C12-C11-C10	2.86	123.48	113.19	3	2
4	A	350	PX4	C8-O5-C9	2.86	106.53	117.12	2	4
4	A	358	PX4	C34-C33-C32	2.86	99.90	114.42	13	2
4	A	332	PX4	P1-O4-C6	2.86	104.92	121.68	12	10
4	A	412	PX4	C25-C24-C23	2.86	103.22	113.62	6	4
4	A	420	PX4	C13-C12-C11	2.86	99.91	114.42	12	2
4	A	360	PX4	O5-C9-O6	2.86	116.38	123.59	14	5
4	A	395	PX4	C26-C25-C24	2.86	123.46	113.19	4	2
4	A	412	PX4	O7-C23-O8	2.86	116.80	123.70	8	3
4	A	417	PX4	C4-N1-C2	2.86	121.60	109.92	5	4
4	A	310	PX4	O5-C9-C10	2.86	120.87	111.91	10	5
4	A	355	PX4	C11-C10-C9	2.85	124.00	113.62	1	4
4	A	363	PX4	C26-C25-C24	2.85	102.93	113.19	3	1
4	A	414	PX4	C4-N1-C3	2.85	116.31	108.97	12	2
4	A	382	PX4	C13-C12-C11	2.85	99.94	114.42	7	1
4	A	313	PX4	C1-C2-N1	2.85	125.29	115.78	1	1
4	A	320	PX4	C16-C15-C14	2.85	99.95	114.42	4	2
4	A	363	PX4	C7-O7-C23	2.85	124.81	117.79	3	3
4	A	341	PX4	C1-C2-N1	2.85	125.29	115.78	1	2
4	A	342	PX4	C31-C30-C29	2.85	99.96	114.42	5	3
4	A	417	PX4	O7-C7-C8	2.85	118.72	108.40	2	8
4	A	310	PX4	O1-P1-O4	2.85	120.97	107.75	14	1
4	A	368	PX4	C7-O7-C23	2.85	124.81	117.79	3	3
4	A	389	PX4	O1-P1-O3	2.85	94.51	107.75	14	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	407	PX4	O7-C23-O8	2.85	116.82	123.70	1	4
4	A	408	PX4	O1-P1-O4	2.85	120.98	107.75	13	2
4	A	427	PX4	O1-P1-O3	2.85	94.51	107.75	3	3
4	A	327	PX4	C8-O5-C9	2.85	106.58	117.12	12	3
4	A	364	PX4	O7-C7-C6	2.85	118.71	108.40	13	4
4	A	366	PX4	O7-C7-C6	2.85	118.71	108.40	3	4
4	A	405	PX4	C4-N1-C2	2.85	98.26	109.92	10	1
4	A	401	PX4	C4-N1-C3	2.85	101.66	108.97	8	2
4	A	350	PX4	C33-C32-C31	2.84	99.98	114.42	4	2
4	A	387	PX4	O5-C9-O6	2.84	116.41	123.59	13	5
4	A	402	PX4	O1-P1-O2	2.84	126.30	112.24	4	5
4	A	345	PX4	O7-C7-C6	2.84	118.69	108.40	10	2
4	A	341	PX4	C20-C19-C18	2.84	100.00	114.42	3	1
4	A	316	PX4	O5-C9-O6	2.84	116.42	123.59	14	3
4	A	381	PX4	C5-N1-C4	2.84	101.67	108.97	1	3
4	A	386	PX4	C18-C17-C16	2.84	100.01	114.42	14	1
4	A	346	PX4	O5-C9-O6	2.84	116.43	123.59	3	4
4	A	346	PX4	C15-C14-C13	2.84	100.02	114.42	10	2
4	A	398	PX4	O1-P1-O4	2.84	120.92	107.75	2	3
4	A	407	PX4	C32-C31-C30	2.84	100.02	114.42	1	1
4	A	409	PX4	O1-P1-O3	2.84	94.56	107.75	12	4
4	A	428	PX4	O7-C7-C8	2.84	118.67	108.40	2	5
4	A	429	PX4	O7-C23-O8	2.84	116.84	123.70	12	2
4	A	385	PX4	O7-C7-C8	2.84	118.67	108.40	10	4
4	A	318	PX4	C16-C15-C14	2.83	100.04	114.42	8	2
4	A	317	PX4	C12-C11-C10	2.83	103.01	113.19	3	2
4	A	326	PX4	C31-C30-C29	2.83	100.04	114.42	11	1
4	A	338	PX4	O1-P1-O3	2.83	94.59	107.75	4	3
4	A	399	PX4	O5-C9-C10	2.83	120.80	111.91	3	5
4	A	363	PX4	C5-N1-C2	2.83	98.33	109.92	4	1
4	A	371	PX4	O5-C9-O6	2.83	116.44	123.59	7	1
4	A	387	PX4	O3-P1-O2	2.83	98.00	109.07	11	3
4	A	422	PX4	C5-N1-C3	2.83	116.25	108.97	10	3
4	A	319	PX4	O3-P1-O2	2.83	98.01	109.07	1	2
4	A	322	PX4	C27-C26-C25	2.83	100.06	114.42	3	2
4	A	370	PX4	C4-N1-C3	2.83	101.70	108.97	2	3
4	A	371	PX4	C3-N1-C2	2.83	121.50	109.92	13	3
4	A	323	PX4	C25-C24-C23	2.83	103.33	113.62	10	3
4	A	373	PX4	P1-O4-C6	2.83	105.09	121.68	8	10
4	A	389	PX4	C30-C29-C28	2.83	100.06	114.42	7	2
4	A	419	PX4	C26-C25-C24	2.83	103.02	113.19	13	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	310	PX4	O7-C7-C8	2.83	118.64	108.40	1	5
4	A	337	PX4	C5-N1-C3	2.83	101.70	108.97	12	4
4	A	342	PX4	C17-C16-C15	2.83	100.07	114.42	14	1
4	A	361	PX4	C11-C10-C9	2.83	103.34	113.62	5	2
4	A	373	PX4	O7-C23-O8	2.83	116.87	123.70	5	4
4	A	393	PX4	C14-C13-C12	2.83	100.07	114.42	12	3
4	A	359	PX4	O6-C9-C10	2.83	112.70	123.73	10	2
4	A	326	PX4	C26-C25-C24	2.82	103.04	113.19	11	2
4	A	328	PX4	O5-C9-C10	2.83	120.77	111.91	5	3
4	A	374	PX4	O1-P1-O3	2.83	94.62	107.75	13	2
4	A	375	PX4	O4-P1-O2	2.82	98.03	109.07	3	2
4	A	377	PX4	C28-C27-C26	2.82	100.08	114.42	5	2
4	A	403	PX4	C16-C15-C14	2.83	100.08	114.42	13	2
4	A	306	PX4	C1-C2-N1	2.82	125.21	115.78	6	2
4	A	422	PX4	O4-P1-O2	2.82	120.10	109.07	8	2
4	A	390	PX4	C12-C11-C10	2.82	103.04	113.19	8	3
4	A	400	PX4	C34-C33-C32	2.82	100.09	114.42	2	2
4	A	413	PX4	C1-C2-N1	2.82	125.20	115.78	8	4
4	A	430	PX4	C12-C11-C10	2.82	123.34	113.19	8	4
4	A	406	PX4	O5-C9-C10	2.82	120.76	111.91	7	1
4	A	430	PX4	O5-C9-C10	2.82	120.76	111.91	13	4
4	A	327	PX4	O1-P1-O2	2.82	126.18	112.24	9	6
4	A	360	PX4	C25-C24-C23	2.82	103.36	113.62	9	2
4	A	379	PX4	C15-C14-C13	2.82	100.11	114.42	8	3
4	A	340	PX4	C8-O5-C9	2.82	127.56	117.12	7	3
4	A	346	PX4	O6-C9-C10	2.82	112.74	123.73	6	1
4	A	354	PX4	C7-O7-C23	2.82	124.73	117.79	1	5
4	A	366	PX4	C5-N1-C3	2.82	116.22	108.97	10	3
4	A	389	PX4	C34-C33-C32	2.82	100.11	114.42	13	1
4	A	383	PX4	P1-O4-C6	2.82	105.16	121.68	6	3
4	A	392	PX4	C7-O7-C23	2.82	124.73	117.79	11	3
4	A	368	PX4	P1-O4-C6	2.82	105.16	121.68	4	8
4	A	316	PX4	C11-C10-C9	2.82	123.86	113.62	14	2
4	A	322	PX4	O1-P1-O4	2.82	120.82	107.75	2	3
4	A	327	PX4	C1-C2-N1	2.81	125.18	115.78	13	5
4	A	344	PX4	C18-C17-C16	2.81	100.14	114.42	12	3
4	A	381	PX4	O1-P1-O4	2.81	120.81	107.75	9	2
4	A	311	PX4	C5-N1-C2	2.81	98.41	109.92	3	3
4	A	356	PX4	C15-C14-C13	2.81	100.15	114.42	14	1
4	A	356	PX4	C8-O5-C9	2.81	106.71	117.12	3	3
4	A	388	PX4	C20-C19-C18	2.81	100.16	114.42	12	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	306	PX4	C28-C27-C26	2.81	100.16	114.42	12	2
4	A	325	PX4	O1-P1-O2	2.81	126.13	112.24	6	7
4	A	364	PX4	C26-C25-C24	2.81	103.09	113.19	6	2
4	A	402	PX4	C20-C19-C18	2.81	100.16	114.42	2	2
4	A	425	PX4	O7-C7-C6	2.81	118.57	108.40	9	2
4	A	429	PX4	C5-N1-C3	2.81	101.75	108.97	3	6
4	A	317	PX4	O1-P1-O2	2.81	126.11	112.24	1	3
4	A	337	PX4	O5-C9-C10	2.81	120.72	111.91	10	1
4	A	328	PX4	O7-C7-C8	2.81	118.56	108.40	10	4
4	A	361	PX4	C5-N1-C2	2.81	121.40	109.92	11	1
4	A	378	PX4	C12-C11-C10	2.81	103.11	113.19	4	1
4	A	380	PX4	C4-N1-C3	2.81	101.76	108.97	6	2
4	A	402	PX4	C4-N1-C2	2.81	121.40	109.92	11	1
4	A	388	PX4	O4-P1-O2	2.80	120.03	109.07	8	2
4	A	414	PX4	O6-C9-C10	2.81	112.79	123.73	12	2
4	A	386	PX4	C5-N1-C4	2.80	101.77	108.97	11	2
4	A	409	PX4	O7-C7-C6	2.80	118.55	108.40	12	3
4	A	313	PX4	C17-C16-C15	2.80	100.20	114.42	11	1
4	A	351	PX4	C4-N1-C2	2.80	98.46	109.92	6	2
4	A	395	PX4	C27-C26-C25	2.80	100.20	114.42	10	2
4	A	306	PX4	C4-N1-C2	2.80	121.37	109.92	14	2
4	A	311	PX4	C1-C2-N1	2.80	125.13	115.78	12	3
4	A	409	PX4	O7-C7-C8	2.80	118.54	108.40	9	8
4	A	409	PX4	C4-N1-C3	2.80	101.77	108.97	9	2
4	A	422	PX4	C8-O5-C9	2.80	106.75	117.12	6	2
4	A	325	PX4	C5-N1-C2	2.80	121.36	109.92	4	2
4	A	358	PX4	C1-C2-N1	2.80	125.12	115.78	8	1
4	A	398	PX4	O6-C9-C10	2.80	112.81	123.73	7	1
4	A	320	PX4	P1-O4-C6	2.80	105.28	121.68	1	10
4	A	355	PX4	O7-C7-C6	2.80	118.53	108.40	13	5
4	A	366	PX4	O5-C9-O6	2.80	116.54	123.59	14	2
4	A	395	PX4	O7-C23-O8	2.80	130.46	123.70	6	4
4	A	402	PX4	C26-C25-C24	2.80	103.14	113.19	2	3
4	A	383	PX4	C7-O7-C23	2.79	110.91	117.79	13	4
4	A	389	PX4	C11-C10-C9	2.79	103.46	113.62	3	2
4	A	362	PX4	O1-P1-O2	2.79	126.05	112.24	14	4
4	A	391	PX4	C5-N1-C3	2.79	101.79	108.97	13	2
4	A	362	PX4	O7-C7-C6	2.79	118.51	108.40	4	4
4	A	388	PX4	O7-C7-C6	2.79	118.51	108.40	13	4
4	A	382	PX4	C12-C11-C10	2.79	103.16	113.19	11	1
4	A	403	PX4	O5-C9-O6	2.79	116.55	123.59	14	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	414	PX4	C20-C19-C18	2.79	100.26	114.42	7	2
4	A	422	PX4	C30-C29-C28	2.79	100.25	114.42	8	2
4	A	327	PX4	O4-P1-O2	2.79	98.17	109.07	8	3
4	A	329	PX4	C27-C26-C25	2.79	128.58	114.42	13	1
4	A	385	PX4	C18-C17-C16	2.79	100.26	114.42	12	3
4	A	359	PX4	O1-P1-O4	2.79	120.70	107.75	13	2
4	A	387	PX4	C4-N1-C3	2.79	101.80	108.97	5	2
4	A	376	PX4	C4-N1-C2	2.79	121.32	109.92	7	2
4	A	407	PX4	O1-P1-O2	2.79	126.03	112.24	1	7
4	A	316	PX4	C18-C17-C16	2.79	100.28	114.42	14	1
4	A	323	PX4	C5-N1-C2	2.79	98.52	109.92	12	3
4	A	420	PX4	C15-C14-C13	2.79	100.28	114.42	8	1
4	A	333	PX4	C13-C12-C11	2.78	100.29	114.42	3	1
4	A	326	PX4	C16-C15-C14	2.78	100.30	114.42	8	1
4	A	329	PX4	C8-O5-C9	2.78	106.82	117.12	6	2
4	A	381	PX4	C16-C15-C14	2.78	100.30	114.42	4	3
4	A	382	PX4	C5-N1-C3	2.78	116.13	108.97	5	2
4	A	400	PX4	C5-N1-C3	2.78	116.12	108.97	4	2
4	A	379	PX4	C3-N1-C2	2.78	98.55	109.92	2	1
4	A	400	PX4	C12-C11-C10	2.78	103.20	113.19	11	2
4	A	410	PX4	C18-C17-C16	2.78	100.31	114.42	14	3
4	A	335	PX4	C14-C13-C12	2.78	100.33	114.42	2	1
4	A	336	PX4	O3-P1-O2	2.78	98.21	109.07	13	5
4	A	308	PX4	C5-N1-C4	2.78	116.11	108.97	4	2
4	A	344	PX4	C32-C31-C30	2.78	100.33	114.42	6	2
4	A	387	PX4	C31-C30-C29	2.78	100.33	114.42	13	1
4	A	389	PX4	C20-C19-C18	2.78	100.33	114.42	10	1
4	A	335	PX4	O1-P1-O2	2.77	125.96	112.24	10	7
4	A	415	PX4	C11-C10-C9	2.77	103.53	113.62	5	2
4	A	420	PX4	O1-P1-O2	2.77	125.96	112.24	12	7
4	A	325	PX4	C30-C29-C28	2.77	100.35	114.42	11	2
4	A	373	PX4	C12-C11-C10	2.77	103.22	113.19	4	1
4	A	424	PX4	C12-C11-C10	2.77	103.22	113.19	2	1
4	A	327	PX4	C30-C29-C28	2.77	100.35	114.42	2	1
4	A	344	PX4	O1-P1-O2	2.77	125.95	112.24	6	6
4	A	388	PX4	C15-C14-C13	2.77	100.35	114.42	7	1
4	A	429	PX4	C11-C10-C9	2.77	103.54	113.62	8	2
4	A	370	PX4	O1-P1-O4	2.77	120.61	107.75	3	2
4	A	372	PX4	C30-C29-C28	2.77	100.36	114.42	9	3
4	A	393	PX4	C33-C32-C31	2.77	100.36	114.42	7	1
4	A	398	PX4	C12-C11-C10	2.77	103.23	113.19	6	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	426	PX4	O5-C9-O6	2.77	116.60	123.59	8	4
4	A	330	PX4	O1-P1-O4	2.77	94.89	107.75	3	1
4	A	341	PX4	C4-N1-C3	2.77	116.09	108.97	1	3
4	A	366	PX4	O1-P1-O2	2.77	125.92	112.24	1	6
4	A	406	PX4	C7-O7-C23	2.77	110.98	117.79	7	2
4	A	416	PX4	O5-C9-C10	2.77	120.59	111.91	7	5
4	A	344	PX4	C33-C32-C31	2.77	100.38	114.42	13	3
4	A	359	PX4	C4-N1-C3	2.77	101.86	108.97	7	1
4	A	379	PX4	C25-C24-C23	2.77	103.56	113.62	3	3
4	A	410	PX4	C1-C2-N1	2.77	125.02	115.78	9	6
4	A	416	PX4	O5-C8-C7	2.77	116.48	108.43	10	5
4	A	426	PX4	C34-C33-C32	2.77	100.38	114.42	12	3
4	A	332	PX4	O1-P1-O4	2.76	120.58	107.75	2	3
4	A	375	PX4	C32-C31-C30	2.76	100.39	114.42	13	2
4	A	385	PX4	O4-P1-O2	2.76	119.87	109.07	13	1
4	A	397	PX4	C8-O5-C9	2.76	106.88	117.12	3	1
4	A	416	PX4	O5-C9-O6	2.76	116.61	123.59	10	4
4	A	328	PX4	O1-P1-O4	2.76	120.58	107.75	7	3
4	A	347	PX4	C7-O7-C23	2.76	110.99	117.79	2	4
4	A	413	PX4	O5-C9-C10	2.76	120.58	111.91	6	2
4	A	424	PX4	C29-C28-C27	2.76	100.39	114.42	6	1
4	A	325	PX4	C27-C26-C25	2.76	100.40	114.42	12	4
4	A	429	PX4	O7-C7-C6	2.76	118.40	108.40	10	3
4	A	393	PX4	C5-N1-C4	2.76	101.88	108.97	10	2
4	A	306	PX4	O5-C9-C10	2.76	120.56	111.91	4	3
4	A	308	PX4	C12-C11-C10	2.76	103.28	113.19	1	6
4	A	308	PX4	O4-P1-O2	2.76	119.84	109.07	12	2
4	A	381	PX4	C8-O5-C9	2.76	106.91	117.12	5	1
4	A	390	PX4	C5-N1-C2	2.76	121.20	109.92	1	3
4	A	377	PX4	C8-O5-C9	2.76	106.91	117.12	9	3
4	A	389	PX4	O3-C1-C2	2.76	123.66	109.16	5	2
4	A	327	PX4	C29-C28-C27	2.76	100.44	114.42	5	2
4	A	334	PX4	P1-O4-C6	2.76	105.52	121.68	13	6
4	A	367	PX4	C12-C11-C10	2.76	103.28	113.19	6	2
4	A	401	PX4	C25-C24-C23	2.76	103.59	113.62	1	3
4	A	379	PX4	O1-P1-O4	2.76	120.54	107.75	14	2
4	A	424	PX4	C16-C15-C14	2.76	100.44	114.42	14	1
4	A	427	PX4	C7-O7-C23	2.76	124.58	117.79	4	4
4	A	315	PX4	O1-P1-O2	2.75	125.86	112.24	9	7
4	A	368	PX4	C4-N1-C2	2.75	121.19	109.92	4	2
4	A	372	PX4	C32-C31-C30	2.75	100.44	114.42	3	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	324	PX4	C1-C2-N1	2.75	124.97	115.78	13	2
4	A	339	PX4	C5-N1-C4	2.75	116.05	108.97	13	1
4	A	378	PX4	C1-C2-N1	2.75	124.97	115.78	7	2
4	A	391	PX4	C4-N1-C2	2.75	121.18	109.92	14	2
4	A	403	PX4	C4-N1-C3	2.75	101.90	108.97	8	4
4	A	311	PX4	C3-N1-C2	2.75	121.17	109.92	3	3
4	A	320	PX4	C26-C25-C24	2.75	103.30	113.19	10	1
4	A	400	PX4	O5-C9-O6	2.75	116.65	123.59	3	3
4	A	327	PX4	C34-C33-C32	2.75	100.47	114.42	10	1
4	A	346	PX4	C1-C2-N1	2.75	124.96	115.78	11	4
4	A	347	PX4	O5-C9-C10	2.75	120.54	111.91	10	6
4	A	407	PX4	O4-P1-O2	2.75	119.81	109.07	14	5
4	A	419	PX4	C11-C10-C9	2.75	103.62	113.62	9	2
4	A	318	PX4	C12-C11-C10	2.75	103.31	113.19	5	2
4	A	377	PX4	O1-P1-O3	2.75	120.51	107.75	1	1
4	A	377	PX4	C4-N1-C2	2.75	98.67	109.92	6	2
4	A	404	PX4	C29-C28-C27	2.75	100.48	114.42	2	1
4	A	429	PX4	C7-O7-C23	2.75	111.03	117.79	10	1
4	A	306	PX4	O4-P1-O2	2.74	119.79	109.07	5	5
4	A	312	PX4	O7-C7-C6	2.75	118.34	108.40	12	3
4	A	357	PX4	C11-C10-C9	2.75	103.64	113.62	4	3
4	A	334	PX4	C14-C13-C12	2.74	100.50	114.42	4	1
4	A	358	PX4	C5-N1-C4	2.74	101.92	108.97	1	3
4	A	361	PX4	O4-P1-O2	2.74	119.79	109.07	9	2
4	A	416	PX4	C19-C18-C17	2.74	100.49	114.42	8	1
4	A	384	PX4	C32-C31-C30	2.74	100.51	114.42	12	1
4	A	389	PX4	C26-C25-C24	2.74	103.34	113.19	12	3
4	A	346	PX4	O3-P1-O2	2.74	98.37	109.07	8	2
4	A	364	PX4	O5-C9-O6	2.74	116.68	123.59	1	2
4	A	367	PX4	O1-P1-O2	2.74	125.78	112.24	14	2
4	A	369	PX4	C12-C11-C10	2.74	123.04	113.19	8	2
4	A	419	PX4	C29-C28-C27	2.74	100.51	114.42	3	1
4	A	314	PX4	C30-C29-C28	2.74	100.53	114.42	3	2
4	A	394	PX4	O7-C7-C8	2.74	118.31	108.40	12	5
4	A	391	PX4	C33-C32-C31	2.74	100.53	114.42	1	3
4	A	416	PX4	C33-C32-C31	2.74	100.53	114.42	10	1
4	A	343	PX4	C4-N1-C2	2.74	121.11	109.92	8	2
4	A	317	PX4	O7-C7-C6	2.73	118.30	108.40	4	6
4	A	367	PX4	C4-N1-C2	2.74	121.11	109.92	7	1
4	A	374	PX4	O5-C9-C10	2.74	120.49	111.91	1	5
4	A	376	PX4	C25-C24-C23	2.73	103.68	113.62	9	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	400	PX4	O3-P1-O2	2.74	98.38	109.07	13	4
4	A	425	PX4	O1-P1-O3	2.74	95.04	107.75	4	3
4	A	322	PX4	C34-C33-C32	2.73	100.55	114.42	7	2
4	A	323	PX4	C32-C31-C30	2.73	100.55	114.42	11	1
4	A	328	PX4	C8-O5-C9	2.73	107.00	117.12	3	2
4	A	338	PX4	C28-C27-C26	2.73	100.55	114.42	11	1
4	A	343	PX4	C5-N1-C4	2.73	101.95	108.97	3	1
4	A	371	PX4	O3-P1-O2	2.73	98.39	109.07	6	5
4	A	358	PX4	O1-P1-O4	2.73	120.42	107.75	9	2
4	A	338	PX4	C5-N1-C4	2.73	101.96	108.97	13	2
4	A	362	PX4	C3-N1-C2	2.73	98.75	109.92	11	2
4	A	367	PX4	O5-C9-C10	2.73	120.48	111.91	5	3
4	A	371	PX4	O8-C23-C24	2.73	113.08	123.73	12	2
4	A	389	PX4	C5-N1-C2	2.73	98.74	109.92	12	3
4	A	407	PX4	C5-N1-C2	2.73	121.09	109.92	11	1
4	A	317	PX4	C4-N1-C2	2.73	121.08	109.92	2	2
4	A	367	PX4	C32-C31-C30	2.73	100.57	114.42	11	1
4	A	419	PX4	C31-C30-C29	2.73	100.57	114.42	14	3
4	A	360	PX4	C19-C18-C17	2.73	100.58	114.42	10	2
4	A	404	PX4	O1-P1-O2	2.73	125.73	112.24	12	2
4	A	422	PX4	O1-P1-O4	2.73	120.42	107.75	6	2
4	A	321	PX4	O4-P1-O2	2.73	98.41	109.07	8	2
4	A	398	PX4	C19-C18-C17	2.73	100.58	114.42	3	1
4	A	323	PX4	C12-C11-C10	2.73	103.39	113.19	4	3
4	A	364	PX4	C4-N1-C2	2.72	121.06	109.92	14	1
4	A	398	PX4	O1-P1-O3	2.73	95.09	107.75	3	4
4	A	416	PX4	O6-C9-C10	2.73	113.10	123.73	14	1
4	A	372	PX4	C5-N1-C4	2.72	101.97	108.97	3	2
4	A	347	PX4	C12-C11-C10	2.72	103.41	113.19	12	5
4	A	421	PX4	C29-C28-C27	2.72	100.60	114.42	3	2
4	A	399	PX4	C26-C25-C24	2.72	103.41	113.19	9	3
4	A	391	PX4	C26-C25-C24	2.72	103.41	113.19	9	2
4	A	420	PX4	O1-P1-O3	2.72	95.11	107.75	1	2
4	A	311	PX4	C27-C26-C25	2.72	100.62	114.42	6	2
4	A	339	PX4	C33-C32-C31	2.72	100.62	114.42	3	3
4	A	353	PX4	C25-C24-C23	2.72	123.51	113.62	7	1
4	A	410	PX4	O5-C9-O6	2.72	116.73	123.59	2	2
4	A	370	PX4	C5-N1-C3	2.72	115.96	108.97	9	4
4	A	406	PX4	O4-P1-O2	2.72	119.69	109.07	14	4
4	A	315	PX4	C1-C2-N1	2.72	124.85	115.78	4	2
4	A	321	PX4	O1-P1-O3	2.72	95.13	107.75	11	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	340	PX4	O3-C1-C2	2.72	123.45	109.16	9	3
4	A	316	PX4	O1-P1-O4	2.72	120.36	107.75	5	2
4	A	322	PX4	C5-N1-C3	2.72	101.99	108.97	14	4
4	A	321	PX4	P1-O4-C6	2.71	105.77	121.68	13	5
4	A	355	PX4	C14-C13-C12	2.71	100.64	114.42	3	1
4	A	394	PX4	C29-C28-C27	2.71	100.64	114.42	6	3
4	A	395	PX4	C11-C10-C9	2.72	103.75	113.62	1	2
4	A	342	PX4	C1-C2-N1	2.71	124.84	115.78	11	3
4	A	321	PX4	C13-C12-C11	2.71	100.66	114.42	7	3
4	A	370	PX4	O1-P1-O2	2.71	125.65	112.24	2	6
4	A	379	PX4	C5-N1-C4	2.71	102.00	108.97	11	3
4	A	381	PX4	O4-P1-O2	2.71	119.67	109.07	3	1
4	A	383	PX4	O3-P1-O2	2.71	98.47	109.07	10	2
4	A	411	PX4	O1-P1-O3	2.71	95.14	107.75	11	2
4	A	425	PX4	C7-O7-C23	2.71	124.47	117.79	4	2
4	A	366	PX4	C12-C11-C10	2.71	103.45	113.19	3	1
4	A	384	PX4	C3-N1-C2	2.71	121.00	109.92	6	2
4	A	422	PX4	C12-C11-C10	2.71	103.45	113.19	4	2
4	A	314	PX4	C1-C2-N1	2.71	124.82	115.78	10	1
4	A	419	PX4	C5-N1-C2	2.71	121.00	109.92	13	1
4	A	318	PX4	C5-N1-C4	2.71	102.01	108.97	6	1
4	A	351	PX4	O4-P1-O2	2.71	119.64	109.07	11	2
4	A	346	PX4	O7-C23-O8	2.71	117.16	123.70	11	2
4	A	353	PX4	O3-P1-O2	2.71	98.49	109.07	4	4
4	A	375	PX4	C12-C11-C10	2.71	103.46	113.19	10	3
4	A	378	PX4	O5-C9-O6	2.71	116.76	123.59	10	3
4	A	344	PX4	C4-N1-C2	2.70	120.98	109.92	11	2
4	A	319	PX4	C11-C10-C9	2.70	103.80	113.62	1	3
4	A	331	PX4	C32-C31-C30	2.70	100.71	114.42	7	1
4	A	358	PX4	O5-C9-O6	2.70	116.78	123.59	8	2
4	A	361	PX4	C13-C12-C11	2.70	100.71	114.42	13	2
4	A	422	PX4	C1-C2-N1	2.70	124.80	115.78	12	1
4	A	308	PX4	C4-N1-C2	2.70	98.87	109.92	1	1
4	A	314	PX4	C8-O5-C9	2.70	107.12	117.12	3	4
4	A	424	PX4	O7-C7-C6	2.70	118.18	108.40	6	1
4	A	403	PX4	O1-P1-O2	2.70	125.59	112.24	11	3
4	A	319	PX4	C14-C13-C12	2.70	100.73	114.42	1	2
4	A	347	PX4	C15-C14-C13	2.70	100.73	114.42	12	1
4	A	412	PX4	C16-C15-C14	2.70	100.73	114.42	14	1
4	A	414	PX4	C11-C10-C9	2.70	103.81	113.62	9	1
4	A	425	PX4	O4-P1-O2	2.70	119.61	109.07	10	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	325	PX4	O1-P1-O3	2.69	95.23	107.75	5	2
4	A	357	PX4	O1-P1-O4	2.69	120.26	107.75	8	3
4	A	380	PX4	C8-O5-C9	2.69	107.15	117.12	1	1
4	A	385	PX4	C25-C24-C23	2.69	103.82	113.62	14	1
4	A	400	PX4	C7-O7-C23	2.69	124.42	117.79	2	3
4	A	399	PX4	C4-N1-C2	2.69	98.90	109.92	3	1
4	A	377	PX4	C31-C30-C29	2.69	100.76	114.42	13	1
4	A	339	PX4	O7-C7-C8	2.69	118.14	108.40	5	3
4	A	391	PX4	O4-P1-O2	2.69	119.58	109.07	2	5
4	A	410	PX4	C5-N1-C4	2.69	102.06	108.97	2	4
4	A	410	PX4	C34-C33-C32	2.69	100.76	114.42	4	1
4	A	349	PX4	C1-C2-N1	2.69	124.76	115.78	5	1
4	A	346	PX4	C14-C13-C12	2.69	100.78	114.42	3	1
4	A	355	PX4	C18-C17-C16	2.69	100.77	114.42	14	2
4	A	397	PX4	C33-C32-C31	2.69	100.78	114.42	2	2
4	A	414	PX4	C17-C16-C15	2.69	100.77	114.42	8	1
4	A	416	PX4	C11-C10-C9	2.69	103.84	113.62	8	2
4	A	423	PX4	C7-O7-C23	2.69	124.41	117.79	2	4
4	A	395	PX4	O5-C9-C10	2.69	120.34	111.91	13	2
4	A	362	PX4	C1-C2-N1	2.68	124.74	115.78	8	3
4	A	376	PX4	C11-C10-C9	2.68	103.86	113.62	1	3
4	A	386	PX4	O7-C23-O8	2.68	117.22	123.70	2	5
4	A	400	PX4	O8-C23-C24	2.68	113.26	123.73	13	1
4	A	422	PX4	C14-C13-C12	2.68	100.80	114.42	14	2
4	A	310	PX4	C34-C33-C32	2.68	100.81	114.42	12	1
4	A	317	PX4	O7-C7-C8	2.68	118.11	108.40	9	2
4	A	337	PX4	O3-C1-C2	2.68	123.27	109.16	2	4
4	A	357	PX4	O3-P1-O2	2.68	98.59	109.07	2	2
4	A	384	PX4	C19-C18-C17	2.68	100.81	114.42	1	1
4	A	383	PX4	C16-C15-C14	2.68	100.81	114.42	4	1
4	A	405	PX4	C8-O5-C9	2.68	107.19	117.12	10	1
4	A	338	PX4	O7-C7-C6	2.68	118.10	108.40	12	4
4	A	404	PX4	C16-C15-C14	2.68	100.82	114.42	3	1
4	A	421	PX4	C19-C18-C17	2.68	100.82	114.42	6	1
4	A	387	PX4	O7-C7-C8	2.68	118.10	108.40	4	5
4	A	406	PX4	C26-C25-C24	2.68	103.56	113.19	4	3
4	A	414	PX4	O1-P1-O3	2.68	120.19	107.75	14	2
4	A	308	PX4	O1-P1-O4	2.68	120.18	107.75	11	2
4	A	310	PX4	C4-N1-C3	2.68	102.09	108.97	11	4
4	A	362	PX4	C7-O7-C23	2.68	124.38	117.79	7	2
4	A	374	PX4	O3-C1-C2	2.68	123.24	109.16	7	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	425	PX4	C12-C11-C10	2.68	122.82	113.19	12	1
4	A	382	PX4	C11-C10-C9	2.68	103.89	113.62	10	2
4	A	393	PX4	C4-N1-C3	2.68	115.86	108.97	11	2
4	A	430	PX4	C14-C13-C12	2.68	100.83	114.42	8	3
4	A	330	PX4	O4-P1-O2	2.67	119.52	109.07	8	1
4	A	377	PX4	O4-P1-O2	2.68	98.61	109.07	1	3
4	A	320	PX4	C12-C11-C10	2.67	103.58	113.19	2	2
4	A	319	PX4	C12-C11-C10	2.67	103.58	113.19	5	3
4	A	353	PX4	C1-C2-N1	2.67	124.70	115.78	1	2
4	A	368	PX4	C14-C13-C12	2.67	100.86	114.42	7	3
4	A	396	PX4	O7-C23-O8	2.67	130.16	123.70	9	2
4	A	404	PX4	C27-C26-C25	2.67	100.86	114.42	2	2
4	A	408	PX4	O3-P1-O2	2.67	98.62	109.07	1	4
4	A	365	PX4	O5-C9-O6	2.67	116.85	123.59	4	5
4	A	370	PX4	C1-C2-N1	2.67	124.70	115.78	11	3
4	A	414	PX4	C26-C25-C24	2.67	103.59	113.19	13	1
4	A	417	PX4	C5-N1-C3	2.67	102.10	108.97	4	3
4	A	370	PX4	O4-P1-O2	2.67	119.50	109.07	11	1
4	A	372	PX4	C31-C30-C29	2.67	100.86	114.42	14	1
4	A	329	PX4	C30-C29-C28	2.67	100.87	114.42	4	2
4	A	360	PX4	C5-N1-C3	2.67	102.11	108.97	7	2
4	A	374	PX4	C29-C28-C27	2.67	100.87	114.42	1	1
4	A	388	PX4	C4-N1-C3	2.67	102.11	108.97	13	2
4	A	406	PX4	O1-P1-O3	2.67	95.35	107.75	14	3
4	A	384	PX4	O6-C9-C10	2.67	113.33	123.73	7	1
4	A	397	PX4	C31-C30-C29	2.67	100.89	114.42	10	4
4	A	407	PX4	O3-P1-O2	2.67	98.64	109.07	2	3
4	A	408	PX4	C28-C27-C26	2.67	100.88	114.42	7	1
4	A	373	PX4	O4-P1-O2	2.66	119.48	109.07	7	6
4	A	377	PX4	O7-C7-C6	2.66	118.05	108.40	6	4
4	A	397	PX4	O1-P1-O2	2.66	125.41	112.24	7	6
4	A	312	PX4	O5-C9-C10	2.66	120.26	111.91	4	3
4	A	376	PX4	C17-C16-C15	2.66	100.91	114.42	14	1
4	A	393	PX4	O3-C1-C2	2.66	123.16	109.16	14	1
4	A	395	PX4	O8-C23-C24	2.66	113.35	123.73	14	1
4	A	320	PX4	O1-P1-O4	2.66	120.10	107.75	7	3
4	A	330	PX4	C4-N1-C3	2.66	115.81	108.97	4	1
4	A	347	PX4	C26-C25-C24	2.66	103.63	113.19	7	3
4	A	349	PX4	C12-C11-C10	2.66	103.63	113.19	1	2
4	A	363	PX4	C13-C12-C11	2.66	100.92	114.42	14	1
4	A	382	PX4	C31-C30-C29	2.66	100.92	114.42	13	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	370	PX4	O3-C1-C2	2.66	123.14	109.16	12	2
4	A	386	PX4	C11-C10-C9	2.66	103.95	113.62	7	2
4	A	399	PX4	C8-O5-C9	2.66	107.27	117.12	11	4
4	A	404	PX4	C4-N1-C2	2.66	120.80	109.92	1	1
4	A	411	PX4	O5-C9-C10	2.66	120.25	111.91	13	4
4	A	386	PX4	C1-C2-N1	2.66	124.66	115.78	14	2
4	A	428	PX4	C20-C19-C18	2.66	100.93	114.42	3	2
4	A	430	PX4	O1-P1-O4	2.66	120.09	107.75	3	3
4	A	310	PX4	C26-C25-C24	2.66	103.64	113.19	2	2
4	A	333	PX4	C26-C25-C24	2.66	103.64	113.19	8	1
4	A	340	PX4	O7-C7-C8	2.66	118.02	108.40	8	5
4	A	363	PX4	C3-N1-C2	2.66	120.78	109.92	6	3
4	A	365	PX4	C4-N1-C3	2.66	115.81	108.97	10	2
4	A	421	PX4	O7-C7-C6	2.66	118.02	108.40	7	2
4	A	309	PX4	O1-P1-O3	2.65	95.42	107.75	3	3
4	A	317	PX4	O3-P1-O2	2.66	98.69	109.07	9	1
4	A	396	PX4	C20-C19-C18	2.66	100.94	114.42	2	2
4	A	402	PX4	O7-C7-C6	2.66	118.02	108.40	13	5
4	A	413	PX4	C7-O7-C23	2.66	111.25	117.79	11	5
4	A	330	PX4	C1-C2-N1	2.65	124.64	115.78	4	4
4	A	332	PX4	C29-C28-C27	2.65	100.95	114.42	11	2
4	A	335	PX4	C8-O5-C9	2.65	107.29	117.12	5	3
4	A	392	PX4	P1-O4-C6	2.65	106.12	121.68	10	5
4	A	347	PX4	C4-N1-C3	2.65	102.15	108.97	11	3
4	A	358	PX4	O1-P1-O3	2.65	95.42	107.75	11	2
4	A	327	PX4	C16-C15-C14	2.65	100.96	114.42	4	1
4	A	328	PX4	O5-C9-O6	2.65	116.90	123.59	14	6
4	A	330	PX4	O3-P1-O2	2.65	98.71	109.07	9	1
4	A	335	PX4	C31-C30-C29	2.65	100.97	114.42	13	1
4	A	346	PX4	O5-C9-C10	2.65	120.23	111.91	6	1
4	A	399	PX4	C16-C15-C14	2.65	100.96	114.42	14	2
4	A	385	PX4	O3-P1-O2	2.65	98.71	109.07	4	1
4	A	418	PX4	C7-O7-C23	2.65	124.31	117.79	10	2
4	A	428	PX4	C7-O7-C23	2.65	124.32	117.79	12	4
4	A	341	PX4	O7-C7-C6	2.65	117.99	108.40	7	4
4	A	372	PX4	C26-C25-C24	2.65	103.67	113.19	7	1
4	A	392	PX4	O1-P1-O4	2.65	120.05	107.75	11	1
4	A	401	PX4	C34-C33-C32	2.65	100.98	114.42	8	1
4	A	402	PX4	C13-C12-C11	2.65	100.98	114.42	2	2
4	A	409	PX4	C12-C11-C10	2.65	103.67	113.19	13	3
4	A	412	PX4	C28-C27-C26	2.65	100.97	114.42	14	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	340	PX4	C27-C26-C25	2.65	100.99	114.42	9	2
4	A	358	PX4	C26-C25-C24	2.65	103.67	113.19	4	1
4	A	394	PX4	C17-C16-C15	2.65	100.99	114.42	10	1
4	A	320	PX4	C25-C24-C23	2.65	104.00	113.62	5	2
4	A	398	PX4	C20-C19-C18	2.65	100.99	114.42	7	1
4	A	420	PX4	O7-C7-C6	2.65	117.98	108.40	11	4
4	A	314	PX4	C20-C19-C18	2.64	101.00	114.42	8	4
4	A	400	PX4	O1-P1-O2	2.64	125.31	112.24	8	6
4	A	404	PX4	O5-C9-O6	2.64	116.92	123.59	2	1
4	A	316	PX4	C14-C13-C12	2.64	101.01	114.42	5	2
4	A	324	PX4	O1-P1-O3	2.64	95.47	107.75	5	2
4	A	326	PX4	O3-C1-C2	2.64	123.06	109.16	11	1
4	A	353	PX4	C5-N1-C3	2.64	102.18	108.97	14	3
4	A	421	PX4	P1-O4-C6	2.64	106.18	121.68	2	10
4	A	421	PX4	C12-C11-C10	2.64	103.69	113.19	5	1
4	A	381	PX4	O5-C9-C10	2.64	120.20	111.91	6	3
4	A	317	PX4	C16-C15-C14	2.64	101.02	114.42	5	2
4	A	369	PX4	C5-N1-C3	2.64	102.18	108.97	11	3
4	A	428	PX4	O3-P1-O2	2.64	98.74	109.07	9	1
4	A	327	PX4	C5-N1-C2	2.64	99.12	109.92	2	2
4	A	326	PX4	C34-C33-C32	2.64	101.03	114.42	7	2
4	A	334	PX4	C11-C10-C9	2.64	104.03	113.62	6	1
4	A	340	PX4	O6-C9-C10	2.64	113.44	123.73	14	4
4	A	374	PX4	C5-N1-C4	2.64	115.76	108.97	14	3
4	A	387	PX4	O8-C23-C24	2.64	113.44	123.73	2	1
4	A	397	PX4	O6-C9-C10	2.64	113.44	123.73	11	2
4	A	317	PX4	C5-N1-C4	2.63	102.20	108.97	13	4
4	A	339	PX4	O5-C9-C10	2.64	120.18	111.91	11	1
4	A	370	PX4	C12-C11-C10	2.64	103.72	113.19	5	2
4	A	393	PX4	O1-P1-O3	2.64	95.50	107.75	5	2
4	A	399	PX4	C13-C12-C11	2.63	101.05	114.42	2	1
4	A	356	PX4	O7-C7-C6	2.63	117.93	108.40	8	4
4	A	317	PX4	C11-C10-C9	2.63	123.19	113.62	6	4
4	A	326	PX4	C17-C16-C15	2.63	101.07	114.42	5	2
4	A	393	PX4	C11-C10-C9	2.63	104.05	113.62	7	1
4	A	404	PX4	C17-C16-C15	2.63	101.06	114.42	1	1
4	A	311	PX4	C18-C17-C16	2.63	101.07	114.42	12	3
4	A	312	PX4	C18-C17-C16	2.63	101.08	114.42	2	2
4	A	314	PX4	C33-C32-C31	2.63	101.08	114.42	4	3
4	A	318	PX4	C11-C10-C9	2.63	104.06	113.62	10	3
4	A	380	PX4	C11-C10-C9	2.63	104.06	113.62	4	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	370	PX4	O7-C7-C6	2.63	117.91	108.40	14	2
4	A	428	PX4	O5-C9-C10	2.63	120.15	111.91	2	4
4	A	417	PX4	C11-C10-C9	2.63	104.07	113.62	3	1
4	A	314	PX4	C28-C27-C26	2.62	101.11	114.42	11	1
4	A	359	PX4	C12-C11-C10	2.62	103.76	113.19	8	2
4	A	370	PX4	C16-C15-C14	2.62	101.12	114.42	4	1
4	A	396	PX4	C29-C28-C27	2.62	101.12	114.42	9	1
4	A	420	PX4	O3-P1-O2	2.62	98.82	109.07	10	3
4	A	424	PX4	O3-P1-O2	2.62	98.82	109.07	11	5
4	A	333	PX4	C25-C24-C23	2.62	104.09	113.62	11	1
4	A	410	PX4	C25-C24-C23	2.62	104.09	113.62	12	2
4	A	338	PX4	C1-C2-N1	2.62	124.52	115.78	7	3
4	A	359	PX4	C5-N1-C3	2.62	102.24	108.97	12	6
4	A	359	PX4	C30-C29-C28	2.62	101.13	114.42	5	1
4	A	366	PX4	C8-O5-C9	2.62	107.42	117.12	10	2
4	A	386	PX4	O4-P1-O2	2.62	119.30	109.07	1	3
4	A	414	PX4	O3-C1-C2	2.62	122.93	109.16	4	2
4	A	330	PX4	C19-C18-C17	2.62	101.14	114.42	13	1
4	A	379	PX4	O3-C1-C2	2.62	122.92	109.16	11	2
4	A	405	PX4	O3-P1-O2	2.62	98.84	109.07	14	2
4	A	414	PX4	O4-P1-O2	2.62	119.29	109.07	1	3
4	A	365	PX4	C26-C25-C24	2.61	103.79	113.19	1	2
4	A	324	PX4	C8-O5-C9	2.61	107.44	117.12	14	3
4	A	398	PX4	C33-C32-C31	2.61	101.16	114.42	9	2
4	A	406	PX4	C1-C2-N1	2.61	124.51	115.78	9	4
4	A	325	PX4	C19-C18-C17	2.61	101.16	114.42	8	2
4	A	348	PX4	C5-N1-C2	2.61	120.61	109.92	2	1
4	A	407	PX4	C28-C27-C26	2.61	101.16	114.42	9	2
4	A	412	PX4	C14-C13-C12	2.61	101.16	114.42	3	1
4	A	348	PX4	C4-N1-C3	2.61	102.26	108.97	6	3
4	A	379	PX4	C20-C19-C18	2.61	101.17	114.42	5	2
4	A	393	PX4	O1-P1-O4	2.61	119.87	107.75	14	2
4	A	409	PX4	C18-C17-C16	2.61	101.17	114.42	1	1
4	A	412	PX4	O3-P1-O2	2.61	98.87	109.07	5	4
4	A	312	PX4	C28-C27-C26	2.61	101.18	114.42	5	4
4	A	319	PX4	C5-N1-C2	2.61	120.59	109.92	14	1
4	A	403	PX4	C5-N1-C2	2.61	120.59	109.92	5	1
4	A	317	PX4	C31-C30-C29	2.61	101.19	114.42	1	2
4	A	397	PX4	C26-C25-C24	2.61	103.82	113.19	13	1
4	A	410	PX4	O1-P1-O4	2.61	119.85	107.75	7	2
4	A	415	PX4	O5-C9-O6	2.61	117.01	123.59	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	310	PX4	C8-O5-C9	2.60	107.47	117.12	14	2
4	A	331	PX4	C12-C11-C10	2.61	103.82	113.19	13	3
4	A	398	PX4	C29-C28-C27	2.61	101.20	114.42	10	1
4	A	404	PX4	C28-C27-C26	2.60	101.21	114.42	9	2
4	A	430	PX4	C26-C25-C24	2.60	103.83	113.19	2	2
4	A	383	PX4	O3-C1-C2	2.60	122.84	109.16	2	2
4	A	390	PX4	C4-N1-C3	2.60	102.28	108.97	3	2
4	A	397	PX4	O4-P1-O2	2.60	119.23	109.07	11	2
4	A	399	PX4	C19-C18-C17	2.60	101.22	114.42	9	3
4	A	424	PX4	C1-C2-N1	2.60	124.47	115.78	5	2
4	A	306	PX4	C4-N1-C3	2.60	102.29	108.97	8	2
4	A	318	PX4	O5-C9-C10	2.60	120.06	111.91	10	2
4	A	362	PX4	C30-C29-C28	2.60	101.22	114.42	11	1
4	A	405	PX4	C13-C12-C11	2.60	101.22	114.42	4	1
4	A	404	PX4	O1-P1-O4	2.60	119.81	107.75	13	2
4	A	407	PX4	C1-C2-N1	2.60	124.46	115.78	12	2
4	A	327	PX4	C11-C10-C9	2.60	104.17	113.62	4	1
4	A	378	PX4	C20-C19-C18	2.60	101.24	114.42	14	1
4	A	406	PX4	C4-N1-C2	2.60	120.54	109.92	13	2
4	A	337	PX4	C3-N1-C2	2.59	99.30	109.92	3	1
4	A	418	PX4	O3-C1-C2	2.60	122.81	109.16	6	3
4	A	311	PX4	C7-O7-C23	2.59	111.41	117.79	5	1
4	A	324	PX4	C11-C10-C9	2.59	104.19	113.62	5	2
4	A	384	PX4	C5-N1-C2	2.59	120.53	109.92	3	3
4	A	400	PX4	C5-N1-C2	2.59	120.53	109.92	2	3
4	A	419	PX4	C12-C11-C10	2.59	103.87	113.19	8	1
4	A	422	PX4	C4-N1-C2	2.59	99.31	109.92	7	3
4	A	348	PX4	C34-C33-C32	2.59	101.27	114.42	9	1
4	A	382	PX4	C3-N1-C2	2.59	99.31	109.92	5	1
4	A	425	PX4	C13-C12-C11	2.59	101.27	114.42	3	2
4	A	306	PX4	O3-P1-O2	2.59	98.95	109.07	8	3
4	A	361	PX4	C34-C33-C32	2.59	101.28	114.42	11	2
4	A	364	PX4	O8-C23-C24	2.59	133.83	123.73	11	2
4	A	377	PX4	C12-C11-C10	2.59	122.50	113.19	7	2
4	A	409	PX4	C1-C2-N1	2.59	124.42	115.78	8	5
4	A	413	PX4	C34-C33-C32	2.59	101.28	114.42	3	3
4	A	428	PX4	O1-P1-O4	2.59	119.77	107.75	13	1
4	A	423	PX4	C31-C30-C29	2.59	101.28	114.42	12	2
4	A	425	PX4	C28-C27-C26	2.59	101.28	114.42	9	2
4	A	426	PX4	C27-C26-C25	2.59	101.28	114.42	7	2
4	A	321	PX4	C5-N1-C4	2.59	115.63	108.97	5	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	374	PX4	O3-P1-O2	2.59	98.96	109.07	12	2
4	A	327	PX4	O5-C9-C10	2.59	120.02	111.91	13	5
4	A	421	PX4	C15-C14-C13	2.59	101.30	114.42	14	2
4	A	330	PX4	O5-C9-C10	2.58	120.02	111.91	6	1
4	A	359	PX4	C1-C2-N1	2.58	124.41	115.78	12	3
4	A	390	PX4	C30-C29-C28	2.58	101.31	114.42	6	1
4	A	397	PX4	O1-P1-O4	2.58	119.74	107.75	14	3
4	A	407	PX4	O6-C9-C10	2.58	113.65	123.73	8	1
4	A	307	PX4	C11-C10-C9	2.58	104.23	113.62	4	2
4	A	313	PX4	C25-C24-C23	2.58	104.23	113.62	3	1
4	A	341	PX4	O5-C9-C10	2.58	120.01	111.91	8	5
4	A	371	PX4	C28-C27-C26	2.58	101.32	114.42	1	1
4	A	408	PX4	C34-C33-C32	2.58	101.32	114.42	5	1
4	A	408	PX4	C18-C17-C16	2.58	101.32	114.42	6	1
4	A	306	PX4	O1-P1-O3	2.58	95.76	107.75	1	3
4	A	320	PX4	O1-P1-O3	2.58	95.77	107.75	8	3
4	A	321	PX4	C5-N1-C2	2.58	120.47	109.92	11	1
4	A	326	PX4	C20-C19-C18	2.58	101.33	114.42	12	1
4	A	340	PX4	C31-C30-C29	2.58	101.34	114.42	10	2
4	A	397	PX4	C19-C18-C17	2.58	101.34	114.42	3	2
4	A	331	PX4	C13-C12-C11	2.57	101.35	114.42	3	1
4	A	361	PX4	O1-P1-O2	2.57	124.96	112.24	14	6
4	A	365	PX4	C3-N1-C2	2.57	99.39	109.92	5	1
4	A	367	PX4	O7-C7-C8	2.57	117.72	108.40	8	2
4	A	337	PX4	C18-C17-C16	2.57	101.37	114.42	7	2
4	A	388	PX4	O3-C1-C2	2.57	122.69	109.16	2	2
4	A	400	PX4	C1-C2-N1	2.57	124.36	115.78	10	2
4	A	332	PX4	C14-C13-C12	2.57	101.38	114.42	9	2
4	A	344	PX4	O1-P1-O3	2.57	95.81	107.75	1	2
4	A	382	PX4	C34-C33-C32	2.57	101.38	114.42	8	1
4	A	396	PX4	C33-C32-C31	2.57	101.38	114.42	13	2
4	A	309	PX4	C8-O5-C9	2.57	107.61	117.12	7	3
4	A	331	PX4	C29-C28-C27	2.57	101.39	114.42	3	1
4	A	412	PX4	C31-C30-C29	2.57	101.39	114.42	4	1
4	A	415	PX4	C29-C28-C27	2.57	101.39	114.42	6	3
4	A	317	PX4	C15-C14-C13	2.57	101.39	114.42	9	2
4	A	372	PX4	C33-C32-C31	2.57	101.40	114.42	7	1
4	A	389	PX4	O3-P1-O2	2.57	99.04	109.07	6	4
4	A	307	PX4	C16-C15-C14	2.56	101.40	114.42	9	1
4	A	309	PX4	C27-C26-C25	2.57	101.40	114.42	5	1
4	A	311	PX4	O5-C9-C10	2.56	119.95	111.91	9	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	313	PX4	C15-C14-C13	2.56	101.41	114.42	13	1
4	A	327	PX4	O1-P1-O4	2.56	119.66	107.75	3	5
4	A	333	PX4	C8-O5-C9	2.56	126.62	117.12	8	3
4	A	345	PX4	C34-C33-C32	2.56	101.40	114.42	3	3
4	A	348	PX4	C32-C31-C30	2.57	101.40	114.42	10	1
4	A	376	PX4	C12-C11-C10	2.56	103.97	113.19	8	1
4	A	412	PX4	O4-P1-O2	2.57	119.09	109.07	5	2
4	A	321	PX4	O7-C7-C6	2.56	117.68	108.40	8	2
4	A	323	PX4	O3-C1-C2	2.56	122.64	109.16	14	2
4	A	325	PX4	C18-C17-C16	2.56	101.41	114.42	13	3
4	A	352	PX4	C15-C14-C13	2.56	101.41	114.42	6	1
4	A	357	PX4	C30-C29-C28	2.56	101.41	114.42	11	2
4	A	339	PX4	O5-C9-O6	2.56	130.06	123.59	10	1
4	A	363	PX4	C31-C30-C29	2.56	101.41	114.42	3	1
4	A	364	PX4	C17-C16-C15	2.56	101.41	114.42	8	1
4	A	408	PX4	C14-C13-C12	2.56	101.41	114.42	9	1
4	A	309	PX4	C30-C29-C28	2.56	101.42	114.42	11	1
4	A	320	PX4	C32-C31-C30	2.56	101.42	114.42	9	1
4	A	367	PX4	O1-P1-O4	2.56	119.64	107.75	11	2
4	A	406	PX4	C4-N1-C3	2.56	102.39	108.97	13	3
4	A	408	PX4	C5-N1-C3	2.56	102.39	108.97	9	2
4	A	429	PX4	C3-N1-C2	2.56	99.43	109.92	10	3
4	A	332	PX4	O7-C7-C6	2.56	117.67	108.40	6	7
4	A	343	PX4	C27-C26-C25	2.56	101.43	114.42	2	1
4	A	352	PX4	O3-P1-O2	2.56	99.07	109.07	5	2
4	A	389	PX4	C1-C2-N1	2.56	124.33	115.78	2	2
4	A	390	PX4	O1-P1-O4	2.56	119.63	107.75	2	1
4	A	412	PX4	C20-C19-C18	2.56	101.43	114.42	1	2
4	A	415	PX4	C17-C16-C15	2.56	101.43	114.42	8	1
4	A	315	PX4	C33-C32-C31	2.56	101.44	114.42	6	1
4	A	317	PX4	O5-C9-O6	2.56	117.14	123.59	1	1
4	A	353	PX4	C12-C11-C10	2.56	122.39	113.19	10	1
4	A	370	PX4	C26-C25-C24	2.56	104.00	113.19	14	3
4	A	426	PX4	C5-N1-C2	2.56	99.45	109.92	4	2
4	A	319	PX4	C27-C26-C25	2.56	101.45	114.42	1	1
4	A	340	PX4	O3-P1-O2	2.55	99.08	109.07	5	4
4	A	360	PX4	O4-P1-O2	2.55	119.05	109.07	9	4
4	A	384	PX4	O1-P1-O3	2.55	95.88	107.75	13	2
4	A	311	PX4	C8-O5-C9	2.55	107.67	117.12	6	2
4	A	312	PX4	C34-C33-C32	2.55	101.47	114.42	5	4
4	A	349	PX4	O4-P1-O2	2.55	99.09	109.07	10	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	370	PX4	O1-P1-O3	2.55	119.60	107.75	14	1
4	A	396	PX4	O3-C1-C2	2.55	122.59	109.16	10	2
4	A	323	PX4	C29-C28-C27	2.55	101.47	114.42	4	2
4	A	345	PX4	C1-C2-N1	2.55	124.30	115.78	9	1
4	A	406	PX4	C34-C33-C32	2.55	101.47	114.42	5	2
4	A	428	PX4	C34-C33-C32	2.55	101.47	114.42	12	3
4	A	358	PX4	C11-C10-C9	2.55	104.34	113.62	12	1
4	A	376	PX4	O7-C7-C6	2.55	117.64	108.40	7	3
4	A	385	PX4	C34-C33-C32	2.55	101.48	114.42	1	1
4	A	390	PX4	O1-P1-O2	2.55	124.85	112.24	10	7
4	A	390	PX4	C28-C27-C26	2.55	101.48	114.42	3	1
4	A	316	PX4	C5-N1-C3	2.55	102.42	108.97	8	3
4	A	328	PX4	C16-C15-C14	2.55	101.49	114.42	3	2
4	A	411	PX4	C7-O7-C23	2.55	124.07	117.79	12	1
4	A	397	PX4	O8-C23-C24	2.55	113.79	123.73	3	2
4	A	417	PX4	C1-C2-N1	2.55	124.29	115.78	2	2
4	A	313	PX4	O1-P1-O3	2.55	95.92	107.75	12	3
4	A	324	PX4	C5-N1-C3	2.55	102.43	108.97	12	3
4	A	349	PX4	C13-C12-C11	2.55	101.50	114.42	3	2
4	A	365	PX4	C11-C10-C9	2.55	122.88	113.62	12	2
4	A	370	PX4	C15-C14-C13	2.55	101.50	114.42	8	1
4	A	391	PX4	O8-C23-C24	2.55	113.80	123.73	3	2
4	A	388	PX4	C19-C18-C17	2.54	101.51	114.42	8	1
4	A	425	PX4	O3-C1-C2	2.55	122.55	109.16	9	1
4	A	332	PX4	O3-P1-O2	2.54	99.13	109.07	2	2
4	A	365	PX4	C15-C14-C13	2.54	101.51	114.42	7	1
4	A	410	PX4	C28-C27-C26	2.54	101.52	114.42	5	1
4	A	414	PX4	C8-O5-C9	2.54	107.70	117.12	4	2
4	A	421	PX4	C13-C12-C11	2.54	101.51	114.42	10	1
4	A	322	PX4	C19-C18-C17	2.54	101.52	114.42	9	2
4	A	332	PX4	C25-C24-C23	2.54	104.38	113.62	4	1
4	A	360	PX4	C15-C14-C13	2.54	101.52	114.42	6	2
4	A	426	PX4	O3-P1-O2	2.54	99.14	109.07	10	3
4	A	331	PX4	C1-C2-N1	2.54	124.26	115.78	1	1
4	A	373	PX4	O7-C7-C6	2.54	117.60	108.40	4	6
4	A	411	PX4	C25-C24-C23	2.54	104.38	113.62	6	3
4	A	422	PX4	C7-O7-C23	2.54	124.04	117.79	11	2
4	A	425	PX4	C26-C25-C24	2.54	104.06	113.19	4	1
4	A	313	PX4	C3-N1-C2	2.54	120.30	109.92	10	1
4	A	316	PX4	C5-N1-C4	2.54	102.45	108.97	4	4
4	A	342	PX4	O1-P1-O4	2.54	119.53	107.75	3	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	336	PX4	C13-C12-C11	2.54	101.55	114.42	13	1
4	A	369	PX4	C17-C16-C15	2.54	101.55	114.42	10	1
4	A	371	PX4	C25-C24-C23	2.54	104.40	113.62	10	3
4	A	333	PX4	O3-C1-C2	2.53	122.49	109.16	3	1
4	A	349	PX4	C31-C30-C29	2.53	101.56	114.42	5	1
4	A	414	PX4	C3-N1-C2	2.54	120.29	109.92	5	3
4	A	376	PX4	C28-C27-C26	2.53	101.56	114.42	2	2
4	A	385	PX4	C12-C11-C10	2.53	104.08	113.19	13	5
4	A	392	PX4	O3-C1-C2	2.53	122.49	109.16	8	2
4	A	415	PX4	C1-C2-N1	2.53	124.24	115.78	1	4
4	A	401	PX4	C28-C27-C26	2.53	101.56	114.42	10	2
4	A	422	PX4	C11-C10-C9	2.53	104.40	113.62	8	1
4	A	311	PX4	C5-N1-C4	2.53	102.46	108.97	14	5
4	A	389	PX4	O4-P1-O2	2.53	118.96	109.07	7	4
4	A	389	PX4	C5-N1-C4	2.53	115.49	108.97	8	4
4	A	376	PX4	C18-C17-C16	2.53	101.58	114.42	11	2
4	A	379	PX4	C31-C30-C29	2.53	101.57	114.42	1	1
4	A	392	PX4	C31-C30-C29	2.53	101.57	114.42	12	1
4	A	422	PX4	C28-C27-C26	2.53	101.56	114.42	4	1
4	A	367	PX4	C17-C16-C15	2.53	101.58	114.42	13	3
4	A	319	PX4	C17-C16-C15	2.53	101.59	114.42	11	1
4	A	333	PX4	C12-C11-C10	2.53	104.10	113.19	6	1
4	A	350	PX4	C19-C18-C17	2.53	101.58	114.42	11	1
4	A	323	PX4	C26-C25-C24	2.53	104.11	113.19	2	2
4	A	355	PX4	C12-C11-C10	2.53	104.10	113.19	2	1
4	A	398	PX4	O3-C1-C2	2.53	122.46	109.16	14	1
4	A	430	PX4	C30-C29-C28	2.53	101.59	114.42	9	1
4	A	318	PX4	O5-C9-O6	2.53	117.22	123.59	1	2
4	A	395	PX4	C31-C30-C29	2.53	101.60	114.42	9	2
4	A	397	PX4	O5-C9-O6	2.53	117.22	123.59	13	3
4	A	398	PX4	C26-C25-C24	2.53	104.11	113.19	12	2
4	A	396	PX4	O3-P1-O2	2.52	99.20	109.07	12	1
4	A	399	PX4	C1-C2-N1	2.53	124.21	115.78	12	2
4	A	330	PX4	C3-N1-C2	2.52	99.59	109.92	1	1
4	A	334	PX4	C25-C24-C23	2.52	104.44	113.62	13	2
4	A	417	PX4	O5-C9-O6	2.52	117.22	123.59	12	6
4	A	372	PX4	O7-C7-C6	2.52	117.54	108.40	5	3
4	A	398	PX4	C11-C10-C9	2.52	104.44	113.62	1	2
4	A	424	PX4	O5-C9-C10	2.52	119.83	111.91	8	3
4	A	307	PX4	O4-P1-O2	2.52	118.92	109.07	12	1
4	A	364	PX4	O6-C9-C10	2.52	113.89	123.73	13	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	312	PX4	C17-C16-C15	2.52	101.63	114.42	12	3
4	A	354	PX4	C27-C26-C25	2.52	101.63	114.42	2	2
4	A	390	PX4	O5-C9-C10	2.52	119.82	111.91	5	3
4	A	408	PX4	C33-C32-C31	2.52	101.63	114.42	6	1
4	A	422	PX4	C17-C16-C15	2.52	101.63	114.42	11	1
4	A	427	PX4	C8-O5-C9	2.52	107.79	117.12	14	1
4	A	313	PX4	C27-C26-C25	2.52	101.64	114.42	9	2
4	A	322	PX4	C1-C2-N1	2.52	124.19	115.78	14	2
4	A	371	PX4	C14-C13-C12	2.52	101.64	114.42	5	3
4	A	386	PX4	C20-C19-C18	2.52	101.64	114.42	6	2
4	A	389	PX4	C7-O7-C23	2.52	123.99	117.79	14	2
4	A	337	PX4	C1-C2-N1	2.52	124.18	115.78	10	3
4	A	342	PX4	C14-C13-C12	2.52	101.65	114.42	14	1
4	A	340	PX4	C3-N1-C2	2.52	99.62	109.92	9	2
4	A	345	PX4	O1-P1-O3	2.52	96.06	107.75	4	4
4	A	318	PX4	C3-N1-C2	2.52	120.21	109.92	9	1
4	A	318	PX4	O4-P1-O2	2.51	99.24	109.07	10	2
4	A	332	PX4	C5-N1-C2	2.51	99.63	109.92	11	1
4	A	417	PX4	C5-N1-C4	2.51	102.51	108.97	10	2
4	A	429	PX4	C4-N1-C3	2.52	115.44	108.97	11	2
4	A	358	PX4	O7-C7-C6	2.51	117.50	108.40	6	4
4	A	368	PX4	C11-C10-C9	2.51	104.48	113.62	5	1
4	A	325	PX4	O3-C1-C2	2.51	122.37	109.16	3	2
4	A	327	PX4	C3-N1-C2	2.51	120.20	109.92	13	1
4	A	338	PX4	C8-O5-C9	2.51	107.82	117.12	2	2
4	A	356	PX4	C13-C12-C11	2.51	101.67	114.42	8	1
4	A	392	PX4	O8-C23-C24	2.51	113.93	123.73	2	1
4	A	399	PX4	C17-C16-C15	2.51	101.67	114.42	13	2
4	A	374	PX4	C27-C26-C25	2.51	101.68	114.42	12	3
4	A	385	PX4	C33-C32-C31	2.51	101.68	114.42	6	1
4	A	386	PX4	C31-C30-C29	2.51	101.68	114.42	7	2
4	A	399	PX4	C15-C14-C13	2.51	101.68	114.42	9	1
4	A	411	PX4	C1-C2-N1	2.51	124.17	115.78	9	3
4	A	324	PX4	C15-C14-C13	2.51	101.69	114.42	10	1
4	A	326	PX4	C25-C24-C23	2.51	104.50	113.62	13	2
4	A	328	PX4	C17-C16-C15	2.51	101.69	114.42	13	1
4	A	332	PX4	C26-C25-C24	2.51	104.17	113.19	5	3
4	A	387	PX4	C19-C18-C17	2.51	101.68	114.42	5	2
4	A	392	PX4	C14-C13-C12	2.51	101.69	114.42	9	1
4	A	415	PX4	C16-C15-C14	2.51	101.68	114.42	3	2
4	A	315	PX4	O3-P1-O2	2.51	99.27	109.07	4	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	347	PX4	C1-C2-N1	2.51	124.15	115.78	9	3
4	A	355	PX4	C13-C12-C11	2.51	101.69	114.42	11	1
4	A	360	PX4	C13-C12-C11	2.51	101.69	114.42	13	1
4	A	394	PX4	C1-C2-N1	2.51	124.15	115.78	12	2
4	A	398	PX4	O8-C23-C24	2.51	113.95	123.73	4	2
4	A	411	PX4	O7-C7-C6	2.51	117.48	108.40	4	4
4	A	312	PX4	O1-P1-O2	2.51	124.63	112.24	6	5
4	A	365	PX4	C30-C29-C28	2.51	101.70	114.42	1	1
4	A	414	PX4	O3-P1-O2	2.51	99.27	109.07	1	2
4	A	312	PX4	C3-N1-C2	2.51	99.67	109.92	9	2
4	A	315	PX4	O6-C9-C10	2.51	113.96	123.73	3	1
4	A	315	PX4	C11-C10-C9	2.51	104.51	113.62	7	1
4	A	329	PX4	C28-C27-C26	2.51	101.71	114.42	6	1
4	A	343	PX4	C29-C28-C27	2.50	101.71	114.42	5	1
4	A	323	PX4	C5-N1-C4	2.50	102.54	108.97	5	3
4	A	368	PX4	O8-C23-C24	2.50	113.96	123.73	13	2
4	A	389	PX4	C16-C15-C14	2.50	101.71	114.42	6	1
4	A	396	PX4	C30-C29-C28	2.50	101.71	114.42	5	1
4	A	315	PX4	C15-C14-C13	2.50	101.72	114.42	3	1
4	A	319	PX4	C20-C19-C18	2.50	101.72	114.42	7	1
4	A	324	PX4	C20-C19-C18	2.50	101.72	114.42	2	4
4	A	361	PX4	C17-C16-C15	2.50	101.72	114.42	5	1
4	A	397	PX4	C29-C28-C27	2.50	101.72	114.42	6	4
4	A	403	PX4	O3-C1-C2	2.50	122.32	109.16	5	1
4	A	407	PX4	C19-C18-C17	2.50	101.72	114.42	4	1
4	A	408	PX4	C17-C16-C15	2.50	101.72	114.42	4	2
4	A	411	PX4	C33-C32-C31	2.50	101.72	114.42	8	2
4	A	419	PX4	C15-C14-C13	2.50	101.72	114.42	8	1
4	A	421	PX4	C5-N1-C4	2.50	102.54	108.97	6	4
4	A	356	PX4	C34-C33-C32	2.50	101.73	114.42	12	1
4	A	363	PX4	O3-P1-O2	2.50	99.29	109.07	10	2
4	A	364	PX4	C5-N1-C2	2.50	120.15	109.92	13	2
4	A	428	PX4	C25-C24-C23	2.50	104.52	113.62	10	1
4	A	335	PX4	C27-C26-C25	2.50	101.74	114.42	14	1
4	A	370	PX4	C33-C32-C31	2.50	101.73	114.42	10	3
4	A	388	PX4	O5-C9-O6	2.50	117.28	123.59	13	1
4	A	392	PX4	O1-P1-O3	2.50	96.13	107.75	11	1
4	A	408	PX4	C11-C10-C9	2.50	104.53	113.62	1	1
4	A	428	PX4	O6-C9-C10	2.50	113.98	123.73	3	2
4	A	343	PX4	O5-C9-O6	2.50	117.29	123.59	5	5
4	A	368	PX4	C5-N1-C2	2.50	99.70	109.92	14	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	402	PX4	C18-C17-C16	2.50	101.75	114.42	6	2
4	A	417	PX4	C3-N1-C2	2.50	99.70	109.92	9	1
4	A	419	PX4	O7-C23-O8	2.50	117.67	123.70	2	2
4	A	308	PX4	C34-C33-C32	2.49	101.76	114.42	11	2
4	A	312	PX4	C27-C26-C25	2.49	101.77	114.42	2	1
4	A	351	PX4	C27-C26-C25	2.49	101.76	114.42	4	2
4	A	318	PX4	C20-C19-C18	2.49	101.78	114.42	14	2
4	A	324	PX4	C26-C25-C24	2.49	104.23	113.19	11	3
4	A	330	PX4	C34-C33-C32	2.49	101.77	114.42	7	1
4	A	345	PX4	C19-C18-C17	2.49	101.77	114.42	11	2
4	A	346	PX4	C31-C30-C29	2.49	101.77	114.42	7	1
4	A	352	PX4	C3-N1-C2	2.49	99.72	109.92	6	2
4	A	360	PX4	C18-C17-C16	2.49	101.77	114.42	1	1
4	A	392	PX4	C17-C16-C15	2.49	101.77	114.42	5	1
4	A	421	PX4	C5-N1-C3	2.49	102.56	108.97	5	1
4	A	426	PX4	O3-C1-C2	2.49	122.28	109.16	9	1
4	A	340	PX4	C4-N1-C2	2.49	120.11	109.92	10	4
4	A	356	PX4	C14-C13-C12	2.49	101.78	114.42	5	2
4	A	372	PX4	C1-C2-N1	2.49	124.09	115.78	13	5
4	A	407	PX4	C34-C33-C32	2.49	101.78	114.42	1	1
4	A	416	PX4	C16-C15-C14	2.49	101.79	114.42	1	1
4	A	343	PX4	C32-C31-C30	2.49	101.79	114.42	2	1
4	A	353	PX4	C26-C25-C24	2.49	104.25	113.19	7	2
4	A	414	PX4	C19-C18-C17	2.49	101.79	114.42	8	1
4	A	341	PX4	C33-C32-C31	2.49	101.80	114.42	5	1
4	A	334	PX4	C1-C2-N1	2.49	124.08	115.78	7	3
4	A	364	PX4	C32-C31-C30	2.49	101.80	114.42	8	1
4	A	395	PX4	C5-N1-C3	2.49	102.58	108.97	13	1
4	A	334	PX4	C5-N1-C2	2.49	120.08	109.92	3	1
4	A	367	PX4	C28-C27-C26	2.49	101.81	114.42	5	1
4	A	384	PX4	C34-C33-C32	2.49	101.81	114.42	3	2
4	A	396	PX4	O4-P1-O2	2.49	118.78	109.07	1	2
4	A	401	PX4	O1-P1-O4	2.49	119.29	107.75	2	3
4	A	402	PX4	C3-N1-C2	2.49	99.75	109.92	2	1
4	A	405	PX4	O5-C9-C10	2.48	119.70	111.91	1	5
4	A	419	PX4	O1-P1-O4	2.48	119.28	107.75	7	2
4	A	428	PX4	O1-P1-O3	2.48	119.28	107.75	7	1
4	A	311	PX4	O8-C23-C24	2.48	114.05	123.73	1	2
4	A	421	PX4	C33-C32-C31	2.48	101.82	114.42	2	1
4	A	339	PX4	C13-C12-C11	2.48	101.83	114.42	13	2
4	A	341	PX4	C12-C11-C10	2.48	122.11	113.19	11	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	351	PX4	C36-C35-C34	2.48	94.59	113.42	14	1
4	A	380	PX4	C5-N1-C4	2.48	102.59	108.97	3	1
4	A	386	PX4	C27-C26-C25	2.48	101.83	114.42	14	2
4	A	399	PX4	O3-C1-C2	2.48	122.21	109.16	9	2
4	A	403	PX4	C11-C10-C9	2.48	104.59	113.62	14	2
4	A	418	PX4	O1-P1-O3	2.48	119.27	107.75	3	1
4	A	339	PX4	O8-C23-C24	2.48	114.06	123.73	3	3
4	A	359	PX4	O5-C9-C10	2.48	119.69	111.91	3	2
4	A	360	PX4	C30-C29-C28	2.48	101.83	114.42	11	1
4	A	412	PX4	O1-P1-O4	2.48	119.27	107.75	4	2
4	A	384	PX4	O7-C7-C6	2.48	117.38	108.40	13	2
4	A	345	PX4	C7-O7-C23	2.48	111.69	117.79	14	3
4	A	351	PX4	C1-C2-N1	2.48	124.05	115.78	13	1
4	A	399	PX4	O3-P1-O2	2.48	99.38	109.07	5	2
4	A	385	PX4	C13-C12-C11	2.48	101.85	114.42	9	2
4	A	411	PX4	C19-C18-C17	2.48	101.85	114.42	9	1
4	A	424	PX4	C33-C32-C31	2.48	101.85	114.42	7	2
4	A	319	PX4	C31-C30-C29	2.48	101.85	114.42	14	1
4	A	321	PX4	C4-N1-C2	2.48	120.05	109.92	13	1
4	A	324	PX4	O5-C9-O6	2.48	117.34	123.59	13	1
4	A	334	PX4	C15-C14-C13	2.48	101.86	114.42	11	1
4	A	353	PX4	O1-P1-O4	2.48	119.25	107.75	9	1
4	A	358	PX4	C18-C17-C16	2.48	101.86	114.42	4	2
4	A	382	PX4	C20-C19-C18	2.48	101.86	114.42	1	2
4	A	397	PX4	C5-N1-C3	2.48	115.34	108.97	10	4
4	A	405	PX4	C33-C32-C31	2.48	101.86	114.42	5	2
4	A	419	PX4	C4-N1-C2	2.48	99.78	109.92	8	1
4	A	361	PX4	C12-C11-C10	2.47	104.30	113.19	7	1
4	A	336	PX4	C25-C24-C23	2.47	104.63	113.62	11	1
4	A	361	PX4	C19-C18-C17	2.47	101.87	114.42	10	1
4	A	307	PX4	C19-C18-C17	2.47	101.88	114.42	14	2
4	A	348	PX4	C7-O7-C23	2.47	111.70	117.79	10	2
4	A	350	PX4	O5-C9-O6	2.47	117.35	123.59	1	2
4	A	353	PX4	O7-C7-C6	2.47	117.36	108.40	6	2
4	A	370	PX4	C18-C17-C16	2.47	101.87	114.42	14	1
4	A	371	PX4	C15-C14-C13	2.47	101.87	114.42	10	3
4	A	382	PX4	C27-C26-C25	2.47	101.87	114.42	13	2
4	A	416	PX4	C17-C16-C15	2.47	101.87	114.42	8	2
4	A	355	PX4	C26-C25-C24	2.47	104.30	113.19	6	1
4	A	390	PX4	C3-N1-C2	2.47	99.80	109.92	5	2
4	A	392	PX4	C26-C25-C24	2.47	104.30	113.19	5	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	394	PX4	C8-O5-C9	2.47	107.97	117.12	12	4
4	A	402	PX4	C15-C14-C13	2.47	101.88	114.42	14	1
4	A	410	PX4	C8-O5-C9	2.47	107.97	117.12	1	1
4	A	314	PX4	C34-C33-C32	2.47	101.89	114.42	3	1
4	A	317	PX4	C25-C24-C23	2.47	104.64	113.62	13	3
4	A	322	PX4	C25-C24-C23	2.47	104.64	113.62	6	1
4	A	361	PX4	C31-C30-C29	2.47	101.89	114.42	9	1
4	A	410	PX4	C31-C30-C29	2.47	101.88	114.42	5	3
4	A	314	PX4	O7-C23-O8	2.47	117.74	123.70	14	3
4	A	347	PX4	C33-C32-C31	2.47	101.89	114.42	11	1
4	A	308	PX4	C29-C28-C27	2.47	101.90	114.42	10	1
4	A	359	PX4	O4-P1-O2	2.47	118.71	109.07	11	1
4	A	363	PX4	C16-C15-C14	2.47	101.90	114.42	13	2
4	A	390	PX4	C11-C10-C9	2.47	104.65	113.62	12	4
4	A	395	PX4	C29-C28-C27	2.47	101.90	114.42	4	1
4	A	398	PX4	C13-C12-C11	2.47	101.90	114.42	7	3
4	A	403	PX4	C20-C19-C18	2.47	101.90	114.42	11	2
4	A	387	PX4	O3-C1-C2	2.47	122.12	109.16	7	2
4	A	389	PX4	C3-N1-C2	2.47	120.00	109.92	14	1
4	A	396	PX4	C16-C15-C14	2.46	101.92	114.42	4	2
4	A	400	PX4	C4-N1-C2	2.46	120.00	109.92	13	2
4	A	404	PX4	O3-C1-C2	2.47	122.13	109.16	8	2
4	A	405	PX4	C5-N1-C2	2.47	120.00	109.92	10	1
4	A	414	PX4	C4-N1-C2	2.47	99.83	109.92	5	1
4	A	358	PX4	C19-C18-C17	2.46	101.91	114.42	2	1
4	A	315	PX4	C4-N1-C2	2.46	119.99	109.92	5	1
4	A	335	PX4	C1-C2-N1	2.46	124.00	115.78	11	4
4	A	362	PX4	C18-C17-C16	2.46	101.92	114.42	9	3
4	A	430	PX4	C31-C30-C29	2.47	101.91	114.42	12	1
4	A	372	PX4	O3-C1-C2	2.46	122.11	109.16	3	1
4	A	378	PX4	O4-P1-O2	2.46	118.69	109.07	4	1
4	A	404	PX4	C32-C31-C30	2.46	101.92	114.42	1	1
4	A	404	PX4	C25-C24-C23	2.46	104.67	113.62	14	2
4	A	421	PX4	C3-N1-C2	2.46	99.84	109.92	12	2
4	A	323	PX4	C13-C12-C11	2.46	101.93	114.42	10	2
4	A	325	PX4	C32-C31-C30	2.46	101.93	114.42	5	1
4	A	340	PX4	C17-C16-C15	2.46	101.94	114.42	8	1
4	A	360	PX4	O3-C1-C2	2.46	122.10	109.16	10	2
4	A	367	PX4	C20-C19-C18	2.46	101.93	114.42	9	2
4	A	404	PX4	C34-C33-C32	2.46	101.93	114.42	7	1
4	A	402	PX4	C4-N1-C3	2.46	102.65	108.97	12	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	411	PX4	C30-C29-C28	2.46	101.94	114.42	13	1
4	A	430	PX4	C20-C19-C18	2.46	101.94	114.42	13	3
4	A	315	PX4	O4-P1-O2	2.46	118.67	109.07	13	1
4	A	325	PX4	C1-C2-N1	2.46	123.99	115.78	14	4
4	A	322	PX4	C33-C32-C31	2.46	101.95	114.42	7	4
4	A	336	PX4	C34-C33-C32	2.46	101.95	114.42	3	2
4	A	375	PX4	C1-C2-N1	2.46	123.99	115.78	13	2
4	A	425	PX4	O8-C23-C24	2.46	114.14	123.73	10	2
4	A	380	PX4	C5-N1-C3	2.46	102.66	108.97	1	1
4	A	385	PX4	C4-N1-C2	2.46	119.97	109.92	11	1
4	A	411	PX4	C27-C26-C25	2.46	101.95	114.42	7	3
4	A	422	PX4	C18-C17-C16	2.46	101.95	114.42	2	2
4	A	367	PX4	C3-N1-C2	2.45	99.87	109.92	5	2
4	A	418	PX4	C15-C14-C13	2.45	101.96	114.42	5	3
4	A	421	PX4	C25-C24-C23	2.45	104.70	113.62	13	1
4	A	312	PX4	C4-N1-C2	2.45	119.95	109.92	12	1
4	A	323	PX4	O1-P1-O3	2.45	96.35	107.75	8	2
4	A	429	PX4	C26-C25-C24	2.45	104.37	113.19	8	2
4	A	357	PX4	O3-C1-C2	2.45	122.05	109.16	2	2
4	A	361	PX4	C27-C26-C25	2.45	101.98	114.42	13	1
4	A	377	PX4	C19-C18-C17	2.45	101.98	114.42	5	2
4	A	399	PX4	C29-C28-C27	2.45	101.98	114.42	5	2
4	A	401	PX4	O6-C9-C10	2.45	114.17	123.73	14	1
4	A	306	PX4	C12-C11-C10	2.45	104.38	113.19	10	3
4	A	375	PX4	C29-C28-C27	2.45	101.99	114.42	2	2
4	A	407	PX4	C12-C11-C10	2.45	104.38	113.19	9	3
4	A	385	PX4	C27-C26-C25	2.45	102.00	114.42	7	2
4	A	413	PX4	C26-C25-C24	2.45	104.39	113.19	6	1
4	A	428	PX4	C12-C11-C10	2.45	104.39	113.19	4	1
4	A	319	PX4	C4-N1-C2	2.45	119.93	109.92	13	1
4	A	339	PX4	C30-C29-C28	2.45	102.01	114.42	5	2
4	A	340	PX4	O5-C9-C10	2.45	119.58	111.91	11	2
4	A	374	PX4	C15-C14-C13	2.45	102.01	114.42	6	1
4	A	376	PX4	C30-C29-C28	2.45	102.00	114.42	14	2
4	A	378	PX4	C7-O7-C23	2.45	111.77	117.79	4	2
4	A	378	PX4	C16-C15-C14	2.45	102.00	114.42	6	3
4	A	311	PX4	O7-C7-C8	2.45	117.25	108.40	7	4
4	A	361	PX4	C26-C25-C24	2.45	104.40	113.19	2	3
4	A	398	PX4	C34-C33-C32	2.45	102.01	114.42	11	1
4	A	326	PX4	O4-P1-O2	2.44	118.62	109.07	1	1
4	A	329	PX4	C13-C12-C11	2.44	102.02	114.42	14	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	340	PX4	C34-C33-C32	2.44	102.02	114.42	7	2
4	A	345	PX4	C30-C29-C28	2.44	102.02	114.42	14	1
4	A	352	PX4	C8-O5-C9	2.44	108.07	117.12	1	3
4	A	381	PX4	C30-C29-C28	2.44	102.02	114.42	5	1
4	A	391	PX4	C16-C15-C14	2.44	102.02	114.42	2	1
4	A	394	PX4	C16-C15-C14	2.44	102.03	114.42	11	1
4	A	405	PX4	C11-C10-C9	2.44	104.74	113.62	1	4
4	A	405	PX4	C18-C17-C16	2.44	102.03	114.42	8	3
4	A	423	PX4	C30-C29-C28	2.44	102.02	114.42	1	1
4	A	360	PX4	C14-C13-C12	2.44	102.03	114.42	9	1
4	A	365	PX4	O7-C23-O8	2.44	117.80	123.70	3	1
4	A	370	PX4	C14-C13-C12	2.44	102.03	114.42	9	1
4	A	413	PX4	O4-P1-O2	2.44	118.61	109.07	14	5
4	A	351	PX4	C5-N1-C4	2.44	115.25	108.97	1	2
4	A	366	PX4	O7-C23-O8	2.44	117.80	123.70	7	5
4	A	419	PX4	C3-N1-C2	2.44	119.91	109.92	4	3
4	A	404	PX4	C11-C10-C9	2.44	104.75	113.62	6	1
4	A	415	PX4	C25-C24-C23	2.44	104.75	113.62	5	1
4	A	424	PX4	O8-C23-C24	2.44	114.21	123.73	10	1
4	A	309	PX4	O5-C9-C10	2.44	119.56	111.91	13	4
4	A	331	PX4	C3-N1-C2	2.44	119.89	109.92	2	1
4	A	365	PX4	C12-C11-C10	2.44	104.42	113.19	6	2
4	A	393	PX4	C26-C25-C24	2.44	104.42	113.19	7	2
4	A	389	PX4	C27-C26-C25	2.44	102.05	114.42	3	1
4	A	395	PX4	C5-N1-C2	2.44	99.94	109.92	12	2
4	A	397	PX4	C30-C29-C28	2.44	102.05	114.42	6	1
4	A	410	PX4	O1-P1-O3	2.44	96.42	107.75	11	1
4	A	325	PX4	O8-C23-C24	2.44	114.23	123.73	6	1
4	A	336	PX4	O3-C1-C2	2.44	121.97	109.16	4	3
4	A	357	PX4	C4-N1-C3	2.44	102.71	108.97	4	5
4	A	387	PX4	C34-C33-C32	2.43	102.06	114.42	12	2
4	A	415	PX4	O8-C23-C24	2.43	114.23	123.73	7	2
4	A	425	PX4	C15-C14-C13	2.44	102.06	114.42	8	1
4	A	314	PX4	C11-C10-C9	2.43	122.47	113.62	10	1
4	A	326	PX4	C13-C12-C11	2.43	102.07	114.42	4	2
4	A	349	PX4	O1-P1-O4	2.43	119.05	107.75	7	1
4	A	359	PX4	O3-C1-C2	2.43	121.96	109.16	14	2
4	A	390	PX4	O7-C7-C8	2.43	117.21	108.40	3	5
4	A	392	PX4	C32-C31-C30	2.43	102.07	114.42	12	1
4	A	393	PX4	C30-C29-C28	2.43	102.08	114.42	8	1
4	A	399	PX4	O4-P1-O2	2.43	99.56	109.07	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	401	PX4	C19-C18-C17	2.43	102.07	114.42	2	2
4	A	420	PX4	O5-C9-O6	2.43	117.45	123.59	2	4
4	A	307	PX4	O1-P1-O3	2.43	96.45	107.75	6	1
4	A	333	PX4	C20-C19-C18	2.43	102.08	114.42	3	1
4	A	334	PX4	C19-C18-C17	2.43	102.08	114.42	4	1
4	A	346	PX4	C3-N1-C2	2.43	99.97	109.92	9	1
4	A	362	PX4	C16-C15-C14	2.43	102.08	114.42	1	2
4	A	363	PX4	C33-C32-C31	2.43	102.08	114.42	8	1
4	A	372	PX4	C28-C27-C26	2.43	102.07	114.42	4	1
4	A	377	PX4	C29-C28-C27	2.43	102.08	114.42	10	1
4	A	384	PX4	C11-C10-C9	2.43	104.77	113.62	3	3
4	A	317	PX4	C8-O5-C9	2.43	108.12	117.12	3	4
4	A	314	PX4	O4-P1-O2	2.43	118.56	109.07	13	1
4	A	348	PX4	O4-P1-O2	2.43	118.56	109.07	8	3
4	A	354	PX4	C31-C30-C29	2.43	102.09	114.42	1	1
4	A	390	PX4	O3-C1-C2	2.43	121.94	109.16	11	2
4	A	425	PX4	C4-N1-C3	2.43	102.72	108.97	5	3
4	A	364	PX4	C25-C24-C23	2.43	104.78	113.62	3	3
4	A	309	PX4	O1-P1-O4	2.43	119.02	107.75	5	3
4	A	351	PX4	O5-C9-C10	2.43	119.53	111.91	8	2
4	A	396	PX4	O5-C9-O6	2.43	117.46	123.59	14	5
4	A	318	PX4	C25-C24-C23	2.43	104.80	113.62	7	3
4	A	319	PX4	O3-C1-C2	2.43	121.92	109.16	4	2
4	A	334	PX4	O4-P1-O2	2.43	99.59	109.07	9	3
4	A	425	PX4	C20-C19-C18	2.43	102.11	114.42	4	1
4	A	421	PX4	C8-O5-C9	2.43	108.14	117.12	1	3
4	A	427	PX4	C34-C33-C32	2.43	102.11	114.42	1	1
4	A	310	PX4	C27-C26-C25	2.42	102.12	114.42	7	1
4	A	308	PX4	C32-C31-C30	2.42	102.13	114.42	5	1
4	A	321	PX4	C3-N1-C2	2.42	100.00	109.92	13	2
4	A	322	PX4	O5-C9-C10	2.42	119.51	111.91	10	4
4	A	322	PX4	C14-C13-C12	2.42	102.13	114.42	8	1
4	A	330	PX4	C4-N1-C2	2.42	100.00	109.92	4	2
4	A	330	PX4	C17-C16-C15	2.42	102.13	114.42	13	1
4	A	331	PX4	C4-N1-C2	2.42	119.83	109.92	13	1
4	A	369	PX4	O5-C9-O6	2.42	117.48	123.59	5	4
4	A	377	PX4	C25-C24-C23	2.42	122.43	113.62	6	2
4	A	411	PX4	C31-C30-C29	2.42	102.13	114.42	5	2
4	A	375	PX4	O3-C1-C2	2.42	121.89	109.16	8	1
4	A	387	PX4	C8-O5-C9	2.42	108.16	117.12	3	3
4	A	391	PX4	C17-C16-C15	2.42	102.14	114.42	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	404	PX4	O6-C9-C10	2.42	114.29	123.73	3	1
4	A	419	PX4	O3-C1-C2	2.42	121.89	109.16	1	2
4	A	428	PX4	C30-C29-C28	2.42	102.14	114.42	4	2
4	A	430	PX4	C4-N1-C2	2.42	100.01	109.92	4	2
4	A	314	PX4	C13-C12-C11	2.42	102.14	114.42	13	1
4	A	351	PX4	C31-C30-C29	2.42	102.15	114.42	4	1
4	A	369	PX4	C15-C14-C13	2.42	102.15	114.42	7	1
4	A	402	PX4	C31-C30-C29	2.42	102.16	114.42	7	1
4	A	407	PX4	C14-C13-C12	2.42	102.15	114.42	9	1
4	A	411	PX4	O3-P1-O2	2.42	99.62	109.07	5	4
4	A	413	PX4	C27-C26-C25	2.42	102.15	114.42	11	2
4	A	417	PX4	C28-C27-C26	2.42	102.15	114.42	6	1
4	A	424	PX4	C5-N1-C4	2.42	102.76	108.97	12	2
4	A	321	PX4	O1-P1-O4	2.42	118.96	107.75	9	2
4	A	321	PX4	C15-C14-C13	2.42	102.16	114.42	7	1
4	A	336	PX4	C4-N1-C2	2.42	119.80	109.92	4	4
4	A	371	PX4	C30-C29-C28	2.42	102.16	114.42	14	1
4	A	373	PX4	C18-C17-C16	2.42	102.16	114.42	10	1
4	A	426	PX4	C33-C32-C31	2.42	102.16	114.42	11	2
4	A	309	PX4	C26-C25-C24	2.41	104.51	113.19	14	2
4	A	354	PX4	O4-P1-O2	2.42	118.50	109.07	9	1
4	A	370	PX4	C30-C29-C28	2.41	102.17	114.42	12	1
4	A	374	PX4	O1-P1-O4	2.41	118.96	107.75	14	1
4	A	388	PX4	C16-C15-C14	2.41	102.17	114.42	9	1
4	A	405	PX4	O1-P1-O4	2.42	118.96	107.75	4	2
4	A	341	PX4	C18-C17-C16	2.41	102.17	114.42	1	2
4	A	347	PX4	C27-C26-C25	2.41	102.18	114.42	14	3
4	A	406	PX4	C19-C18-C17	2.41	102.18	114.42	7	2
4	A	415	PX4	O3-C1-C2	2.41	121.85	109.16	5	1
4	A	359	PX4	C16-C15-C14	2.41	102.18	114.42	7	1
4	A	373	PX4	O1-P1-O4	2.41	96.55	107.75	13	3
4	A	387	PX4	O7-C7-C6	2.41	117.13	108.40	2	2
4	A	395	PX4	C4-N1-C2	2.41	119.78	109.92	6	3
4	A	408	PX4	C25-C24-C23	2.41	104.85	113.62	13	2
4	A	414	PX4	C15-C14-C13	2.41	102.19	114.42	14	1
4	A	417	PX4	O7-C7-C6	2.41	117.13	108.40	5	4
4	A	427	PX4	C29-C28-C27	2.41	102.18	114.42	13	2
4	A	306	PX4	P1-O4-C6	2.41	107.55	121.68	11	4
4	A	323	PX4	C1-C2-N1	2.41	123.82	115.78	10	3
4	A	348	PX4	C8-O5-C9	2.41	108.20	117.12	9	3
4	A	377	PX4	C17-C16-C15	2.41	102.19	114.42	7	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	393	PX4	C25-C24-C23	2.41	104.86	113.62	3	1
4	A	319	PX4	C29-C28-C27	2.41	102.20	114.42	11	1
4	A	322	PX4	C3-N1-C2	2.41	119.77	109.92	8	4
4	A	333	PX4	O7-C23-O8	2.41	117.88	123.70	10	2
4	A	402	PX4	C34-C33-C32	2.41	102.20	114.42	9	1
4	A	328	PX4	C30-C29-C28	2.41	102.21	114.42	1	2
4	A	348	PX4	C16-C15-C14	2.41	102.21	114.42	9	3
4	A	370	PX4	C8-O5-C9	2.41	108.21	117.12	6	2
4	A	386	PX4	C17-C16-C15	2.41	102.21	114.42	5	2
4	A	413	PX4	O6-C9-C10	2.41	114.34	123.73	6	1
4	A	427	PX4	C11-C10-C9	2.41	122.38	113.62	14	1
4	A	327	PX4	C17-C16-C15	2.40	102.22	114.42	5	2
4	A	334	PX4	O1-P1-O4	2.41	118.92	107.75	8	2
4	A	348	PX4	O6-C9-C10	2.41	114.35	123.73	13	1
4	A	405	PX4	C12-C11-C10	2.41	104.54	113.19	5	2
4	A	430	PX4	C15-C14-C13	2.41	102.21	114.42	13	1
4	A	313	PX4	C5-N1-C3	2.40	102.80	108.97	2	1
4	A	333	PX4	C15-C14-C13	2.40	102.23	114.42	1	1
4	A	402	PX4	C32-C31-C30	2.40	102.22	114.42	12	1
4	A	416	PX4	O3-C1-C2	2.40	121.80	109.16	11	3
4	A	416	PX4	C25-C24-C23	2.40	104.88	113.62	5	2
4	A	418	PX4	C17-C16-C15	2.40	102.22	114.42	8	1
4	A	376	PX4	C26-C25-C24	2.40	104.56	113.19	7	2
4	A	383	PX4	C33-C32-C31	2.40	102.23	114.42	5	2
4	A	423	PX4	C17-C16-C15	2.40	102.23	114.42	6	4
4	A	309	PX4	C12-C11-C10	2.40	104.56	113.19	6	2
4	A	311	PX4	C25-C24-C23	2.40	104.89	113.62	7	2
4	A	379	PX4	C33-C32-C31	2.40	102.23	114.42	2	1
4	A	386	PX4	C28-C27-C26	2.40	102.23	114.42	3	2
4	A	360	PX4	O1-P1-O4	2.40	118.89	107.75	5	1
4	A	386	PX4	C25-C24-C23	2.40	104.89	113.62	5	2
4	A	387	PX4	C30-C29-C28	2.40	102.24	114.42	5	1
4	A	393	PX4	C3-N1-C2	2.40	100.09	109.92	5	1
4	A	423	PX4	C8-O5-C9	2.40	108.23	117.12	13	1
4	A	365	PX4	C27-C26-C25	2.40	102.25	114.42	4	3
4	A	348	PX4	C27-C26-C25	2.40	102.25	114.42	13	1
4	A	351	PX4	C5-N1-C3	2.40	102.81	108.97	12	2
4	A	428	PX4	C13-C12-C11	2.40	102.25	114.42	12	2
4	A	352	PX4	C33-C32-C31	2.40	102.25	114.42	2	1
4	A	354	PX4	C34-C33-C32	2.40	102.26	114.42	8	1
4	A	356	PX4	C20-C19-C18	2.40	102.26	114.42	7	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	366	PX4	C19-C18-C17	2.40	102.25	114.42	12	2
4	A	335	PX4	C25-C24-C23	2.40	104.91	113.62	14	1
4	A	396	PX4	C27-C26-C25	2.40	102.26	114.42	13	1
4	A	375	PX4	O5-C9-O6	2.39	117.55	123.59	6	1
4	A	401	PX4	C15-C14-C13	2.39	102.27	114.42	1	2
4	A	405	PX4	C25-C24-C23	2.39	104.91	113.62	5	1
4	A	407	PX4	C26-C25-C24	2.39	104.58	113.19	6	2
4	A	330	PX4	C31-C30-C29	2.39	102.28	114.42	9	3
4	A	329	PX4	C26-C25-C24	2.39	104.59	113.19	10	4
4	A	375	PX4	C16-C15-C14	2.39	102.28	114.42	13	2
4	A	376	PX4	C15-C14-C13	2.39	102.28	114.42	8	1
4	A	379	PX4	C12-C11-C10	2.39	104.59	113.19	10	2
4	A	391	PX4	C29-C28-C27	2.39	102.28	114.42	7	1
4	A	308	PX4	C5-N1-C2	2.39	119.70	109.92	9	1
4	A	328	PX4	C13-C12-C11	2.39	102.29	114.42	10	2
4	A	334	PX4	C26-C25-C24	2.39	104.60	113.19	5	1
4	A	345	PX4	C17-C16-C15	2.39	102.28	114.42	6	2
4	A	412	PX4	C27-C26-C25	2.39	102.28	114.42	7	1
4	A	416	PX4	O7-C23-O8	2.39	117.92	123.70	7	5
4	A	345	PX4	C28-C27-C26	2.39	102.29	114.42	13	3
4	A	375	PX4	O8-C23-C24	2.39	133.06	123.73	8	2
4	A	425	PX4	C30-C29-C28	2.39	102.29	114.42	7	1
4	A	336	PX4	C8-O5-C9	2.39	108.27	117.12	3	2
4	A	307	PX4	C13-C12-C11	2.39	102.30	114.42	9	1
4	A	337	PX4	O3-P1-O2	2.39	99.74	109.07	3	2
4	A	344	PX4	C28-C27-C26	2.39	102.30	114.42	10	1
4	A	355	PX4	C1-C2-N1	2.39	123.76	115.78	11	3
4	A	314	PX4	C4-N1-C2	2.39	119.68	109.92	11	1
4	A	316	PX4	C16-C15-C14	2.39	102.31	114.42	10	1
4	A	326	PX4	C4-N1-C2	2.39	119.68	109.92	6	2
4	A	371	PX4	C26-C25-C24	2.39	104.61	113.19	14	2
4	A	372	PX4	C3-N1-C2	2.39	119.68	109.92	3	1
4	A	395	PX4	C12-C11-C10	2.39	104.61	113.19	10	3
4	A	407	PX4	O1-P1-O3	2.39	96.67	107.75	2	2
4	A	414	PX4	C30-C29-C28	2.39	102.31	114.42	7	3
4	A	314	PX4	O7-C7-C8	2.38	117.03	108.40	12	2
4	A	306	PX4	C8-O5-C9	2.38	108.30	117.12	1	2
4	A	355	PX4	C27-C26-C25	2.38	102.33	114.42	2	3
4	A	374	PX4	C19-C18-C17	2.38	102.32	114.42	3	2
4	A	369	PX4	C20-C19-C18	2.38	102.33	114.42	7	1
4	A	399	PX4	O8-C23-C24	2.38	114.43	123.73	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	401	PX4	O4-P1-O2	2.38	118.38	109.07	6	1
4	A	430	PX4	C17-C16-C15	2.38	102.32	114.42	10	1
4	A	311	PX4	O3-C1-C2	2.38	121.68	109.16	2	2
4	A	337	PX4	C8-O5-C9	2.38	108.30	117.12	1	2
4	A	368	PX4	O4-P1-O2	2.38	99.76	109.07	14	2
4	A	373	PX4	C28-C27-C26	2.38	102.33	114.42	6	1
4	A	386	PX4	O6-C9-C10	2.38	114.44	123.73	3	1
4	A	418	PX4	C29-C28-C27	2.38	102.33	114.42	7	1
4	A	420	PX4	C28-C27-C26	2.38	102.34	114.42	7	2
4	A	424	PX4	C32-C31-C30	2.38	102.33	114.42	7	1
4	A	426	PX4	O6-C9-C10	2.38	114.44	123.73	12	1
4	A	313	PX4	C16-C15-C14	2.38	102.35	114.42	12	2
4	A	375	PX4	C5-N1-C2	2.38	119.65	109.92	2	2
4	A	397	PX4	C13-C12-C11	2.38	102.34	114.42	4	4
4	A	326	PX4	C32-C31-C30	2.38	102.35	114.42	14	1
4	A	376	PX4	C27-C26-C25	2.38	102.35	114.42	11	1
4	A	317	PX4	O1-P1-O3	2.38	118.79	107.75	14	2
4	A	387	PX4	C18-C17-C16	2.38	102.35	114.42	5	2
4	A	403	PX4	C29-C28-C27	2.38	102.35	114.42	10	2
4	A	392	PX4	C15-C14-C13	2.38	102.36	114.42	4	2
4	A	380	PX4	O4-P1-O2	2.37	118.35	109.07	10	4
4	A	399	PX4	C33-C32-C31	2.38	102.36	114.42	10	2
4	A	413	PX4	O1-P1-O4	2.38	118.78	107.75	5	1
4	A	333	PX4	O1-P1-O4	2.38	118.78	107.75	12	1
4	A	332	PX4	C15-C14-C13	2.37	102.38	114.42	5	1
4	A	333	PX4	O8-C23-C24	2.37	114.47	123.73	8	1
4	A	393	PX4	C4-N1-C2	2.37	119.63	109.92	5	1
4	A	402	PX4	O4-P1-O2	2.37	118.34	109.07	3	2
4	A	310	PX4	C29-C28-C27	2.37	102.38	114.42	6	1
4	A	390	PX4	C19-C18-C17	2.37	102.38	114.42	11	2
4	A	405	PX4	C34-C33-C32	2.37	102.38	114.42	2	1
4	A	423	PX4	O1-P1-O4	2.37	118.77	107.75	1	4
4	A	307	PX4	C20-C19-C18	2.37	102.39	114.42	9	1
4	A	365	PX4	O1-P1-O3	2.37	96.74	107.75	2	1
4	A	370	PX4	C28-C27-C26	2.37	102.40	114.42	2	1
4	A	373	PX4	C34-C33-C32	2.37	102.39	114.42	11	1
4	A	381	PX4	C28-C27-C26	2.37	102.39	114.42	10	2
4	A	392	PX4	C3-N1-C2	2.37	119.61	109.92	8	2
4	A	334	PX4	C3-N1-C2	2.37	100.23	109.92	12	1
4	A	364	PX4	C15-C14-C13	2.37	102.40	114.42	14	1
4	A	373	PX4	C14-C13-C12	2.37	102.40	114.42	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	387	PX4	C11-C10-C9	2.37	105.01	113.62	4	1
4	A	388	PX4	C18-C17-C16	2.37	102.40	114.42	5	1
4	A	419	PX4	C8-O5-C9	2.37	108.35	117.12	13	1
4	A	355	PX4	O1-P1-O3	2.37	96.75	107.75	6	1
4	A	356	PX4	C3-N1-C2	2.37	119.60	109.92	3	1
4	A	415	PX4	C34-C33-C32	2.37	102.41	114.42	6	2
4	A	430	PX4	C25-C24-C23	2.37	105.01	113.62	7	1
4	A	345	PX4	C15-C14-C13	2.37	102.42	114.42	13	2
4	A	426	PX4	O5-C8-C7	2.37	115.32	108.43	3	5
4	A	429	PX4	C29-C28-C27	2.37	102.41	114.42	8	1
4	A	307	PX4	C32-C31-C30	2.36	102.43	114.42	5	1
4	A	392	PX4	C19-C18-C17	2.36	102.43	114.42	7	1
4	A	312	PX4	O6-C9-C10	2.36	114.52	123.73	10	1
4	A	306	PX4	C34-C33-C32	2.36	102.44	114.42	4	1
4	A	320	PX4	C13-C12-C11	2.36	102.44	114.42	5	1
4	A	337	PX4	C33-C32-C31	2.36	102.44	114.42	5	2
4	A	342	PX4	C8-O5-C9	2.36	108.38	117.12	1	1
4	A	347	PX4	C5-N1-C3	2.36	115.05	108.97	10	2
4	A	348	PX4	C26-C25-C24	2.36	104.70	113.19	5	3
4	A	428	PX4	C32-C31-C30	2.36	102.43	114.42	11	3
4	A	343	PX4	O3-C1-C2	2.36	121.57	109.16	10	1
4	A	351	PX4	C11-C10-C9	2.36	105.04	113.62	7	2
4	A	381	PX4	C12-C11-C10	2.36	104.70	113.19	1	4
4	A	321	PX4	C18-C17-C16	2.36	102.46	114.42	4	1
4	A	346	PX4	C5-N1-C2	2.36	100.27	109.92	3	1
4	A	414	PX4	C14-C13-C12	2.36	102.45	114.42	6	2
4	A	416	PX4	C5-N1-C2	2.36	119.56	109.92	11	2
4	A	307	PX4	C5-N1-C2	2.36	119.55	109.92	3	1
4	A	356	PX4	O1-P1-O3	2.36	118.69	107.75	1	1
4	A	332	PX4	C4-N1-C3	2.35	102.92	108.97	3	1
4	A	358	PX4	C29-C28-C27	2.35	102.47	114.42	6	2
4	A	379	PX4	O8-C23-C24	2.36	114.54	123.73	14	2
4	A	412	PX4	C4-N1-C2	2.36	119.55	109.92	1	1
4	A	331	PX4	C25-C24-C23	2.35	122.18	113.62	1	1
4	A	347	PX4	C34-C33-C32	2.35	102.48	114.42	10	2
4	A	322	PX4	O6-C9-C10	2.35	114.56	123.73	3	1
4	A	322	PX4	C8-O5-C9	2.35	108.41	117.12	9	1
4	A	329	PX4	C19-C18-C17	2.35	102.48	114.42	6	1
4	A	350	PX4	C16-C15-C14	2.35	102.48	114.42	5	1
4	A	404	PX4	C30-C29-C28	2.35	102.48	114.42	12	1
4	A	384	PX4	C29-C28-C27	2.35	102.49	114.42	10	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	391	PX4	C8-O5-C9	2.35	108.41	117.12	13	1
4	A	308	PX4	O5-C9-O6	2.35	117.66	123.59	13	2
4	A	309	PX4	C5-N1-C2	2.35	100.30	109.92	4	3
4	A	310	PX4	C28-C27-C26	2.35	102.49	114.42	13	1
4	A	340	PX4	C32-C31-C30	2.35	102.50	114.42	5	1
4	A	348	PX4	C17-C16-C15	2.35	102.49	114.42	4	1
4	A	360	PX4	C11-C10-C9	2.35	105.08	113.62	1	2
4	A	396	PX4	C12-C11-C10	2.35	104.75	113.19	7	1
4	A	420	PX4	C26-C25-C24	2.35	104.75	113.19	1	1
4	A	329	PX4	O3-C1-C2	2.35	121.51	109.16	6	1
4	A	352	PX4	C16-C15-C14	2.35	102.51	114.42	1	1
4	A	370	PX4	C7-O7-C23	2.35	123.57	117.79	9	2
4	A	390	PX4	C20-C19-C18	2.35	102.51	114.42	4	1
4	A	423	PX4	C13-C12-C11	2.35	102.51	114.42	9	1
4	A	360	PX4	C32-C31-C30	2.34	102.52	114.42	6	1
4	A	314	PX4	C14-C13-C12	2.34	102.54	114.42	7	1
4	A	329	PX4	C15-C14-C13	2.34	102.53	114.42	12	3
4	A	356	PX4	C19-C18-C17	2.34	102.53	114.42	3	2
4	A	362	PX4	C32-C31-C30	2.34	102.53	114.42	2	1
4	A	375	PX4	C8-O5-C9	2.34	108.44	117.12	12	1
4	A	425	PX4	C32-C31-C30	2.34	102.53	114.42	7	1
4	A	388	PX4	C5-N1-C3	2.34	102.95	108.97	4	4
4	A	388	PX4	C25-C24-C23	2.34	105.11	113.62	9	1
4	A	390	PX4	C4-N1-C2	2.34	119.49	109.92	2	1
4	A	394	PX4	C5-N1-C2	2.34	100.34	109.92	2	3
4	A	312	PX4	C32-C31-C30	2.34	102.55	114.42	12	1
4	A	342	PX4	C5-N1-C2	2.34	119.49	109.92	9	1
4	A	357	PX4	C14-C13-C12	2.34	102.55	114.42	2	1
4	A	368	PX4	O3-P1-O2	2.34	99.93	109.07	11	1
4	A	381	PX4	O3-C1-C2	2.34	121.46	109.16	3	1
4	A	387	PX4	C29-C28-C27	2.34	102.55	114.42	6	2
4	A	389	PX4	O7-C7-C6	2.34	116.87	108.40	13	2
4	A	406	PX4	C12-C11-C10	2.34	104.78	113.19	4	1
4	A	418	PX4	C31-C30-C29	2.34	102.54	114.42	6	1
4	A	307	PX4	C34-C33-C32	2.34	102.55	114.42	3	1
4	A	307	PX4	O5-C9-C10	2.34	119.24	111.91	4	1
4	A	331	PX4	O4-P1-O2	2.34	118.20	109.07	6	1
4	A	335	PX4	C16-C15-C14	2.34	126.29	114.42	4	2
4	A	417	PX4	C17-C16-C15	2.34	102.55	114.42	6	2
4	A	353	PX4	C19-C18-C17	2.34	102.56	114.42	14	1
4	A	318	PX4	O7-C23-O8	2.34	118.06	123.70	14	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	342	PX4	C33-C32-C31	2.34	102.57	114.42	4	1
4	A	348	PX4	O1-P1-O2	2.34	123.79	112.24	14	4
4	A	361	PX4	O1-P1-O3	2.34	118.60	107.75	12	1
4	A	354	PX4	C32-C31-C30	2.33	102.57	114.42	6	2
4	A	363	PX4	C28-C27-C26	2.34	102.57	114.42	6	1
4	A	394	PX4	C34-C33-C32	2.34	102.56	114.42	3	2
4	A	308	PX4	C8-O5-C9	2.33	108.48	117.12	1	1
4	A	313	PX4	O5-C9-C10	2.33	119.23	111.91	11	2
4	A	318	PX4	C31-C30-C29	2.33	102.58	114.42	13	1
4	A	325	PX4	O6-C9-C10	2.33	114.63	123.73	9	1
4	A	313	PX4	O3-C1-C2	2.33	121.43	109.16	11	2
4	A	385	PX4	C14-C13-C12	2.33	102.58	114.42	11	1
4	A	335	PX4	C28-C27-C26	2.33	102.58	114.42	6	1
4	A	424	PX4	C17-C16-C15	2.33	102.58	114.42	7	1
4	A	371	PX4	C32-C31-C30	2.33	102.59	114.42	2	1
4	A	378	PX4	C17-C16-C15	2.33	102.59	114.42	14	1
4	A	400	PX4	O6-C9-C10	2.33	114.64	123.73	12	2
4	A	415	PX4	O5-C9-C10	2.33	119.22	111.91	6	2
4	A	313	PX4	C30-C29-C28	2.33	102.61	114.42	1	2
4	A	343	PX4	C20-C19-C18	2.33	102.61	114.42	14	1
4	A	357	PX4	C12-C11-C10	2.33	104.82	113.19	5	1
4	A	365	PX4	O4-P1-O2	2.33	118.17	109.07	3	1
4	A	425	PX4	O5-C9-O6	2.33	117.71	123.59	5	2
4	A	328	PX4	C33-C32-C31	2.33	102.61	114.42	9	1
4	A	330	PX4	C5-N1-C3	2.33	114.96	108.97	12	1
4	A	370	PX4	C29-C28-C27	2.33	102.61	114.42	10	1
4	A	401	PX4	C27-C26-C25	2.33	102.61	114.42	10	2
4	A	314	PX4	C19-C18-C17	2.33	102.62	114.42	14	1
4	A	322	PX4	C28-C27-C26	2.32	102.62	114.42	5	2
4	A	328	PX4	C18-C17-C16	2.32	102.63	114.42	13	1
4	A	357	PX4	C5-N1-C2	2.32	119.42	109.92	5	1
4	A	362	PX4	C33-C32-C31	2.32	102.63	114.42	7	2
4	A	364	PX4	C3-N1-C2	2.32	100.41	109.92	13	1
4	A	406	PX4	C18-C17-C16	2.32	102.63	114.42	3	1
4	A	415	PX4	C15-C14-C13	2.32	102.63	114.42	14	3
4	A	316	PX4	O7-C7-C8	2.32	116.81	108.40	9	1
4	A	370	PX4	O5-C9-O6	2.32	117.73	123.59	2	2
4	A	408	PX4	O4-P1-O2	2.32	118.13	109.07	6	1
4	A	409	PX4	C8-O5-C9	2.32	108.53	117.12	1	1
4	A	425	PX4	C5-N1-C2	2.32	119.41	109.92	4	1
4	A	399	PX4	C12-C11-C10	2.32	104.85	113.19	10	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	423	PX4	C33-C32-C31	2.32	102.65	114.42	12	1
4	A	349	PX4	C11-C10-C9	2.32	105.19	113.62	10	2
4	A	330	PX4	C12-C11-C10	2.32	104.86	113.19	4	2
4	A	348	PX4	C33-C32-C31	2.32	102.66	114.42	3	1
4	A	393	PX4	C20-C19-C18	2.32	102.65	114.42	3	2
4	A	377	PX4	O1-P1-O4	2.32	118.51	107.75	11	1
4	A	382	PX4	C29-C28-C27	2.32	102.66	114.42	11	2
4	A	403	PX4	C34-C33-C32	2.32	102.66	114.42	4	1
4	A	391	PX4	C25-C24-C23	2.32	105.19	113.62	11	2
4	A	411	PX4	C15-C14-C13	2.32	102.66	114.42	2	1
4	A	401	PX4	C3-N1-C2	2.32	100.44	109.92	2	2
4	A	420	PX4	O4-P1-O2	2.32	118.12	109.07	1	2
4	A	315	PX4	C8-O5-C9	2.31	108.55	117.12	4	1
4	A	352	PX4	C18-C17-C16	2.31	102.67	114.42	9	1
4	A	339	PX4	C17-C16-C15	2.31	102.69	114.42	2	1
4	A	346	PX4	C30-C29-C28	2.31	102.68	114.42	8	2
4	A	422	PX4	C34-C33-C32	2.31	102.68	114.42	2	1
4	A	429	PX4	C5-N1-C2	2.31	119.38	109.92	5	1
4	A	352	PX4	C14-C13-C12	2.31	102.69	114.42	11	1
4	A	374	PX4	C5-N1-C2	2.31	119.38	109.92	10	1
4	A	423	PX4	C4-N1-C2	2.31	100.47	109.92	6	2
4	A	423	PX4	C32-C31-C30	2.31	102.69	114.42	12	1
4	A	426	PX4	C26-C25-C24	2.31	121.50	113.19	3	2
4	A	342	PX4	C34-C33-C32	2.31	102.70	114.42	14	2
4	A	351	PX4	C13-C12-C11	2.31	126.15	114.42	11	3
4	A	359	PX4	C33-C32-C31	2.31	102.70	114.42	4	2
4	A	364	PX4	O3-P1-O2	2.31	100.04	109.07	4	2
4	A	396	PX4	C11-C10-C9	2.31	105.22	113.62	7	3
4	A	394	PX4	C14-C13-C12	2.31	102.70	114.42	11	1
4	A	401	PX4	O8-C23-C24	2.31	114.72	123.73	5	1
4	A	412	PX4	C26-C25-C24	2.31	104.89	113.19	2	4
4	A	368	PX4	C3-N1-C2	2.31	119.36	109.92	1	1
4	A	383	PX4	C19-C18-C17	2.31	102.71	114.42	3	1
4	A	392	PX4	C8-O5-C9	2.31	108.58	117.12	1	1
4	A	310	PX4	C13-C12-C11	2.31	102.72	114.42	5	2
4	A	326	PX4	O7-C23-O8	2.31	118.13	123.70	12	3
4	A	409	PX4	C14-C13-C12	2.31	102.72	114.42	4	2
4	A	405	PX4	C27-C26-C25	2.30	102.73	114.42	12	1
4	A	409	PX4	O4-P1-O2	2.31	118.07	109.07	11	1
4	A	418	PX4	C27-C26-C25	2.31	102.72	114.42	11	1
4	A	349	PX4	C32-C31-C30	2.30	102.73	114.42	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	352	PX4	C5-N1-C4	2.30	114.90	108.97	3	2
4	A	379	PX4	O4-P1-O2	2.30	118.07	109.07	11	1
4	A	367	PX4	O3-C1-C2	2.30	121.27	109.16	8	1
4	A	388	PX4	O1-P1-O4	2.30	118.44	107.75	6	2
4	A	392	PX4	C16-C15-C14	2.30	102.73	114.42	4	1
4	A	312	PX4	C5-N1-C4	2.30	103.06	108.97	14	2
4	A	313	PX4	O1-P1-O4	2.30	118.44	107.75	1	1
4	A	341	PX4	C31-C30-C29	2.30	102.74	114.42	4	1
4	A	392	PX4	O4-P1-O2	2.30	118.07	109.07	7	1
4	A	421	PX4	C14-C13-C12	2.30	102.74	114.42	7	2
4	A	342	PX4	C16-C15-C14	2.30	102.75	114.42	14	2
4	A	344	PX4	O3-C1-C2	2.30	121.26	109.16	12	2
4	A	350	PX4	C5-N1-C4	2.30	103.06	108.97	12	2
4	A	353	PX4	C11-C10-C9	2.30	105.25	113.62	6	1
4	A	371	PX4	C11-C10-C9	2.30	105.25	113.62	5	1
4	A	376	PX4	O1-P1-O4	2.30	118.43	107.75	10	1
4	A	381	PX4	C17-C16-C15	2.30	102.74	114.42	10	1
4	A	405	PX4	C3-N1-C2	2.30	100.50	109.92	4	3
4	A	319	PX4	C4-N1-C3	2.30	103.07	108.97	3	1
4	A	329	PX4	C12-C11-C10	2.30	104.93	113.19	6	1
4	A	388	PX4	C14-C13-C12	2.30	102.75	114.42	14	2
4	A	417	PX4	C15-C14-C13	2.30	102.75	114.42	8	1
4	A	325	PX4	C11-C10-C9	2.30	105.27	113.62	12	1
4	A	343	PX4	C16-C15-C14	2.30	102.76	114.42	14	1
4	A	346	PX4	C32-C31-C30	2.30	102.77	114.42	4	1
4	A	366	PX4	O1-P1-O3	2.30	118.42	107.75	10	1
4	A	385	PX4	C5-N1-C2	2.30	119.32	109.92	4	2
4	A	396	PX4	C14-C13-C12	2.30	102.76	114.42	2	1
4	A	416	PX4	C34-C33-C32	2.30	102.77	114.42	11	3
4	A	364	PX4	C30-C29-C28	2.30	102.77	114.42	11	1
4	A	371	PX4	O6-C9-C10	2.30	114.78	123.73	12	2
4	A	375	PX4	C27-C26-C25	2.29	102.78	114.42	1	1
4	A	394	PX4	C20-C19-C18	2.30	102.77	114.42	7	1
4	A	383	PX4	C17-C16-C15	2.29	102.78	114.42	5	3
4	A	418	PX4	C19-C18-C17	2.29	102.78	114.42	3	1
4	A	424	PX4	O6-C9-C10	2.30	114.78	123.73	13	1
4	A	428	PX4	C33-C32-C31	2.30	102.77	114.42	1	1
4	A	325	PX4	C5-N1-C4	2.29	103.08	108.97	12	1
4	A	344	PX4	C27-C26-C25	2.29	102.78	114.42	7	2
4	A	350	PX4	C34-C33-C32	2.29	102.79	114.42	11	1
4	A	387	PX4	C1-C2-N1	2.29	123.44	115.78	3	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	390	PX4	C1-C2-N1	2.29	123.44	115.78	2	3
4	A	328	PX4	O6-C9-C10	2.29	114.79	123.73	6	1
4	A	335	PX4	O1-P1-O4	2.29	97.11	107.75	11	1
4	A	336	PX4	C19-C18-C17	2.29	102.80	114.42	2	2
4	A	354	PX4	C19-C18-C17	2.29	102.80	114.42	13	1
4	A	363	PX4	O5-C9-C10	2.29	119.10	111.91	3	1
4	A	371	PX4	C33-C32-C31	2.29	102.79	114.42	11	2
4	A	403	PX4	C12-C11-C10	2.29	104.95	113.19	13	1
4	A	374	PX4	C8-O5-C9	2.29	108.64	117.12	4	3
4	A	323	PX4	C14-C13-C12	2.29	102.81	114.42	3	1
4	A	375	PX4	O6-C9-C10	2.29	114.80	123.73	7	1
4	A	388	PX4	C17-C16-C15	2.29	102.81	114.42	2	1
4	A	394	PX4	C33-C32-C31	2.29	102.81	114.42	5	1
4	A	363	PX4	C8-O5-C9	2.29	108.65	117.12	7	1
4	A	371	PX4	C18-C17-C16	2.29	102.81	114.42	13	1
4	A	317	PX4	C14-C13-C12	2.28	102.83	114.42	14	1
4	A	319	PX4	C33-C32-C31	2.29	102.82	114.42	2	1
4	A	341	PX4	O8-C23-C24	2.29	114.81	123.73	10	2
4	A	397	PX4	C27-C26-C25	2.29	102.82	114.42	8	1
4	A	402	PX4	C19-C18-C17	2.29	102.81	114.42	13	1
4	A	407	PX4	C5-N1-C3	2.29	114.85	108.97	11	1
4	A	425	PX4	C31-C30-C29	2.29	102.82	114.42	2	2
4	A	428	PX4	C28-C27-C26	2.29	102.81	114.42	2	1
4	A	347	PX4	C13-C12-C11	2.28	102.83	114.42	13	1
4	A	350	PX4	C3-N1-C2	2.29	119.27	109.92	2	1
4	A	371	PX4	C12-C11-C10	2.28	104.98	113.19	9	2
4	A	408	PX4	C13-C12-C11	2.28	102.83	114.42	3	2
4	A	321	PX4	C5-N1-C3	2.28	103.11	108.97	5	3
4	A	329	PX4	O8-C23-C24	2.28	114.83	123.73	4	1
4	A	383	PX4	C31-C30-C29	2.28	102.84	114.42	13	1
4	A	371	PX4	C20-C19-C18	2.28	102.85	114.42	12	3
4	A	390	PX4	O8-C23-C24	2.28	114.83	123.73	9	2
4	A	402	PX4	C5-N1-C2	2.28	100.58	109.92	13	1
4	A	310	PX4	C16-C15-C14	2.28	102.85	114.42	13	2
4	A	333	PX4	C30-C29-C28	2.28	102.85	114.42	10	1
4	A	330	PX4	O3-C1-C2	2.28	121.15	109.16	6	1
4	A	352	PX4	C28-C27-C26	2.28	102.85	114.42	12	1
4	A	413	PX4	C33-C32-C31	2.28	102.85	114.42	1	1
4	A	352	PX4	C12-C11-C10	2.28	105.00	113.19	13	1
4	A	320	PX4	O7-C23-O8	2.28	118.20	123.70	2	1
4	A	358	PX4	O3-C1-C2	2.28	121.14	109.16	12	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	405	PX4	C20-C19-C18	2.28	102.86	114.42	1	2
4	A	376	PX4	C16-C15-C14	2.28	102.87	114.42	5	1
4	A	382	PX4	O3-C1-C2	2.28	121.14	109.16	9	2
4	A	392	PX4	O5-C9-C10	2.28	119.05	111.91	3	2
4	A	410	PX4	C27-C26-C25	2.28	102.86	114.42	3	1
4	A	306	PX4	C3-N1-C2	2.28	100.60	109.92	9	2
4	A	312	PX4	C11-C10-C9	2.28	105.35	113.62	7	2
4	A	317	PX4	O7-C23-O8	2.28	118.20	123.70	13	2
4	A	316	PX4	C34-C33-C32	2.28	102.88	114.42	9	1
4	A	353	PX4	C18-C17-C16	2.28	102.87	114.42	7	1
4	A	306	PX4	C26-C25-C24	2.27	105.02	113.19	11	4
4	A	316	PX4	C29-C28-C27	2.27	102.88	114.42	3	1
4	A	347	PX4	C14-C13-C12	2.27	102.88	114.42	2	2
4	A	359	PX4	C26-C25-C24	2.27	105.02	113.19	10	1
4	A	308	PX4	C18-C17-C16	2.27	102.89	114.42	10	1
4	A	316	PX4	O5-C9-C10	2.27	119.04	111.91	8	2
4	A	409	PX4	C29-C28-C27	2.27	102.89	114.42	13	1
4	A	378	PX4	C30-C29-C28	2.27	102.89	114.42	13	1
4	A	415	PX4	C14-C13-C12	2.27	102.89	114.42	2	2
4	A	349	PX4	O8-C23-C24	2.27	114.87	123.73	8	1
4	A	358	PX4	C31-C30-C29	2.27	102.90	114.42	10	2
4	A	364	PX4	C31-C30-C29	2.27	102.90	114.42	4	1
4	A	421	PX4	C32-C31-C30	2.27	102.90	114.42	11	1
4	A	320	PX4	C20-C19-C18	2.27	102.90	114.42	1	1
4	A	337	PX4	C4-N1-C3	2.27	103.14	108.97	9	1
4	A	362	PX4	C25-C24-C23	2.27	105.37	113.62	4	1
4	A	373	PX4	C5-N1-C2	2.27	100.64	109.92	4	1
4	A	386	PX4	C32-C31-C30	2.27	102.91	114.42	7	1
4	A	415	PX4	C8-O5-C9	2.27	108.72	117.12	11	2
4	A	306	PX4	C29-C28-C27	2.27	102.92	114.42	9	3
4	A	317	PX4	C20-C19-C18	2.27	102.92	114.42	9	1
4	A	326	PX4	O5-C9-O6	2.27	117.87	123.59	6	2
4	A	339	PX4	C16-C15-C14	2.27	102.92	114.42	13	1
4	A	345	PX4	O6-C9-C10	2.27	114.89	123.73	2	1
4	A	345	PX4	C18-C17-C16	2.27	102.92	114.42	7	2
4	A	364	PX4	O1-P1-O3	2.27	97.22	107.75	8	2
4	A	384	PX4	C30-C29-C28	2.27	102.92	114.42	2	1
4	A	309	PX4	C4-N1-C2	2.26	119.18	109.92	1	2
4	A	354	PX4	O5-C9-C10	2.27	119.02	111.91	11	2
4	A	387	PX4	C33-C32-C31	2.26	102.93	114.42	5	3
4	A	388	PX4	C32-C31-C30	2.26	102.93	114.42	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	397	PX4	C11-C10-C9	2.26	105.39	113.62	8	1
4	A	427	PX4	C20-C19-C18	2.27	102.92	114.42	2	2
4	A	334	PX4	C27-C26-C25	2.26	102.93	114.42	7	1
4	A	334	PX4	C7-O7-C23	2.26	123.36	117.79	8	2
4	A	362	PX4	C14-C13-C12	2.26	102.94	114.42	7	1
4	A	363	PX4	C1-C2-N1	2.26	123.33	115.78	6	2
4	A	387	PX4	O1-P1-O4	2.26	118.25	107.75	12	1
4	A	389	PX4	C15-C14-C13	2.26	102.94	114.42	3	1
4	A	392	PX4	C20-C19-C18	2.26	102.94	114.42	2	1
4	A	328	PX4	C20-C19-C18	2.26	102.94	114.42	13	1
4	A	358	PX4	O7-C7-C8	2.26	116.59	108.40	1	4
4	A	362	PX4	O6-C9-C10	2.26	114.91	123.73	11	1
4	A	370	PX4	C3-N1-C2	2.26	100.66	109.92	13	1
4	A	306	PX4	O3-C1-C2	2.26	121.04	109.16	5	1
4	A	315	PX4	C13-C12-C11	2.26	102.95	114.42	9	1
4	A	345	PX4	C33-C32-C31	2.26	102.95	114.42	14	1
4	A	349	PX4	C3-N1-C2	2.26	119.17	109.92	8	2
4	A	398	PX4	C3-N1-C2	2.26	119.17	109.92	4	1
4	A	350	PX4	C25-C24-C23	2.26	105.40	113.62	9	3
4	A	363	PX4	C14-C13-C12	2.26	102.95	114.42	8	1
4	A	367	PX4	C18-C17-C16	2.26	102.95	114.42	4	2
4	A	384	PX4	O1-P1-O4	2.26	118.24	107.75	8	1
4	A	391	PX4	C11-C10-C9	2.26	105.40	113.62	5	2
4	A	336	PX4	C28-C27-C26	2.26	102.96	114.42	1	2
4	A	359	PX4	C13-C12-C11	2.26	102.96	114.42	11	1
4	A	359	PX4	C8-O5-C9	2.26	108.76	117.12	13	1
4	A	418	PX4	C20-C19-C18	2.26	102.96	114.42	5	1
4	A	406	PX4	C32-C31-C30	2.26	102.96	114.42	5	2
4	A	407	PX4	C18-C17-C16	2.26	102.96	114.42	7	1
4	A	310	PX4	C11-C10-C9	2.26	121.82	113.62	2	1
4	A	322	PX4	C12-C11-C10	2.26	105.08	113.19	6	1
4	A	329	PX4	C16-C15-C14	2.26	102.97	114.42	13	1
4	A	336	PX4	C3-N1-C2	2.26	119.15	109.92	5	1
4	A	341	PX4	C19-C18-C17	2.26	102.97	114.42	7	2
4	A	386	PX4	C30-C29-C28	2.26	102.97	114.42	10	2
4	A	422	PX4	C32-C31-C30	2.26	102.97	114.42	10	1
4	A	343	PX4	C3-N1-C2	2.26	119.15	109.92	6	1
4	A	345	PX4	C32-C31-C30	2.25	102.98	114.42	4	2
4	A	397	PX4	C32-C31-C30	2.26	102.98	114.42	11	1
4	A	400	PX4	C19-C18-C17	2.26	102.97	114.42	4	1
4	A	409	PX4	C5-N1-C2	2.25	119.14	109.92	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	348	PX4	C4-N1-C2	2.25	119.14	109.92	5	2
4	A	377	PX4	C32-C31-C30	2.25	102.99	114.42	14	2
4	A	403	PX4	C13-C12-C11	2.25	102.99	114.42	11	2
4	A	405	PX4	C19-C18-C17	2.25	102.99	114.42	7	1
4	A	417	PX4	C14-C13-C12	2.25	102.98	114.42	3	1
4	A	315	PX4	C25-C24-C23	2.25	105.44	113.62	8	1
4	A	326	PX4	C28-C27-C26	2.25	103.00	114.42	2	1
4	A	347	PX4	C20-C19-C18	2.25	103.00	114.42	9	1
4	A	348	PX4	C1-C2-N1	2.25	123.30	115.78	10	1
4	A	369	PX4	C5-N1-C2	2.25	119.13	109.92	14	1
4	A	385	PX4	C20-C19-C18	2.25	102.99	114.42	6	1
4	A	384	PX4	C27-C26-C25	2.25	103.00	114.42	12	3
4	A	373	PX4	C32-C31-C30	2.25	103.00	114.42	6	1
4	A	425	PX4	C3-N1-C2	2.25	119.12	109.92	2	1
4	A	360	PX4	O1-P1-O3	2.25	97.30	107.75	13	1
4	A	388	PX4	O6-C9-C10	2.25	114.97	123.73	5	1
4	A	390	PX4	O7-C7-C6	2.25	116.54	108.40	10	3
4	A	420	PX4	O3-C1-C2	2.25	120.98	109.16	10	2
4	A	427	PX4	C16-C15-C14	2.25	103.01	114.42	12	1
4	A	351	PX4	C28-C27-C26	2.25	103.02	114.42	1	1
4	A	314	PX4	O3-P1-O2	2.25	100.30	109.07	13	1
4	A	337	PX4	C12-C11-C10	2.25	105.12	113.19	13	4
4	A	364	PX4	C13-C12-C11	2.25	103.02	114.42	10	2
4	A	338	PX4	C30-C29-C28	2.24	103.03	114.42	5	2
4	A	391	PX4	O5-C9-C10	2.25	118.95	111.91	6	2
4	A	341	PX4	C4-N1-C2	2.24	119.10	109.92	14	1
4	A	367	PX4	O8-C23-C24	2.24	114.98	123.73	9	1
4	A	402	PX4	O1-P1-O4	2.25	118.17	107.75	9	2
4	A	406	PX4	C16-C15-C14	2.24	103.03	114.42	10	2
4	A	313	PX4	C28-C27-C26	2.24	103.04	114.42	5	1
4	A	337	PX4	C16-C15-C14	2.24	103.04	114.42	14	1
4	A	349	PX4	C15-C14-C13	2.24	103.04	114.42	8	3
4	A	365	PX4	O7-C7-C6	2.24	116.52	108.40	5	5
4	A	384	PX4	C18-C17-C16	2.24	103.04	114.42	2	1
4	A	406	PX4	C27-C26-C25	2.24	103.05	114.42	4	1
4	A	412	PX4	C18-C17-C16	2.24	103.04	114.42	10	2
4	A	424	PX4	C26-C25-C24	2.24	105.13	113.19	5	1
4	A	319	PX4	C32-C31-C30	2.24	103.06	114.42	13	1
4	A	335	PX4	C5-N1-C4	2.24	114.73	108.97	14	2
4	A	353	PX4	C30-C29-C28	2.24	103.06	114.42	13	2
4	A	362	PX4	O8-C23-C24	2.24	115.00	123.73	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	399	PX4	C27-C26-C25	2.24	103.05	114.42	14	1
4	A	358	PX4	O5-C9-C10	2.24	118.93	111.91	8	3
4	A	363	PX4	C4-N1-C2	2.24	100.76	109.92	14	1
4	A	404	PX4	C5-N1-C2	2.24	119.08	109.92	9	3
4	A	326	PX4	C15-C14-C13	2.24	103.07	114.42	4	2
4	A	328	PX4	C31-C30-C29	2.24	103.07	114.42	8	1
4	A	383	PX4	C34-C33-C32	2.24	103.07	114.42	1	1
4	A	425	PX4	C17-C16-C15	2.24	103.06	114.42	14	1
4	A	334	PX4	C18-C17-C16	2.24	103.07	114.42	8	1
4	A	334	PX4	O7-C7-C8	2.24	116.50	108.40	12	1
4	A	335	PX4	C4-N1-C2	2.24	100.76	109.92	8	1
4	A	343	PX4	C18-C17-C16	2.24	103.07	114.42	10	2
4	A	358	PX4	C25-C24-C23	2.24	105.48	113.62	7	1
4	A	331	PX4	C17-C16-C15	2.23	103.08	114.42	11	1
4	A	332	PX4	C11-C10-C9	2.24	105.49	113.62	14	1
4	A	337	PX4	C29-C28-C27	2.24	103.08	114.42	4	2
4	A	341	PX4	C8-O5-C9	2.24	108.84	117.12	6	2
4	A	365	PX4	C25-C24-C23	2.24	105.49	113.62	9	3
4	A	404	PX4	C18-C17-C16	2.23	103.08	114.42	8	1
4	A	422	PX4	O8-C23-C24	2.23	115.02	123.73	11	1
4	A	323	PX4	C31-C30-C29	2.23	103.09	114.42	7	2
4	A	372	PX4	C13-C12-C11	2.23	103.09	114.42	5	1
4	A	321	PX4	C28-C27-C26	2.23	103.10	114.42	8	1
4	A	355	PX4	C29-C28-C27	2.23	103.09	114.42	11	1
4	A	384	PX4	C13-C12-C11	2.23	103.09	114.42	13	2
4	A	406	PX4	C5-N1-C4	2.23	103.23	108.97	2	2
4	A	412	PX4	C32-C31-C30	2.23	103.09	114.42	12	1
4	A	386	PX4	C3-N1-C2	2.23	100.79	109.92	8	1
4	A	420	PX4	C14-C13-C12	2.23	103.10	114.42	12	1
4	A	311	PX4	O6-C9-C10	2.23	115.03	123.73	4	1
4	A	329	PX4	C18-C17-C16	2.23	103.11	114.42	3	2
4	A	346	PX4	C16-C15-C14	2.23	103.10	114.42	14	1
4	A	351	PX4	C3-N1-C2	2.23	119.03	109.92	3	2
4	A	356	PX4	C32-C31-C30	2.23	103.11	114.42	2	1
4	A	320	PX4	C18-C17-C16	2.23	103.12	114.42	7	1
4	A	325	PX4	C17-C16-C15	2.23	103.12	114.42	11	2
4	A	325	PX4	C33-C32-C31	2.23	103.12	114.42	14	1
4	A	338	PX4	C13-C12-C11	2.23	103.12	114.42	5	1
4	A	393	PX4	C16-C15-C14	2.23	103.11	114.42	11	1
4	A	400	PX4	C20-C19-C18	2.23	103.11	114.42	9	1
4	A	421	PX4	C28-C27-C26	2.23	103.11	114.42	10	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	383	PX4	C32-C31-C30	2.23	103.12	114.42	13	1
4	A	408	PX4	C26-C25-C24	2.23	105.19	113.19	13	1
4	A	318	PX4	C17-C16-C15	2.23	103.13	114.42	7	2
4	A	335	PX4	O5-C9-C10	2.23	118.89	111.91	9	3
4	A	343	PX4	C15-C14-C13	2.23	103.13	114.42	3	1
4	A	320	PX4	C5-N1-C2	2.22	119.02	109.92	9	1
4	A	338	PX4	C20-C19-C18	2.22	103.14	114.42	10	1
4	A	350	PX4	C12-C11-C10	2.22	105.19	113.19	5	1
4	A	351	PX4	C17-C16-C15	2.22	103.13	114.42	4	1
4	A	379	PX4	C34-C33-C32	2.22	103.13	114.42	12	2
4	A	394	PX4	C3-N1-C2	2.23	100.81	109.92	13	2
4	A	404	PX4	C26-C25-C24	2.23	105.19	113.19	7	2
4	A	347	PX4	C5-N1-C2	2.22	119.01	109.92	14	1
4	A	355	PX4	C30-C29-C28	2.22	103.14	114.42	12	1
4	A	392	PX4	C34-C33-C32	2.22	103.14	114.42	2	2
4	A	402	PX4	C16-C15-C14	2.22	103.13	114.42	8	2
4	A	412	PX4	C33-C32-C31	2.22	103.13	114.42	6	1
4	A	310	PX4	O6-C9-C10	2.22	115.07	123.73	6	1
4	A	321	PX4	C14-C13-C12	2.22	103.15	114.42	6	1
4	A	368	PX4	C4-N1-C3	2.22	114.69	108.97	14	2
4	A	389	PX4	C18-C17-C16	2.22	103.14	114.42	14	1
4	A	396	PX4	C26-C25-C24	2.22	105.20	113.19	9	1
4	A	418	PX4	C5-N1-C2	2.22	119.01	109.92	4	1
4	A	420	PX4	C34-C33-C32	2.22	103.14	114.42	11	1
4	A	422	PX4	C27-C26-C25	2.22	103.15	114.42	1	1
4	A	337	PX4	O1-P1-O4	2.22	118.06	107.75	4	1
4	A	341	PX4	O3-C1-C2	2.22	120.84	109.16	13	2
4	A	351	PX4	O3-P1-O2	2.22	100.39	109.07	9	1
4	A	307	PX4	C8-O5-C9	2.22	108.91	117.12	8	1
4	A	309	PX4	C34-C33-C32	2.22	103.16	114.42	2	1
4	A	363	PX4	O3-C1-C2	2.22	120.83	109.16	5	1
4	A	319	PX4	C25-C24-C23	2.22	105.56	113.62	3	1
4	A	320	PX4	C4-N1-C2	2.22	100.84	109.92	14	1
4	A	340	PX4	C33-C32-C31	2.22	103.16	114.42	10	1
4	A	364	PX4	O7-C7-C8	2.22	116.44	108.40	8	3
4	A	420	PX4	C8-O5-C9	2.22	108.90	117.12	1	2
4	A	339	PX4	C14-C13-C12	2.22	103.17	114.42	13	1
4	A	354	PX4	C29-C28-C27	2.22	103.17	114.42	3	1
4	A	361	PX4	O3-C1-C2	2.22	120.82	109.16	10	1
4	A	364	PX4	C11-C10-C9	2.22	105.56	113.62	7	2
4	A	419	PX4	C16-C15-C14	2.22	103.16	114.42	11	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	327	PX4	C5-N1-C4	2.22	103.28	108.97	14	1
4	A	329	PX4	C17-C16-C15	2.22	103.18	114.42	12	1
4	A	344	PX4	C30-C29-C28	2.22	103.18	114.42	8	1
4	A	349	PX4	C28-C27-C26	2.22	103.17	114.42	9	3
4	A	358	PX4	C5-N1-C2	2.22	118.98	109.92	5	1
4	A	391	PX4	O1-P1-O3	2.22	97.45	107.75	11	1
4	A	413	PX4	C14-C13-C12	2.22	103.17	114.42	8	1
4	A	308	PX4	C15-C14-C13	2.21	103.19	114.42	11	1
4	A	368	PX4	C32-C31-C30	2.21	103.18	114.42	13	1
4	A	388	PX4	C4-N1-C2	2.21	118.97	109.92	7	2
4	A	400	PX4	C26-C25-C24	2.21	105.23	113.19	3	2
4	A	382	PX4	O1-P1-O3	2.21	97.47	107.75	13	1
4	A	398	PX4	C25-C24-C23	2.21	105.57	113.62	1	2
4	A	400	PX4	O1-P1-O3	2.21	97.47	107.75	3	1
4	A	400	PX4	C29-C28-C27	2.21	103.19	114.42	10	1
4	A	425	PX4	C1-C2-N1	2.21	123.17	115.78	9	1
4	A	312	PX4	O3-C1-C2	2.21	120.79	109.16	3	1
4	A	314	PX4	O5-C9-C10	2.21	118.85	111.91	14	1
4	A	341	PX4	O1-P1-O3	2.21	97.47	107.75	14	1
4	A	352	PX4	C29-C28-C27	2.21	103.20	114.42	2	2
4	A	355	PX4	C33-C32-C31	2.21	103.20	114.42	3	2
4	A	355	PX4	C16-C15-C14	2.21	103.20	114.42	7	1
4	A	417	PX4	C31-C30-C29	2.21	103.20	114.42	11	3
4	A	420	PX4	C16-C15-C14	2.21	103.20	114.42	1	4
4	A	380	PX4	O3-C1-C2	2.21	120.78	109.16	3	2
4	A	381	PX4	C13-C12-C11	2.21	103.21	114.42	1	1
4	A	394	PX4	C12-C11-C10	2.21	105.25	113.19	11	2
4	A	407	PX4	C33-C32-C31	2.21	103.21	114.42	7	1
4	A	424	PX4	C4-N1-C3	2.21	114.66	108.97	8	2
4	A	328	PX4	O1-P1-O3	2.21	97.49	107.75	12	2
4	A	409	PX4	C30-C29-C28	2.21	103.21	114.42	11	1
4	A	412	PX4	C19-C18-C17	2.21	103.21	114.42	1	1
4	A	356	PX4	O4-P1-O2	2.21	100.44	109.07	12	2
4	A	412	PX4	C11-C10-C9	2.21	105.59	113.62	4	1
4	A	315	PX4	C5-N1-C2	2.20	118.94	109.92	14	1
4	A	330	PX4	C11-C10-C9	2.21	105.60	113.62	13	1
4	A	364	PX4	O1-P1-O4	2.21	117.99	107.75	4	1
4	A	393	PX4	O4-P1-O2	2.21	117.69	109.07	9	1
4	A	422	PX4	C20-C19-C18	2.21	103.22	114.42	9	1
4	A	384	PX4	C8-O5-C9	2.21	108.95	117.12	7	1
4	A	324	PX4	C30-C29-C28	2.20	103.23	114.42	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	343	PX4	C17-C16-C15	2.20	103.23	114.42	2	1
4	A	394	PX4	C27-C26-C25	2.21	103.23	114.42	5	2
4	A	422	PX4	C13-C12-C11	2.21	103.23	114.42	4	1
4	A	343	PX4	C5-N1-C2	2.20	100.90	109.92	7	2
4	A	413	PX4	O3-P1-O2	2.20	117.68	109.07	10	2
4	A	306	PX4	C18-C17-C16	2.20	103.25	114.42	6	1
4	A	403	PX4	C14-C13-C12	2.20	103.25	114.42	1	2
4	A	427	PX4	O3-C1-C2	2.20	120.74	109.16	12	1
4	A	316	PX4	O3-C1-C2	2.20	120.74	109.16	7	2
4	A	329	PX4	C32-C31-C30	2.20	103.25	114.42	12	1
4	A	373	PX4	C19-C18-C17	2.20	103.25	114.42	6	2
4	A	400	PX4	C15-C14-C13	2.20	103.25	114.42	5	1
4	A	394	PX4	C26-C25-C24	2.20	105.28	113.19	11	2
4	A	411	PX4	C17-C16-C15	2.20	103.26	114.42	3	1
4	A	306	PX4	C25-C24-C23	2.20	105.62	113.62	7	1
4	A	322	PX4	C11-C10-C9	2.20	105.62	113.62	2	1
4	A	331	PX4	C20-C19-C18	2.20	103.27	114.42	6	1
4	A	375	PX4	C34-C33-C32	2.20	103.26	114.42	5	2
4	A	378	PX4	O1-P1-O4	2.20	117.95	107.75	7	1
4	A	413	PX4	C18-C17-C16	2.20	103.26	114.42	3	1
4	A	315	PX4	O1-P1-O4	2.20	117.95	107.75	11	1
4	A	390	PX4	C34-C33-C32	2.20	103.27	114.42	1	2
4	A	327	PX4	C26-C25-C24	2.20	121.08	113.19	2	2
4	A	332	PX4	O3-C1-C2	2.19	120.70	109.16	3	1
4	A	337	PX4	C34-C33-C32	2.19	103.28	114.42	7	1
4	A	389	PX4	O6-C9-C10	2.20	115.17	123.73	9	1
4	A	322	PX4	C20-C19-C18	2.19	103.29	114.42	10	1
4	A	339	PX4	C29-C28-C27	2.19	103.29	114.42	9	1
4	A	397	PX4	C4-N1-C2	2.19	100.94	109.92	2	1
4	A	341	PX4	O4-P1-O2	2.19	117.64	109.07	2	2
4	A	358	PX4	C7-O7-C23	2.19	112.39	117.79	3	4
4	A	361	PX4	C30-C29-C28	2.19	103.29	114.42	6	1
4	A	354	PX4	C14-C13-C12	2.19	103.30	114.42	3	1
4	A	379	PX4	C11-C10-C9	2.19	105.65	113.62	11	1
4	A	415	PX4	O6-C9-C10	2.19	115.18	123.73	9	1
4	A	421	PX4	C5-N1-C2	2.19	118.89	109.92	11	1
4	A	334	PX4	C30-C29-C28	2.19	103.31	114.42	7	1
4	A	357	PX4	C3-N1-C2	2.19	118.88	109.92	1	2
4	A	378	PX4	C5-N1-C2	2.19	100.95	109.92	1	1
4	A	427	PX4	O1-P1-O4	2.19	117.92	107.75	7	1
4	A	366	PX4	O3-C1-C2	2.19	120.68	109.16	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	320	PX4	C19-C18-C17	2.19	103.32	114.42	1	2
4	A	328	PX4	C29-C28-C27	2.19	103.31	114.42	10	2
4	A	339	PX4	C5-N1-C3	2.19	103.35	108.97	6	1
4	A	338	PX4	O1-P1-O4	2.19	117.90	107.75	8	2
4	A	385	PX4	O1-P1-O4	2.19	117.91	107.75	4	1
4	A	380	PX4	C1-C2-N1	2.19	123.08	115.78	3	3
4	A	380	PX4	C30-C29-C28	2.19	103.32	114.42	10	1
4	A	427	PX4	C27-C26-C25	2.19	103.32	114.42	1	1
4	A	430	PX4	C1-C2-N1	2.19	123.08	115.78	6	4
4	A	321	PX4	C16-C15-C14	2.19	103.33	114.42	8	3
4	A	417	PX4	C32-C31-C30	2.19	103.33	114.42	2	1
4	A	423	PX4	C25-C24-C23	2.19	121.57	113.62	8	2
4	A	335	PX4	C29-C28-C27	2.18	103.34	114.42	13	2
4	A	353	PX4	C29-C28-C27	2.18	103.34	114.42	4	1
4	A	320	PX4	O6-C9-C10	2.18	115.22	123.73	14	1
4	A	357	PX4	C26-C25-C24	2.18	121.04	113.19	11	1
4	A	376	PX4	C20-C19-C18	2.18	103.34	114.42	13	1
4	A	384	PX4	C20-C19-C18	2.18	125.51	114.42	13	1
4	A	411	PX4	O4-P1-O2	2.18	117.60	109.07	6	1
4	A	427	PX4	C17-C16-C15	2.18	103.35	114.42	12	2
4	A	429	PX4	C28-C27-C26	2.18	103.34	114.42	8	1
4	A	306	PX4	C5-N1-C2	2.18	118.83	109.92	13	1
4	A	312	PX4	C31-C30-C29	2.18	103.36	114.42	5	1
4	A	315	PX4	C30-C29-C28	2.18	103.35	114.42	7	2
4	A	330	PX4	C25-C24-C23	2.18	105.69	113.62	5	1
4	A	334	PX4	O8-C23-C24	2.18	115.22	123.73	14	2
4	A	353	PX4	C14-C13-C12	2.18	103.36	114.42	14	1
4	A	383	PX4	C28-C27-C26	2.18	103.36	114.42	14	1
4	A	355	PX4	C4-N1-C2	2.18	118.83	109.92	12	1
4	A	362	PX4	O3-P1-O2	2.18	100.55	109.07	3	1
4	A	392	PX4	C5-N1-C2	2.18	101.00	109.92	14	1
4	A	419	PX4	C20-C19-C18	2.18	103.36	114.42	10	1
4	A	309	PX4	C14-C13-C12	2.18	103.37	114.42	4	1
4	A	317	PX4	C19-C18-C17	2.18	103.38	114.42	4	1
4	A	335	PX4	C5-N1-C2	2.18	118.83	109.92	12	1
4	A	323	PX4	C20-C19-C18	2.18	103.38	114.42	3	1
4	A	328	PX4	C27-C26-C25	2.18	103.37	114.42	4	1
4	A	341	PX4	C30-C29-C28	2.18	103.37	114.42	6	2
4	A	345	PX4	C13-C12-C11	2.18	103.37	114.42	6	1
4	A	333	PX4	C4-N1-C2	2.18	118.82	109.92	3	1
4	A	338	PX4	O6-C9-C10	2.18	115.24	123.73	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	341	PX4	C27-C26-C25	2.18	103.38	114.42	10	1
4	A	350	PX4	C14-C13-C12	2.18	103.38	114.42	6	1
4	A	375	PX4	C14-C13-C12	2.18	103.38	114.42	3	1
4	A	377	PX4	C26-C25-C24	2.18	121.01	113.19	2	1
4	A	395	PX4	C22-C21-C20	2.18	96.91	113.42	6	1
4	A	398	PX4	C4-N1-C2	2.18	118.82	109.92	7	1
4	A	407	PX4	C11-C10-C9	2.18	105.71	113.62	12	1
4	A	421	PX4	O3-C1-C2	2.18	120.60	109.16	6	1
4	A	425	PX4	O1-P1-O4	2.18	117.85	107.75	7	1
4	A	341	PX4	C29-C28-C27	2.17	103.39	114.42	4	2
4	A	348	PX4	C31-C30-C29	2.17	103.38	114.42	10	1
4	A	360	PX4	C5-N1-C2	2.17	101.02	109.92	6	1
4	A	320	PX4	C8-O5-C9	2.17	109.07	117.12	6	1
4	A	324	PX4	C13-C12-C11	2.17	103.39	114.42	14	2
4	A	347	PX4	O3-C1-C2	2.17	120.59	109.16	5	1
4	A	351	PX4	C34-C33-C32	2.17	103.39	114.42	14	1
4	A	360	PX4	C4-N1-C2	2.17	118.81	109.92	10	1
4	A	376	PX4	C5-N1-C2	2.17	118.81	109.92	3	2
4	A	402	PX4	C14-C13-C12	2.17	103.39	114.42	7	2
4	A	316	PX4	C8-O5-C9	2.17	109.08	117.12	8	1
4	A	323	PX4	C17-C16-C15	2.17	103.40	114.42	14	1
4	A	362	PX4	C15-C14-C13	2.17	103.40	114.42	12	1
4	A	424	PX4	C18-C17-C16	2.17	103.39	114.42	9	1
4	A	344	PX4	C8-O5-C9	2.17	125.16	117.12	13	3
4	A	345	PX4	C29-C28-C27	2.17	103.40	114.42	4	2
4	A	365	PX4	C22-C21-C20	2.17	96.94	113.42	13	1
4	A	383	PX4	C5-N1-C2	2.17	118.79	109.92	12	1
4	A	409	PX4	O5-C9-C10	2.17	118.72	111.91	2	1
4	A	335	PX4	C20-C19-C18	2.17	103.42	114.42	7	1
4	A	352	PX4	C20-C19-C18	2.17	103.43	114.42	8	1
4	A	360	PX4	O8-C23-C24	2.17	115.28	123.73	7	1
4	A	366	PX4	C33-C32-C31	2.17	103.42	114.42	12	2
4	A	368	PX4	C16-C15-C14	2.17	103.42	114.42	14	2
4	A	406	PX4	C5-N1-C3	2.17	114.55	108.97	2	1
4	A	430	PX4	O1-P1-O3	2.17	97.68	107.75	8	1
4	A	315	PX4	C14-C13-C12	2.17	103.43	114.42	13	2
4	A	416	PX4	C20-C19-C18	2.17	103.43	114.42	1	1
4	A	325	PX4	C4-N1-C2	2.16	118.77	109.92	7	1
4	A	325	PX4	C34-C33-C32	2.16	103.44	114.42	8	1
4	A	331	PX4	O3-C1-C2	2.16	120.54	109.16	2	1
4	A	359	PX4	C28-C27-C26	2.16	103.45	114.42	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	422	PX4	C25-C24-C23	2.16	105.75	113.62	6	1
4	A	319	PX4	C1-C2-N1	2.16	122.99	115.78	10	3
4	A	319	PX4	O6-C9-C10	2.16	115.30	123.73	12	1
4	A	341	PX4	O6-C9-C10	2.16	115.31	123.73	7	1
4	A	349	PX4	C8-O5-C9	2.16	125.12	117.12	14	1
4	A	366	PX4	C26-C25-C24	2.16	105.42	113.19	4	2
4	A	336	PX4	C33-C32-C31	2.16	103.46	114.42	1	2
4	A	349	PX4	O6-C9-C10	2.16	115.31	123.73	14	1
4	A	350	PX4	C28-C27-C26	2.16	103.46	114.42	13	1
4	A	365	PX4	C20-C19-C18	2.16	103.46	114.42	3	1
4	A	369	PX4	C29-C28-C27	2.16	103.46	114.42	13	2
4	A	400	PX4	C11-C10-C9	2.16	105.76	113.62	2	2
4	A	378	PX4	C19-C18-C17	2.16	103.46	114.42	4	1
4	A	395	PX4	C20-C19-C18	2.16	103.46	114.42	10	1
4	A	416	PX4	C30-C29-C28	2.16	103.46	114.42	7	1
4	A	423	PX4	C5-N1-C4	2.16	114.53	108.97	11	1
4	A	428	PX4	C8-O5-C9	2.16	109.12	117.12	9	1
4	A	365	PX4	C34-C33-C32	2.16	103.46	114.42	7	1
4	A	319	PX4	O1-P1-O4	2.16	97.72	107.75	14	1
4	A	366	PX4	C5-N1-C4	2.16	103.43	108.97	5	2
4	A	367	PX4	C15-C14-C13	2.16	103.47	114.42	10	1
4	A	368	PX4	O3-C1-C2	2.16	120.51	109.16	5	1
4	A	383	PX4	C1-C2-N1	2.16	122.99	115.78	9	2
4	A	378	PX4	C15-C14-C13	2.16	103.48	114.42	11	1
4	A	404	PX4	C12-C11-C10	2.16	120.95	113.19	13	1
4	A	335	PX4	C11-C10-C9	2.16	105.78	113.62	2	2
4	A	395	PX4	C8-O5-C9	2.16	109.14	117.12	11	2
4	A	403	PX4	C25-C24-C23	2.16	105.78	113.62	11	1
4	A	326	PX4	C5-N1-C2	2.15	101.11	109.92	8	2
4	A	333	PX4	O6-C9-C10	2.15	132.13	123.73	11	1
4	A	359	PX4	C17-C16-C15	2.15	103.49	114.42	14	1
4	A	407	PX4	O1-P1-O4	2.16	117.75	107.75	5	1
4	A	419	PX4	C30-C29-C28	2.16	103.48	114.42	8	1
4	A	322	PX4	C5-N1-C4	2.15	103.44	108.97	8	1
4	A	331	PX4	C31-C30-C29	2.15	103.50	114.42	6	3
4	A	341	PX4	C14-C13-C12	2.15	103.49	114.42	10	2
4	A	398	PX4	C30-C29-C28	2.15	103.49	114.42	5	1
4	A	350	PX4	C26-C25-C24	2.15	105.45	113.19	3	2
4	A	355	PX4	O6-C9-C10	2.15	115.33	123.73	2	2
4	A	384	PX4	O3-C1-C2	2.15	120.48	109.16	5	1
4	A	427	PX4	C18-C17-C16	2.15	103.50	114.42	12	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	325	PX4	C16-C15-C14	2.15	103.51	114.42	1	1
4	A	357	PX4	C17-C16-C15	2.15	103.50	114.42	12	1
4	A	395	PX4	C3-N1-C2	2.15	118.72	109.92	7	1
4	A	310	PX4	C25-C24-C23	2.15	121.44	113.62	7	1
4	A	349	PX4	C18-C17-C16	2.15	103.52	114.42	12	1
4	A	361	PX4	C18-C17-C16	2.15	103.52	114.42	5	1
4	A	370	PX4	C19-C18-C17	2.15	103.52	114.42	12	1
4	A	403	PX4	C31-C30-C29	2.15	103.52	114.42	13	2
4	A	429	PX4	C16-C15-C14	2.15	103.52	114.42	10	1
4	A	375	PX4	C7-O7-C23	2.15	112.51	117.79	12	4
4	A	380	PX4	C15-C14-C13	2.15	103.53	114.42	5	1
4	A	415	PX4	C18-C17-C16	2.15	103.53	114.42	8	1
4	A	427	PX4	C28-C27-C26	2.15	103.53	114.42	4	1
4	A	355	PX4	C34-C33-C32	2.14	103.54	114.42	14	1
4	A	338	PX4	O8-C23-C24	2.14	115.37	123.73	4	2
4	A	429	PX4	C30-C29-C28	2.14	103.54	114.42	10	1
4	A	366	PX4	C27-C26-C25	2.14	103.55	114.42	11	2
4	A	399	PX4	C20-C19-C18	2.14	103.55	114.42	1	1
4	A	401	PX4	C31-C30-C29	2.14	103.55	114.42	6	2
4	A	408	PX4	O3-C1-C2	2.14	120.43	109.16	2	1
4	A	423	PX4	C18-C17-C16	2.14	103.54	114.42	8	3
4	A	328	PX4	C19-C18-C17	2.14	103.56	114.42	4	1
4	A	339	PX4	C1-C2-N1	2.14	122.92	115.78	9	2
4	A	395	PX4	C13-C12-C11	2.14	103.56	114.42	10	2
4	A	422	PX4	C3-N1-C2	2.14	118.68	109.92	3	1
4	A	347	PX4	C8-O5-C9	2.14	109.20	117.12	7	2
4	A	357	PX4	O8-C23-C24	2.14	115.39	123.73	9	1
4	A	389	PX4	C32-C31-C30	2.14	103.56	114.42	11	1
4	A	420	PX4	C33-C32-C31	2.14	103.57	114.42	11	1
4	A	325	PX4	C15-C14-C13	2.14	103.58	114.42	7	1
4	A	343	PX4	O1-P1-O4	2.14	97.82	107.75	1	1
4	A	360	PX4	C29-C28-C27	2.14	103.58	114.42	2	1
4	A	360	PX4	C16-C15-C14	2.14	103.57	114.42	5	1
4	A	375	PX4	C33-C32-C31	2.14	103.58	114.42	14	2
4	A	376	PX4	O8-C23-C24	2.14	115.39	123.73	2	1
4	A	390	PX4	C8-O5-C9	2.14	109.21	117.12	5	1
4	A	409	PX4	C17-C16-C15	2.14	103.58	114.42	11	1
4	A	419	PX4	C32-C31-C30	2.14	103.57	114.42	9	1
4	A	367	PX4	C33-C32-C31	2.14	103.58	114.42	5	1
4	A	368	PX4	C18-C17-C16	2.14	103.58	114.42	5	1
4	A	369	PX4	C27-C26-C25	2.14	103.58	114.42	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	424	PX4	C31-C30-C29	2.14	103.58	114.42	12	1
4	A	425	PX4	C8-O5-C9	2.14	109.21	117.12	14	2
4	A	313	PX4	C8-O5-C9	2.13	109.22	117.12	12	2
4	A	315	PX4	C31-C30-C29	2.13	103.59	114.42	12	2
4	A	428	PX4	C4-N1-C2	2.14	118.65	109.92	4	1
4	A	311	PX4	C16-C15-C14	2.13	103.59	114.42	6	2
4	A	317	PX4	C34-C33-C32	2.13	103.59	114.42	6	1
4	A	363	PX4	O1-P1-O3	2.13	97.83	107.75	12	1
4	A	401	PX4	O3-C1-C2	2.13	120.38	109.16	7	1
4	A	416	PX4	O8-C23-C24	2.13	115.41	123.73	9	1
4	A	424	PX4	C11-C10-C9	2.13	105.86	113.62	12	1
4	A	425	PX4	C18-C17-C16	2.13	103.59	114.42	9	1
4	A	427	PX4	C14-C13-C12	2.13	103.59	114.42	10	1
4	A	402	PX4	C25-C24-C23	2.13	105.86	113.62	12	2
4	A	403	PX4	C15-C14-C13	2.13	103.60	114.42	8	1
4	A	429	PX4	C1-C2-N1	2.13	122.90	115.78	11	2
4	A	430	PX4	C33-C32-C31	2.13	103.59	114.42	5	1
4	A	316	PX4	C1-C2-N1	2.13	122.90	115.78	12	1
4	A	321	PX4	C4-N1-C3	2.13	103.49	108.97	2	2
4	A	306	PX4	C31-C30-C29	2.13	103.61	114.42	10	1
4	A	322	PX4	C17-C16-C15	2.13	103.61	114.42	12	1
4	A	340	PX4	C13-C12-C11	2.13	103.61	114.42	14	1
4	A	342	PX4	C18-C17-C16	2.13	103.61	114.42	5	2
4	A	382	PX4	C18-C17-C16	2.13	103.60	114.42	8	3
4	A	396	PX4	C13-C12-C11	2.13	103.61	114.42	6	1
4	A	315	PX4	O3-C1-C2	2.13	120.35	109.16	8	1
4	A	348	PX4	C3-N1-C2	2.13	101.21	109.92	2	1
4	A	350	PX4	O1-P1-O3	2.13	117.63	107.75	13	1
4	A	351	PX4	C30-C29-C28	2.13	103.62	114.42	8	2
4	A	387	PX4	C32-C31-C30	2.13	103.62	114.42	8	1
4	A	392	PX4	C27-C26-C25	2.13	103.62	114.42	9	1
4	A	413	PX4	C17-C16-C15	2.13	103.61	114.42	5	1
4	A	339	PX4	C8-O5-C9	2.13	109.25	117.12	4	1
4	A	358	PX4	C12-C11-C10	2.13	105.54	113.19	8	1
4	A	409	PX4	C16-C15-C14	2.13	103.62	114.42	10	1
4	A	407	PX4	C17-C16-C15	2.13	103.63	114.42	4	1
4	A	419	PX4	C25-C24-C23	2.13	105.88	113.62	1	1
4	A	340	PX4	C20-C19-C18	2.13	103.63	114.42	2	1
4	A	344	PX4	C11-C10-C9	2.13	105.89	113.62	3	1
4	A	359	PX4	C5-N1-C2	2.13	118.61	109.92	13	1
4	A	363	PX4	C11-C10-C9	2.13	105.89	113.62	11	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	377	PX4	C13-C12-C11	2.13	103.64	114.42	8	1
4	A	417	PX4	O3-C1-C2	2.13	120.34	109.16	1	1
4	A	332	PX4	C32-C31-C30	2.12	103.64	114.42	9	1
4	A	336	PX4	C14-C13-C12	2.12	103.64	114.42	3	2
4	A	339	PX4	C31-C30-C29	2.12	103.64	114.42	6	2
4	A	361	PX4	C1-C2-N1	2.12	122.87	115.78	8	1
4	A	362	PX4	C28-C27-C26	2.12	103.64	114.42	9	1
4	A	368	PX4	C19-C18-C17	2.12	103.64	114.42	6	2
4	A	324	PX4	C28-C27-C26	2.12	103.65	114.42	13	1
4	A	334	PX4	C32-C31-C30	2.12	103.65	114.42	1	1
4	A	336	PX4	C27-C26-C25	2.12	103.65	114.42	2	2
4	A	356	PX4	C5-N1-C2	2.12	101.23	109.92	7	1
4	A	366	PX4	C25-C24-C23	2.12	105.90	113.62	5	1
4	A	369	PX4	O1-P1-O3	2.12	97.89	107.75	3	1
4	A	369	PX4	C34-C33-C32	2.12	103.66	114.42	2	1
4	A	373	PX4	C3-N1-C2	2.12	118.60	109.92	8	1
4	A	374	PX4	C25-C24-C23	2.12	105.91	113.62	2	1
4	A	385	PX4	C19-C18-C17	2.12	103.66	114.42	12	1
4	A	386	PX4	C5-N1-C2	2.12	118.59	109.92	12	2
4	A	395	PX4	C17-C16-C15	2.12	103.65	114.42	14	1
4	A	309	PX4	C3-N1-C2	2.12	118.59	109.92	4	1
4	A	311	PX4	C31-C30-C29	2.12	103.66	114.42	10	1
4	A	357	PX4	C32-C31-C30	2.12	103.67	114.42	2	1
4	A	362	PX4	C11-C10-C9	2.12	105.92	113.62	13	1
4	A	425	PX4	C33-C32-C31	2.12	103.67	114.42	10	1
4	A	307	PX4	C25-C24-C23	2.12	105.92	113.62	10	3
4	A	310	PX4	C20-C19-C18	2.12	103.67	114.42	13	1
4	A	320	PX4	C31-C30-C29	2.12	103.68	114.42	1	2
4	A	320	PX4	C15-C14-C13	2.12	103.68	114.42	6	1
4	A	395	PX4	C25-C24-C23	2.12	121.32	113.62	11	1
4	A	421	PX4	O1-P1-O3	2.12	117.58	107.75	5	1
4	A	351	PX4	C20-C19-C18	2.12	103.69	114.42	1	1
4	A	353	PX4	C17-C16-C15	2.12	103.69	114.42	7	1
4	A	376	PX4	C19-C18-C17	2.11	103.69	114.42	12	1
4	A	384	PX4	C26-C25-C24	2.11	105.59	113.19	4	1
4	A	308	PX4	O3-C1-C2	2.11	120.28	109.16	10	1
4	A	345	PX4	C4-N1-C2	2.11	101.27	109.92	8	1
4	A	349	PX4	C14-C13-C12	2.11	103.70	114.42	6	1
4	A	350	PX4	O6-C9-C10	2.11	115.49	123.73	10	1
4	A	407	PX4	C15-C14-C13	2.11	103.70	114.42	6	1
4	A	409	PX4	O6-C9-C10	2.11	115.49	123.73	1	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	409	PX4	C27-C26-C25	2.11	103.70	114.42	6	2
4	A	411	PX4	C28-C27-C26	2.11	103.69	114.42	9	1
4	A	419	PX4	C33-C32-C31	2.11	103.69	114.42	2	1
4	A	323	PX4	C28-C27-C26	2.11	103.70	114.42	1	1
4	A	358	PX4	C33-C32-C31	2.11	103.70	114.42	13	1
4	A	362	PX4	C31-C30-C29	2.11	103.70	114.42	8	1
4	A	375	PX4	C11-C10-C9	2.11	105.94	113.62	9	1
4	A	390	PX4	C25-C24-C23	2.11	105.94	113.62	14	1
4	A	396	PX4	C18-C17-C16	2.11	103.70	114.42	12	1
4	A	335	PX4	O8-C23-C24	2.11	115.50	123.73	7	1
4	A	344	PX4	C19-C18-C17	2.11	103.71	114.42	6	1
4	A	366	PX4	O8-C23-C24	2.11	115.50	123.73	4	1
4	A	322	PX4	C15-C14-C13	2.11	103.72	114.42	11	1
4	A	379	PX4	C17-C16-C15	2.11	103.72	114.42	13	3
4	A	416	PX4	C3-N1-C2	2.11	101.28	109.92	12	2
4	A	315	PX4	O1-P1-O3	2.11	97.96	107.75	13	1
4	A	316	PX4	C13-C12-C11	2.11	103.73	114.42	10	1
4	A	334	PX4	C29-C28-C27	2.11	103.72	114.42	11	2
4	A	351	PX4	O3-C1-C2	2.11	120.25	109.16	10	1
4	A	352	PX4	C19-C18-C17	2.11	103.72	114.42	9	1
4	A	353	PX4	O5-C9-O6	2.11	118.27	123.59	11	2
4	A	357	PX4	C33-C32-C31	2.11	103.72	114.42	7	3
4	A	322	PX4	C4-N1-C2	2.11	101.29	109.92	13	1
4	A	406	PX4	C25-C24-C23	2.11	105.96	113.62	10	1
4	A	424	PX4	O4-P1-O2	2.11	117.30	109.07	11	1
4	A	427	PX4	C19-C18-C17	2.11	103.72	114.42	12	1
4	A	365	PX4	O8-C23-C24	2.11	115.51	123.73	14	1
4	A	320	PX4	C17-C16-C15	2.11	103.74	114.42	10	1
4	A	366	PX4	C34-C33-C32	2.11	103.73	114.42	10	1
4	A	377	PX4	C5-N1-C2	2.10	118.53	109.92	7	1
4	A	374	PX4	C13-C12-C11	2.10	103.75	114.42	10	1
4	A	380	PX4	C12-C11-C10	2.10	105.63	113.19	8	2
4	A	426	PX4	C13-C12-C11	2.11	103.74	114.42	13	1
4	A	343	PX4	C33-C32-C31	2.10	103.75	114.42	10	2
4	A	313	PX4	C34-C33-C32	2.10	103.75	114.42	10	2
4	A	345	PX4	C12-C11-C10	2.10	120.75	113.19	2	2
4	A	378	PX4	C5-N1-C3	2.10	114.38	108.97	7	3
4	A	323	PX4	O8-C23-C24	2.10	115.54	123.73	10	1
4	A	374	PX4	C3-N1-C2	2.10	118.51	109.92	11	1
4	A	314	PX4	C26-C25-C24	2.10	105.65	113.19	4	1
4	A	347	PX4	C30-C29-C28	2.10	103.77	114.42	14	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	372	PX4	C18-C17-C16	2.10	103.78	114.42	11	1
4	A	381	PX4	C32-C31-C30	2.10	103.78	114.42	13	1
4	A	382	PX4	C32-C31-C30	2.10	103.77	114.42	1	1
4	A	320	PX4	C33-C32-C31	2.10	103.78	114.42	4	1
4	A	321	PX4	C20-C19-C18	2.10	103.78	114.42	1	2
4	A	387	PX4	C14-C13-C12	2.10	103.78	114.42	14	3
4	A	402	PX4	O3-C1-C2	2.10	120.19	109.16	7	1
4	A	394	PX4	C18-C17-C16	2.10	103.79	114.42	11	1
4	A	401	PX4	C30-C29-C28	2.10	103.78	114.42	10	2
4	A	423	PX4	C5-N1-C2	2.10	101.34	109.92	13	1
4	A	327	PX4	O3-C1-C2	2.10	120.18	109.16	2	2
4	A	344	PX4	C5-N1-C2	2.10	118.49	109.92	11	1
4	A	404	PX4	C33-C32-C31	2.10	103.79	114.42	2	2
4	A	426	PX4	C11-C10-C9	2.10	106.00	113.62	14	1
4	A	353	PX4	C27-C26-C25	2.09	103.79	114.42	4	1
4	A	393	PX4	C31-C30-C29	2.09	103.80	114.42	2	1
4	A	397	PX4	C16-C15-C14	2.09	103.79	114.42	8	1
4	A	427	PX4	C31-C30-C29	2.09	103.79	114.42	10	1
4	A	306	PX4	C14-C13-C12	2.09	103.81	114.42	10	1
4	A	325	PX4	C28-C27-C26	2.09	103.81	114.42	7	1
4	A	357	PX4	O4-P1-O2	2.09	100.89	109.07	8	1
4	A	366	PX4	C18-C17-C16	2.09	103.81	114.42	5	1
4	A	317	PX4	O6-C9-C10	2.09	115.58	123.73	3	1
4	A	342	PX4	C25-C24-C23	2.09	106.02	113.62	2	1
4	A	355	PX4	C8-O5-C9	2.09	109.38	117.12	8	1
4	A	391	PX4	C13-C12-C11	2.09	103.81	114.42	14	1
4	A	396	PX4	C8-O5-C9	2.09	109.38	117.12	3	1
4	A	308	PX4	C19-C18-C17	2.09	103.82	114.42	9	1
4	A	310	PX4	C4-N1-C2	2.09	118.47	109.92	11	2
4	A	332	PX4	C3-N1-C2	2.09	118.46	109.92	14	1
4	A	380	PX4	C14-C13-C12	2.09	103.82	114.42	8	1
4	A	388	PX4	C3-N1-C2	2.09	101.37	109.92	8	1
4	A	410	PX4	O8-C23-C24	2.09	115.58	123.73	10	1
4	A	353	PX4	C5-N1-C2	2.09	118.46	109.92	11	2
4	A	358	PX4	C32-C31-C30	2.09	103.83	114.42	4	1
4	A	366	PX4	C14-C13-C12	2.09	103.82	114.42	5	1
4	A	373	PX4	C29-C28-C27	2.09	103.83	114.42	12	2
4	A	400	PX4	C13-C12-C11	2.09	103.83	114.42	8	1
4	A	412	PX4	O8-C23-C24	2.09	115.59	123.73	11	1
4	A	416	PX4	O1-P1-O3	2.09	98.05	107.75	4	2
4	A	418	PX4	O4-P1-O2	2.09	100.91	109.07	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	424	PX4	C20-C19-C18	2.09	103.83	114.42	12	1
4	A	429	PX4	C4-N1-C2	2.09	118.46	109.92	6	1
4	A	416	PX4	C32-C31-C30	2.09	103.83	114.42	1	1
4	A	354	PX4	O6-C9-C10	2.09	115.60	123.73	11	1
4	A	310	PX4	O4-P1-O2	2.08	117.21	109.07	12	1
4	A	326	PX4	C19-C18-C17	2.08	103.84	114.42	8	1
4	A	335	PX4	O3-C1-C2	2.08	120.12	109.16	14	1
4	A	369	PX4	C28-C27-C26	2.08	103.84	114.42	1	1
4	A	319	PX4	C7-O7-C23	2.08	112.67	117.79	14	1
4	A	337	PX4	C20-C19-C18	2.08	103.85	114.42	5	1
4	A	337	PX4	C11-C10-C9	2.08	106.05	113.62	8	1
4	A	366	PX4	C5-N1-C2	2.08	118.44	109.92	1	1
4	A	381	PX4	C31-C30-C29	2.08	103.85	114.42	9	1
4	A	423	PX4	C27-C26-C25	2.08	103.85	114.42	13	1
4	A	338	PX4	C16-C15-C14	2.08	103.86	114.42	8	1
4	A	360	PX4	C28-C27-C26	2.08	103.86	114.42	3	1
4	A	349	PX4	C19-C18-C17	2.08	103.87	114.42	13	1
4	A	352	PX4	C27-C26-C25	2.08	103.86	114.42	8	1
4	A	376	PX4	C14-C13-C12	2.08	103.86	114.42	12	1
4	A	380	PX4	O1-P1-O4	2.08	117.41	107.75	9	1
4	A	386	PX4	C34-C33-C32	2.08	103.87	114.42	14	1
4	A	389	PX4	C13-C12-C11	2.08	103.87	114.42	4	1
4	A	306	PX4	C15-C14-C13	2.08	103.88	114.42	4	1
4	A	311	PX4	C29-C28-C27	2.08	103.88	114.42	9	1
4	A	324	PX4	C3-N1-C2	2.08	101.41	109.92	2	1
4	A	383	PX4	C14-C13-C12	2.08	103.88	114.42	11	1
4	A	325	PX4	C25-C24-C23	2.08	106.07	113.62	3	1
4	A	316	PX4	O8-C23-C24	2.07	115.64	123.73	3	1
4	A	327	PX4	C36-C35-C34	2.08	97.67	113.42	10	1
4	A	334	PX4	C33-C32-C31	2.08	103.89	114.42	8	1
4	A	366	PX4	C4-N1-C2	2.08	118.41	109.92	4	1
4	A	378	PX4	C8-O5-C9	2.07	109.44	117.12	2	1
4	A	378	PX4	C14-C13-C12	2.07	103.89	114.42	7	1
4	A	378	PX4	C18-C17-C16	2.08	103.89	114.42	10	1
4	A	418	PX4	C33-C32-C31	2.08	103.89	114.42	12	2
4	A	418	PX4	C11-C10-C9	2.07	106.08	113.62	6	1
4	A	430	PX4	O3-C1-C2	2.07	120.07	109.16	13	1
4	A	352	PX4	O4-P1-O2	2.07	117.17	109.07	2	1
4	A	384	PX4	O3-P1-O2	2.07	100.97	109.07	12	1
4	A	386	PX4	C12-C11-C10	2.07	105.74	113.19	3	2
4	A	429	PX4	C20-C19-C18	2.07	103.90	114.42	6	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	395	PX4	C28-C27-C26	2.07	103.91	114.42	11	2
4	A	353	PX4	O1-P1-O3	2.07	98.13	107.75	2	2
4	A	359	PX4	C34-C33-C32	2.07	103.92	114.42	5	1
4	A	363	PX4	O4-P1-O2	2.07	100.98	109.07	11	1
4	A	406	PX4	C29-C28-C27	2.07	103.91	114.42	10	2
4	A	420	PX4	O8-C23-C24	2.07	115.65	123.73	13	1
4	A	378	PX4	C11-C10-C9	2.07	106.09	113.62	5	1
4	A	386	PX4	O1-P1-O3	2.07	117.35	107.75	12	1
4	A	415	PX4	C4-N1-C2	2.07	118.38	109.92	1	1
4	A	366	PX4	C32-C31-C30	2.07	103.93	114.42	13	2
4	A	382	PX4	C25-C24-C23	2.07	121.14	113.62	8	1
4	A	383	PX4	C15-C14-C13	2.07	103.93	114.42	1	1
4	A	389	PX4	C4-N1-C2	2.07	118.38	109.92	14	1
4	A	402	PX4	C8-O5-C9	2.07	124.78	117.12	8	1
4	A	409	PX4	C4-N1-C2	2.07	118.38	109.92	14	2
4	A	421	PX4	C20-C19-C18	2.07	103.93	114.42	4	1
4	A	315	PX4	C19-C18-C17	2.07	103.93	114.42	12	2
4	A	320	PX4	C29-C28-C27	2.07	103.93	114.42	7	1
4	A	354	PX4	C16-C15-C14	2.07	103.94	114.42	10	1
4	A	338	PX4	C15-C14-C13	2.06	103.94	114.42	6	1
4	A	355	PX4	O3-C1-C2	2.07	120.02	109.16	9	1
4	A	399	PX4	C31-C30-C29	2.07	103.94	114.42	2	1
4	A	430	PX4	C16-C15-C14	2.07	103.94	114.42	14	1
4	A	342	PX4	C29-C28-C27	2.06	103.95	114.42	5	1
4	A	364	PX4	C27-C26-C25	2.06	103.94	114.42	7	3
4	A	318	PX4	C27-C26-C25	2.06	103.95	114.42	12	2
4	A	327	PX4	C25-C24-C23	2.06	121.12	113.62	13	1
4	A	369	PX4	O3-P1-O2	2.06	101.00	109.07	14	2
4	A	389	PX4	C19-C18-C17	2.06	103.95	114.42	14	1
4	A	410	PX4	C32-C31-C30	2.06	103.95	114.42	3	1
4	A	346	PX4	O1-P1-O4	2.06	117.32	107.75	3	2
4	A	347	PX4	O6-C9-C10	2.06	115.69	123.73	2	1
4	A	348	PX4	C14-C13-C12	2.06	103.96	114.42	8	1
4	A	401	PX4	C33-C32-C31	2.06	103.96	114.42	12	1
4	A	408	PX4	C15-C14-C13	2.06	103.96	114.42	2	1
4	A	409	PX4	C11-C10-C9	2.06	121.12	113.62	7	1
4	A	412	PX4	C5-N1-C2	2.06	118.35	109.92	5	1
4	A	396	PX4	C28-C27-C26	2.06	103.97	114.42	6	1
4	A	396	PX4	C34-C33-C32	2.06	103.96	114.42	14	1
4	A	418	PX4	C5-N1-C4	2.06	114.27	108.97	1	2
4	A	370	PX4	C13-C12-C11	2.06	103.97	114.42	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	397	PX4	C5-N1-C2	2.06	118.34	109.92	12	1
4	A	399	PX4	C14-C13-C12	2.06	103.97	114.42	7	2
4	A	418	PX4	C16-C15-C14	2.06	103.97	114.42	13	2
4	A	424	PX4	O1-P1-O4	2.06	117.31	107.75	5	1
4	A	317	PX4	O4-P1-O2	2.06	117.11	109.07	12	2
4	A	334	PX4	C12-C11-C10	2.06	120.59	113.19	9	1
4	A	339	PX4	O3-P1-O2	2.06	101.03	109.07	6	3
4	A	367	PX4	C13-C12-C11	2.06	103.98	114.42	9	1
4	A	379	PX4	O6-C9-C10	2.06	115.71	123.73	5	1
4	A	400	PX4	C30-C29-C28	2.06	103.98	114.42	9	1
4	A	419	PX4	C34-C33-C32	2.06	103.98	114.42	12	1
4	A	422	PX4	C29-C28-C27	2.06	103.98	114.42	11	1
4	A	429	PX4	C13-C12-C11	2.06	103.98	114.42	1	1
4	A	322	PX4	C16-C15-C14	2.06	103.99	114.42	6	1
4	A	335	PX4	C17-C16-C15	2.06	103.99	114.42	13	1
4	A	333	PX4	C34-C33-C32	2.05	124.86	114.42	2	1
4	A	338	PX4	C3-N1-C2	2.06	101.51	109.92	11	1
4	A	374	PX4	C14-C13-C12	2.06	103.99	114.42	7	1
4	A	372	PX4	C5-N1-C2	2.05	118.32	109.92	6	1
4	A	391	PX4	C19-C18-C17	2.05	104.00	114.42	3	1
4	A	393	PX4	C27-C26-C25	2.05	103.99	114.42	2	1
4	A	401	PX4	C8-O5-C9	2.05	124.73	117.12	1	1
4	A	405	PX4	C26-C25-C24	2.05	105.81	113.19	1	1
4	A	418	PX4	C4-N1-C2	2.06	101.51	109.92	14	1
4	A	326	PX4	C30-C29-C28	2.05	104.00	114.42	3	1
4	A	364	PX4	C14-C13-C12	2.05	104.00	114.42	3	1
4	A	422	PX4	C26-C25-C24	2.05	105.81	113.19	3	1
4	A	311	PX4	C11-C10-C9	2.05	106.16	113.62	13	1
4	A	322	PX4	C13-C12-C11	2.05	104.01	114.42	3	1
4	A	326	PX4	O1-P1-O4	2.05	117.28	107.75	5	1
4	A	359	PX4	O1-P1-O3	2.05	98.21	107.75	4	1
4	A	419	PX4	C17-C16-C15	2.05	104.00	114.42	4	1
4	A	425	PX4	C16-C15-C14	2.05	104.00	114.42	7	1
4	A	427	PX4	O8-C23-C24	2.05	115.72	123.73	13	1
4	A	333	PX4	C32-C31-C30	2.05	104.01	114.42	10	1
4	A	349	PX4	C4-N1-C2	2.05	101.52	109.92	7	1
4	A	350	PX4	C11-C10-C9	2.05	106.16	113.62	9	1
4	A	323	PX4	C16-C15-C14	2.05	104.02	114.42	6	1
4	A	347	PX4	C16-C15-C14	2.05	104.02	114.42	10	1
4	A	363	PX4	C19-C18-C17	2.05	104.02	114.42	4	1
4	A	368	PX4	C34-C33-C32	2.05	104.01	114.42	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	403	PX4	O6-C9-C10	2.05	115.73	123.73	8	1
4	A	406	PX4	C20-C19-C18	2.05	104.01	114.42	6	1
4	A	364	PX4	C18-C17-C16	2.05	104.02	114.42	7	1
4	A	306	PX4	C33-C32-C31	2.05	104.03	114.42	4	1
4	A	347	PX4	C28-C27-C26	2.05	104.03	114.42	10	1
4	A	385	PX4	C1-C2-N1	2.05	108.94	115.78	11	1
4	A	425	PX4	O6-C9-C10	2.05	115.74	123.73	9	1
4	A	375	PX4	C13-C12-C11	2.05	104.04	114.42	9	1
4	A	428	PX4	C29-C28-C27	2.05	104.03	114.42	7	1
4	A	308	PX4	C3-N1-C2	2.04	118.28	109.92	6	3
4	A	321	PX4	C33-C32-C31	2.05	104.04	114.42	4	1
4	A	328	PX4	C34-C33-C32	2.04	104.04	114.42	8	1
4	A	344	PX4	C20-C19-C18	2.04	104.04	114.42	3	1
4	A	366	PX4	C11-C10-C9	2.05	106.18	113.62	13	1
4	A	306	PX4	C30-C29-C28	2.04	104.06	114.42	9	1
4	A	321	PX4	C25-C24-C23	2.04	106.19	113.62	13	1
4	A	330	PX4	C13-C12-C11	2.04	104.05	114.42	4	1
4	A	351	PX4	C5-N1-C2	2.04	118.28	109.92	9	2
4	A	381	PX4	C11-C10-C9	2.04	106.18	113.62	5	1
4	A	409	PX4	O8-C23-C24	2.04	115.75	123.73	1	1
4	A	426	PX4	C32-C31-C30	2.04	104.05	114.42	1	1
4	A	372	PX4	C25-C24-C23	2.04	106.19	113.62	2	1
4	A	331	PX4	C33-C32-C31	2.04	104.06	114.42	13	1
4	A	378	PX4	C34-C33-C32	2.04	104.05	114.42	9	1
4	A	357	PX4	C34-C33-C32	2.04	104.06	114.42	2	1
4	A	332	PX4	C33-C32-C31	2.04	104.07	114.42	11	1
4	A	350	PX4	C32-C31-C30	2.04	104.07	114.42	6	1
4	A	358	PX4	C8-O5-C9	2.04	109.56	117.12	6	1
4	A	366	PX4	C17-C16-C15	2.04	104.06	114.42	9	1
4	A	368	PX4	C17-C16-C15	2.04	104.06	114.42	7	1
4	A	337	PX4	C15-C14-C13	2.04	104.07	114.42	10	1
4	A	374	PX4	C32-C31-C30	2.04	104.07	114.42	4	1
4	A	377	PX4	C34-C33-C32	2.04	104.07	114.42	2	1
4	A	378	PX4	C13-C12-C11	2.04	104.07	114.42	7	1
4	A	401	PX4	C14-C13-C12	2.04	104.07	114.42	13	1
4	A	404	PX4	C13-C12-C11	2.04	104.06	114.42	3	1
4	A	428	PX4	C1-C2-N1	2.04	122.59	115.78	7	1
4	A	306	PX4	C19-C18-C17	2.04	104.08	114.42	7	1
4	A	345	PX4	C27-C26-C25	2.04	104.08	114.42	6	1
4	A	364	PX4	C12-C11-C10	2.04	105.86	113.19	7	1
4	A	405	PX4	C17-C16-C15	2.04	104.07	114.42	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	428	PX4	C27-C26-C25	2.04	104.08	114.42	3	1
4	A	342	PX4	C32-C31-C30	2.04	104.08	114.42	2	1
4	A	365	PX4	C4-N1-C2	2.04	118.25	109.92	5	1
4	A	321	PX4	C30-C29-C28	2.03	104.10	114.42	8	1
4	A	325	PX4	C26-C25-C24	2.03	105.88	113.19	2	1
4	A	355	PX4	O1-P1-O4	2.03	117.19	107.75	2	1
4	A	411	PX4	O3-C1-C2	2.03	119.86	109.16	6	1
4	A	420	PX4	C27-C26-C25	2.03	104.10	114.42	12	1
4	A	383	PX4	C8-O5-C9	2.03	124.64	117.12	13	1
4	A	394	PX4	O3-C1-C2	2.03	119.85	109.16	14	1
4	A	402	PX4	C33-C32-C31	2.03	104.11	114.42	5	1
4	A	412	PX4	C3-N1-C2	2.03	118.23	109.92	8	1
4	A	418	PX4	C1-C2-N1	2.03	122.56	115.78	5	2
4	A	314	PX4	C5-N1-C2	2.03	118.23	109.92	1	1
4	A	328	PX4	C5-N1-C2	2.03	118.23	109.92	5	1
4	A	334	PX4	C4-N1-C2	2.03	118.22	109.92	7	1
4	A	351	PX4	C25-C24-C23	2.03	121.00	113.62	12	1
4	A	365	PX4	C32-C31-C30	2.03	104.12	114.42	10	1
4	A	370	PX4	C27-C26-C25	2.03	104.12	114.42	4	1
4	A	413	PX4	O8-C23-C24	2.03	115.81	123.73	13	1
4	A	418	PX4	C25-C24-C23	2.03	106.24	113.62	4	1
4	A	321	PX4	C27-C26-C25	2.03	104.12	114.42	13	1
4	A	312	PX4	C5-N1-C2	2.03	118.21	109.92	10	1
4	A	330	PX4	C35-C34-C33	2.03	96.48	115.30	13	1
4	A	371	PX4	C31-C30-C29	2.03	104.14	114.42	7	1
4	A	385	PX4	C32-C31-C30	2.03	104.14	114.42	2	1
4	A	389	PX4	C25-C24-C23	2.03	120.99	113.62	5	1
4	A	429	PX4	C8-O5-C9	2.03	124.63	117.12	2	1
4	A	307	PX4	O8-C23-C24	2.03	131.63	123.73	7	1
4	A	311	PX4	O1-P1-O3	2.02	117.15	107.75	11	1
4	A	318	PX4	O3-C1-C2	2.03	119.81	109.16	9	1
4	A	323	PX4	C30-C29-C28	2.02	104.14	114.42	12	1
4	A	349	PX4	C25-C24-C23	2.03	106.25	113.62	14	1
4	A	420	PX4	C18-C17-C16	2.03	104.14	114.42	14	1
4	A	309	PX4	C19-C18-C17	2.02	104.15	114.42	4	1
4	A	343	PX4	C26-C25-C24	2.02	105.91	113.19	6	1
4	A	360	PX4	C3-N1-C2	2.02	118.20	109.92	8	1
4	A	381	PX4	C20-C19-C18	2.02	104.15	114.42	4	1
4	A	398	PX4	C31-C30-C29	2.02	104.15	114.42	11	1
4	A	408	PX4	C20-C19-C18	2.02	104.15	114.42	9	1
4	A	375	PX4	C15-C14-C13	2.02	104.16	114.42	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	411	PX4	C29-C28-C27	2.02	104.15	114.42	2	1
4	A	353	PX4	C8-O5-C9	2.02	109.63	117.12	7	1
4	A	383	PX4	C27-C26-C25	2.02	104.16	114.42	9	1
4	A	415	PX4	C20-C19-C18	2.02	104.16	114.42	9	1
4	A	426	PX4	C4-N1-C3	2.02	103.77	108.97	6	1
4	A	352	PX4	O6-C9-C10	2.02	115.85	123.73	6	1
4	A	358	PX4	C28-C27-C26	2.02	104.16	114.42	1	1
4	A	362	PX4	O1-P1-O4	2.02	117.14	107.75	1	1
4	A	384	PX4	C4-N1-C2	2.02	101.65	109.92	9	1
4	A	399	PX4	O1-P1-O4	2.02	117.14	107.75	8	1
4	A	318	PX4	C30-C29-C28	2.02	104.17	114.42	11	1
4	A	364	PX4	C20-C19-C18	2.02	104.17	114.42	9	2
4	A	384	PX4	C15-C14-C13	2.02	104.17	114.42	14	1
4	A	392	PX4	C29-C28-C27	2.02	104.17	114.42	9	1
4	A	405	PX4	C15-C14-C13	2.02	104.16	114.42	11	1
4	A	306	PX4	C13-C12-C11	2.02	104.17	114.42	7	1
4	A	308	PX4	C13-C12-C11	2.02	104.18	114.42	8	1
4	A	309	PX4	C29-C28-C27	2.02	104.18	114.42	13	1
4	A	312	PX4	C14-C13-C12	2.02	104.18	114.42	14	1
4	A	333	PX4	C28-C27-C26	2.02	104.18	114.42	11	1
4	A	337	PX4	O1-P1-O3	2.02	98.37	107.75	3	1
4	A	343	PX4	C8-O5-C9	2.02	109.65	117.12	2	1
4	A	362	PX4	C34-C33-C32	2.02	104.18	114.42	10	1
4	A	402	PX4	O8-C23-C24	2.02	115.86	123.73	7	1
4	A	403	PX4	C28-C27-C26	2.02	104.18	114.42	13	1
4	A	427	PX4	C15-C14-C13	2.02	104.18	114.42	14	1
4	A	314	PX4	O1-P1-O4	2.02	117.11	107.75	13	1
4	A	325	PX4	C20-C19-C18	2.02	104.19	114.42	2	1
4	A	368	PX4	C30-C29-C28	2.02	104.19	114.42	10	1
4	A	405	PX4	C30-C29-C28	2.02	104.19	114.42	14	1
4	A	417	PX4	C18-C17-C16	2.02	104.19	114.42	6	1
4	A	421	PX4	C18-C17-C16	2.02	104.19	114.42	14	1
4	A	308	PX4	C28-C27-C26	2.01	104.20	114.42	11	1
4	A	310	PX4	C3-N1-C2	2.01	101.67	109.92	3	1
4	A	379	PX4	C16-C15-C14	2.01	104.20	114.42	2	1
4	A	306	PX4	C17-C16-C15	2.01	104.20	114.42	5	1
4	A	414	PX4	C34-C33-C32	2.01	104.20	114.42	11	1
4	A	415	PX4	C26-C25-C24	2.01	105.95	113.19	1	1
4	A	426	PX4	C3-N1-C2	2.01	101.68	109.92	12	1
4	A	323	PX4	C15-C14-C13	2.01	104.21	114.42	1	1
4	A	333	PX4	C11-C10-C9	2.01	106.31	113.62	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	349	PX4	C17-C16-C15	2.01	104.22	114.42	10	1
4	A	370	PX4	C34-C33-C32	2.01	104.21	114.42	9	1
4	A	403	PX4	C19-C18-C17	2.01	104.22	114.42	1	1
4	A	421	PX4	O6-C9-C10	2.01	115.89	123.73	1	1
4	A	423	PX4	O3-C1-C2	2.01	119.74	109.16	2	1
4	A	362	PX4	C5-N1-C2	2.01	118.14	109.92	2	1
4	A	430	PX4	C32-C31-C30	2.01	104.22	114.42	8	1
4	A	337	PX4	O7-C7-C8	2.01	115.68	108.40	14	1
4	A	336	PX4	C16-C15-C14	2.01	104.23	114.42	10	1
4	A	346	PX4	C28-C27-C26	2.01	104.23	114.42	12	1
4	A	388	PX4	C31-C30-C29	2.01	104.23	114.42	6	1
4	A	412	PX4	C29-C28-C27	2.01	104.23	114.42	1	1
4	A	426	PX4	C14-C13-C12	2.01	104.23	114.42	2	1
4	A	358	PX4	C27-C26-C25	2.01	104.24	114.42	2	1
4	A	359	PX4	C19-C18-C17	2.01	104.24	114.42	9	1
4	A	383	PX4	C12-C11-C10	2.01	105.98	113.19	3	1
4	A	403	PX4	C30-C29-C28	2.01	104.24	114.42	7	1
4	A	408	PX4	O6-C9-C10	2.01	115.91	123.73	5	1
4	A	312	PX4	C20-C19-C18	2.00	104.25	114.42	13	1
4	A	317	PX4	C28-C27-C26	2.00	104.25	114.42	14	1
4	A	316	PX4	C19-C18-C17	2.00	104.26	114.42	9	1
4	A	361	PX4	C15-C14-C13	2.00	104.25	114.42	14	1
4	A	351	PX4	C15-C14-C13	2.00	104.26	114.42	14	1
4	A	396	PX4	C32-C31-C30	2.00	104.26	114.42	14	1
4	A	401	PX4	C29-C28-C27	2.00	104.25	114.42	2	1
4	A	406	PX4	C8-O5-C9	2.00	109.70	117.12	6	1
4	A	326	PX4	C18-C17-C16	2.00	104.27	114.42	3	1
4	A	327	PX4	C4-N1-C2	2.00	118.10	109.92	10	1
4	A	342	PX4	O8-C23-C24	2.00	115.92	123.73	14	1
4	A	354	PX4	C5-N1-C2	2.00	101.73	109.92	5	1
4	A	379	PX4	O1-P1-O3	2.00	98.45	107.75	11	1
4	A	379	PX4	C30-C29-C28	2.00	104.27	114.42	11	1
4	A	393	PX4	O5-C9-C10	2.00	118.19	111.91	12	1
4	A	422	PX4	C31-C30-C29	2.00	104.27	114.42	4	1
4	A	423	PX4	C19-C18-C17	2.00	104.27	114.42	11	1
4	A	425	PX4	C27-C26-C25	2.00	104.27	114.42	3	1

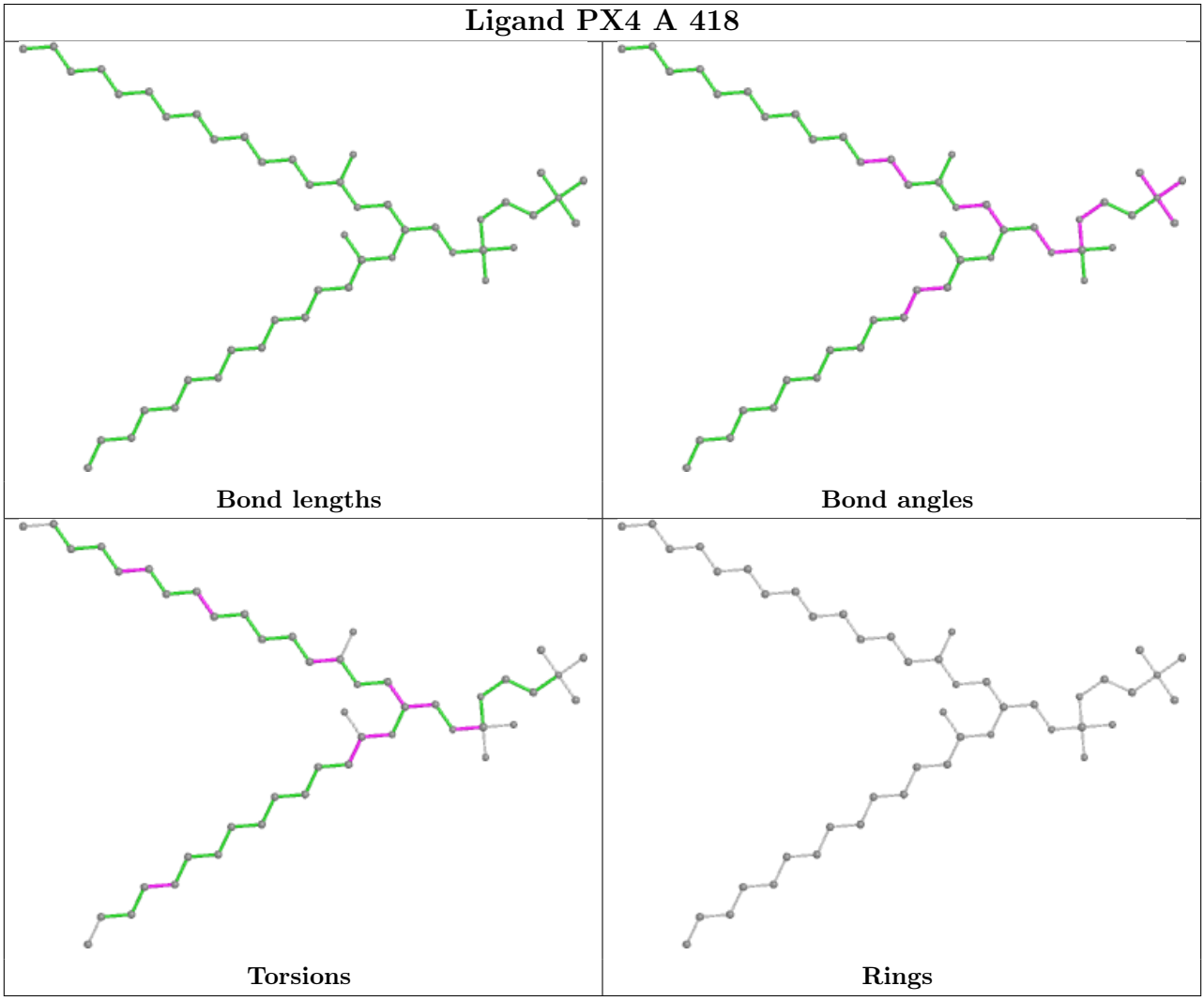
There are no chirality outliers.

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

Mol	Chain	Res	Type	Atoms	Models (Total)
4	A	371	PX4	O8-C23-O7-C7	13
4	A	307	PX4	O8-C23-O7-C7	7

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.



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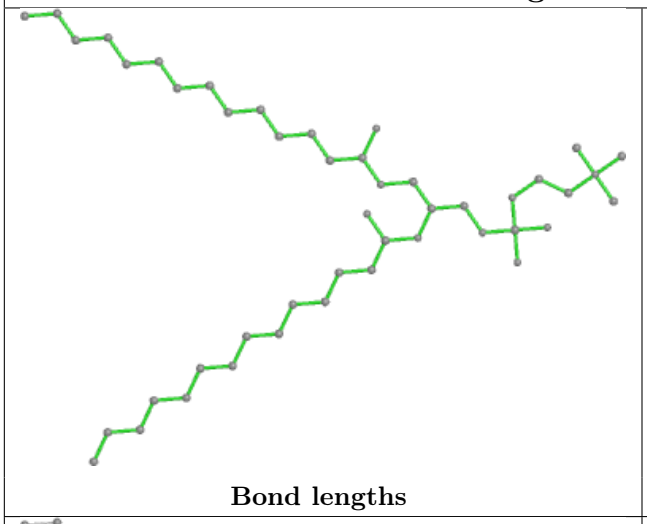
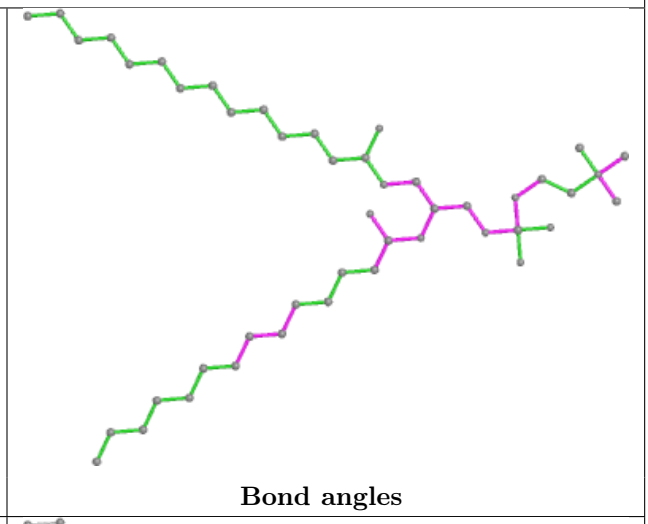
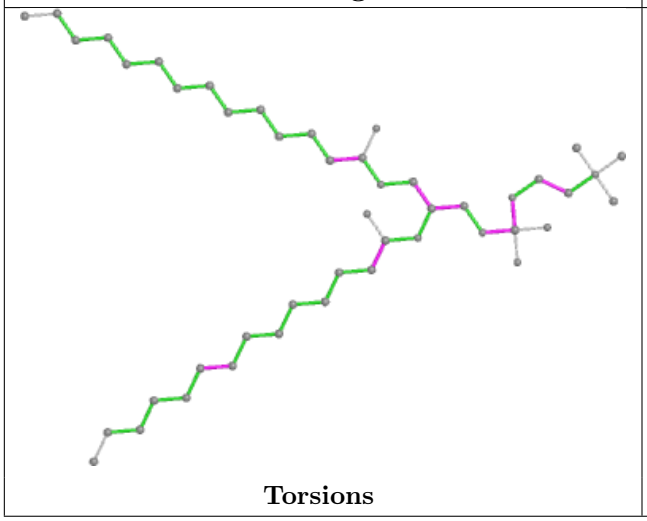


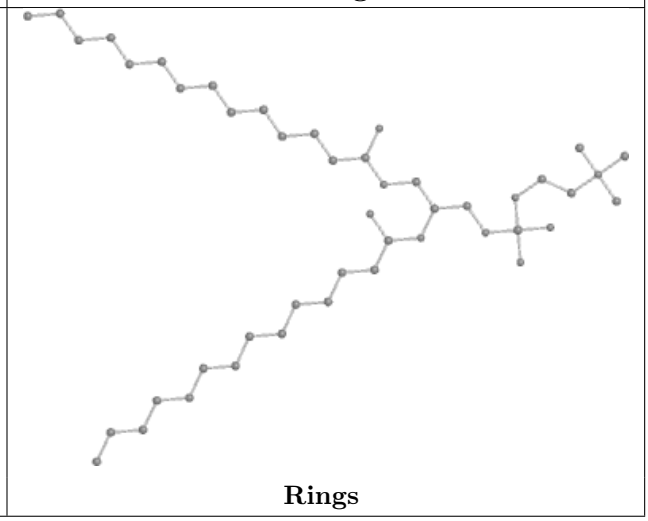
Bond lengths



Bond angles



Torsions



Rings

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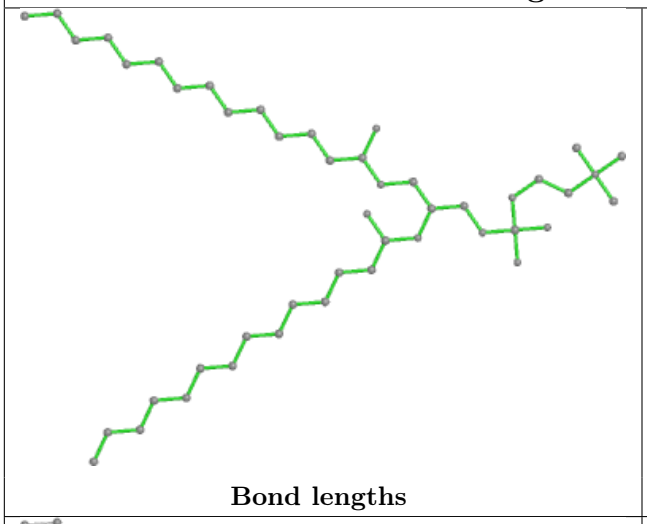
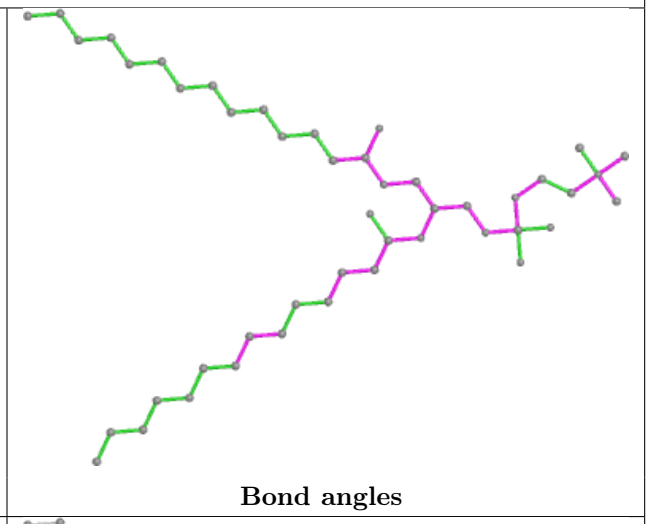
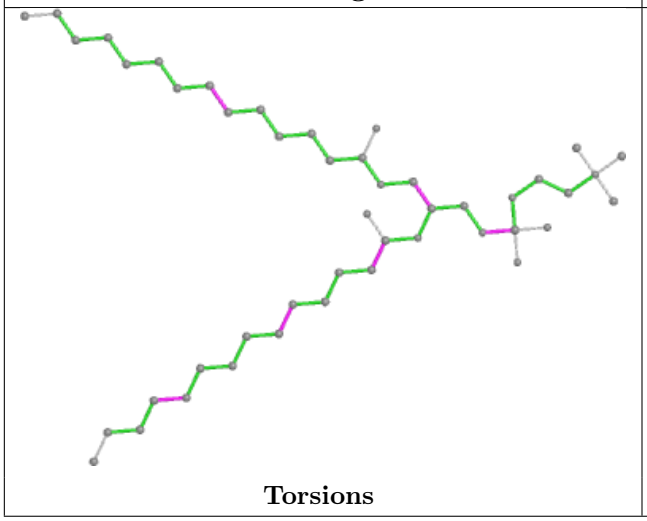


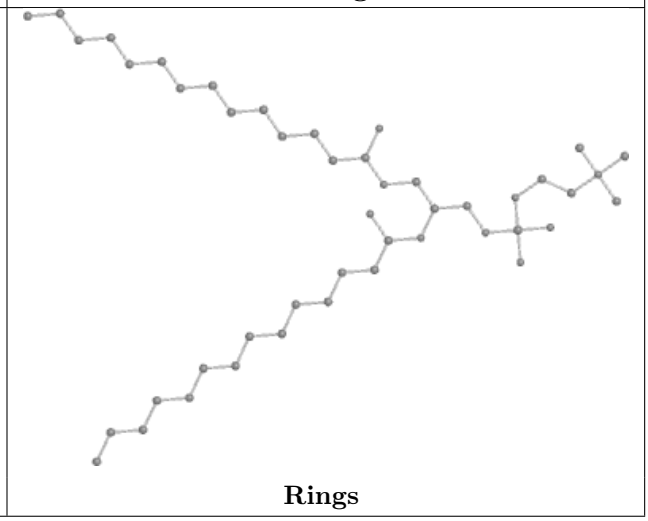
Bond lengths



Bond angles

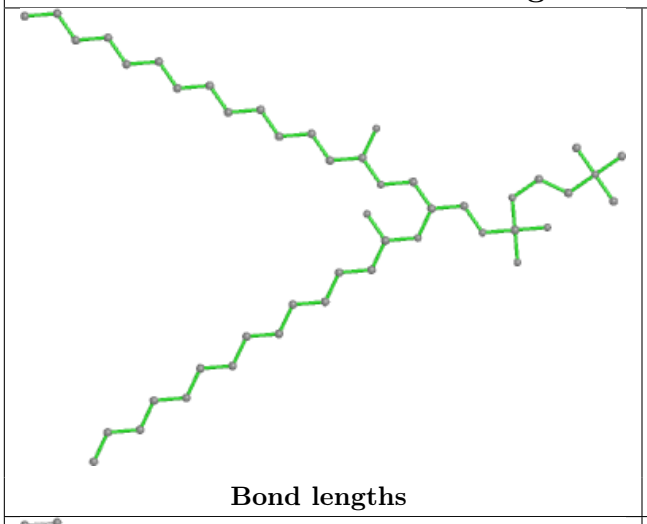


Torsions

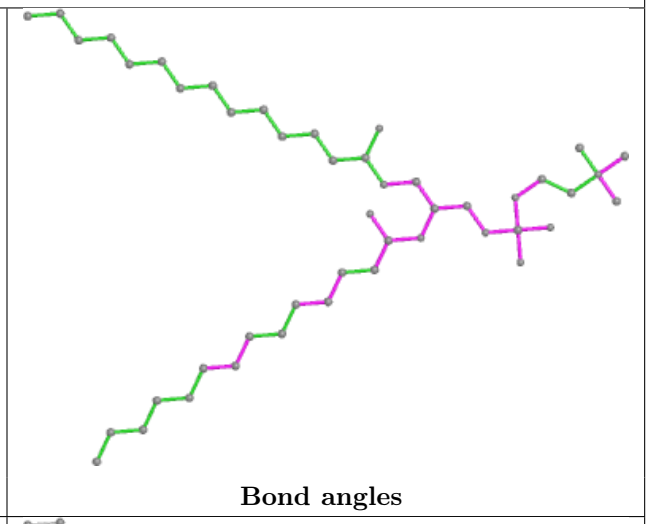


Rings

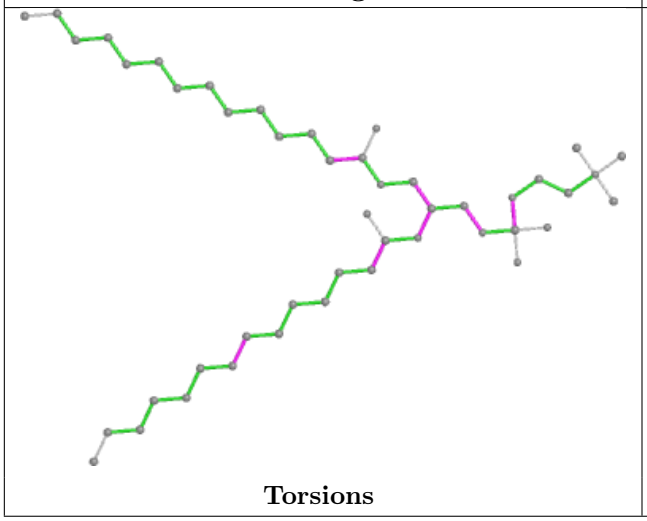
Ligand PX4 A 354



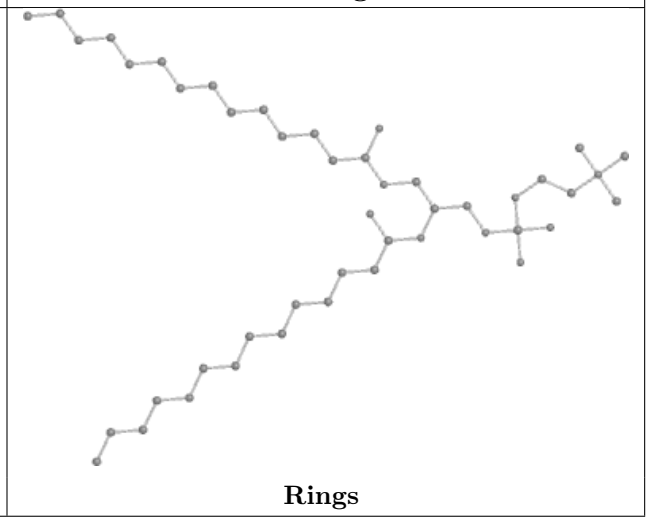
Bond lengths



Bond angles

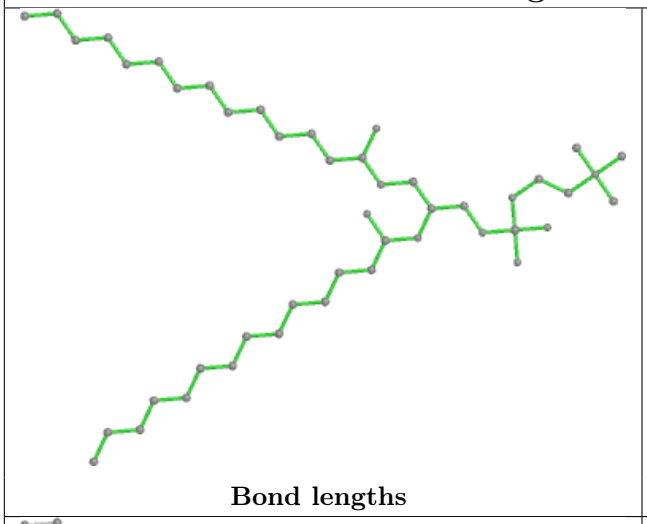


Torsions

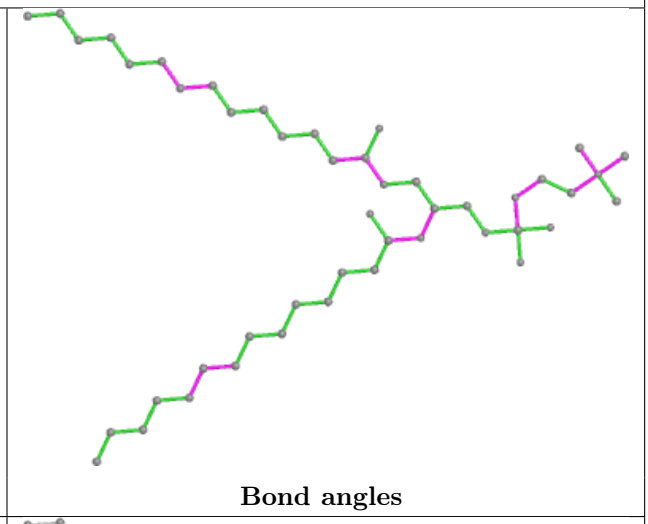


Rings

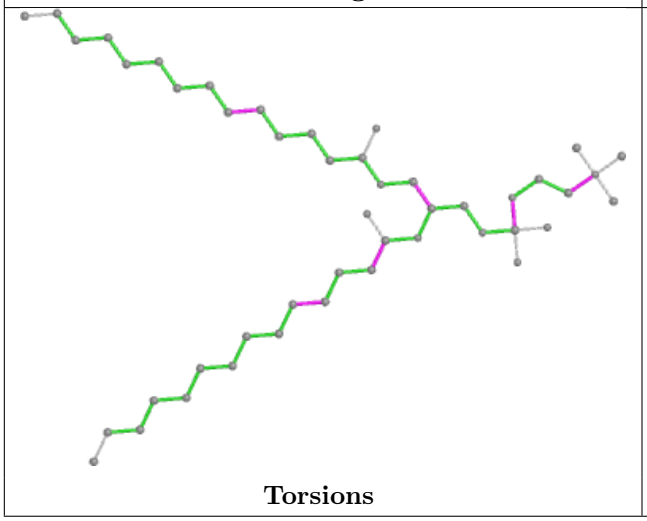
Ligand PX4 A 404



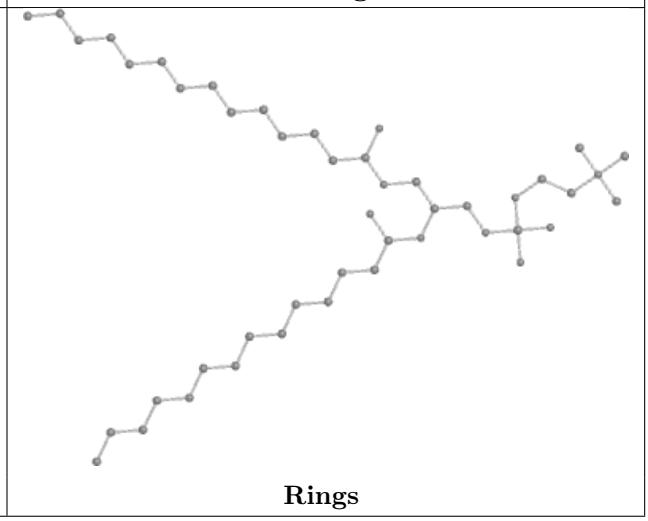
Bond lengths



Bond angles

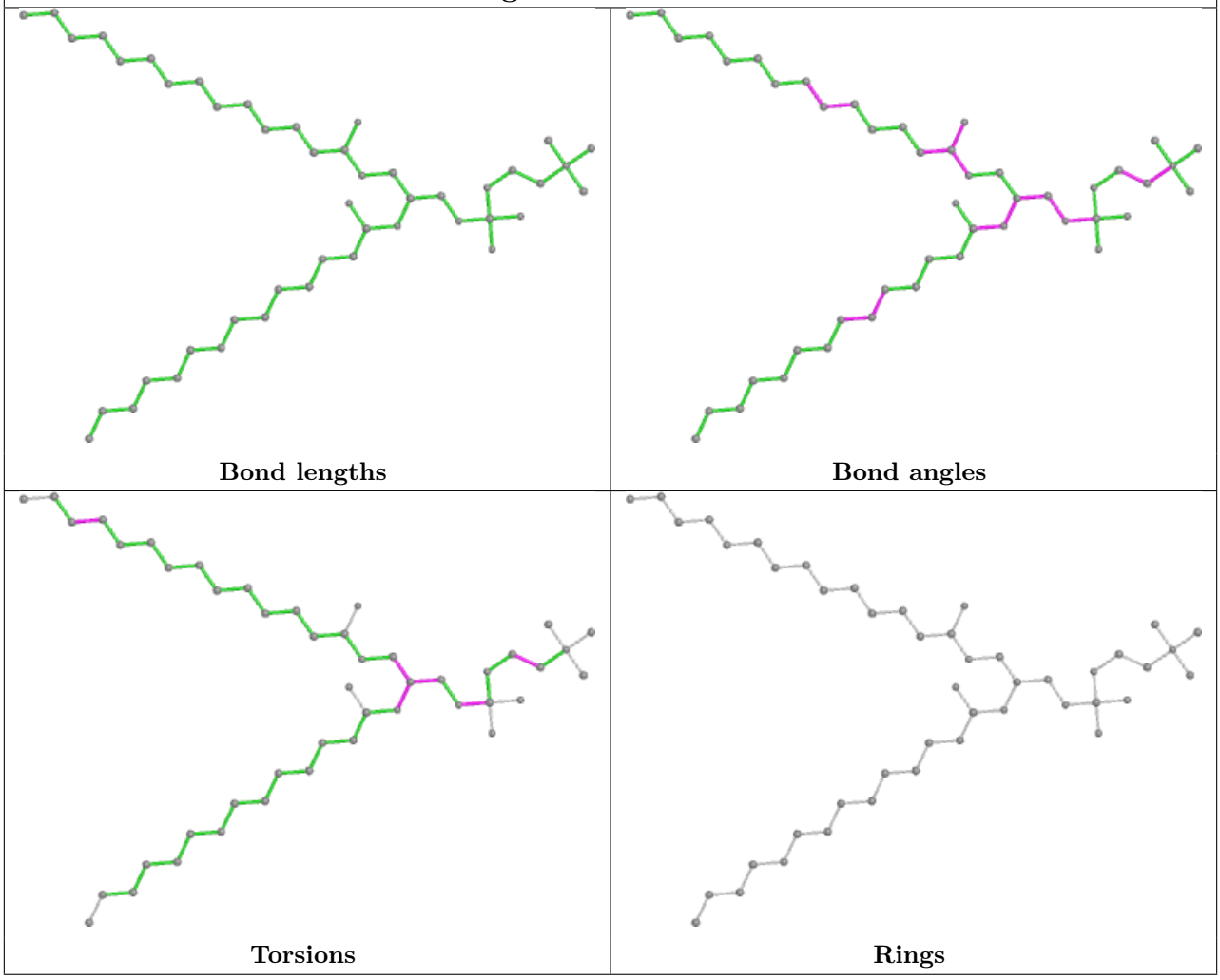


Torsions

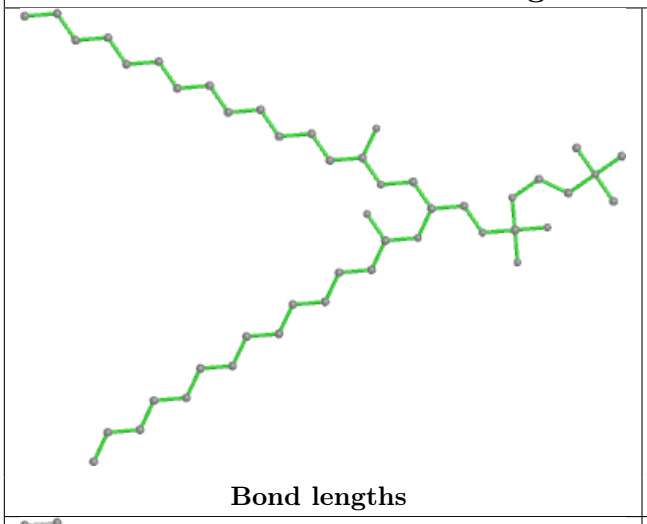


Rings

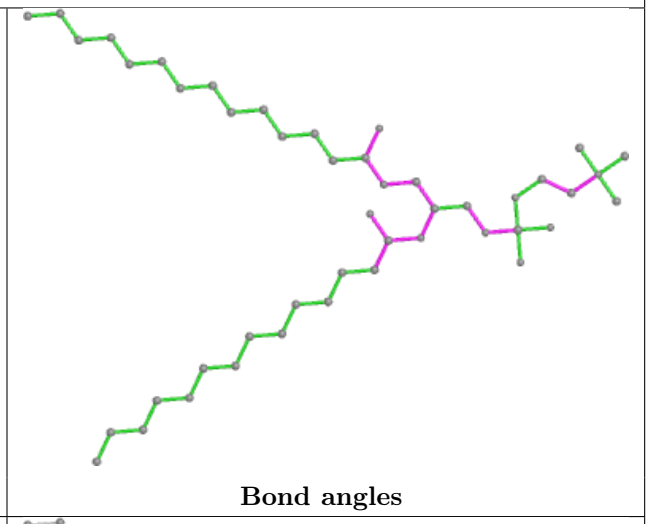
Ligand PX4 A 333



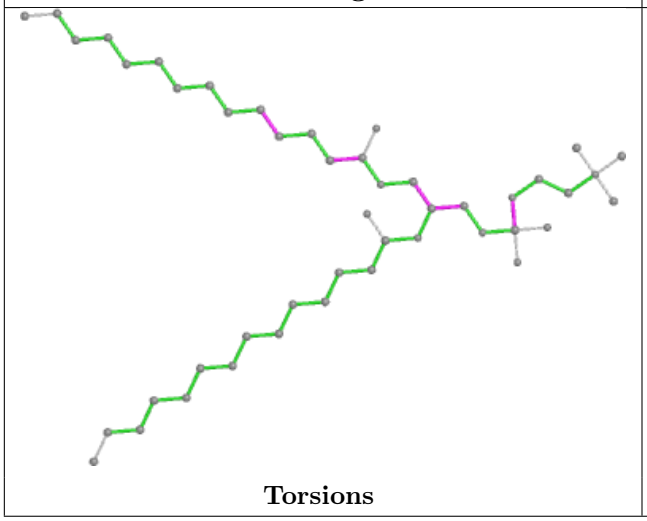
Ligand PX4 A 310



Bond lengths



Bond angles



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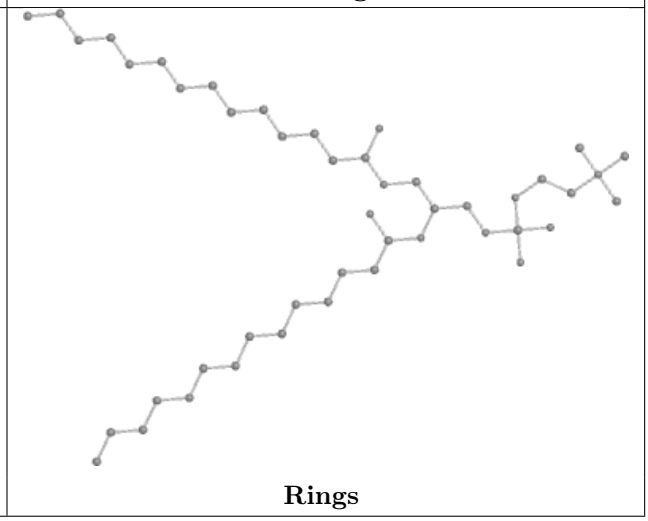
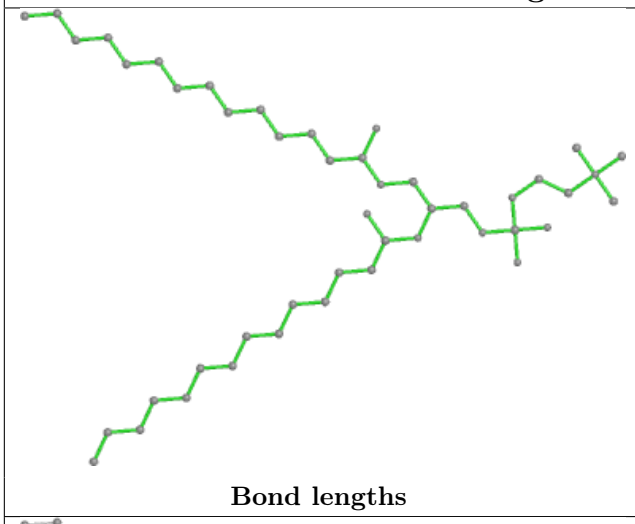


Rings

Ligand PX4 A 397



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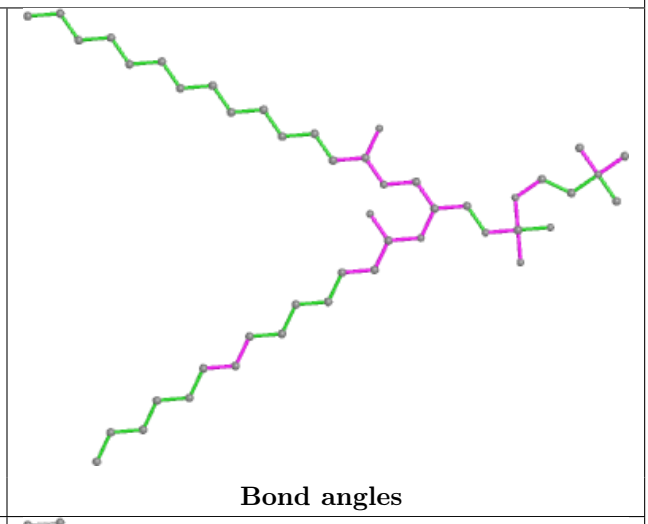
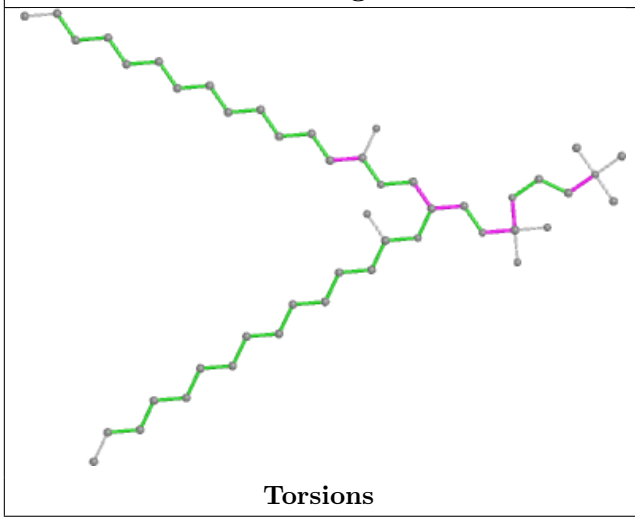
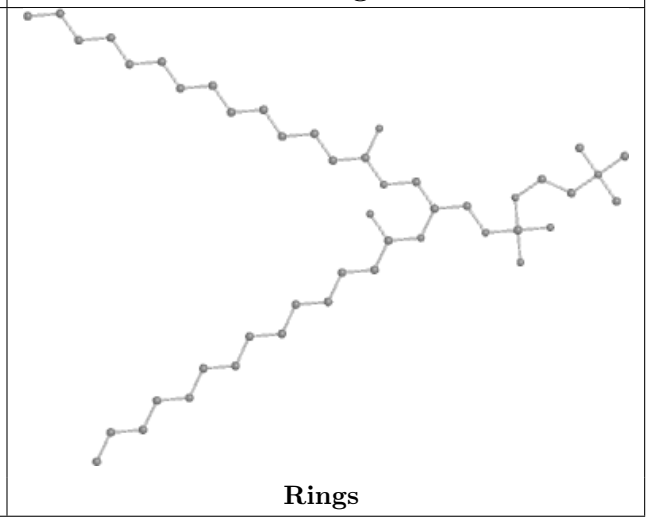


Bond angles

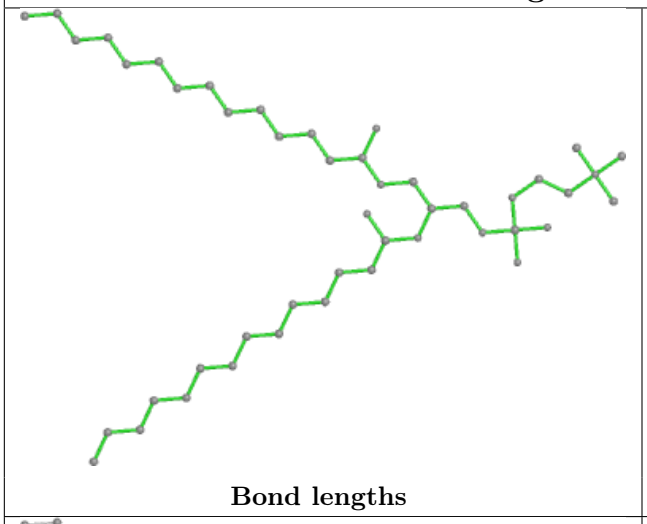


Torsions



Rings

Ligand PX4 A 349



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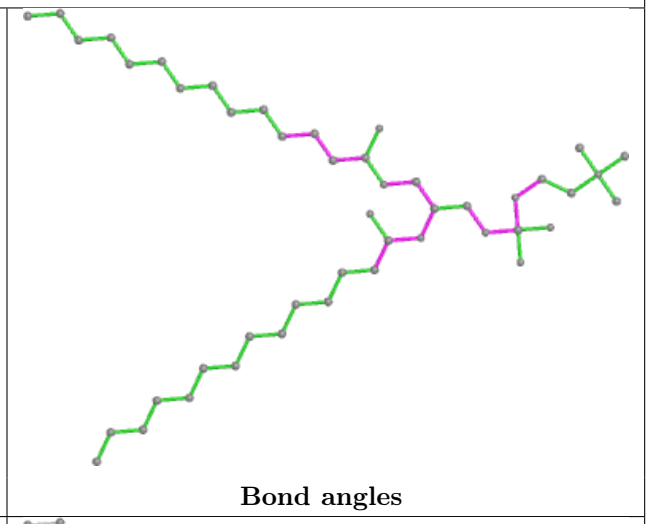
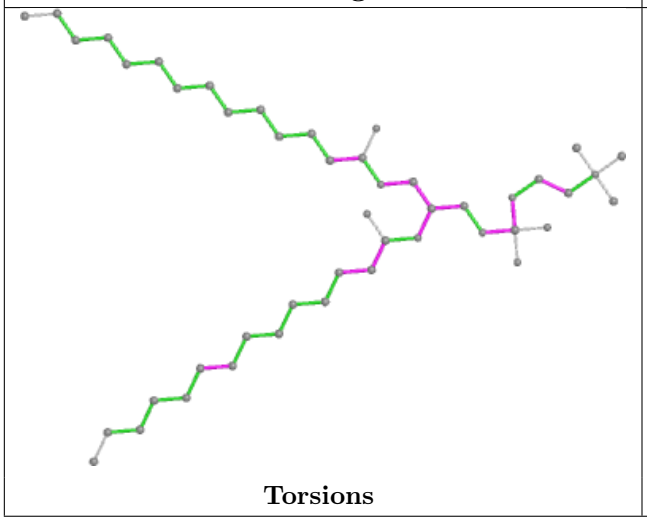


Bond angles



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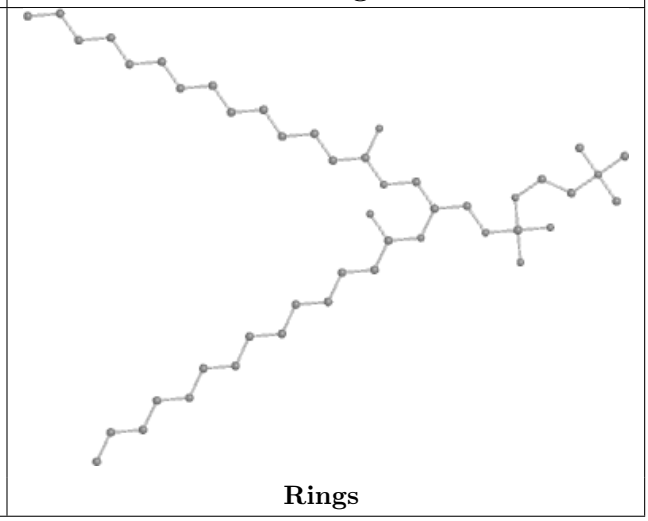
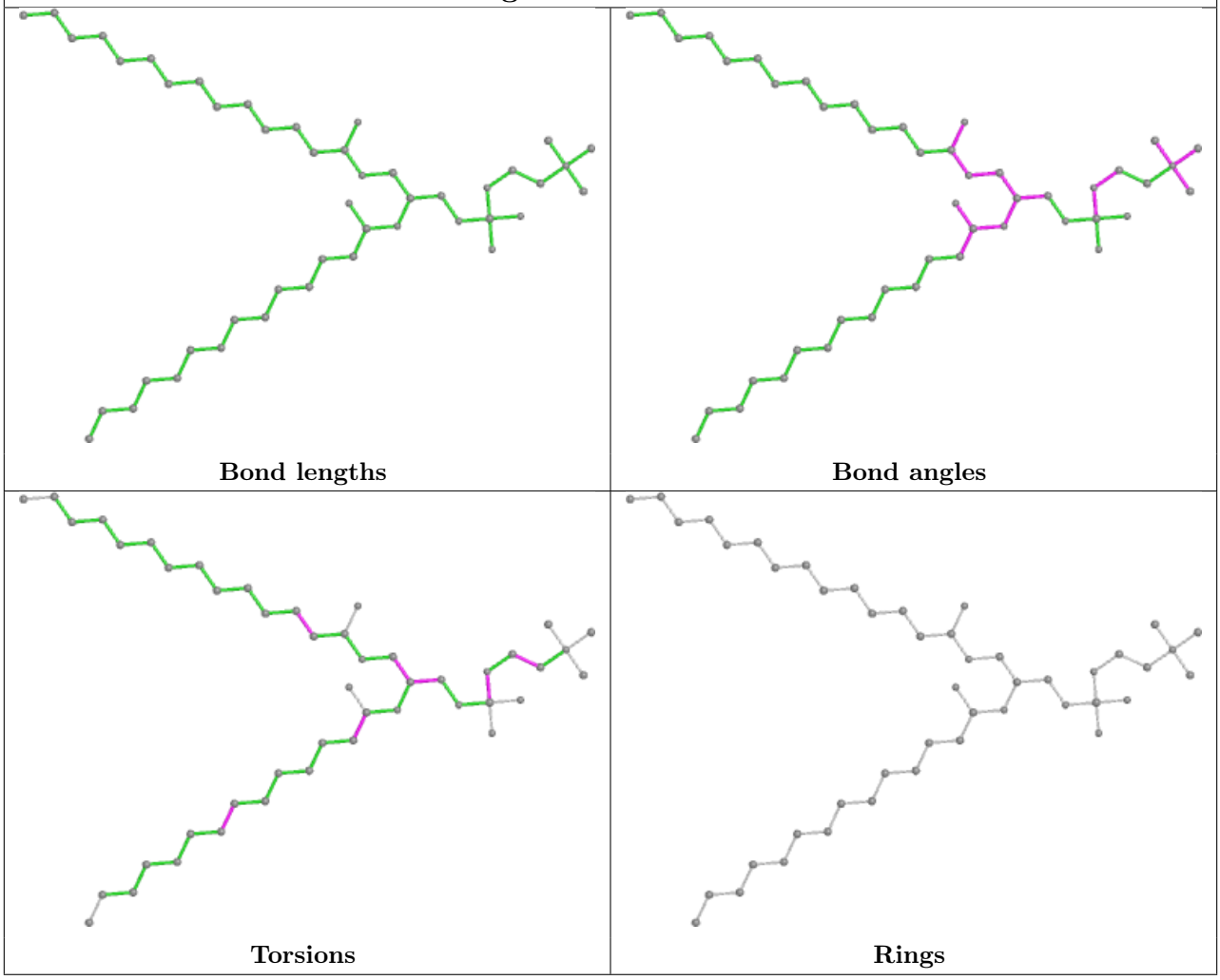
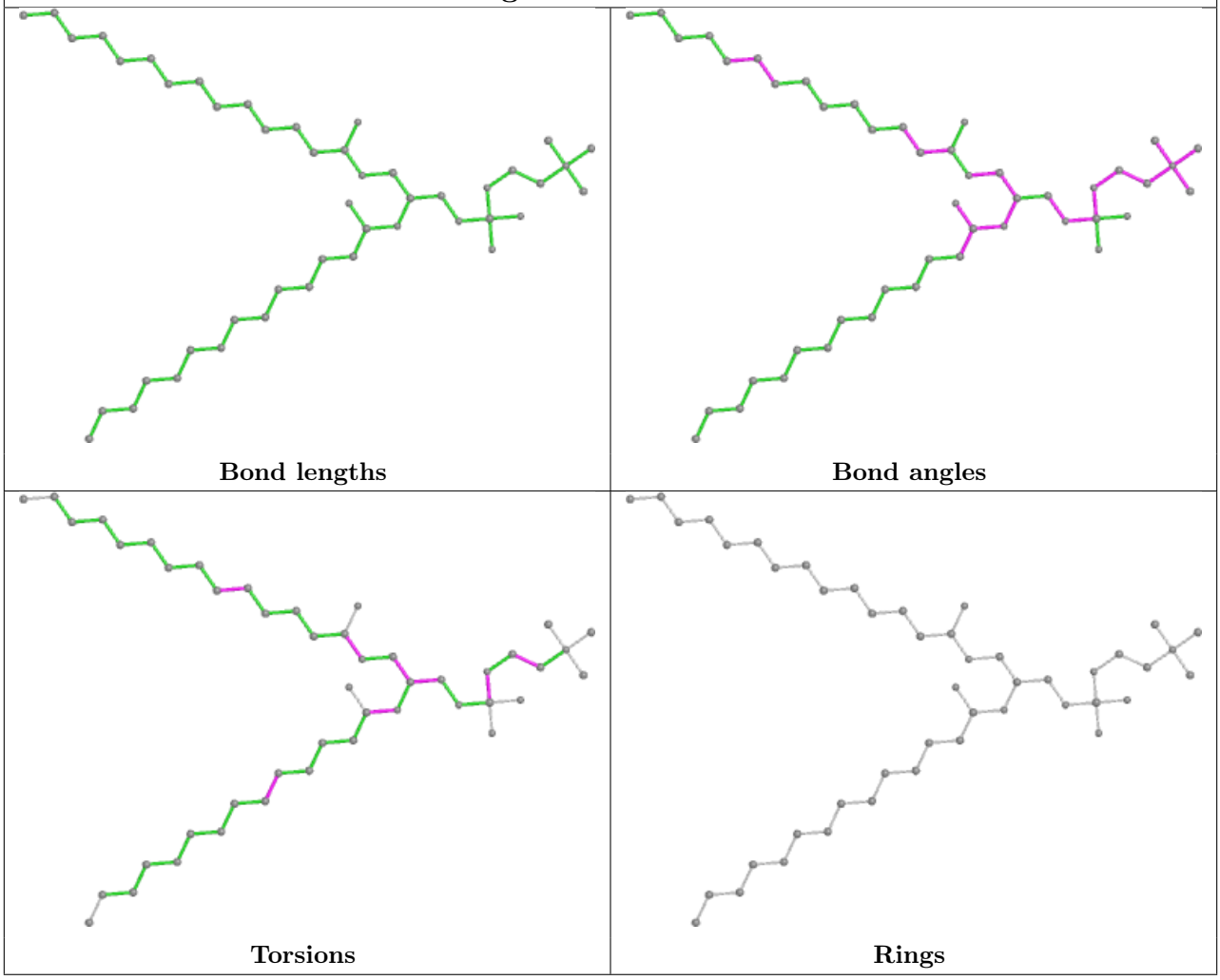


Rings

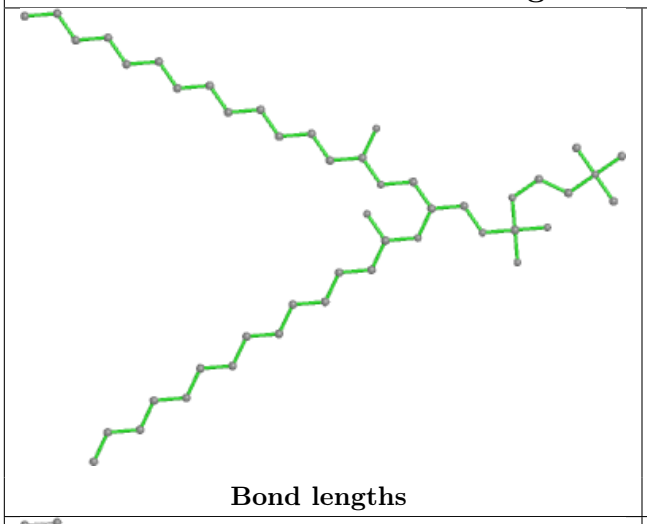
Ligand PX4 A 348



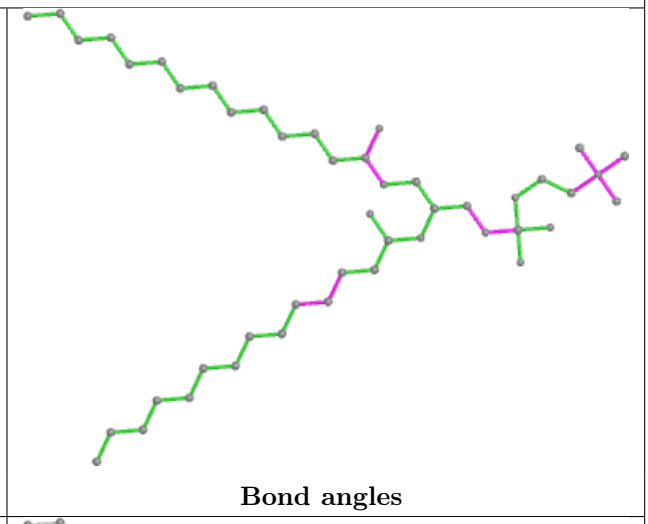
Ligand PX4 A 341



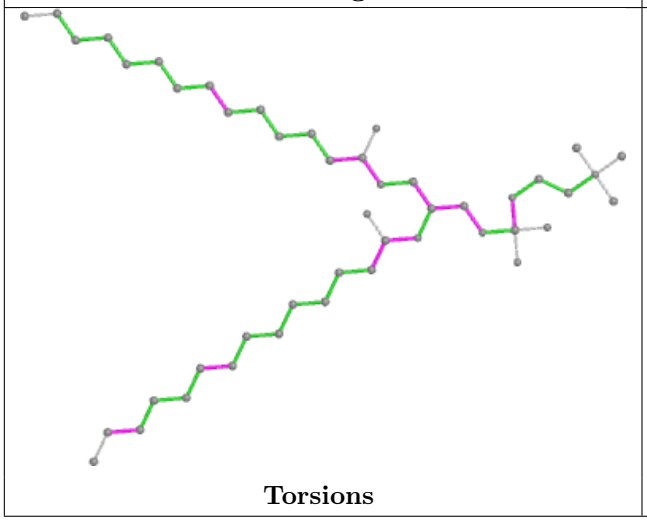
Ligand PX4 A 364



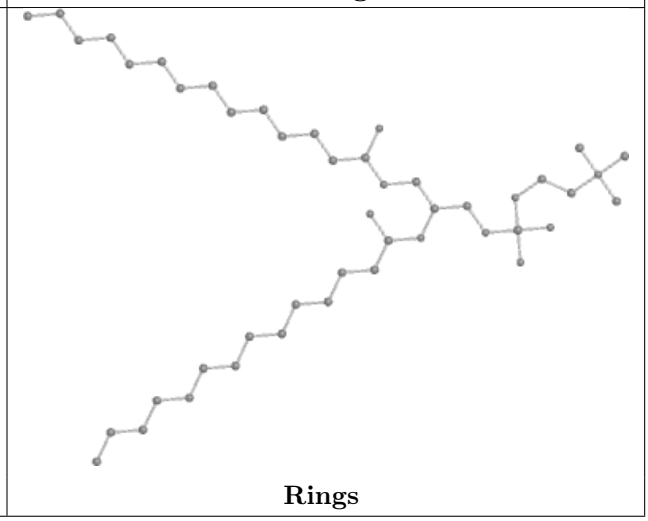
Bond lengths



Bond angles

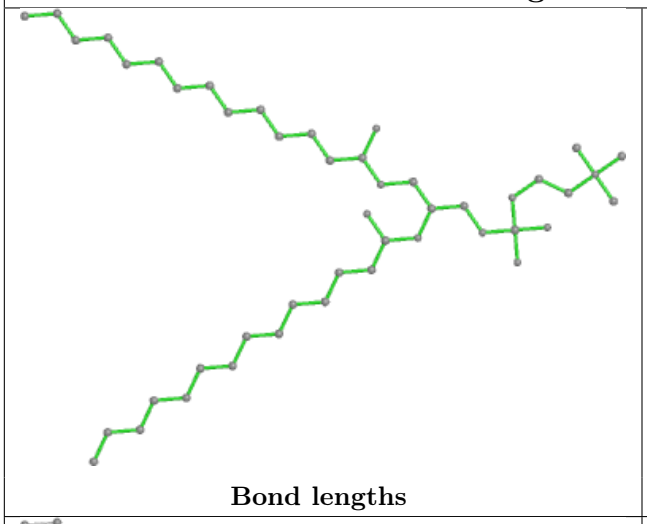


Torsions



Rings

Ligand PX4 A 424



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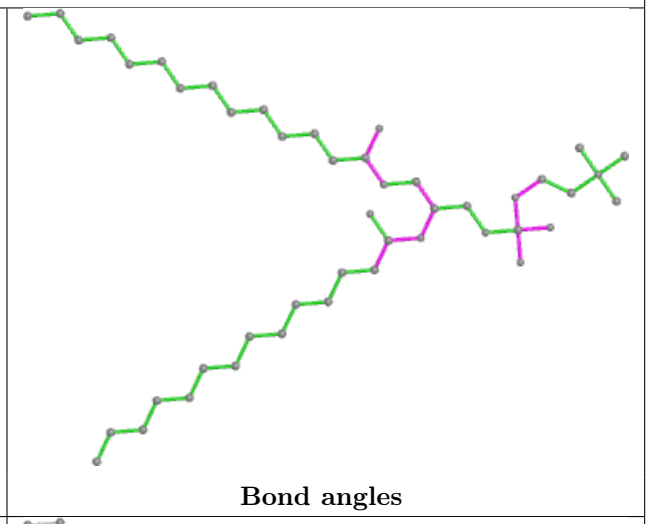
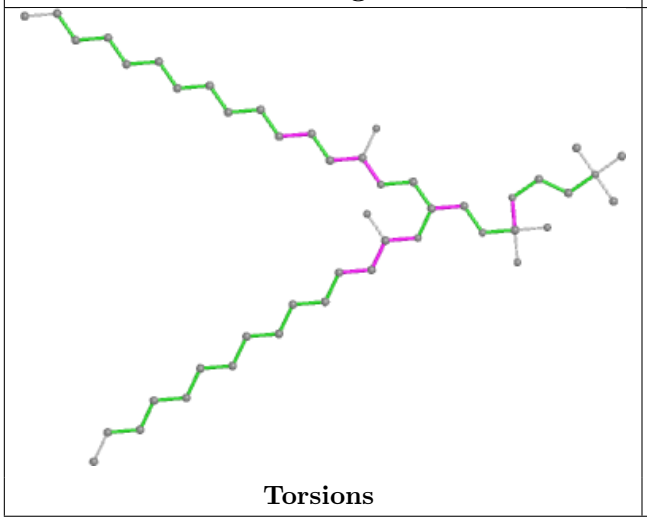


Bond angles



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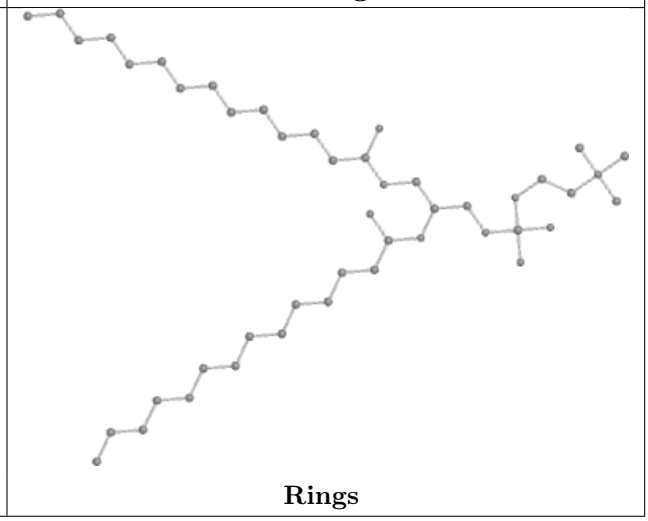
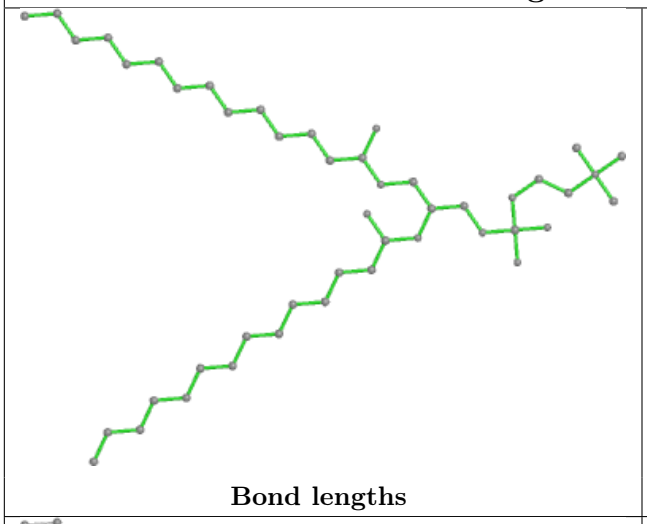


Rings

Ligand PX4 A 383



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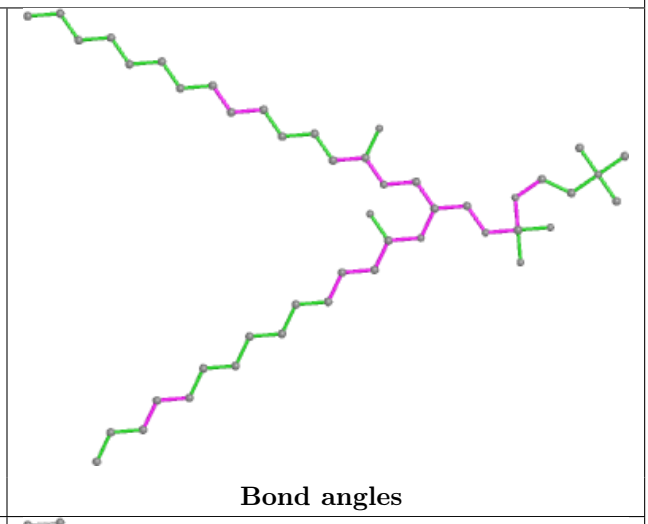
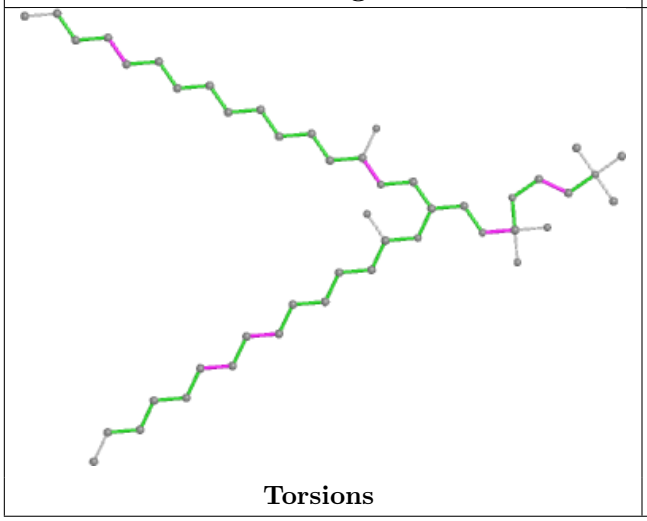


Bond angles



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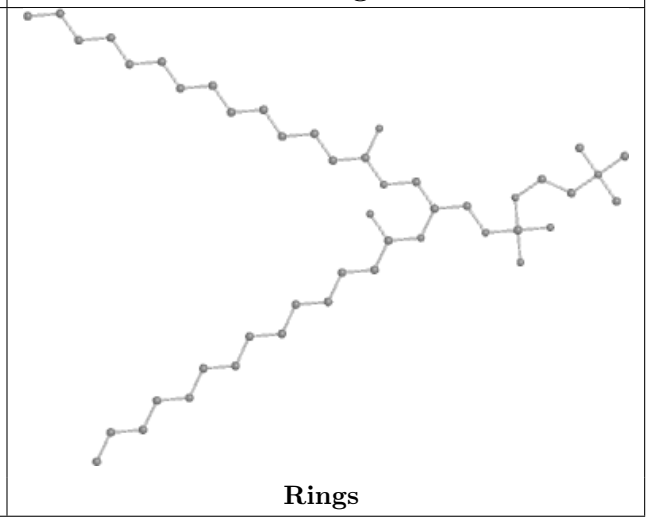
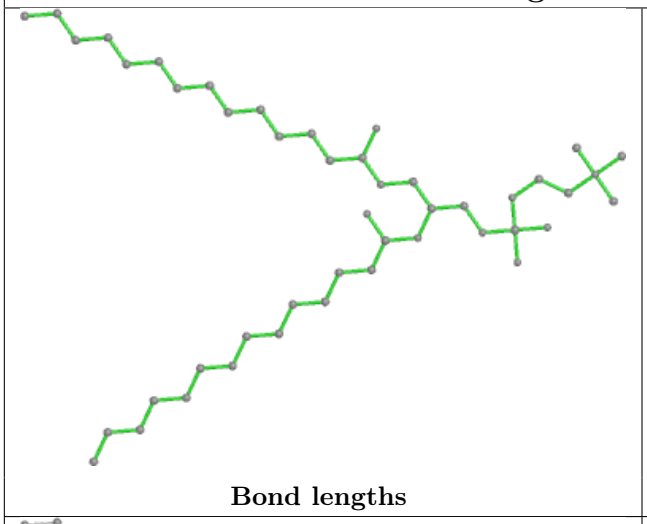
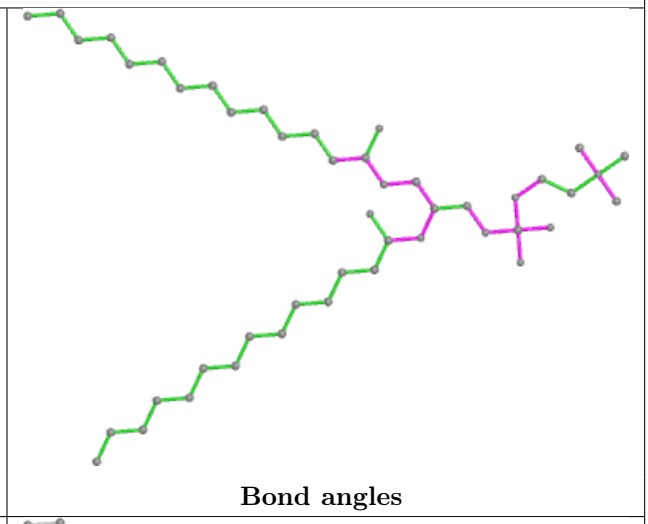


Rings

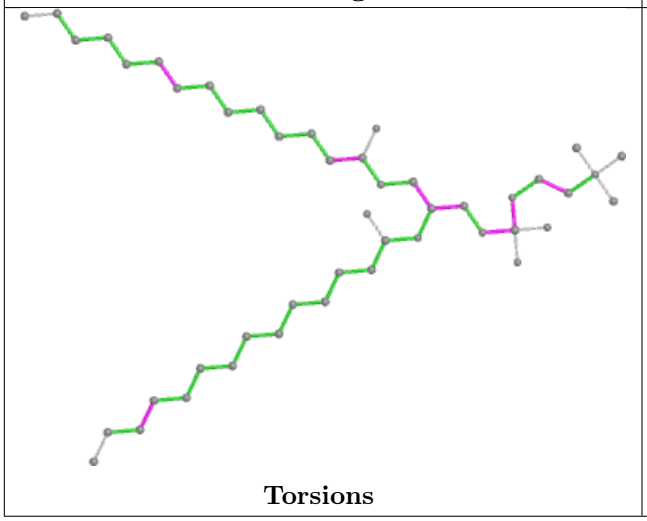
Ligand PX4 A 380



Bond lengths



Bond angles



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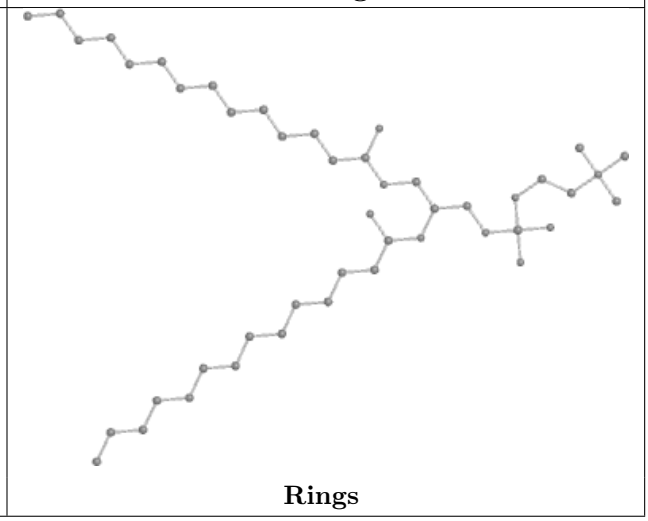
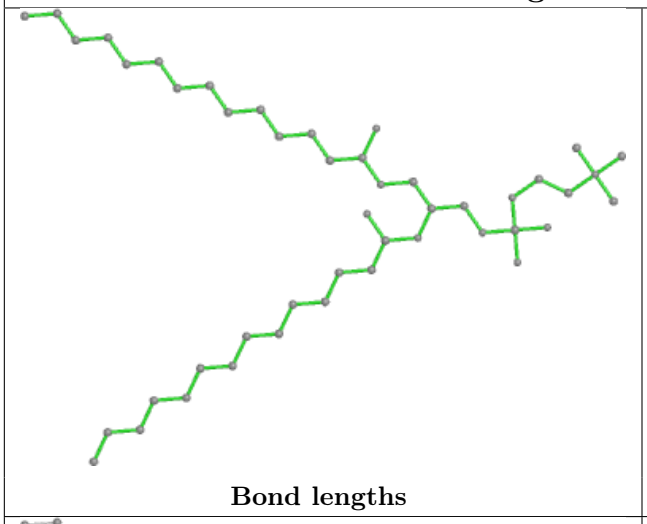


Rings

Ligand PX4 A 338



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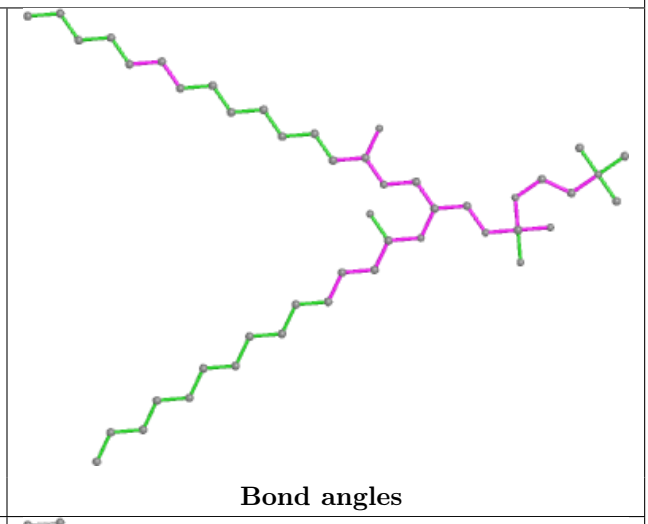
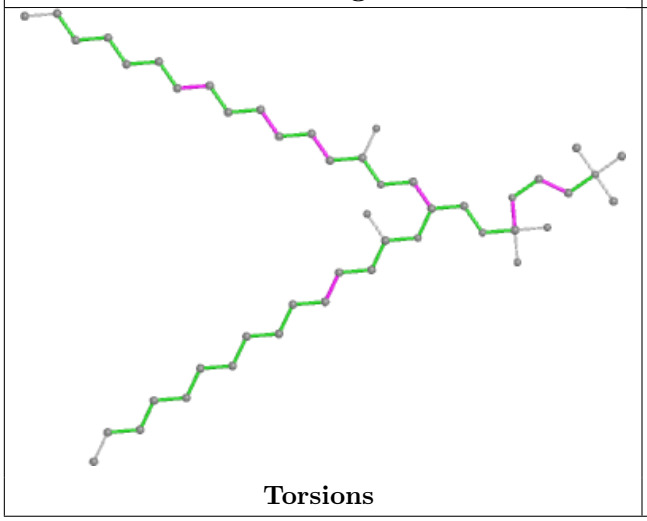


Bond angles



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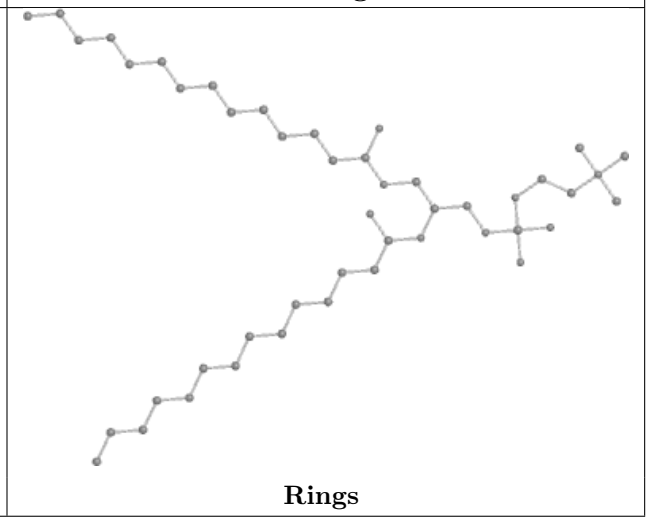
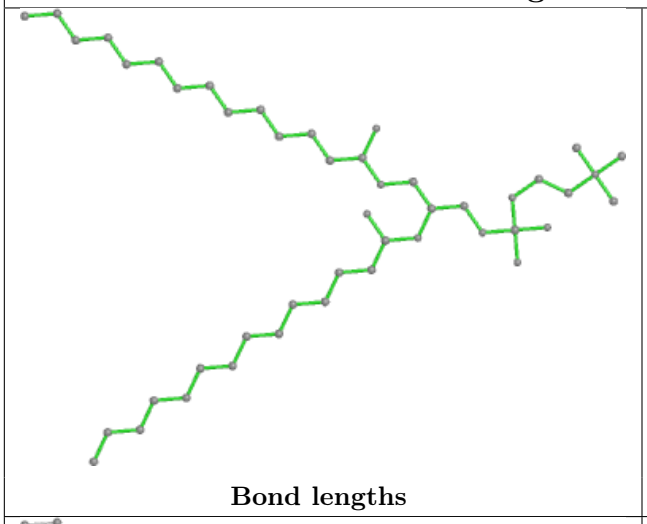


Rings

Ligand PX4 A 355



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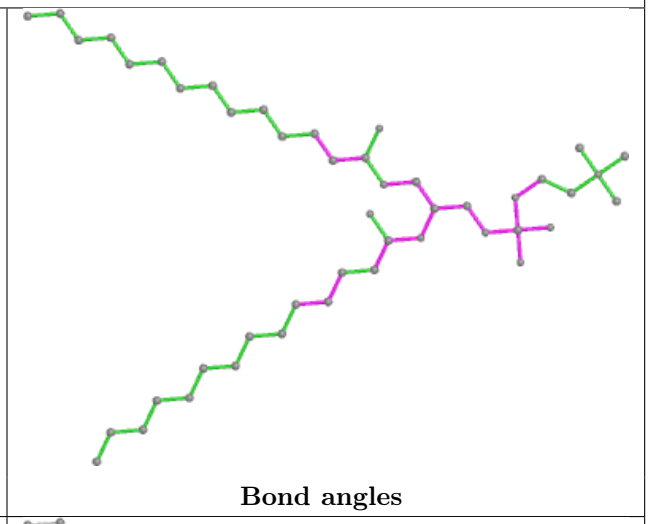
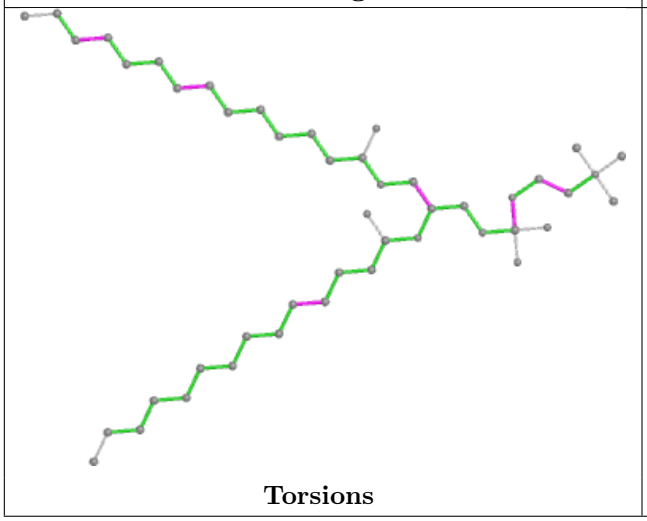


Bond angles



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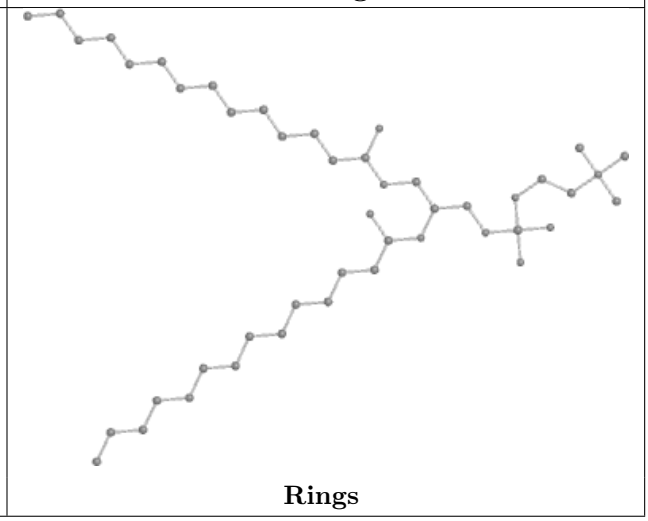
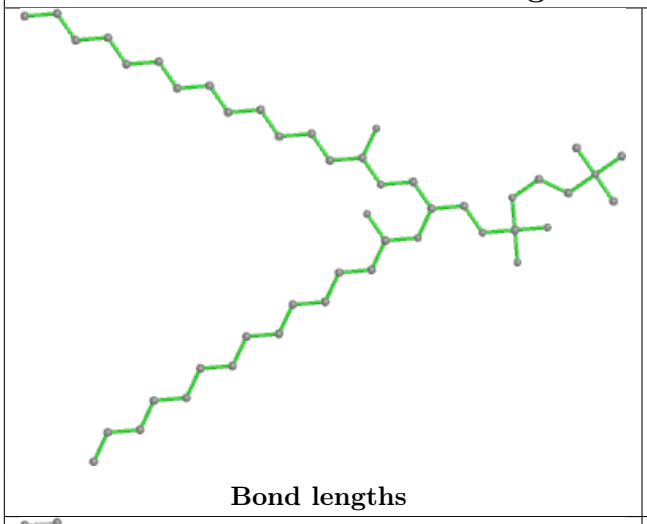


Rings

Ligand PX4 A 306



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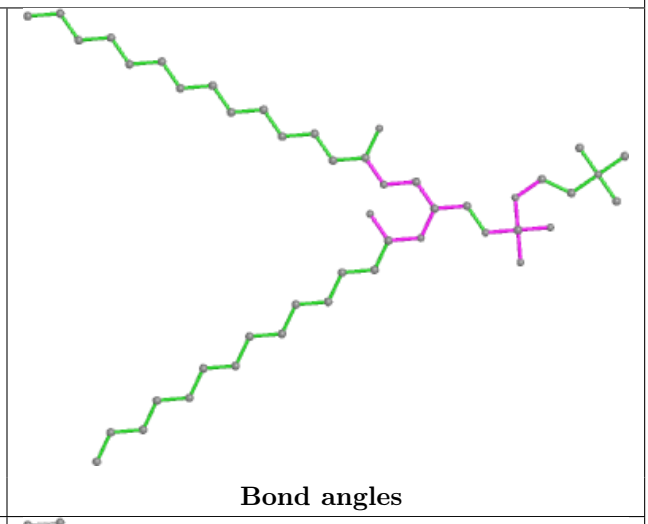
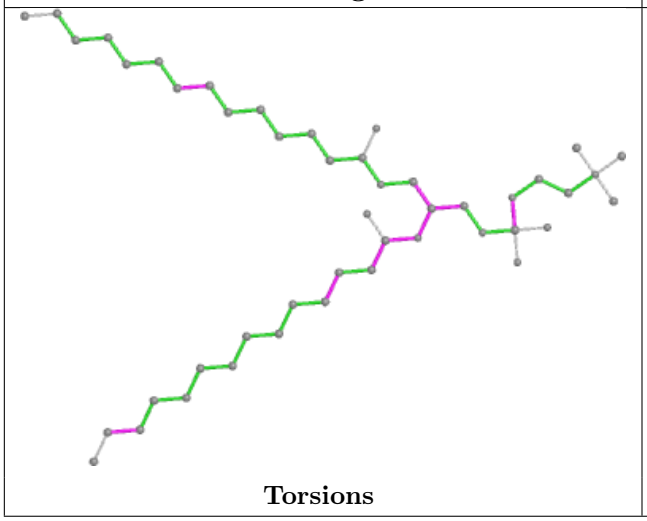


Bond angles



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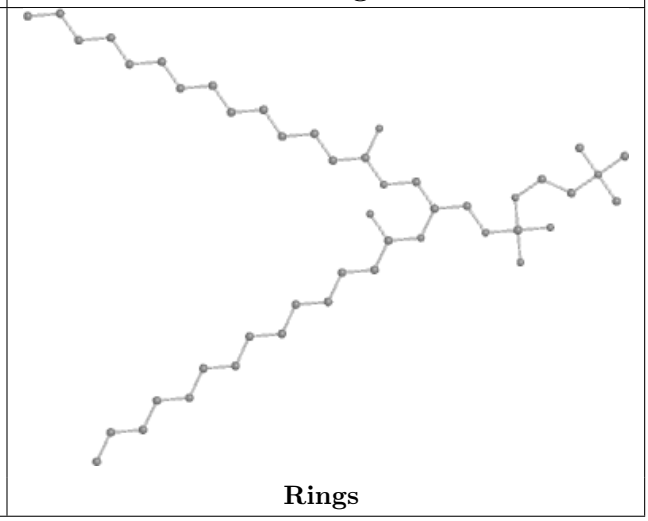
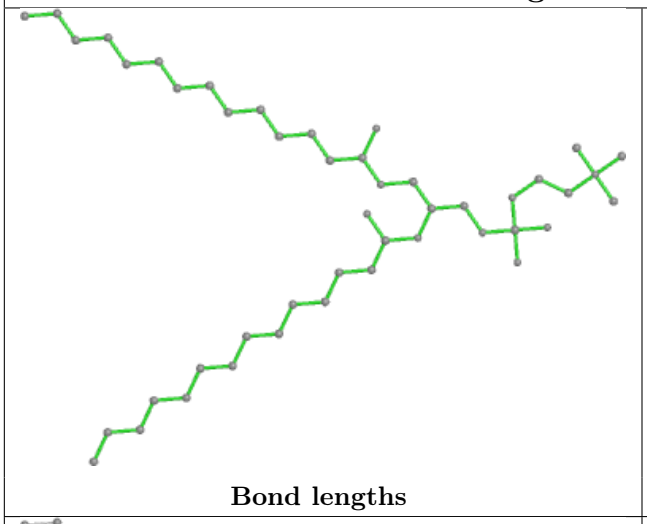


Rings

Ligand PX4 A 368



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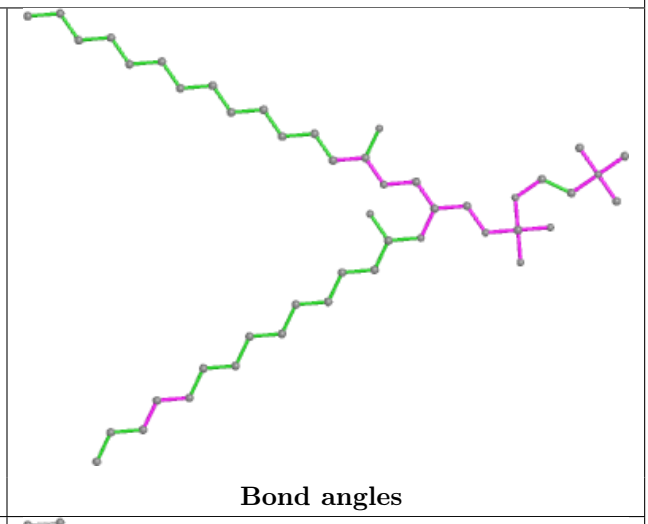
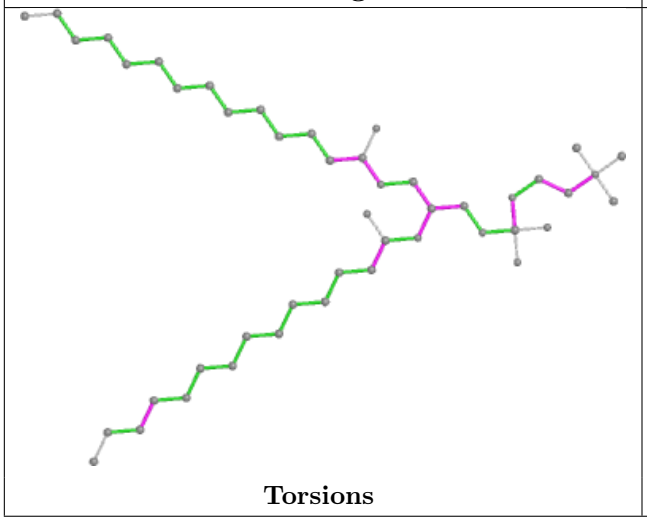


Bond angles



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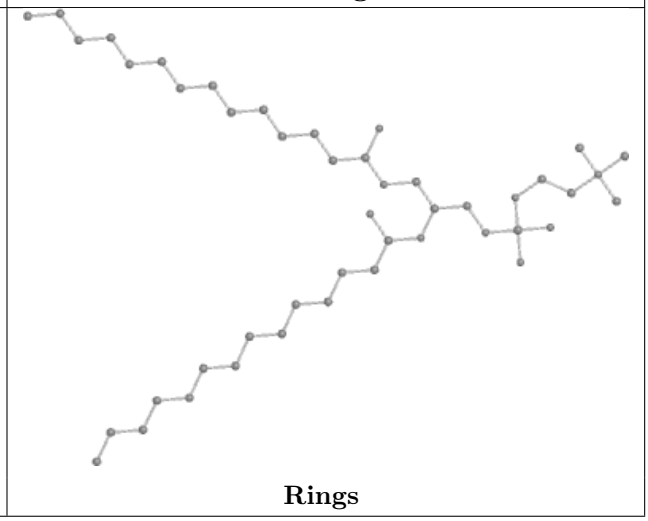
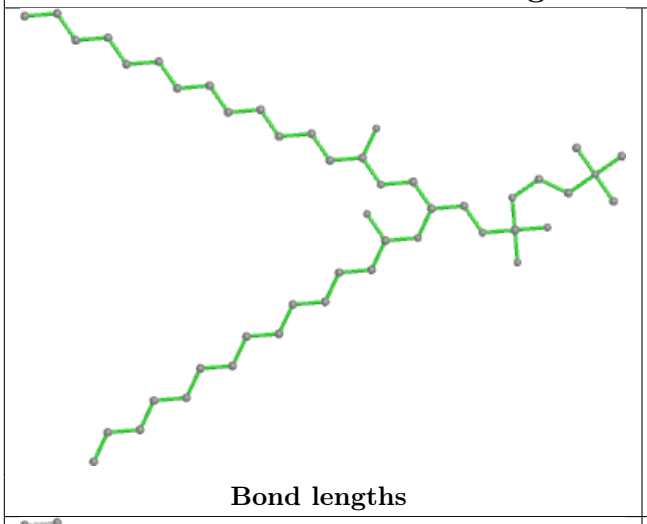
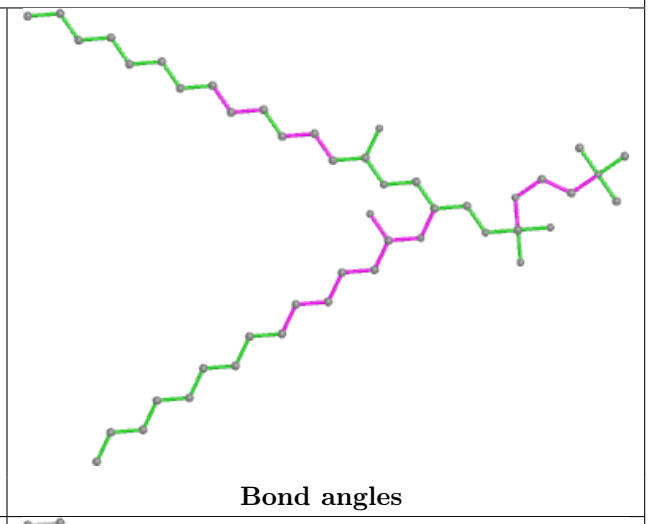


Rings

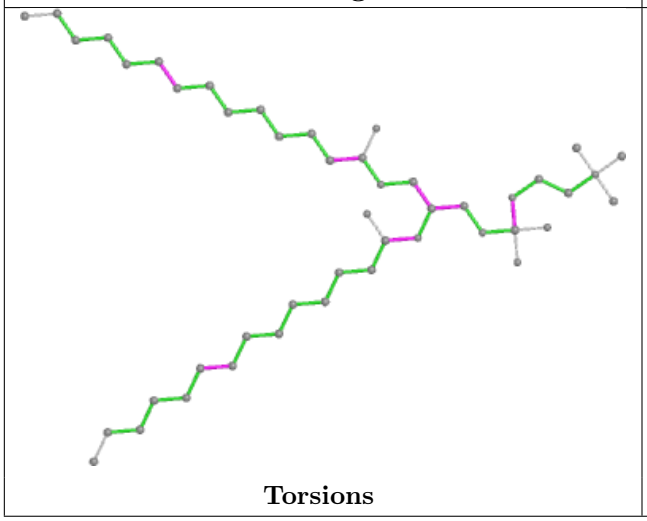
Ligand PX4 A 323



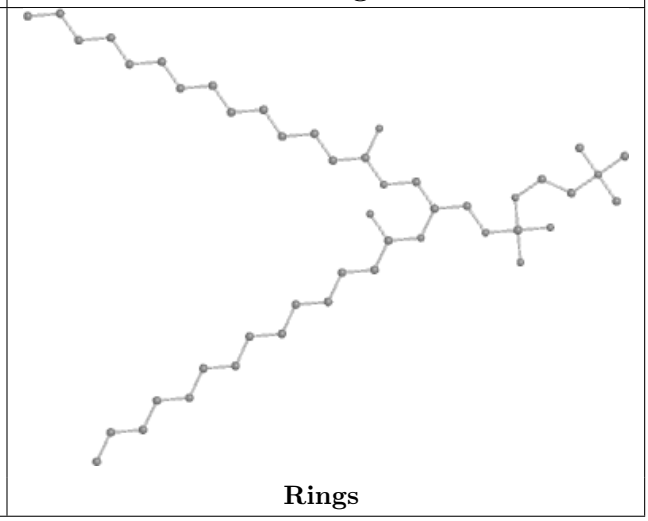
Bond lengths



Bond angles

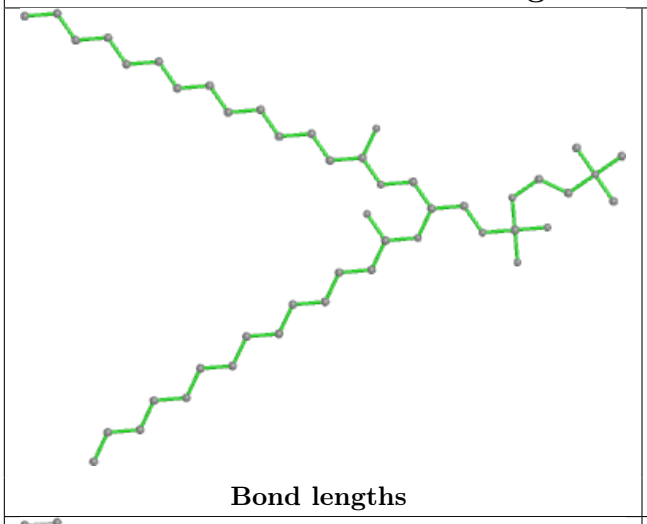


Torsions



Rings

Ligand PX4 A 339



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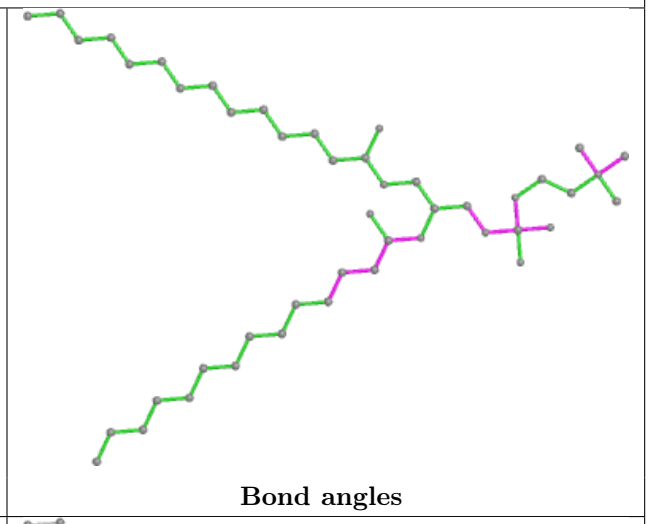

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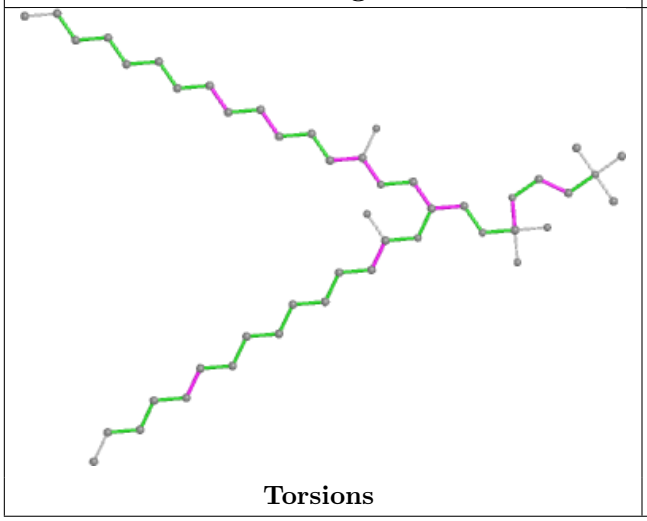

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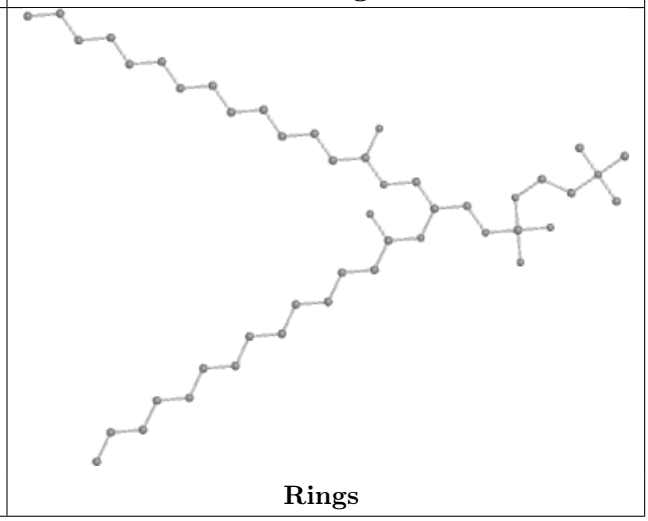
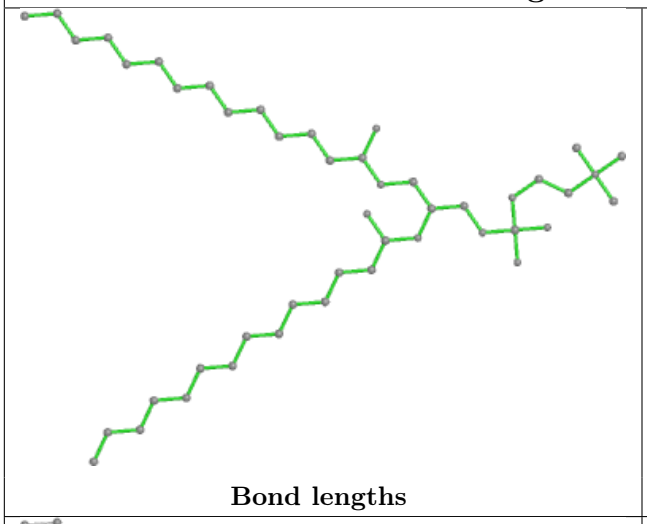


Rings

Ligand PX4 A 369



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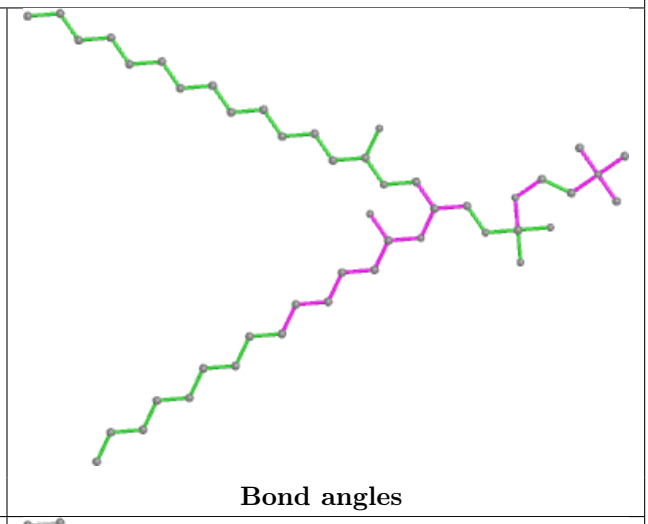
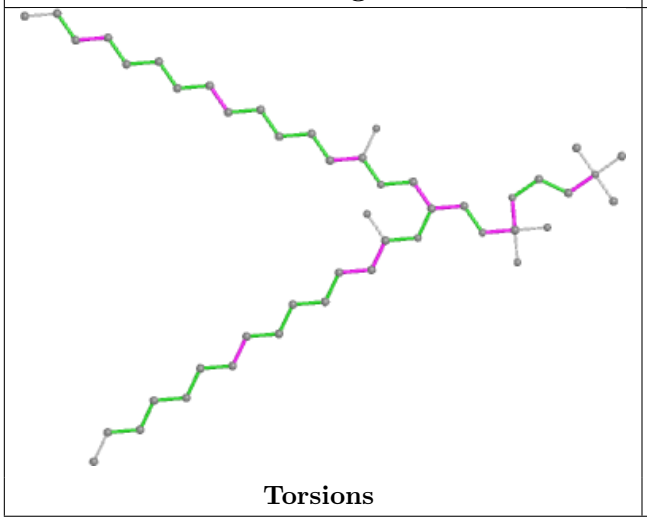


Bond angles



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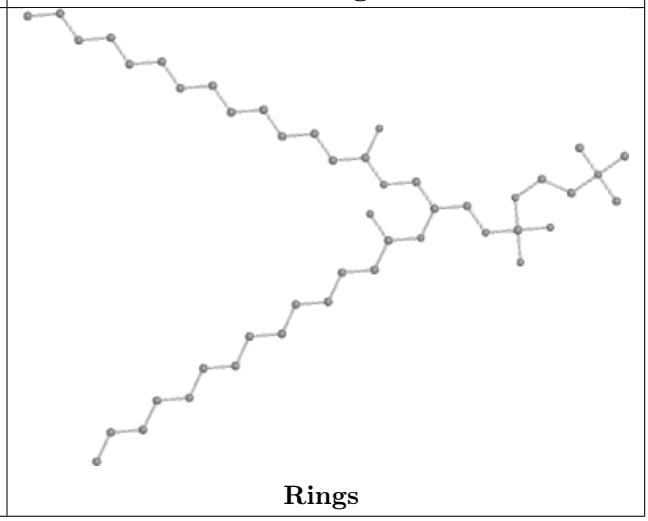
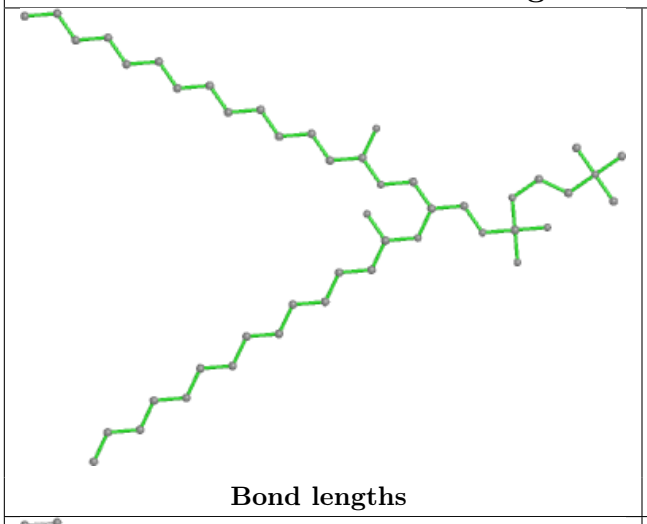


Rings

Ligand PX4 A 307



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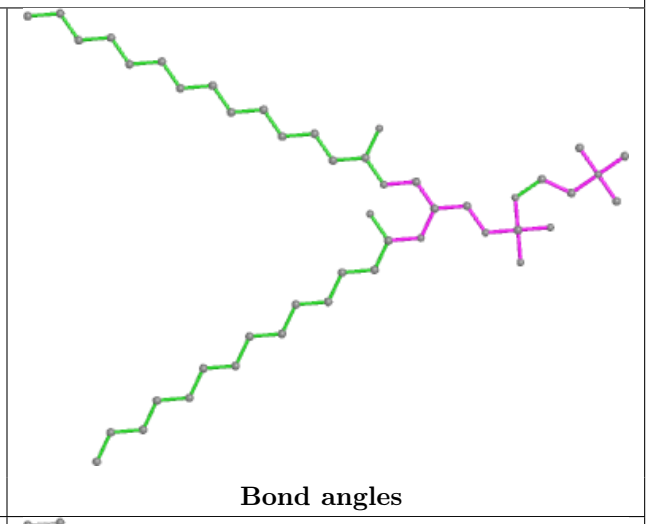

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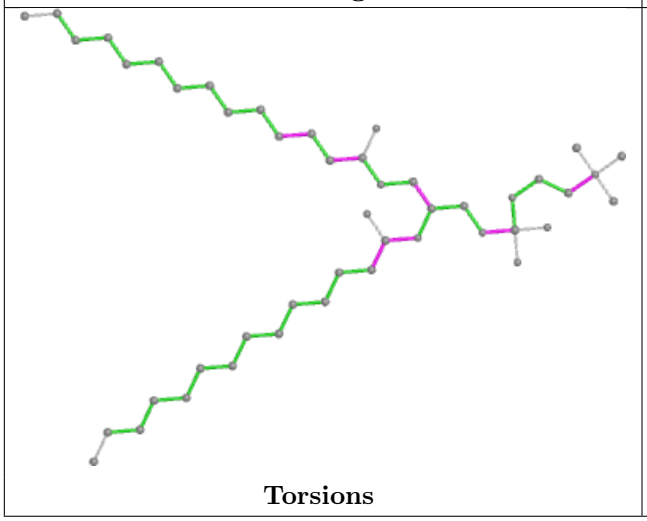

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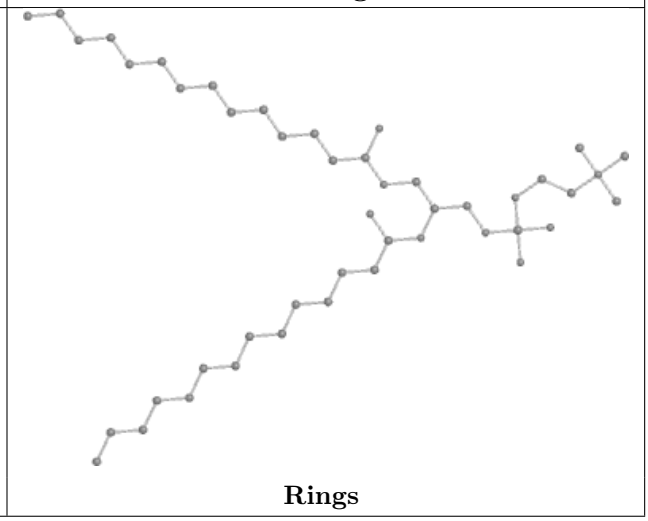
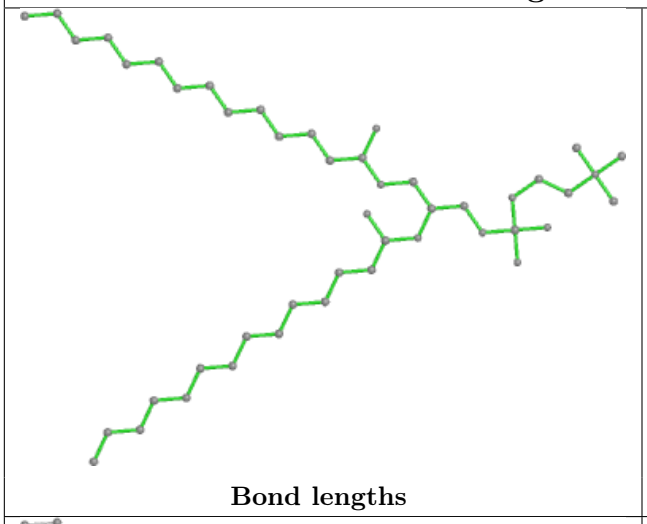


Rings

Ligand PX4 A 390



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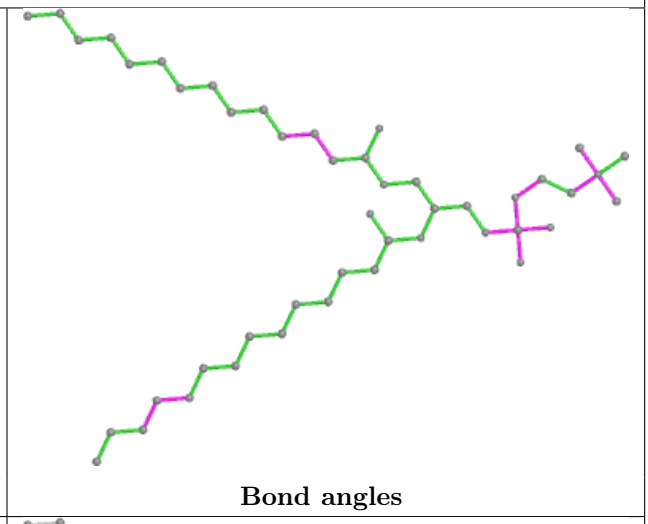
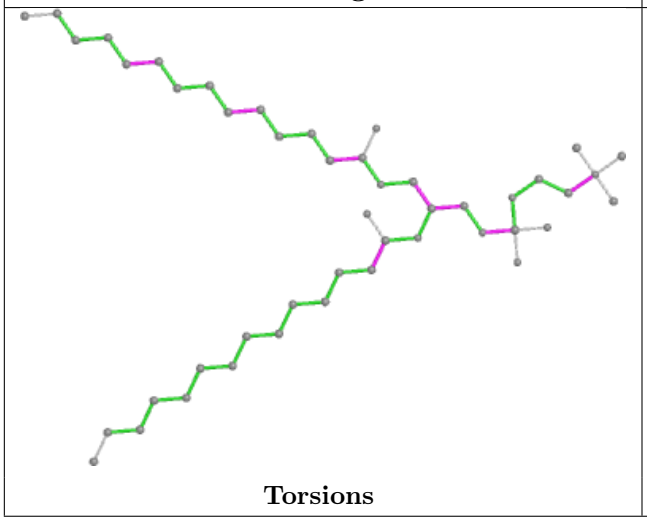


Bond angles



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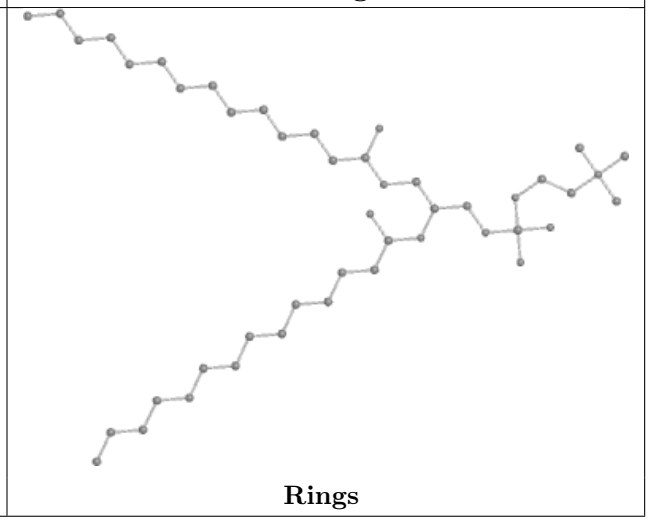
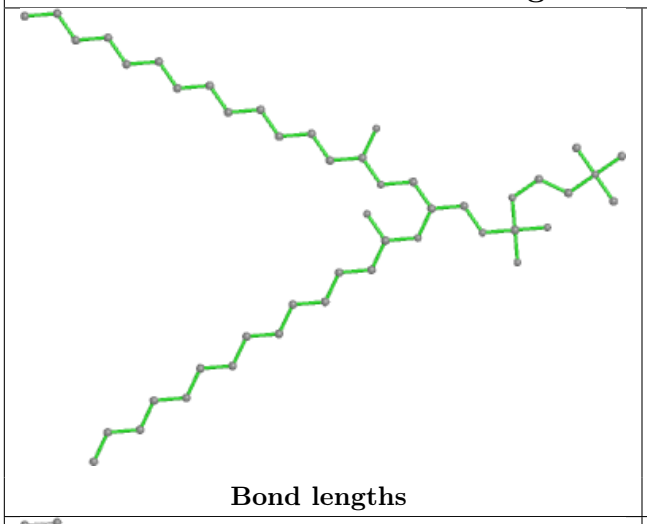


Rings

Ligand PX4 A 378



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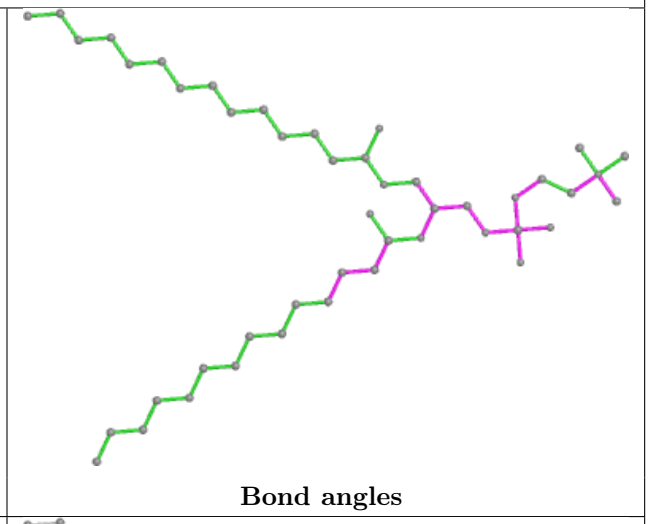
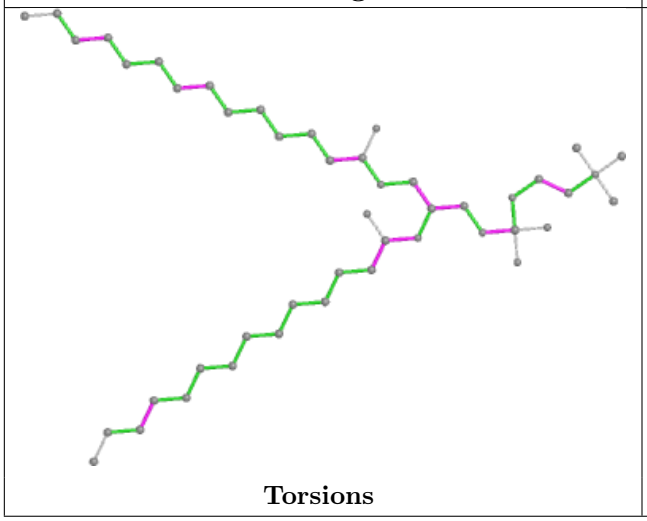


Bond angles



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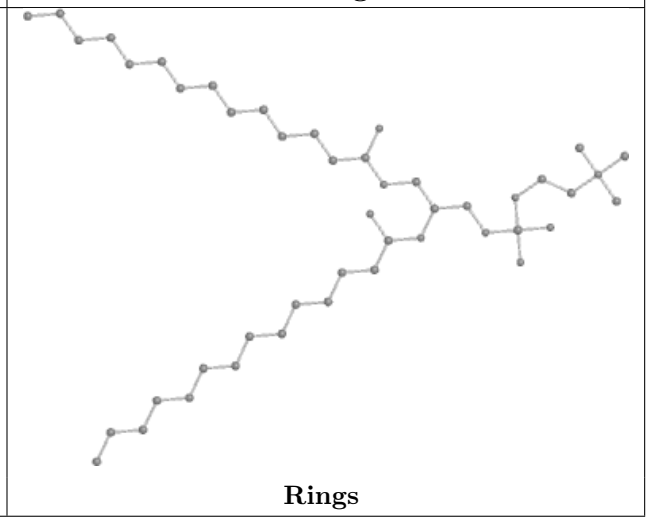
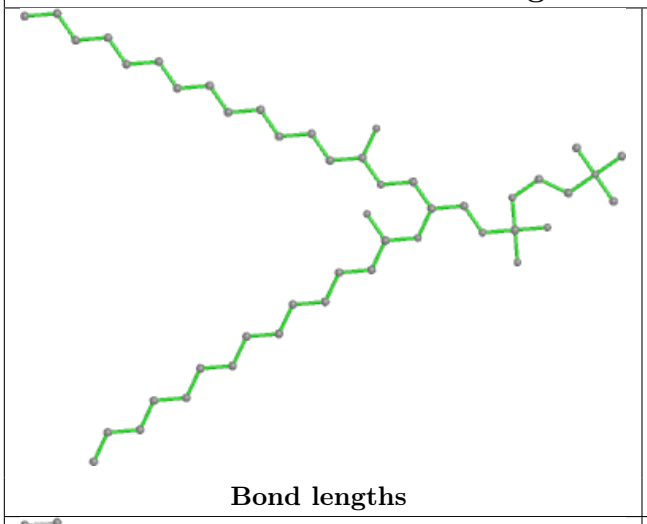


Rings

Ligand PX4 A 414



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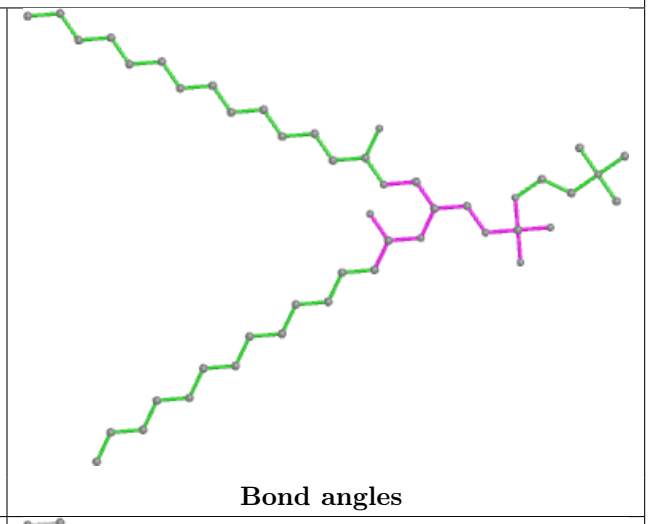

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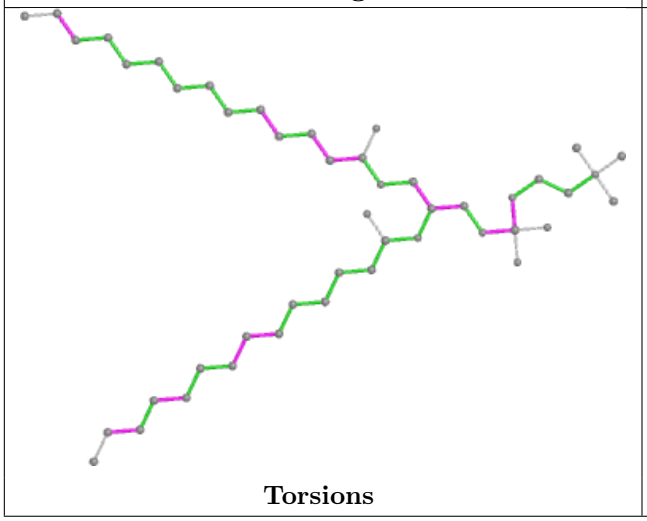

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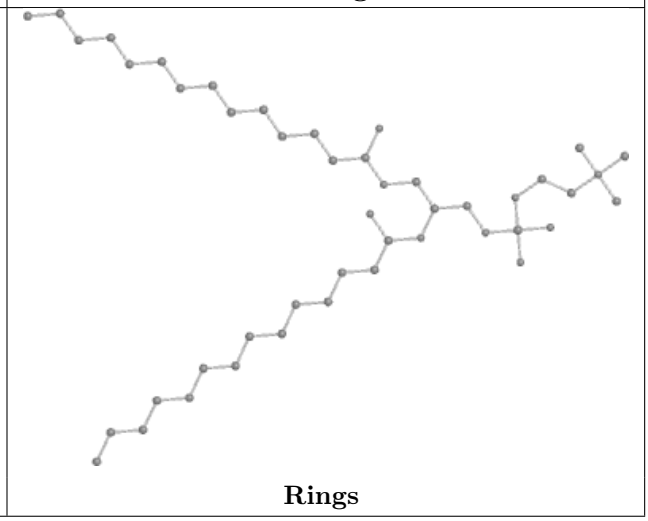
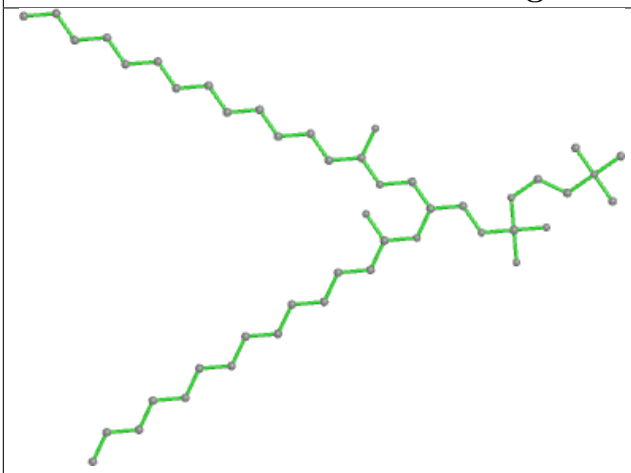


Rings

Ligand PX4 A 315



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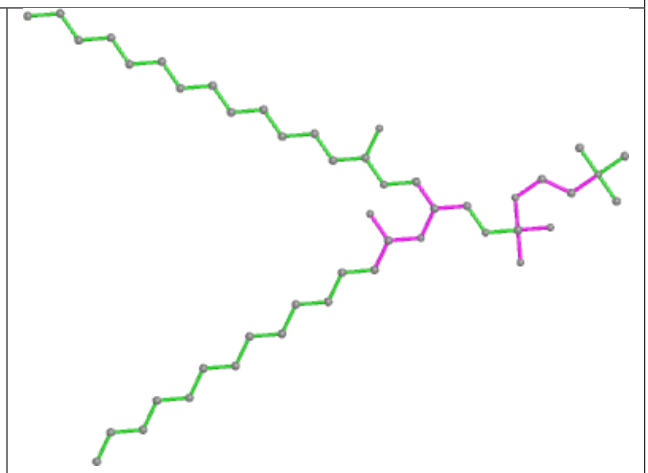
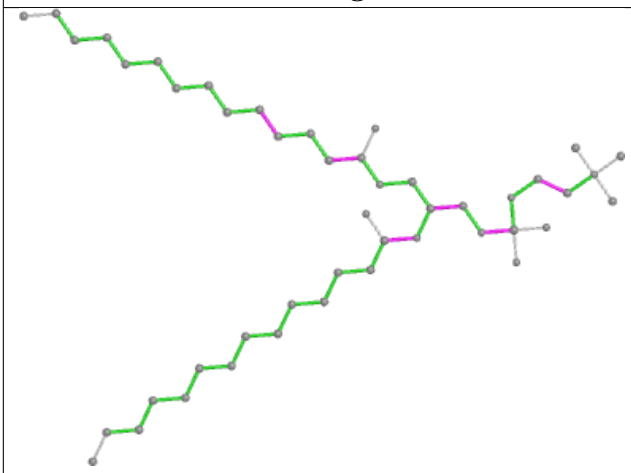


Bond angles



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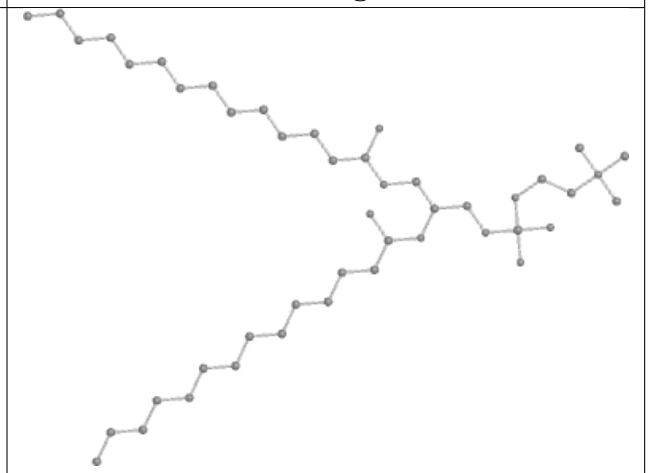
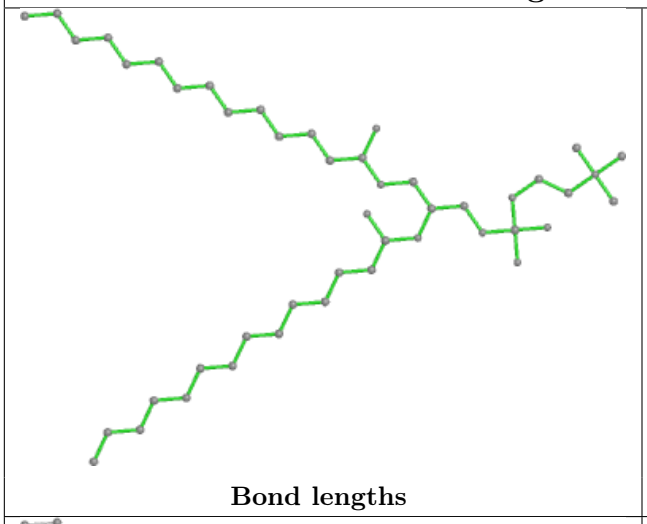


Rings

Ligand PX4 A 366



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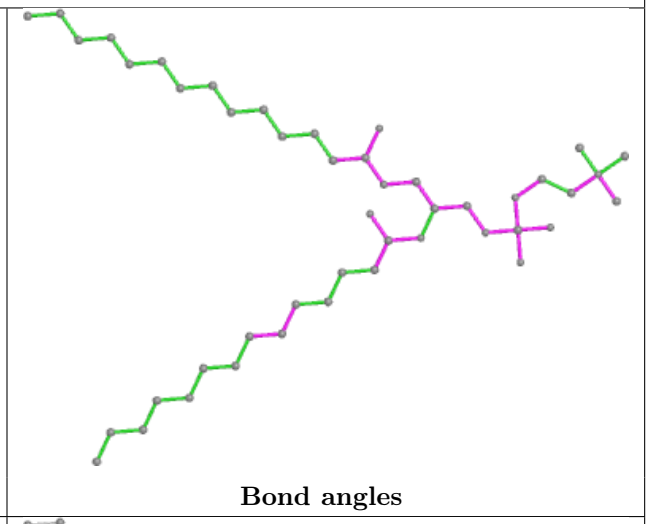

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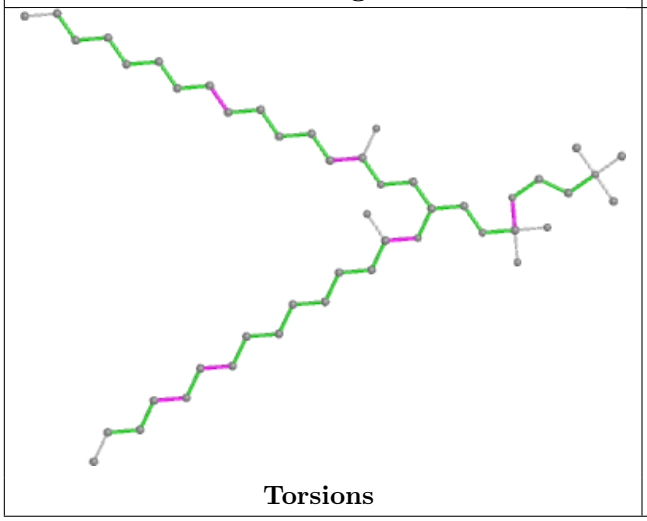

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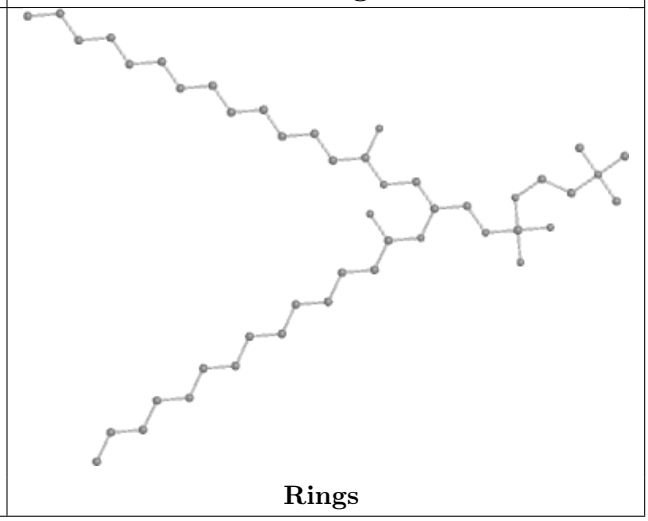
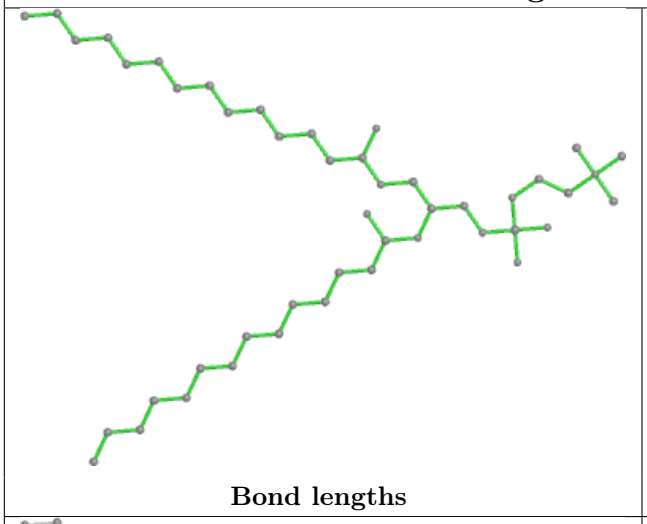


Rings

Ligand PX4 A 325



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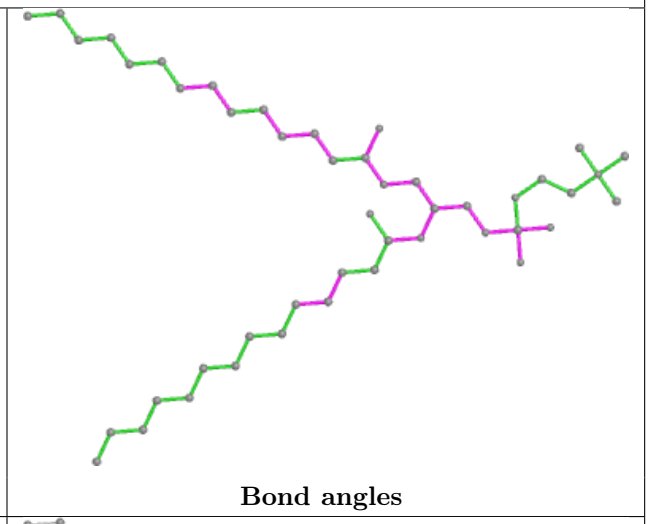
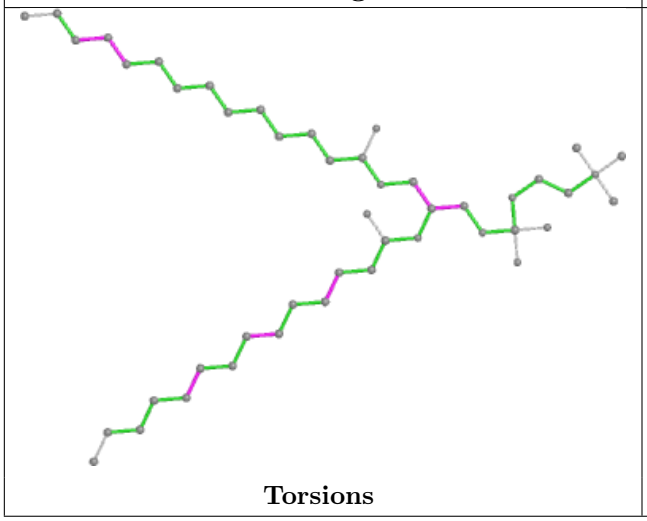


Bond angles



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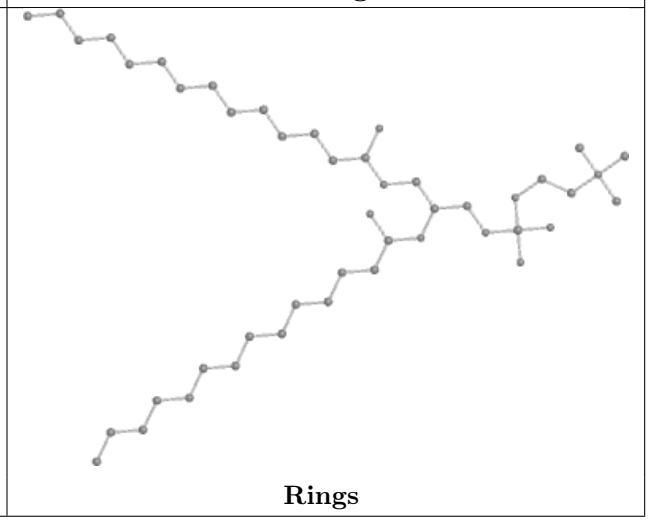
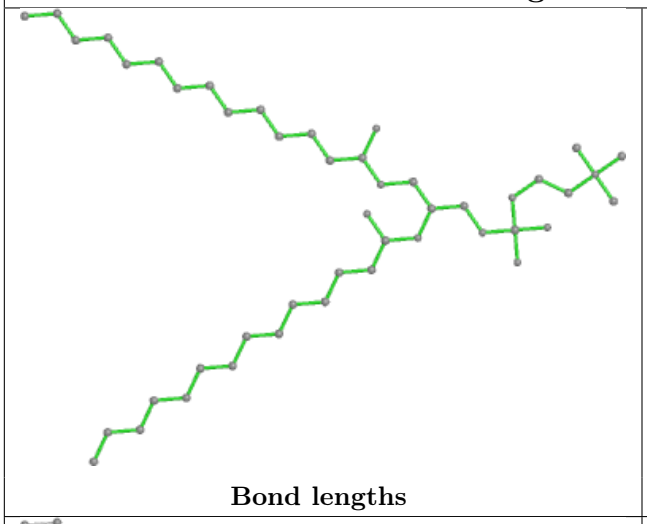


Rings

Ligand PX4 A 346



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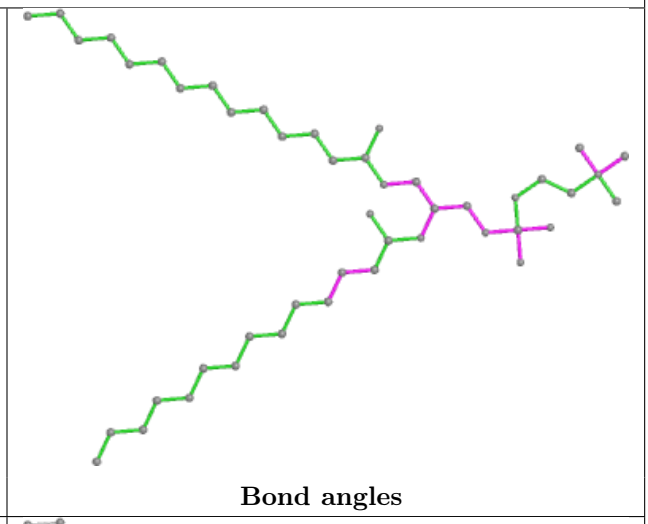
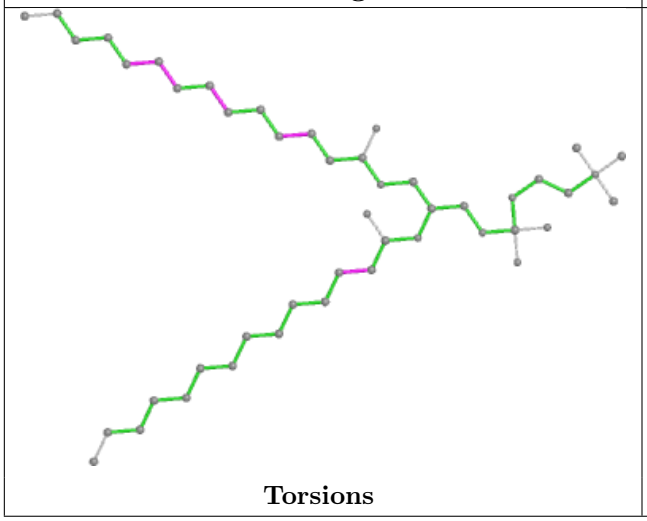


Bond angles



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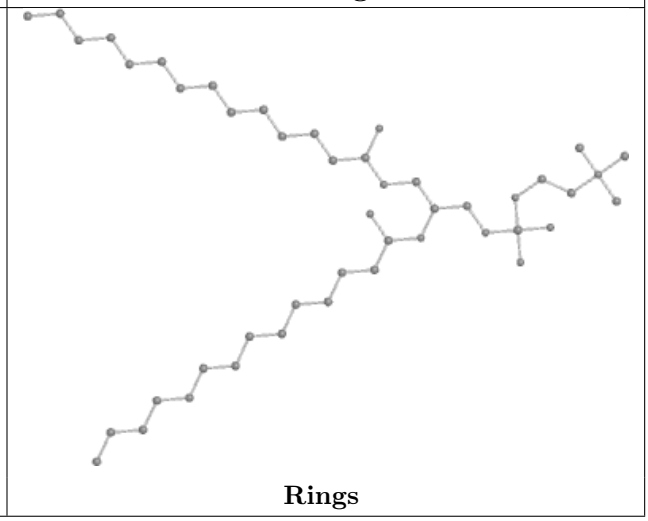
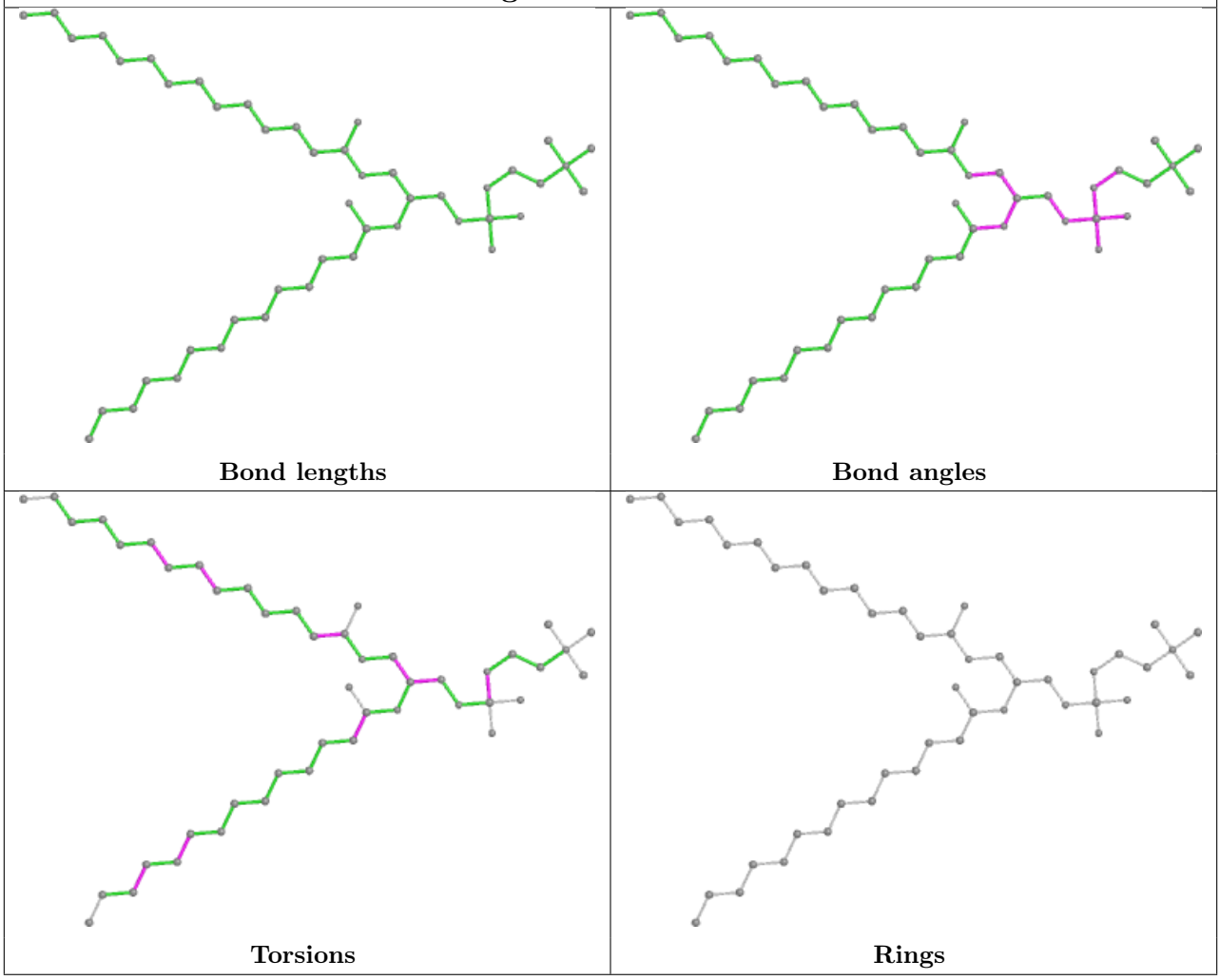
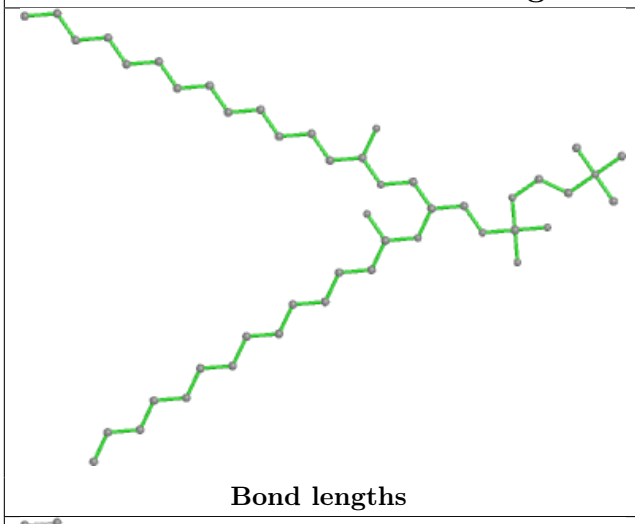


Rings

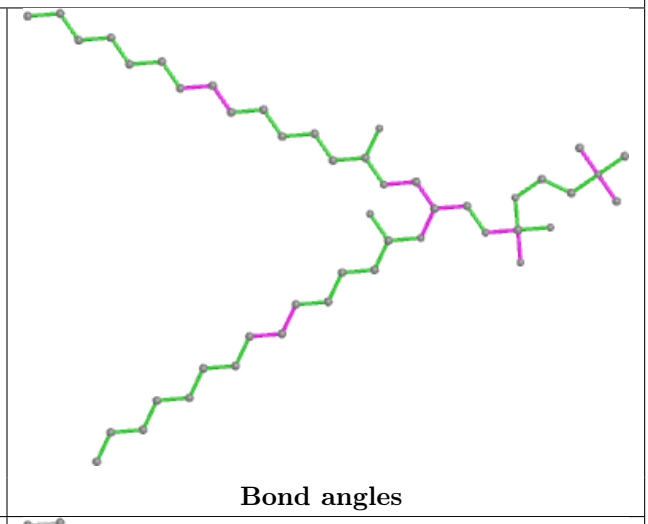
Ligand PX4 A 363



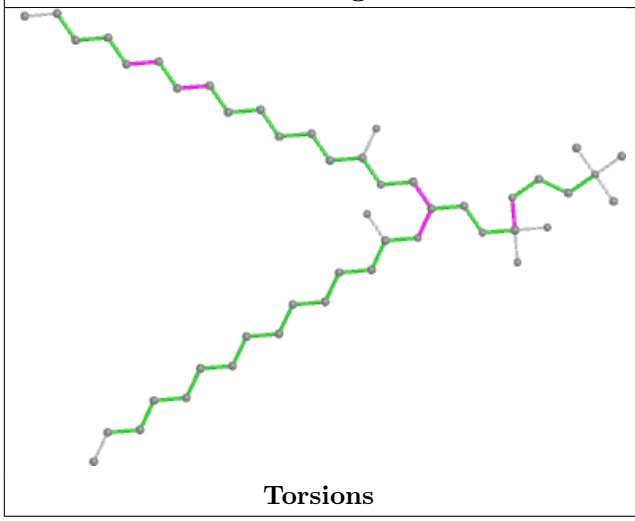
Ligand PX4 A 362



Bond lengths



Bond angles



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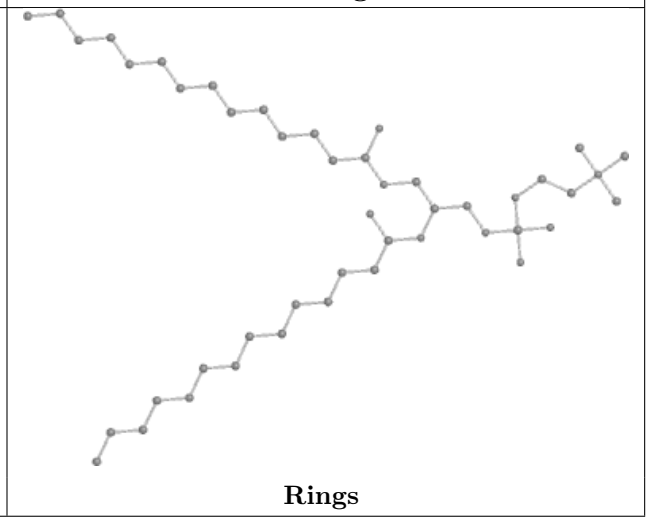
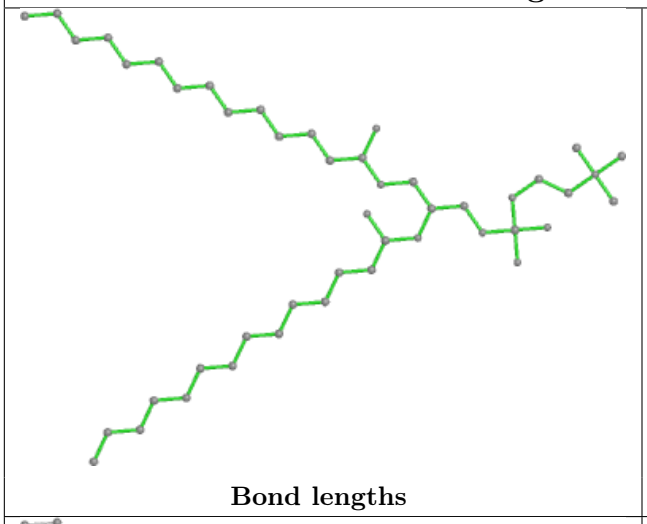
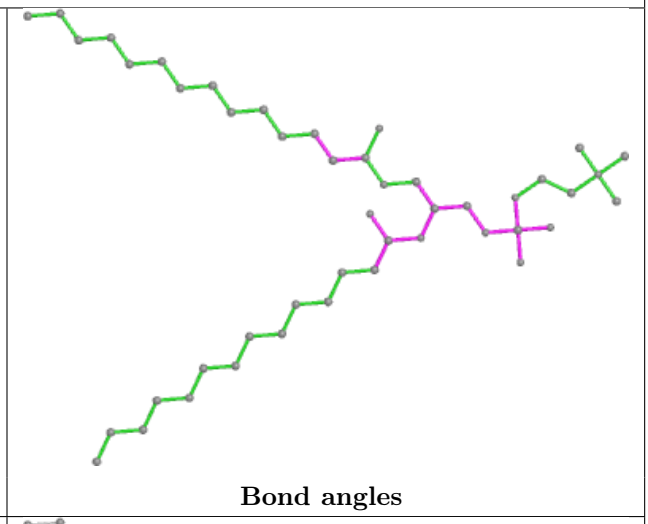


Rings

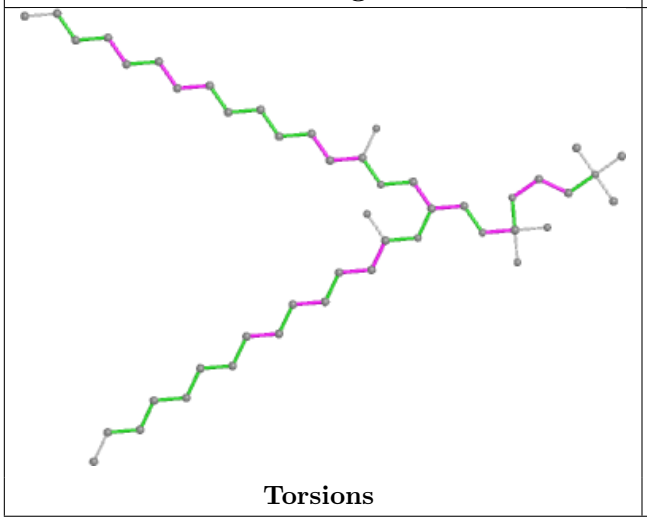
Ligand PX4 A 408



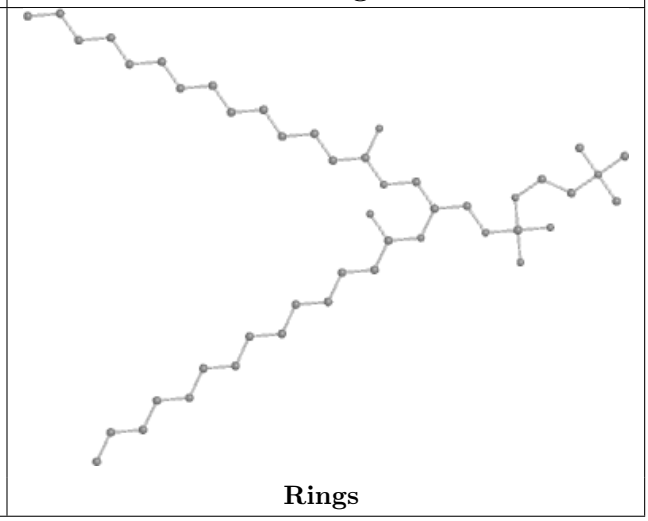
Bond lengths



Bond angles

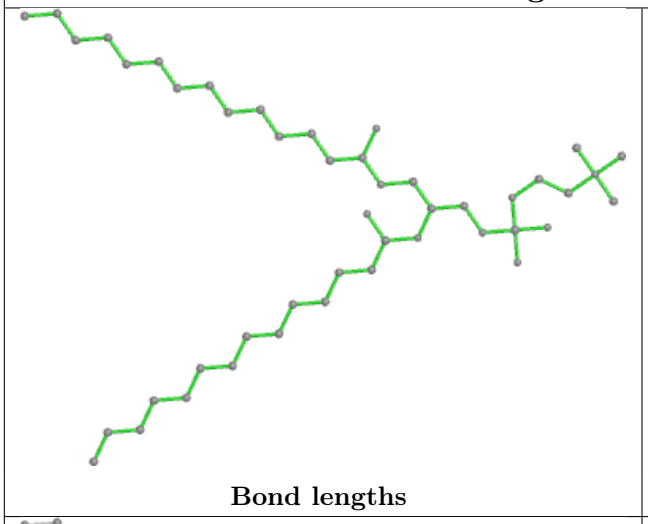


Torsions

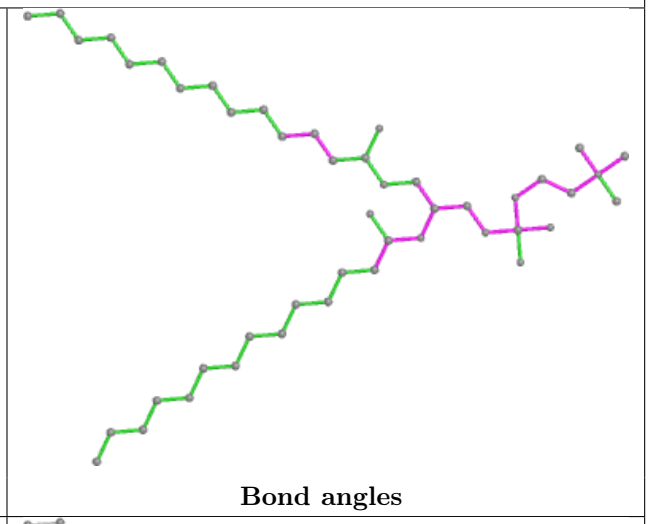


Rings

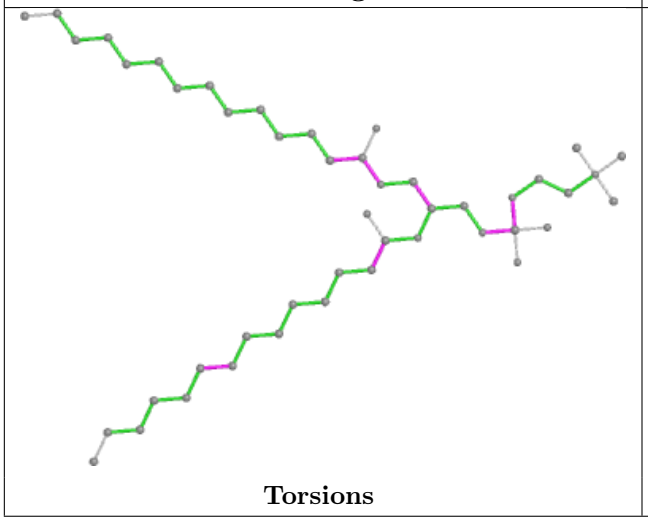
Ligand PX4 A 430



Bond lengths



Bond angles



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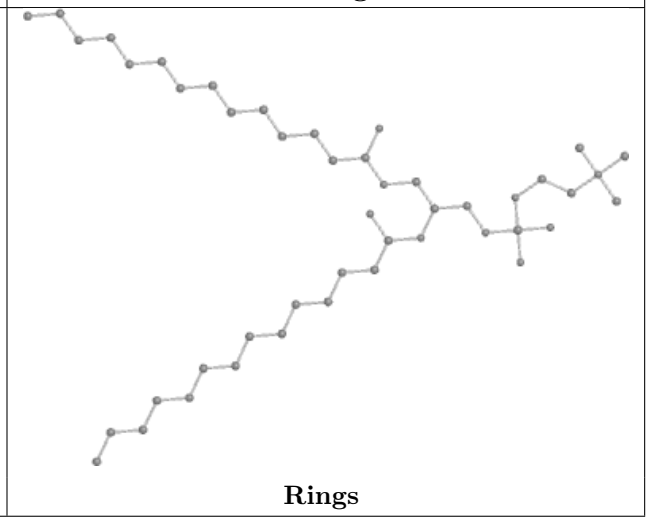
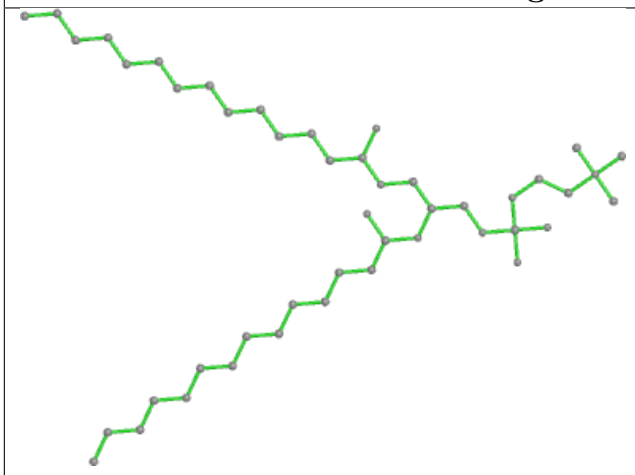


Rings

Ligand PX4 A 316



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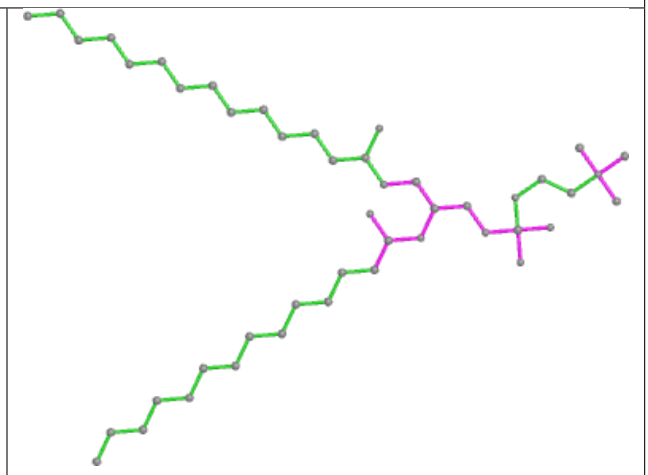
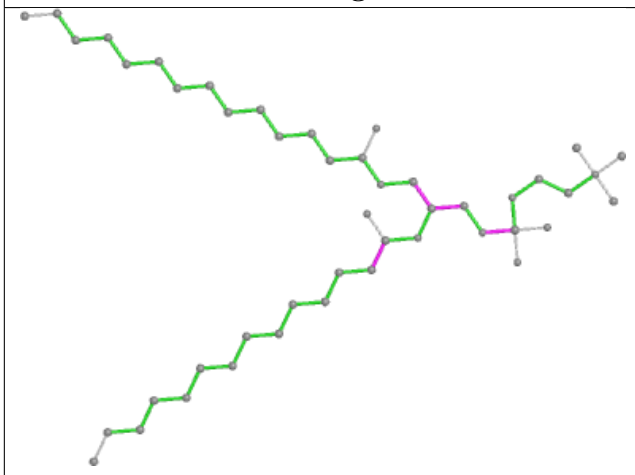


Bond angles



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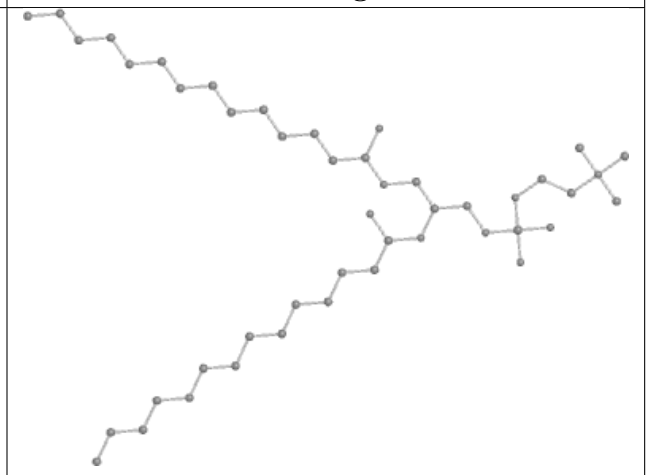
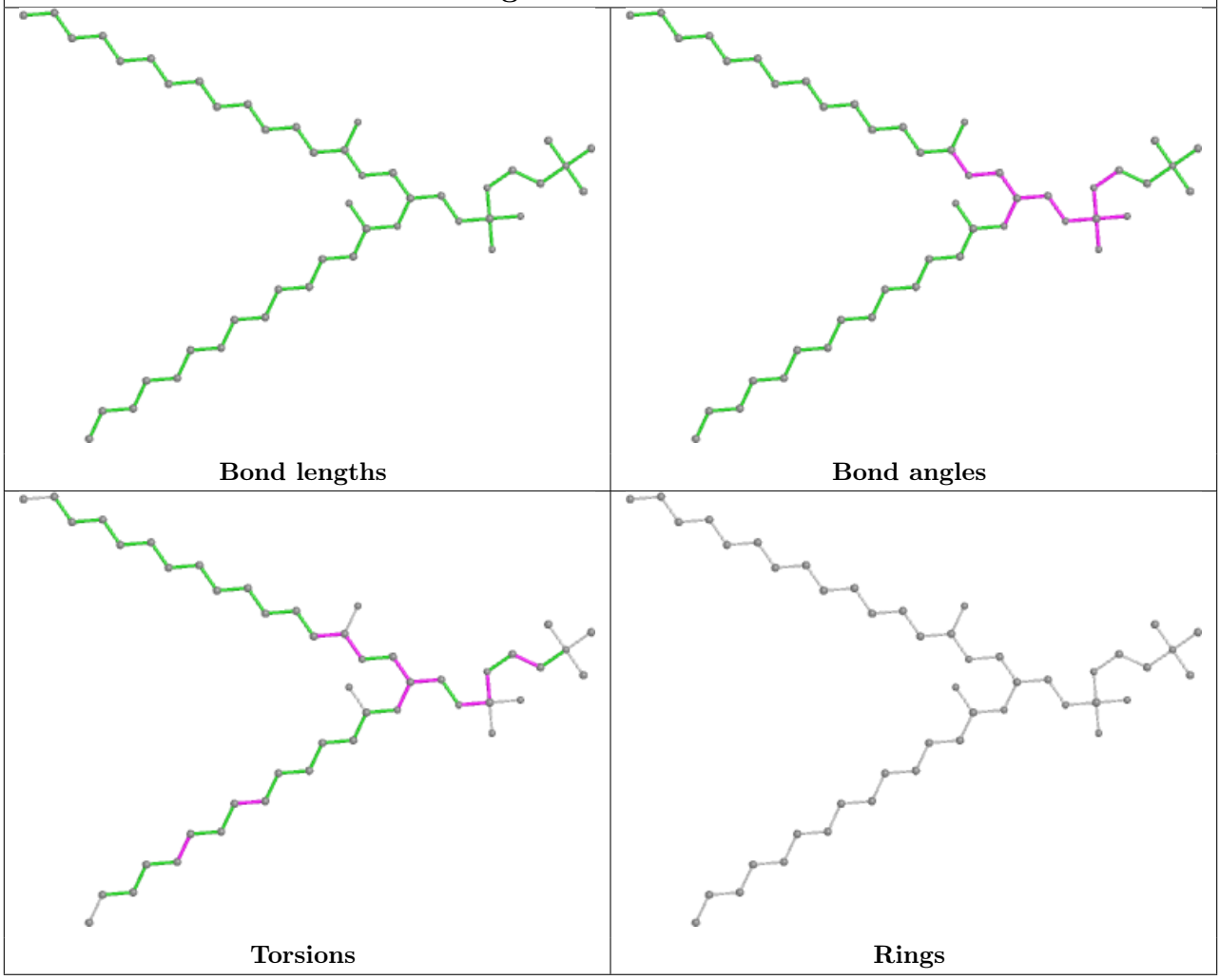
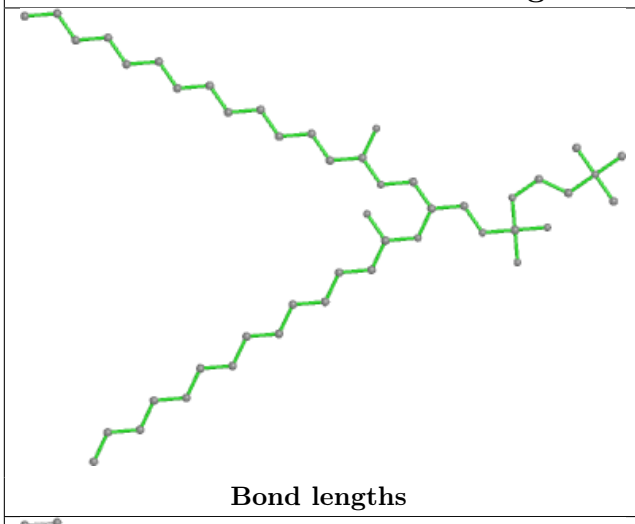


Rings

Ligand PX4 A 400



Ligand PX4 A 359



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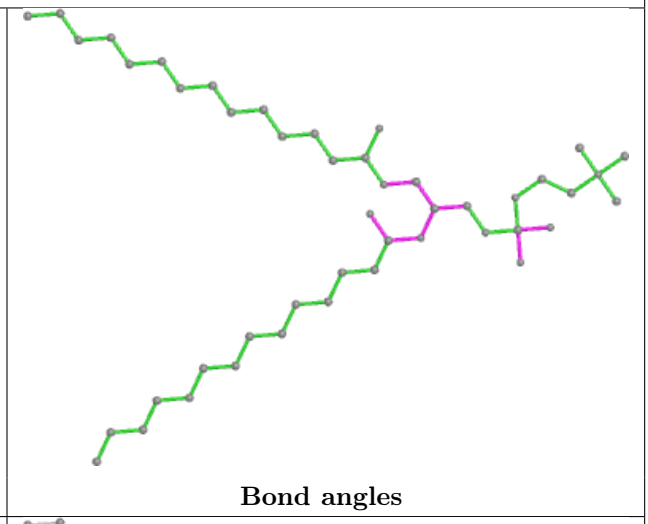
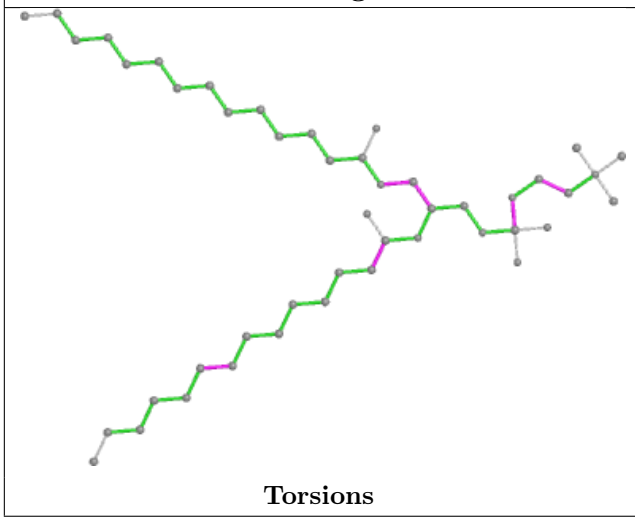


Bond angles



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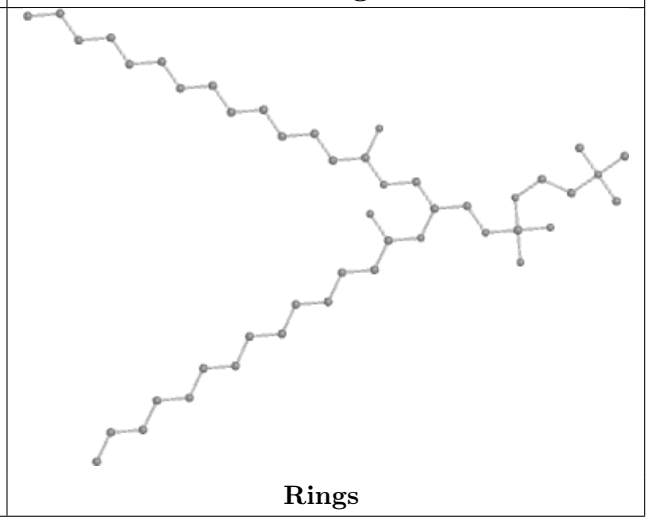
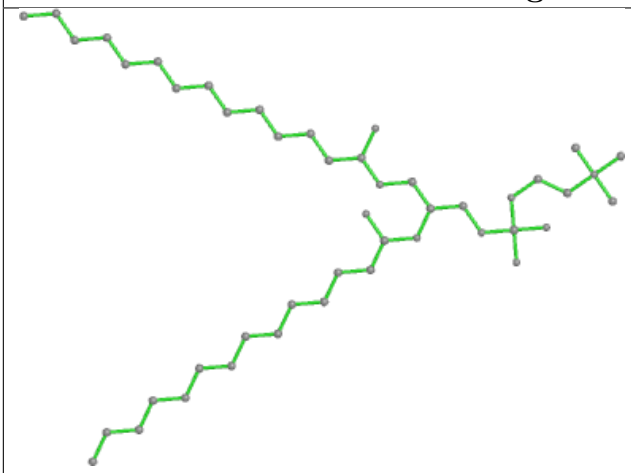


Rings

Ligand PX4 A 379



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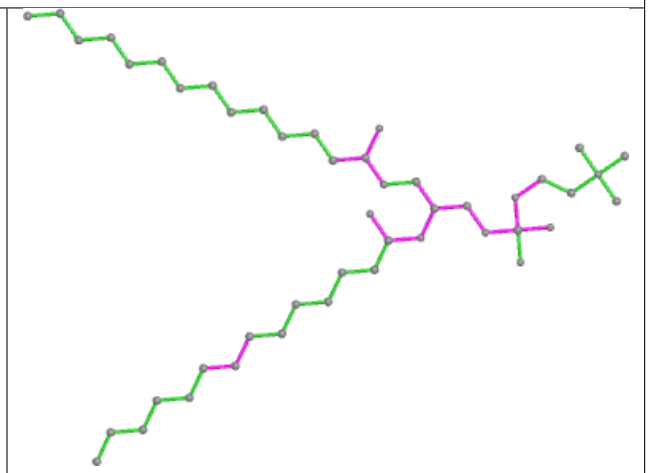
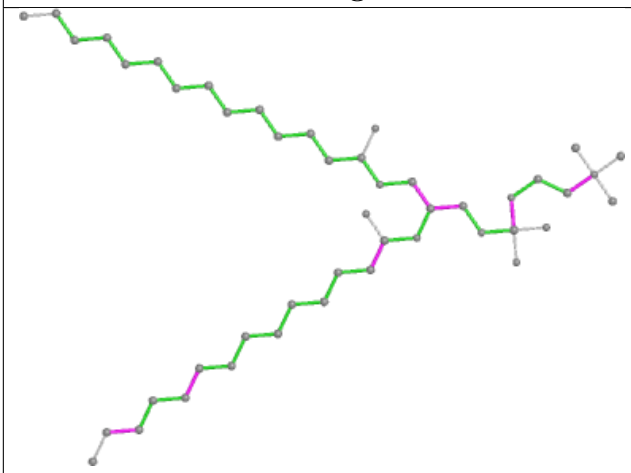


Bond angles



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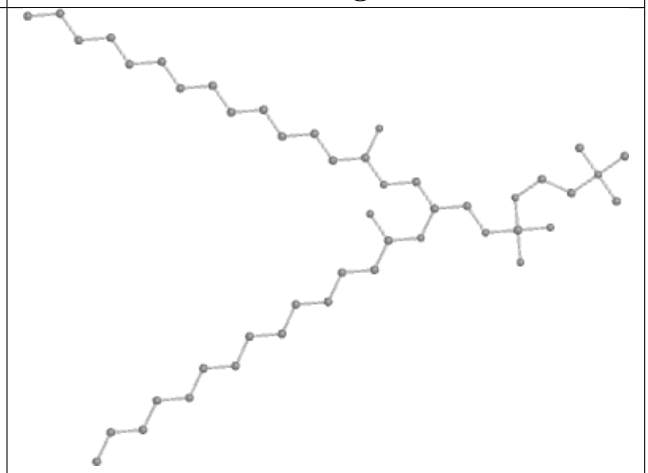
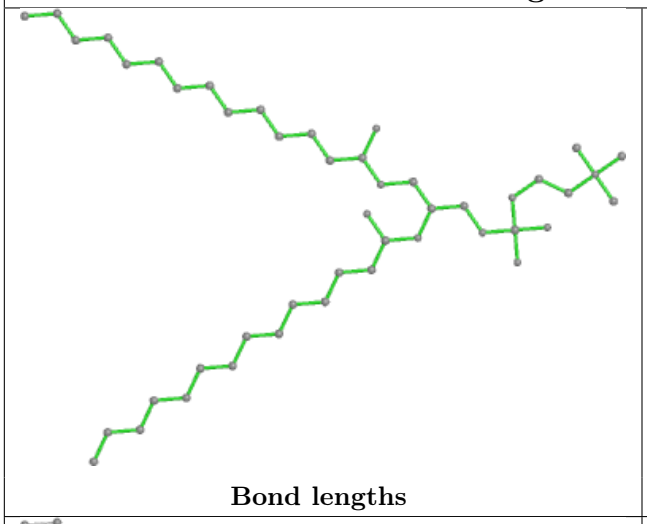


Rings

Ligand PX4 A 372



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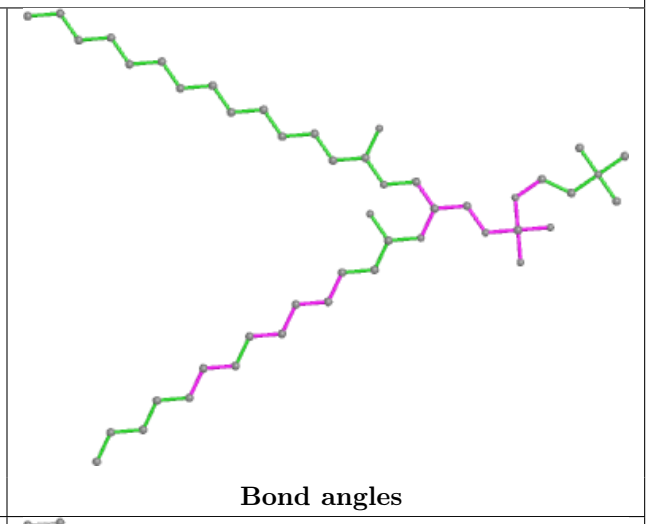
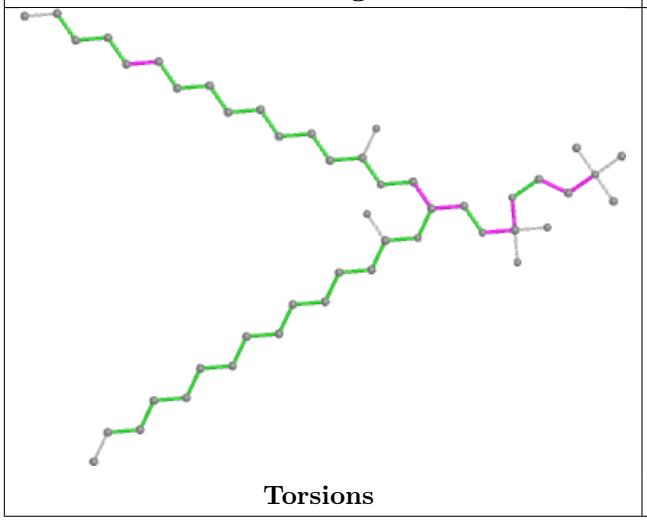


Bond angles



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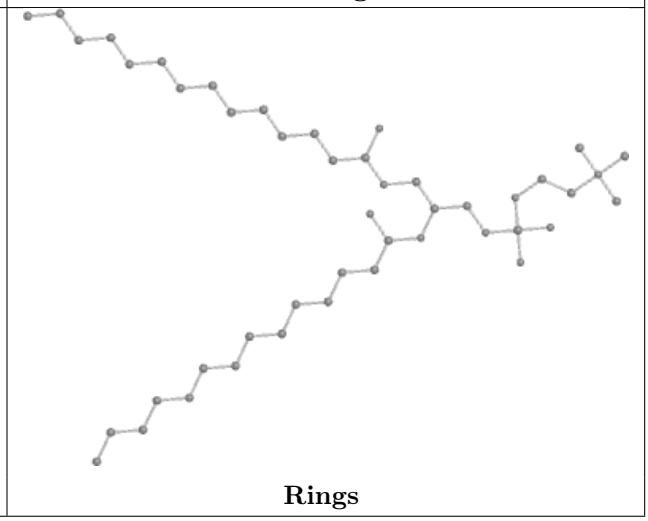
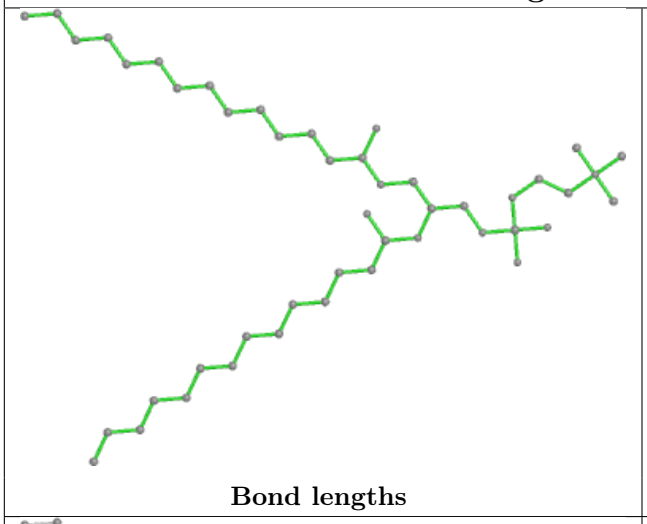


Rings

Ligand PX4 A 386



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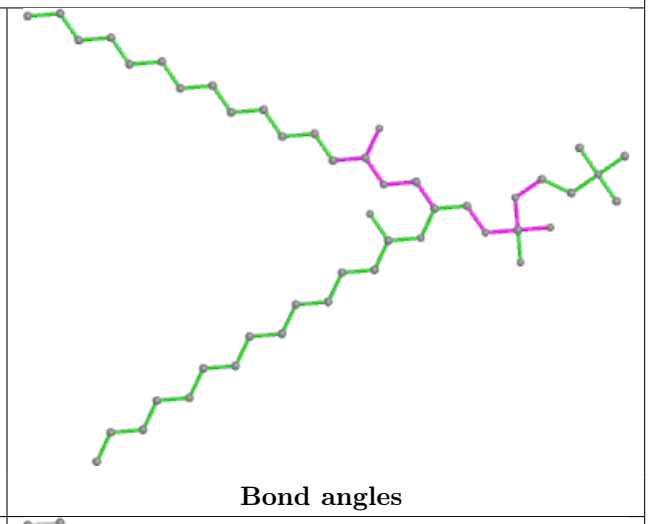
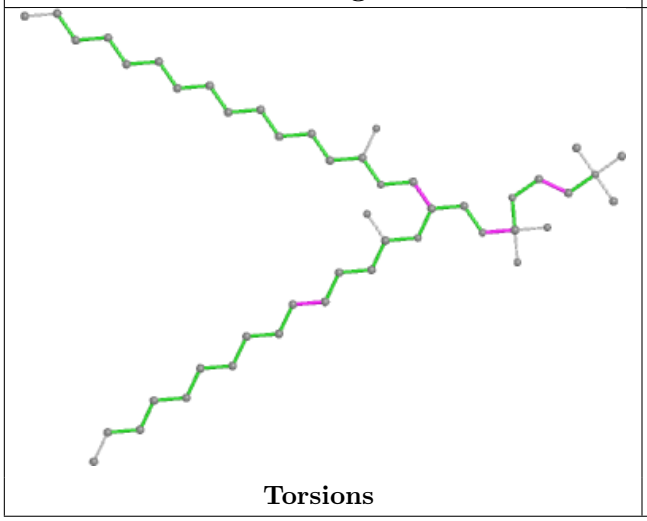


Bond angles



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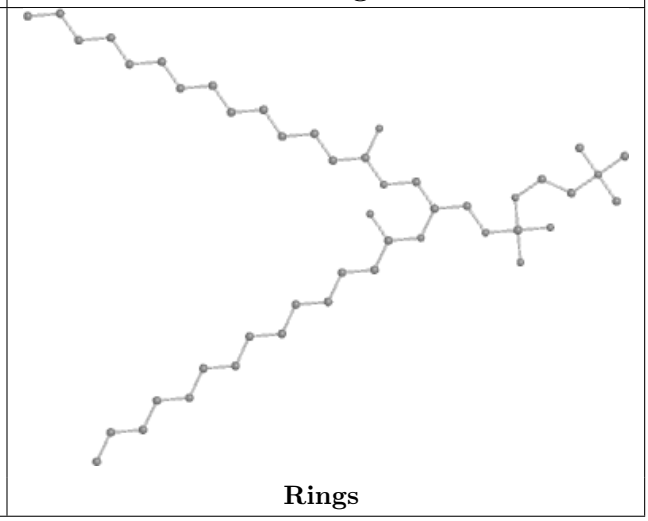
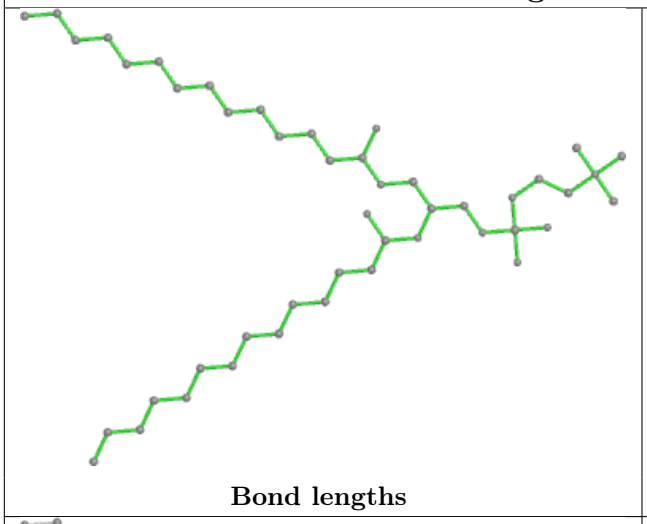


Rings

Ligand PX4 A 427



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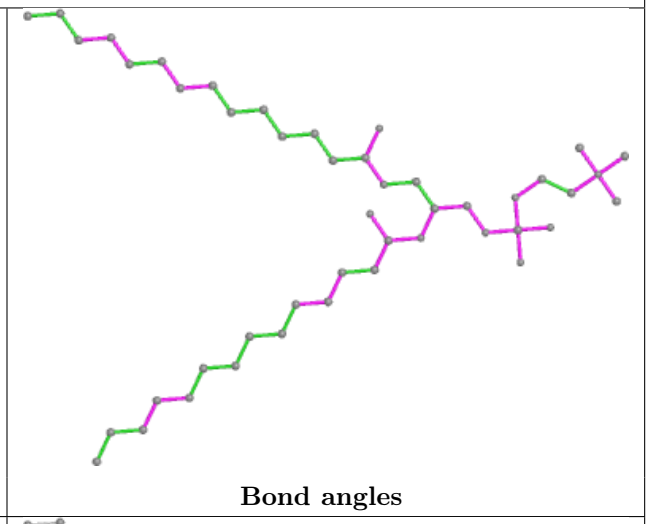

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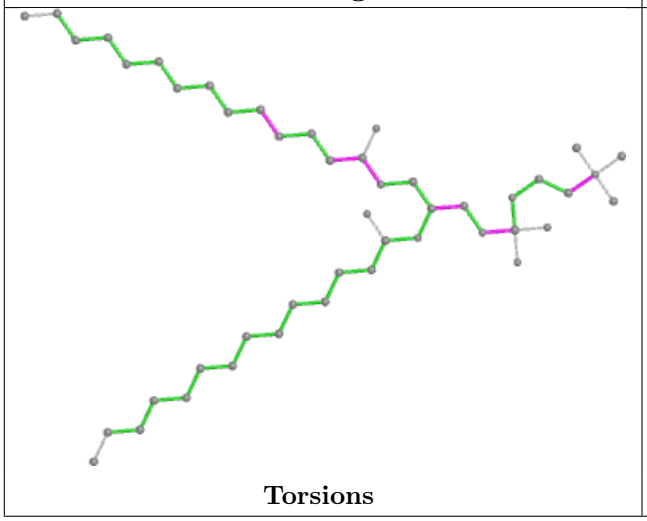

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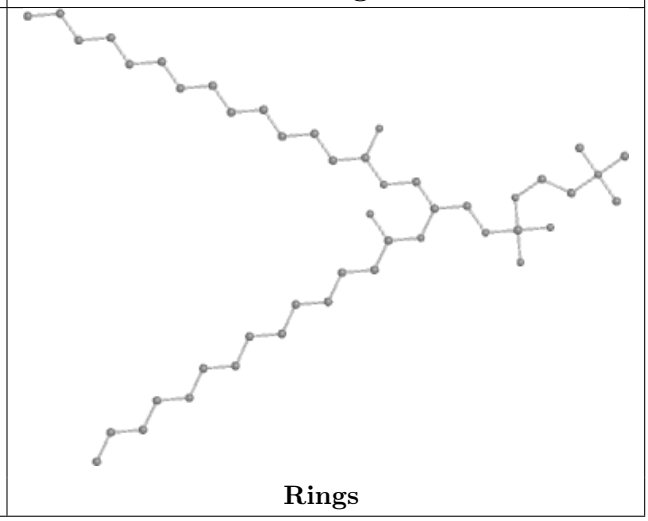
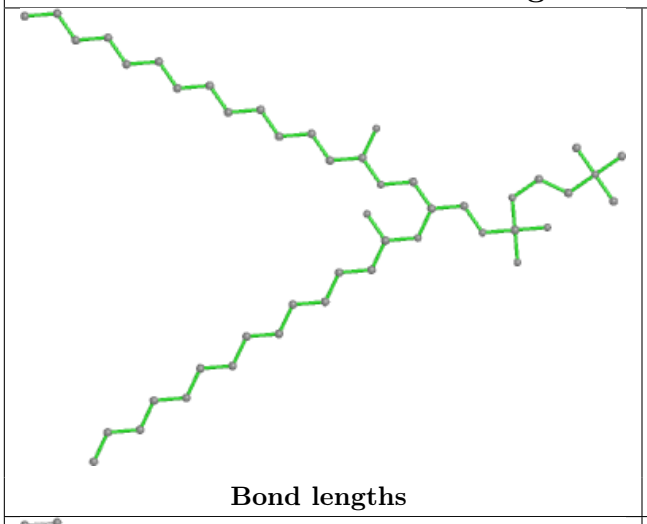


Rings

Ligand PX4 A 356



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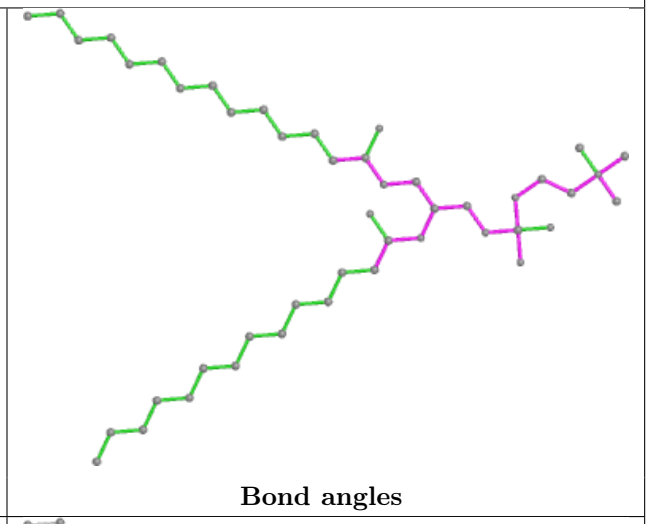
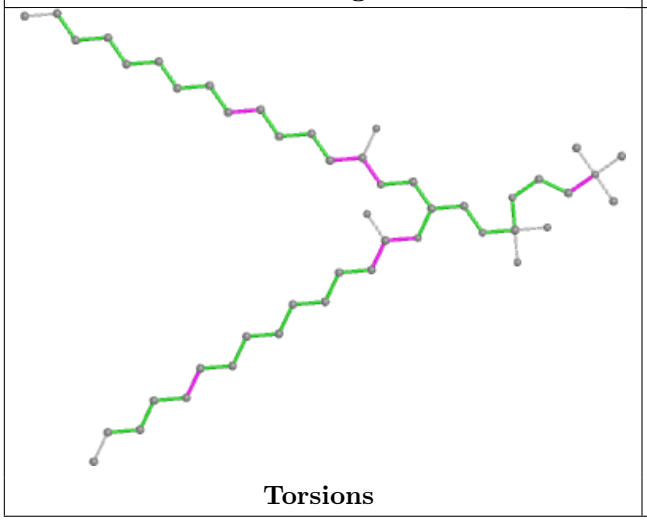


Bond angles



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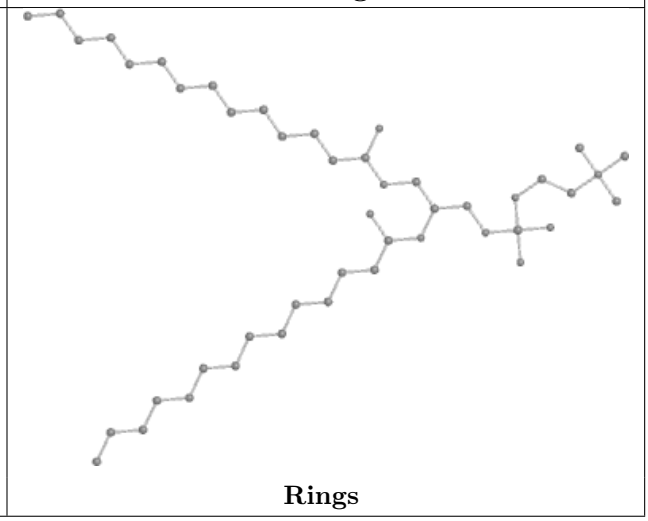
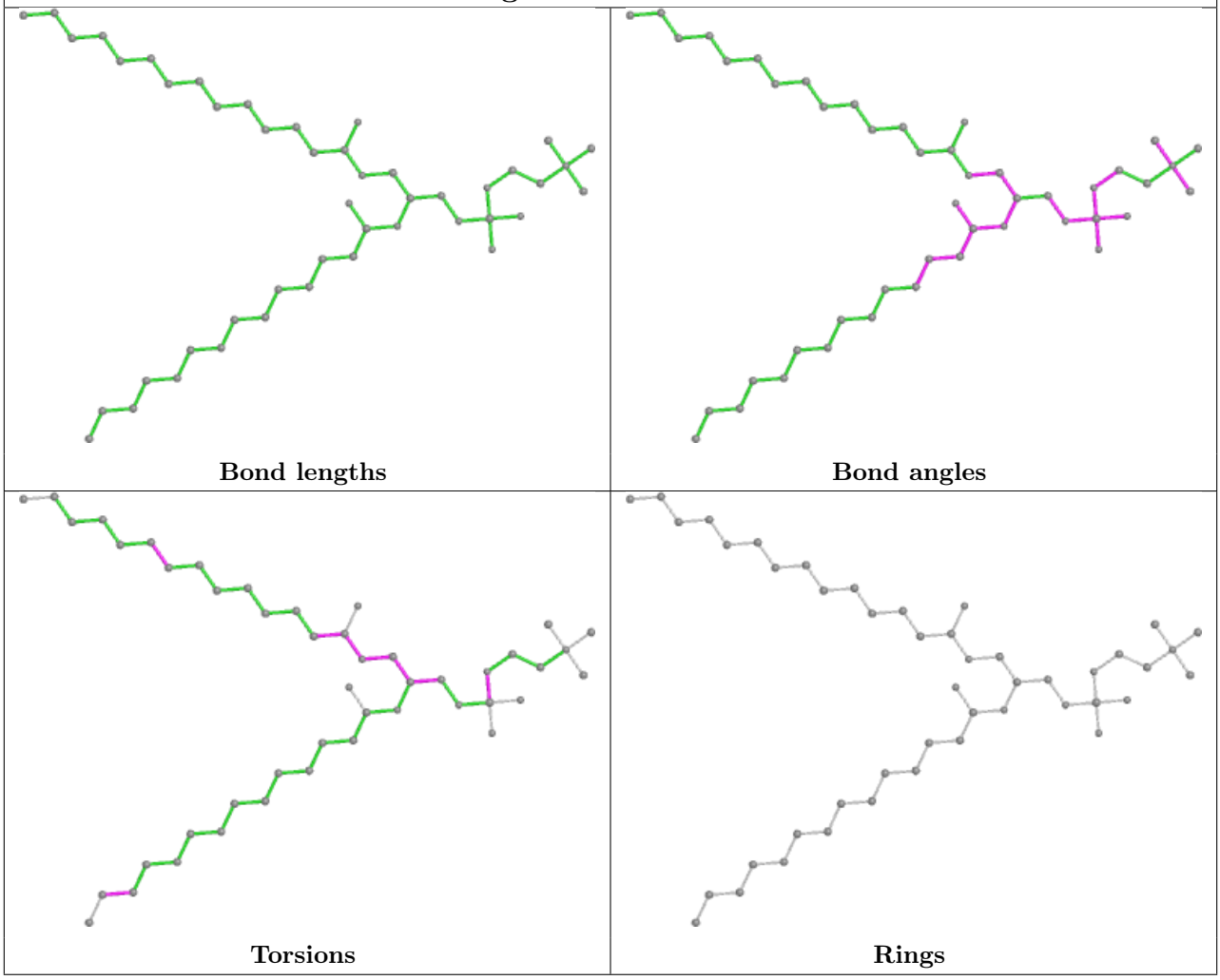
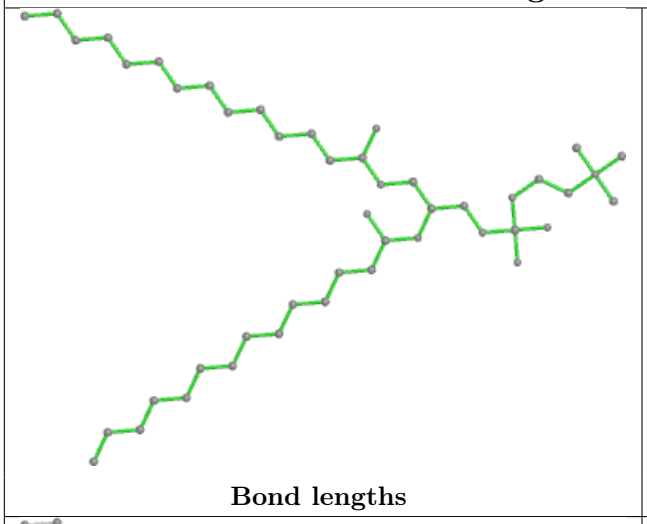


Rings

Ligand PX4 A 389



Ligand PX4 A 324



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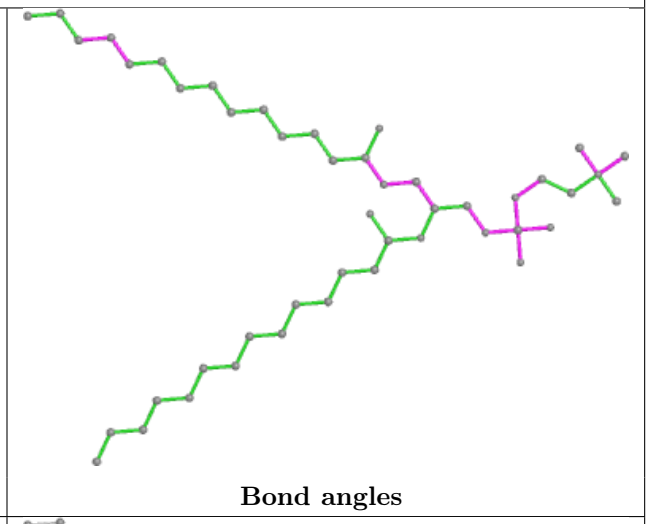
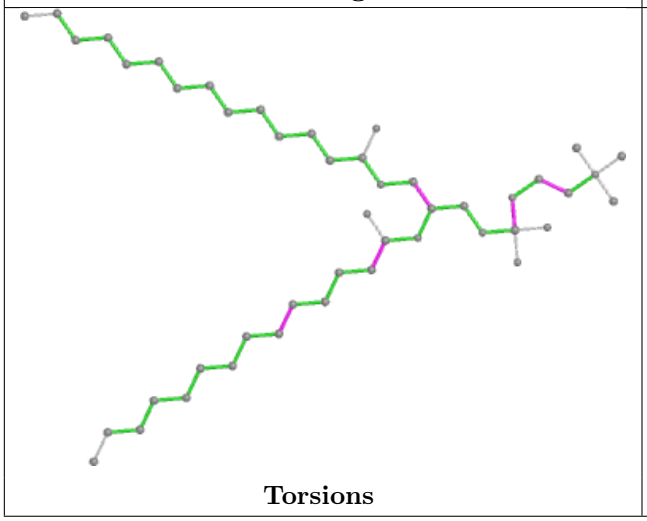


Bond angles



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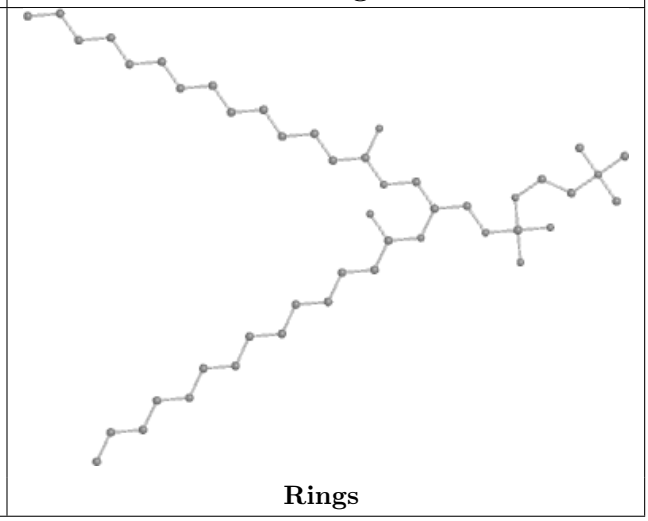
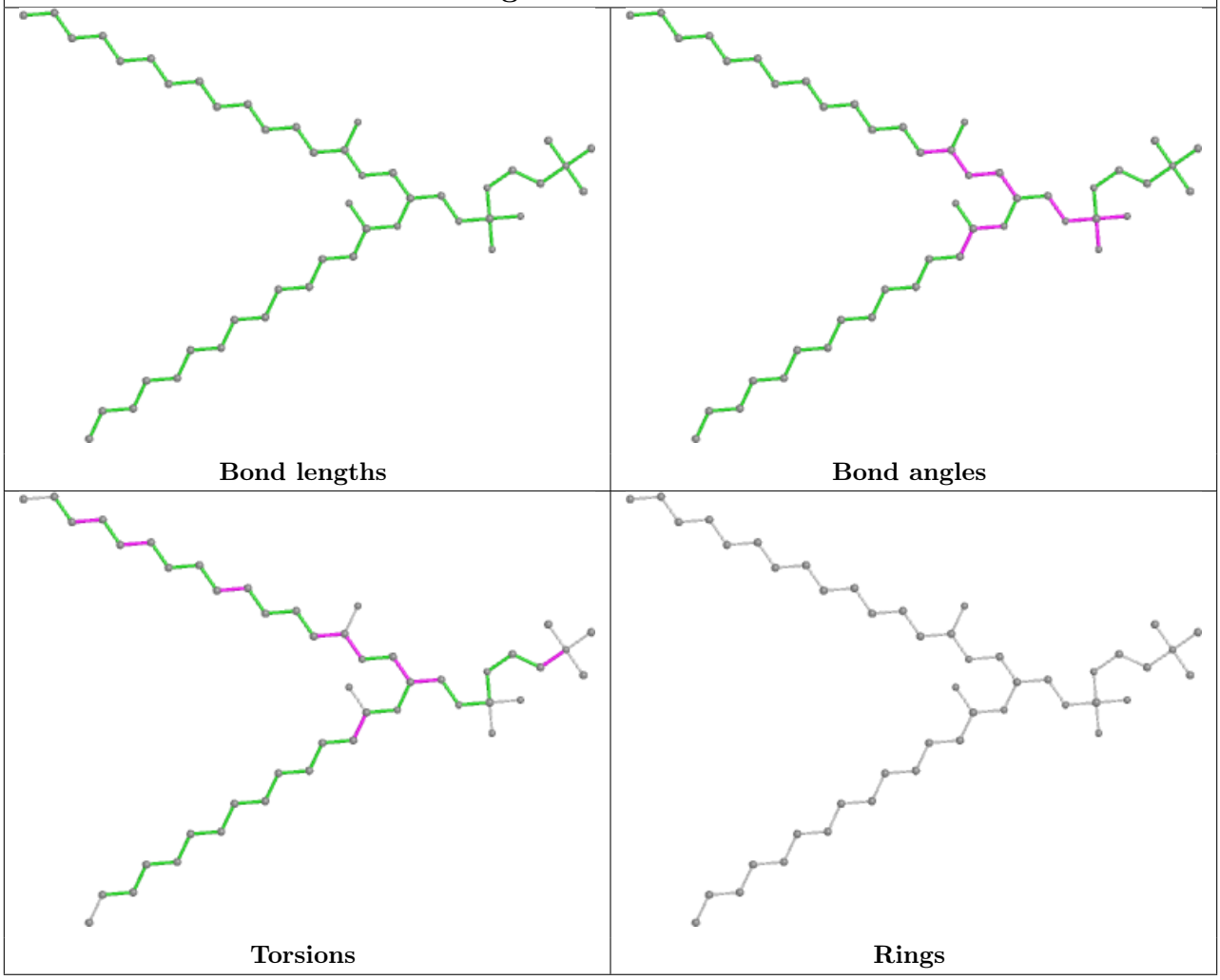
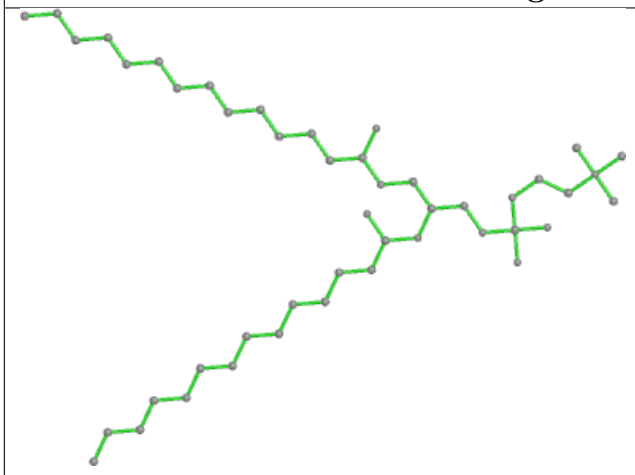


Rings

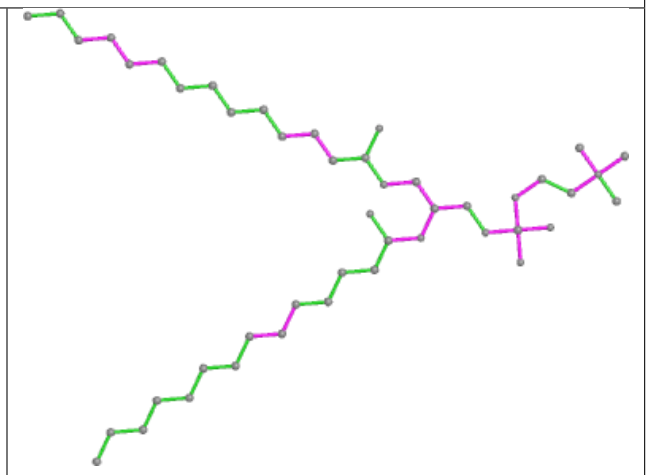
Ligand PX4 A 335



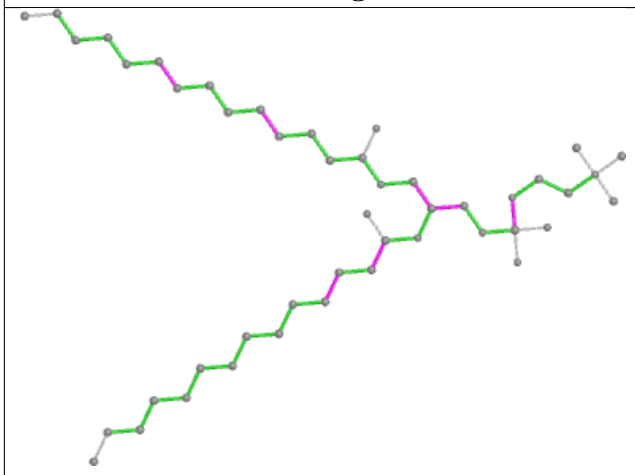
Ligand PX4 A 412



Bond lengths



Bond angles



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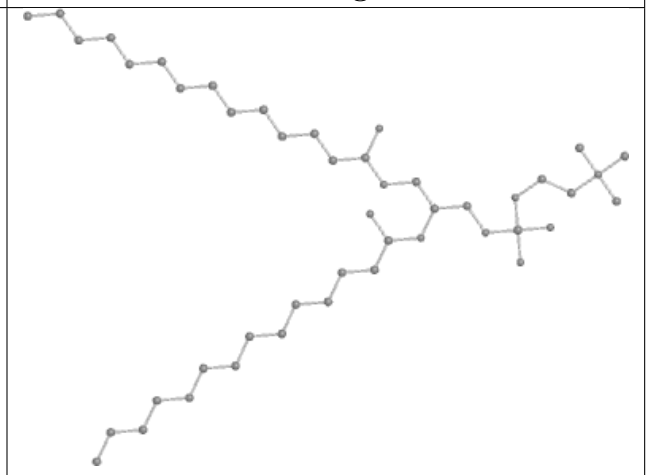
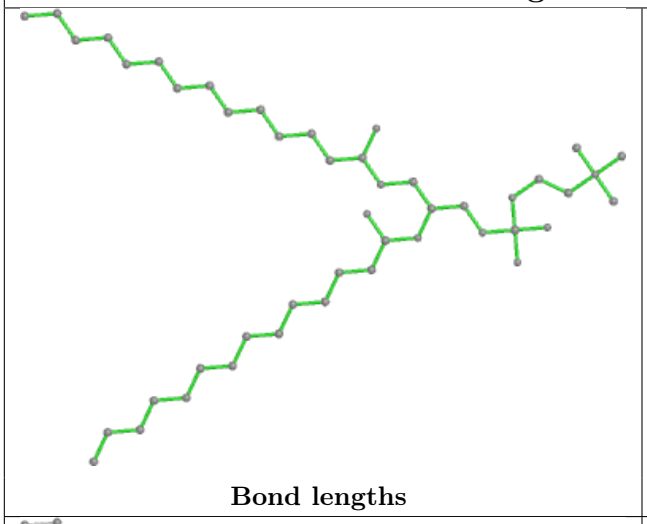
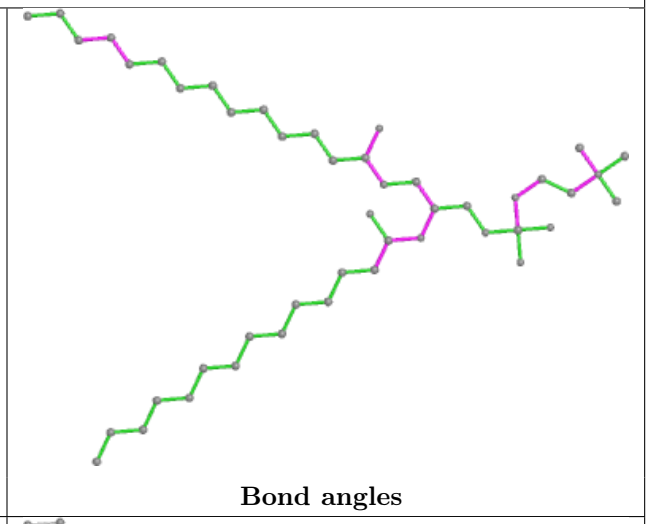


Rings

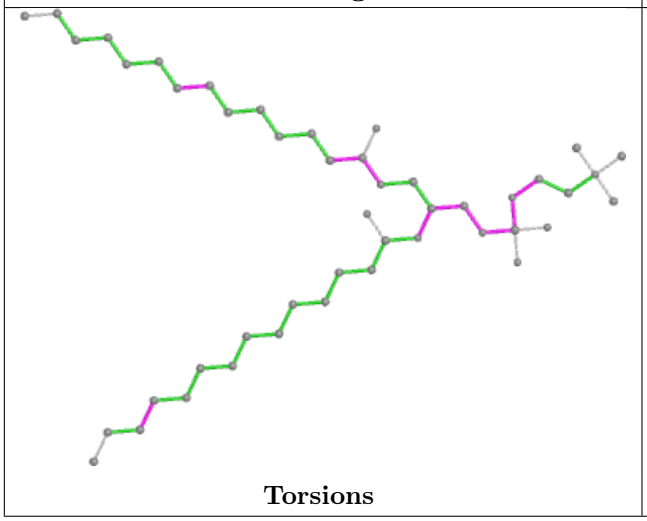
Ligand PX4 A 321



Bond lengths



Bond angles



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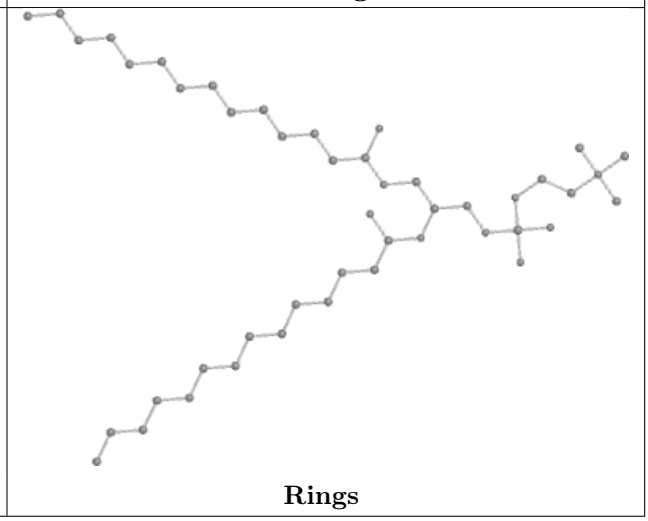
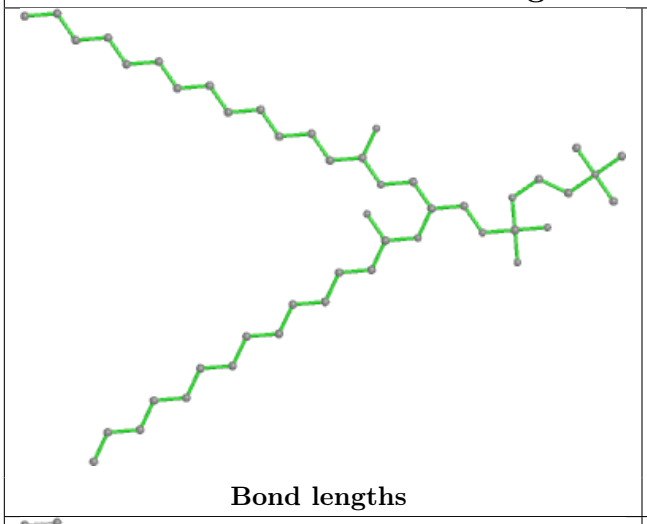
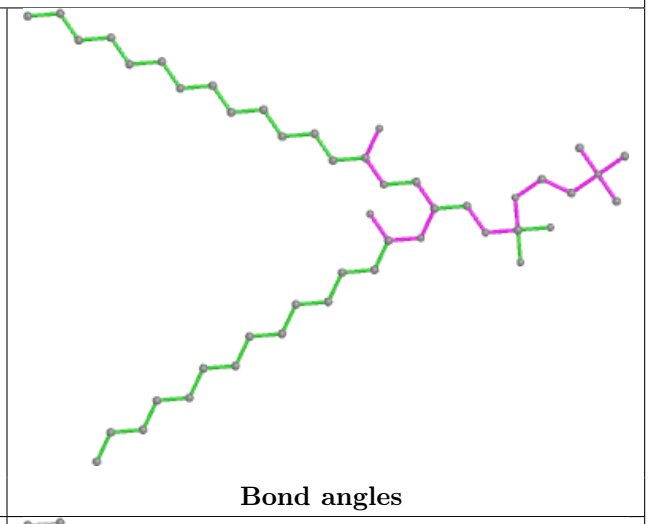


Rings

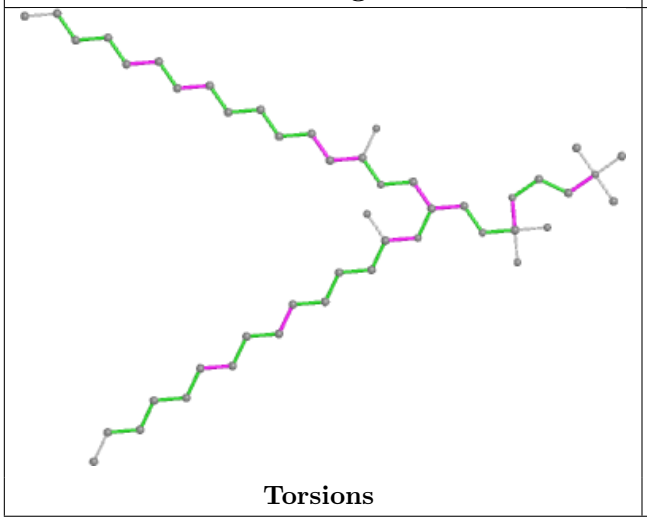
Ligand PX4 A 357



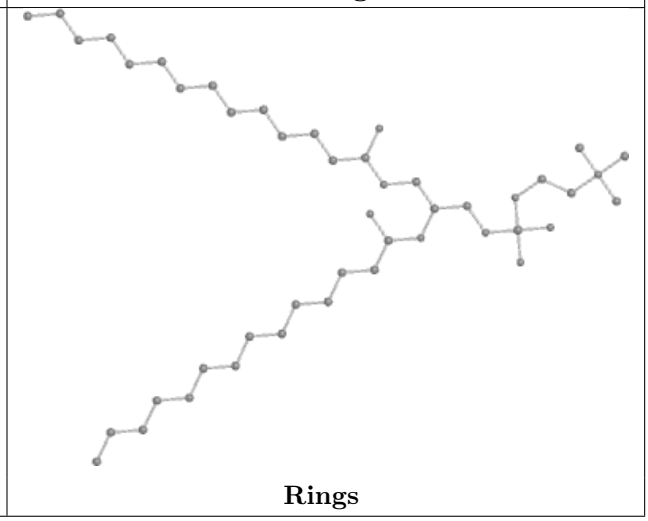
Bond lengths



Bond angles

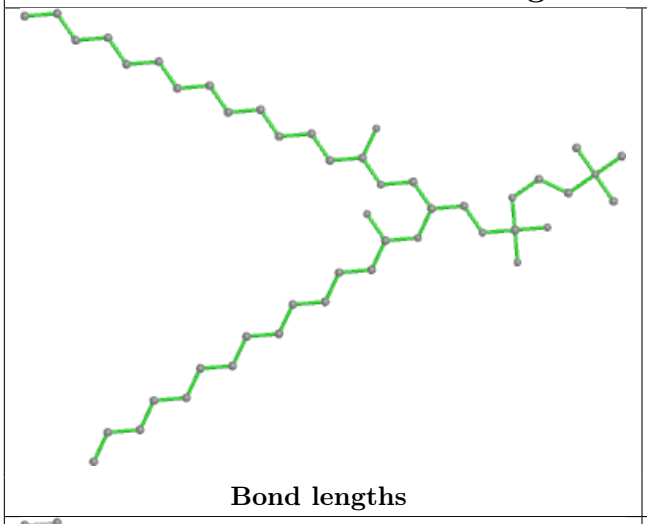


Torsions



Rings

Ligand PX4 A 422



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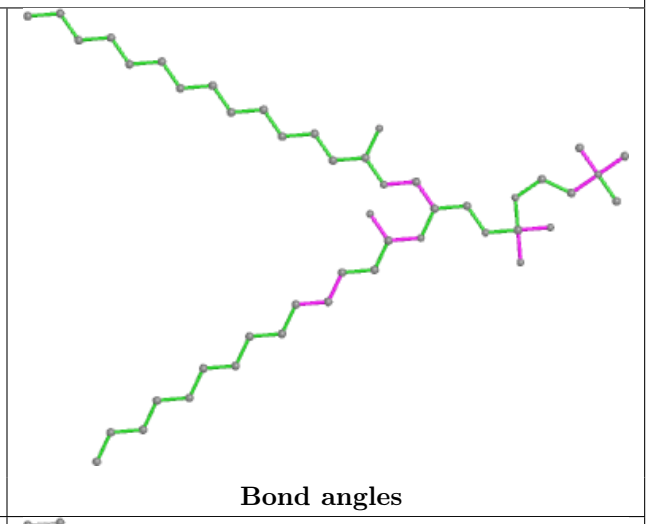

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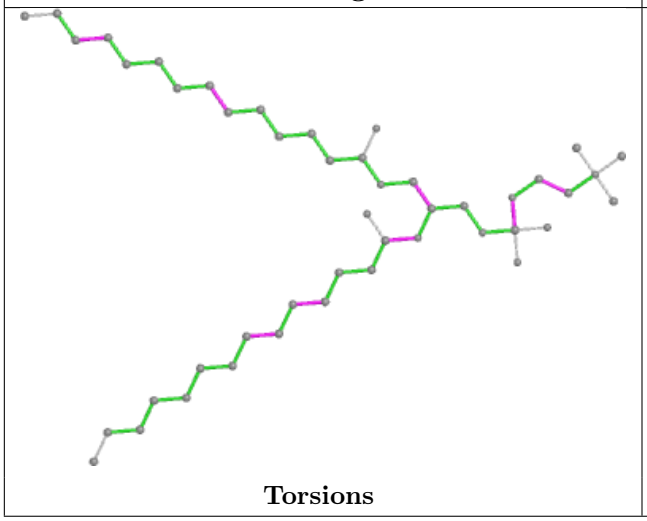

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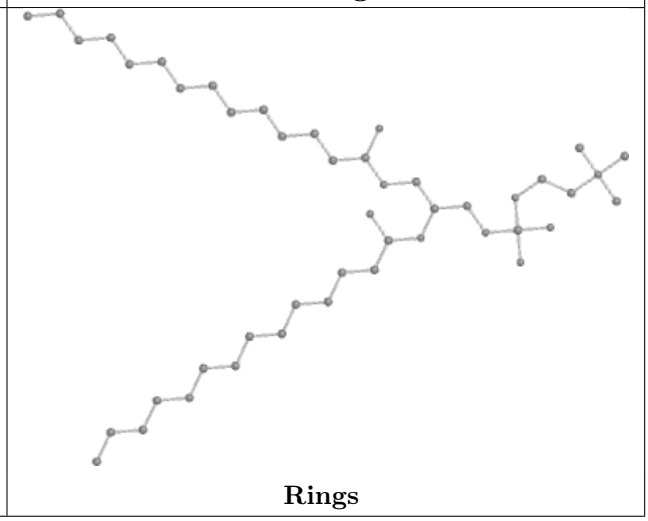
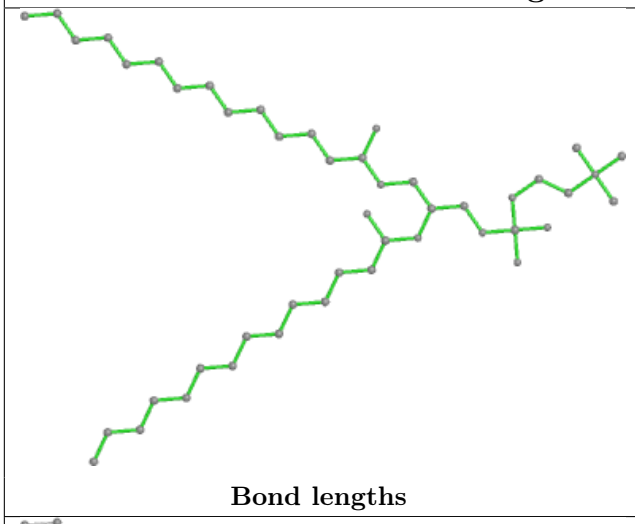


Rings

Ligand PX4 A 371



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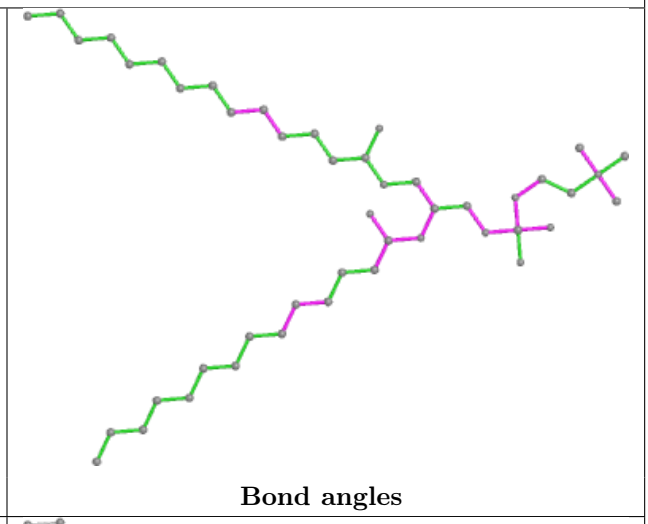

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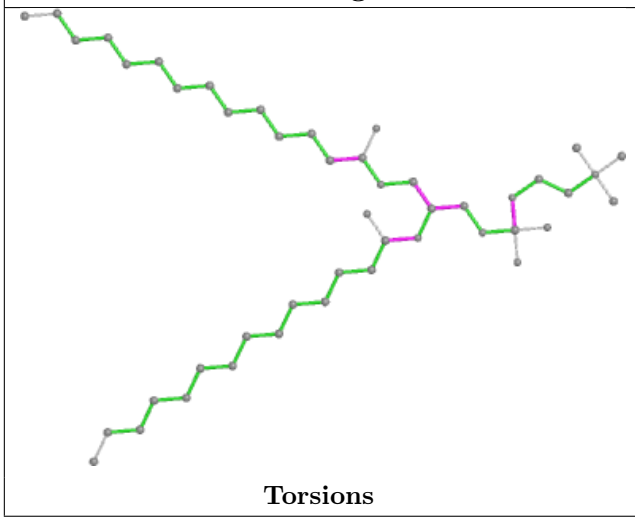

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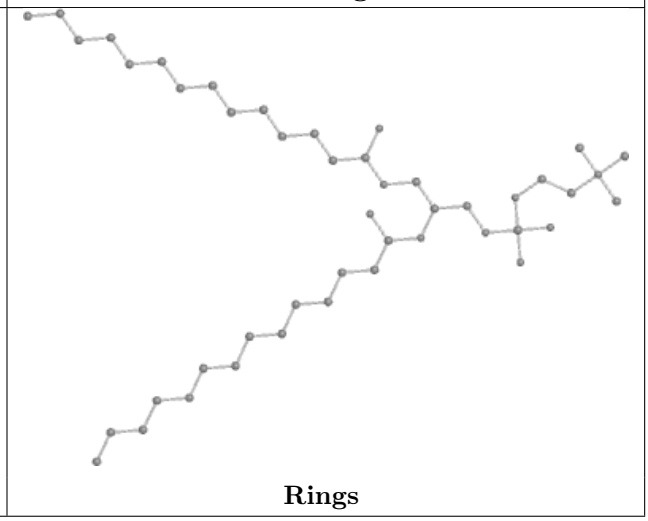
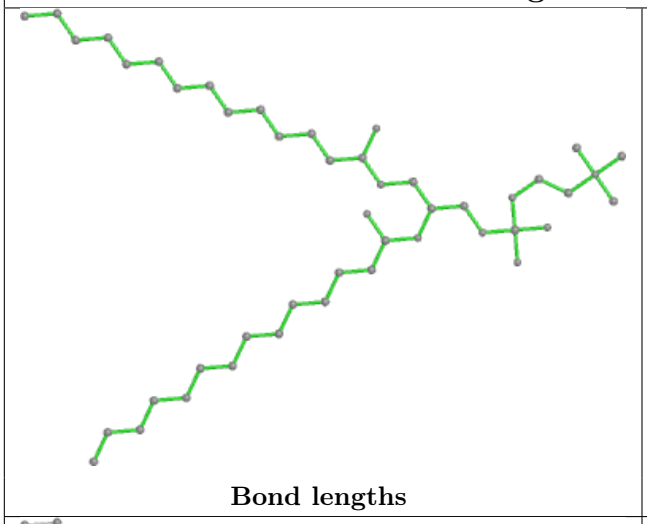


Rings

Ligand PX4 A 327



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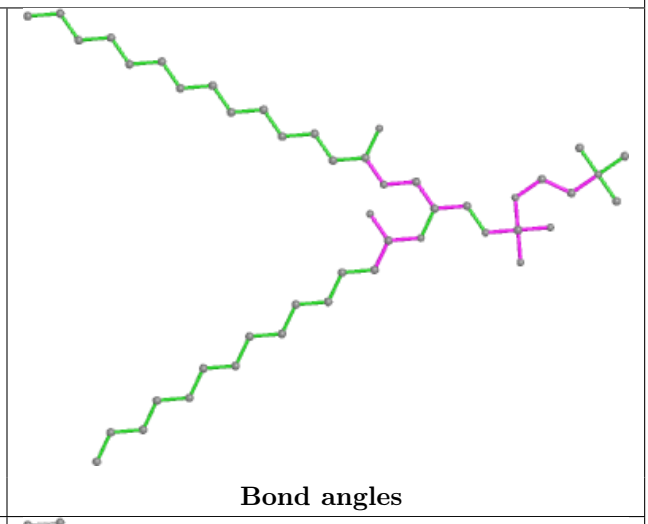

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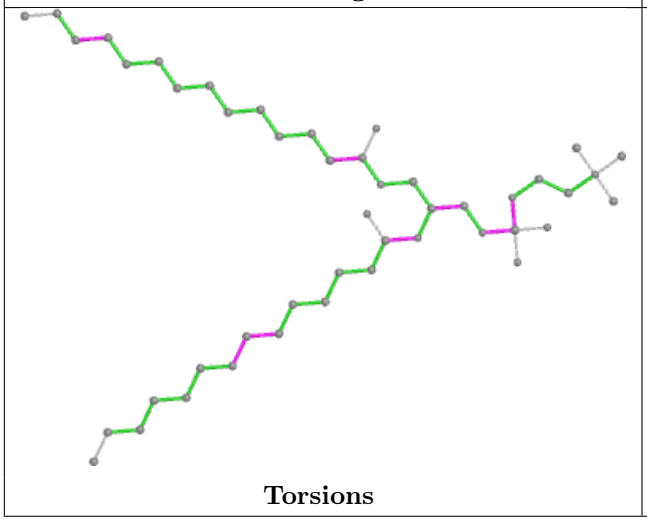

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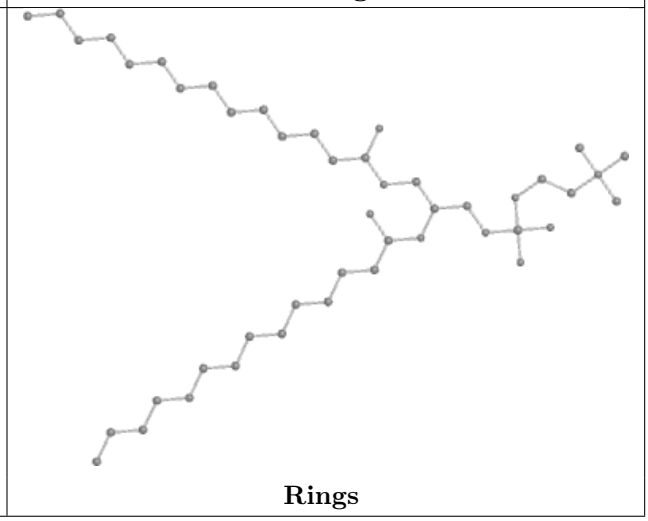
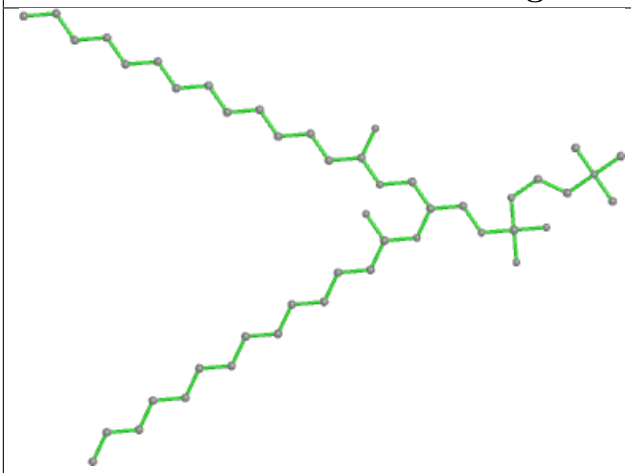


Rings

Ligand PX4 A 337



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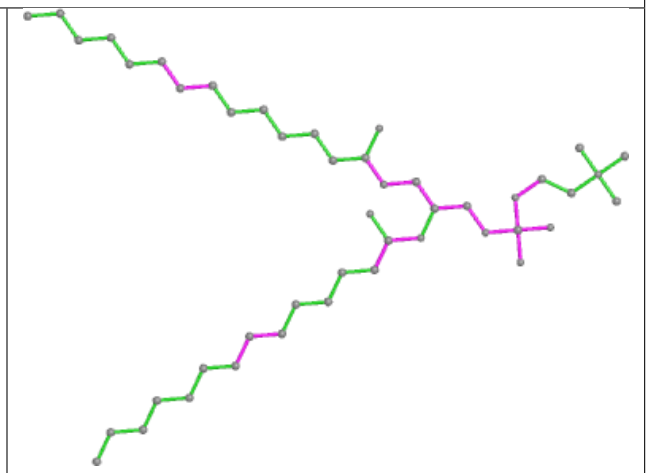
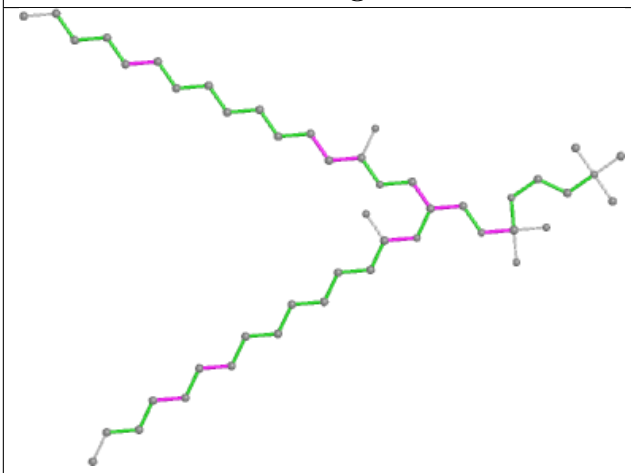


Bond angles



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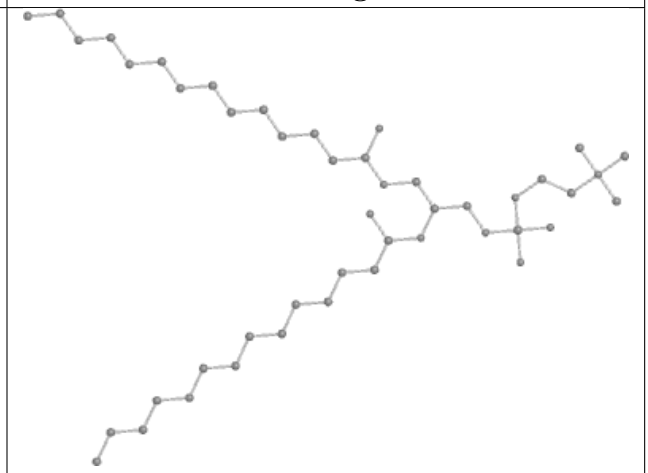
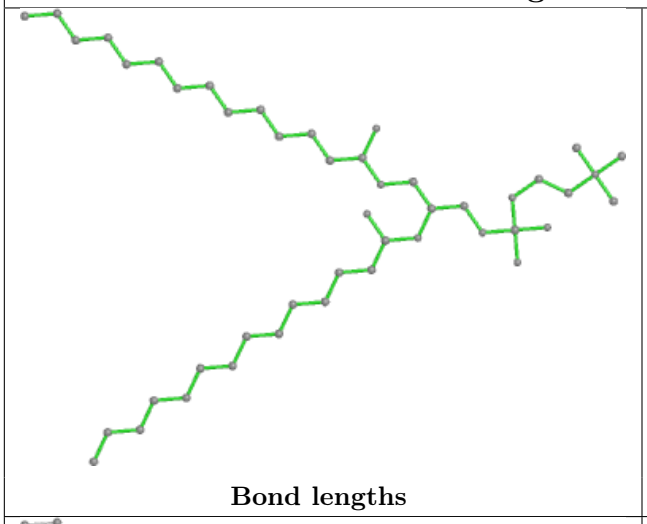


Rings

Ligand PX4 A 376



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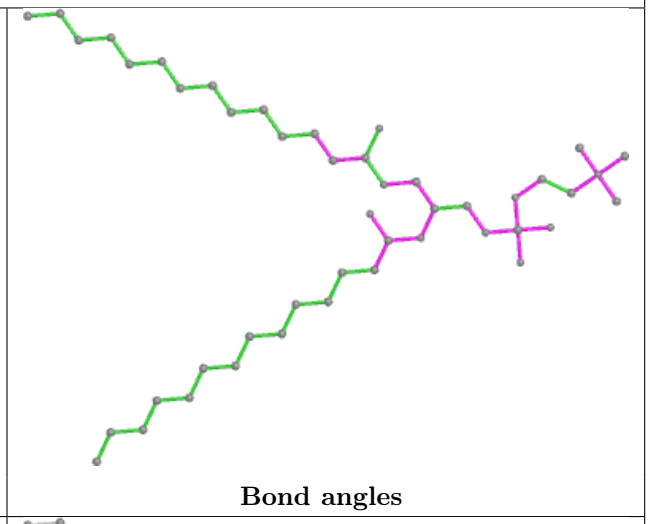
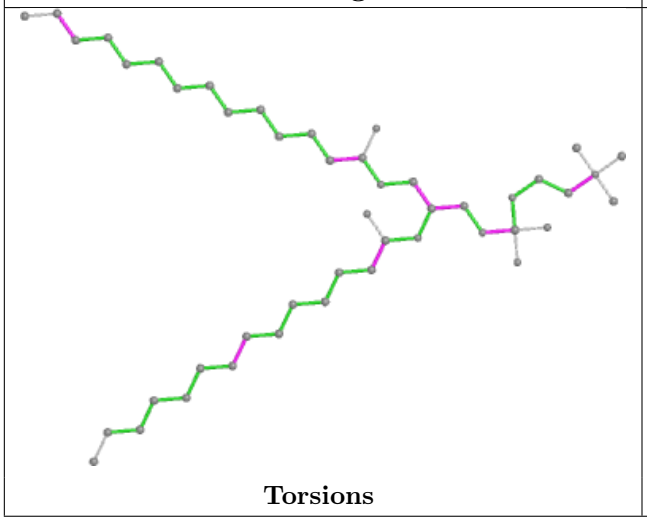


Bond angles



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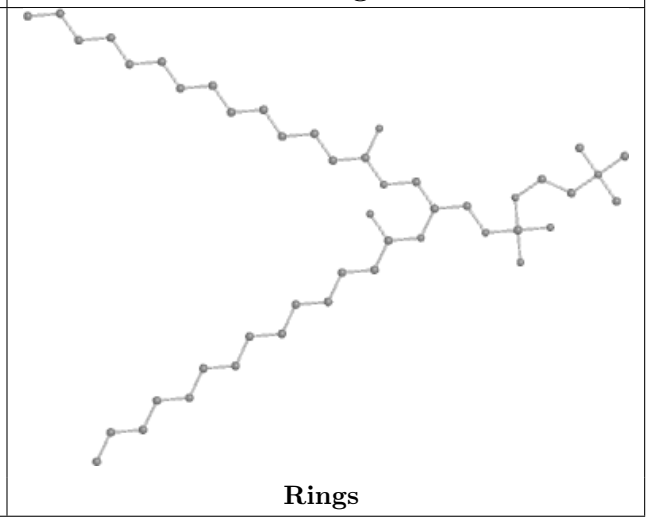
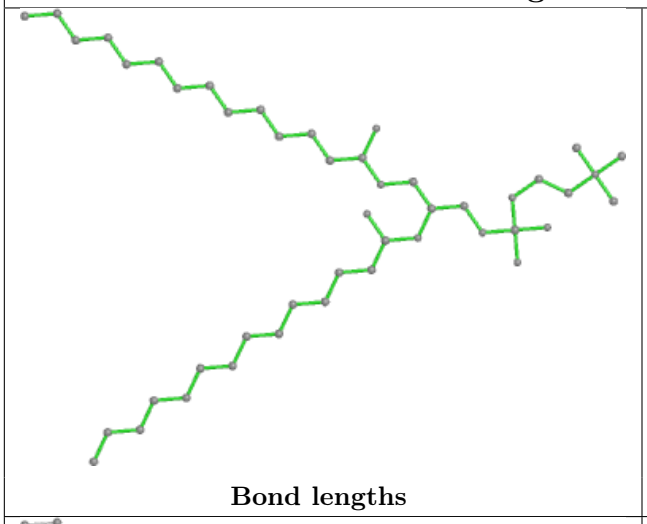


Rings

Ligand PX4 A 342



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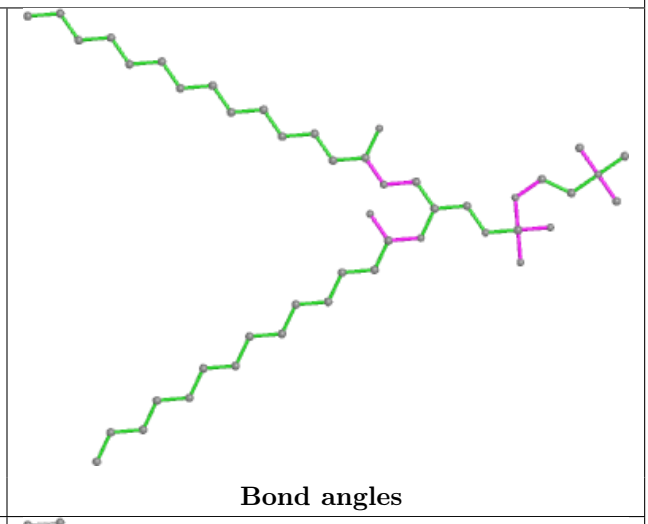
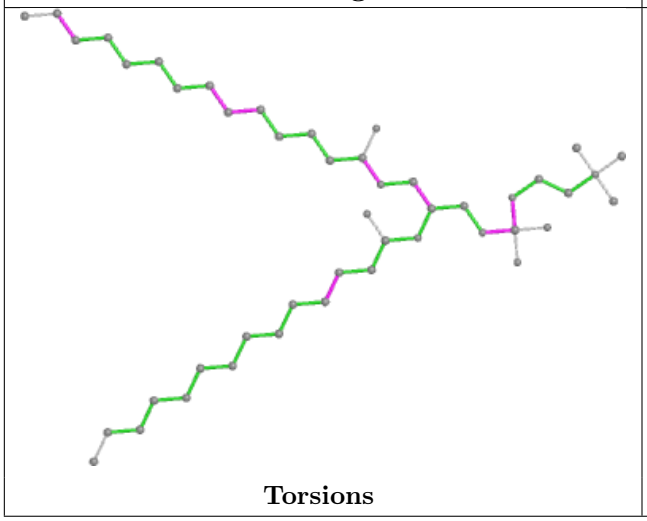


Bond angles



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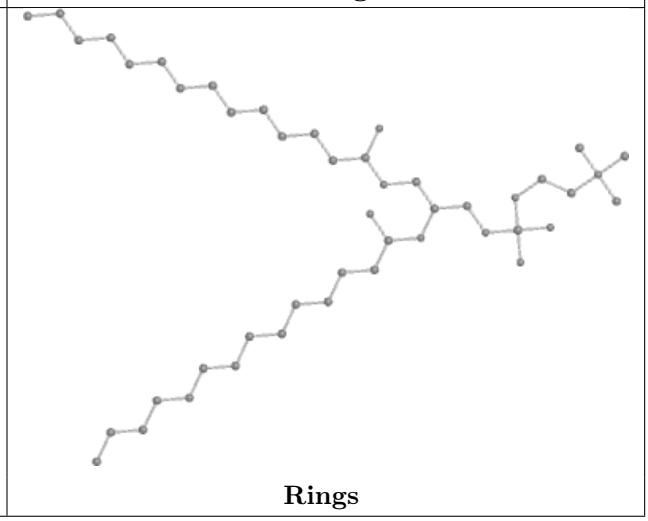
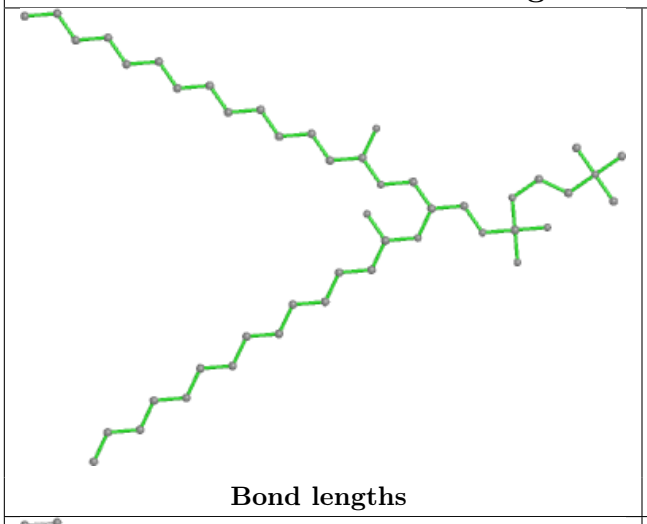


Rings

Ligand PX4 A 420



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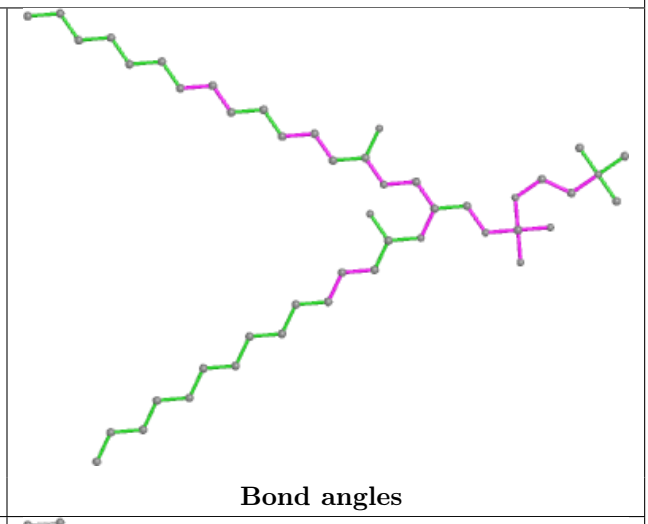
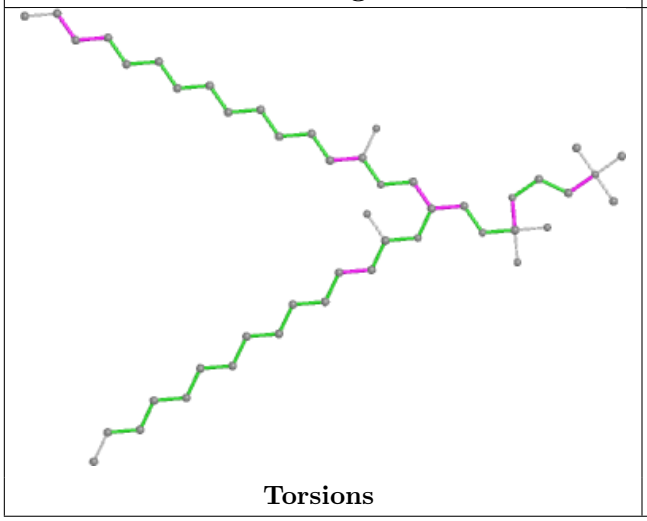


Bond angles



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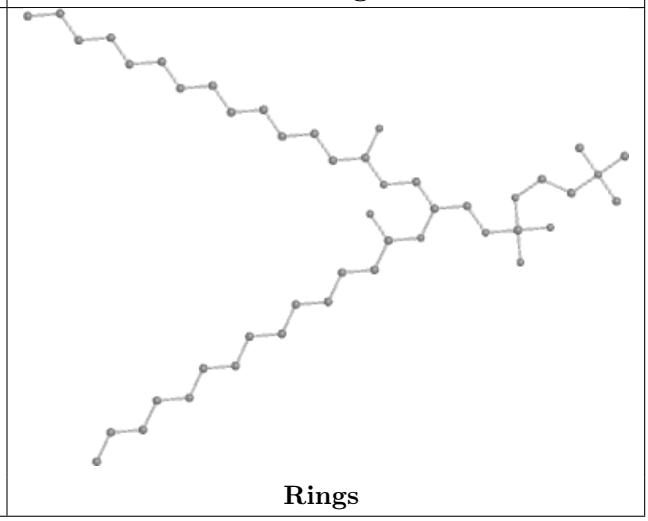
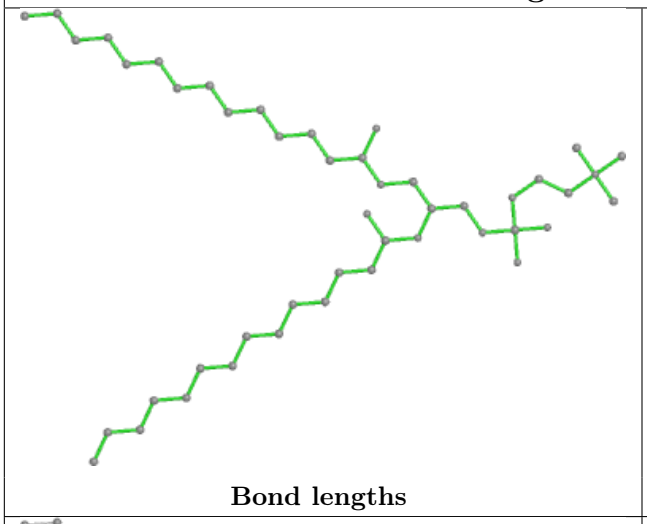


Rings

Ligand PX4 A 411



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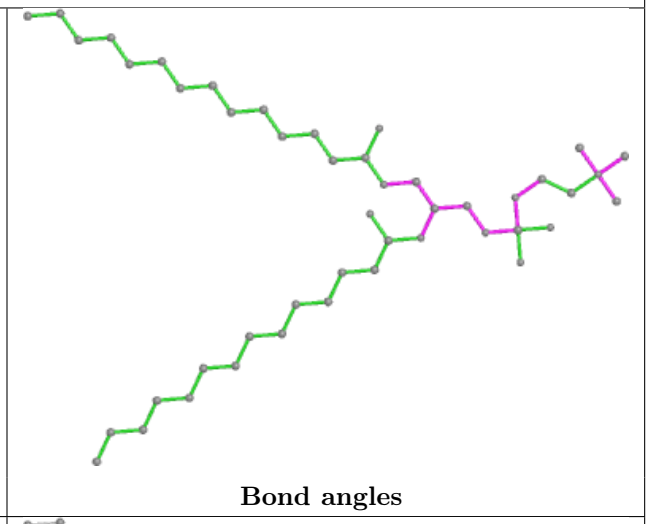
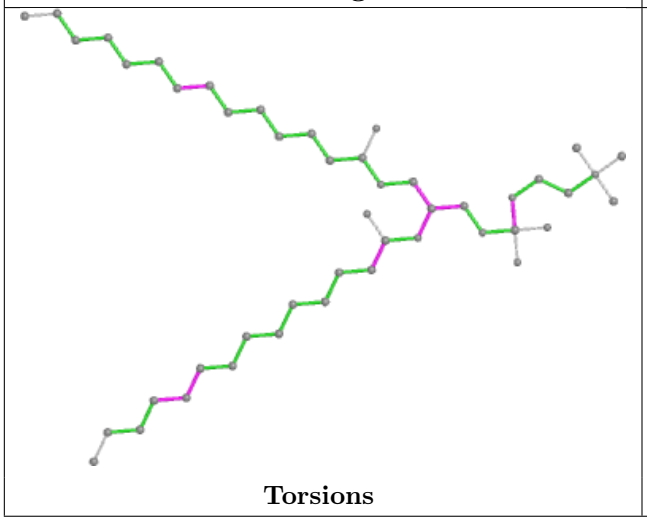


Bond angles



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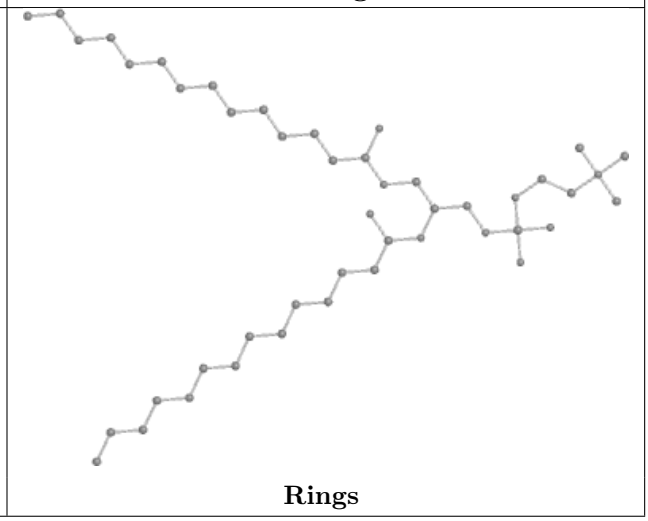
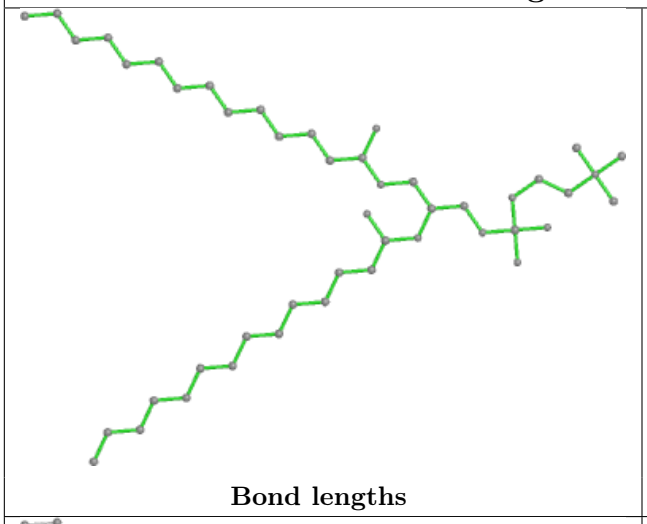


Rings

Ligand PX4 A 317



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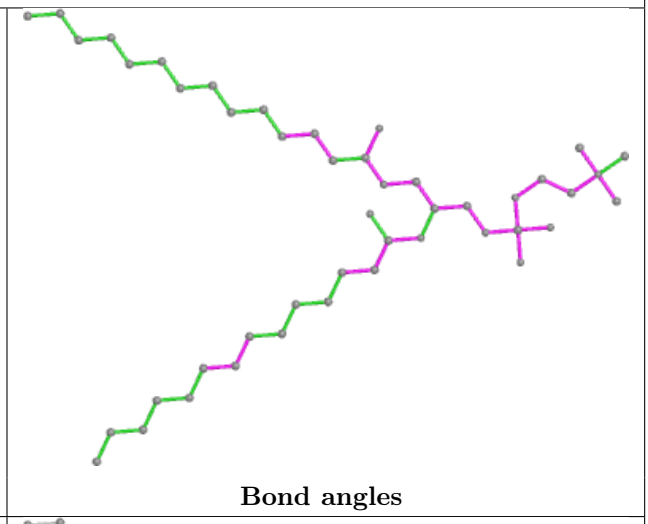
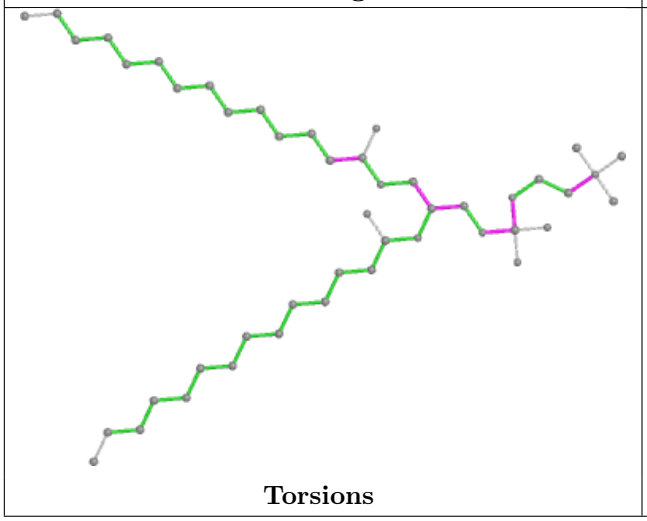


Bond angles



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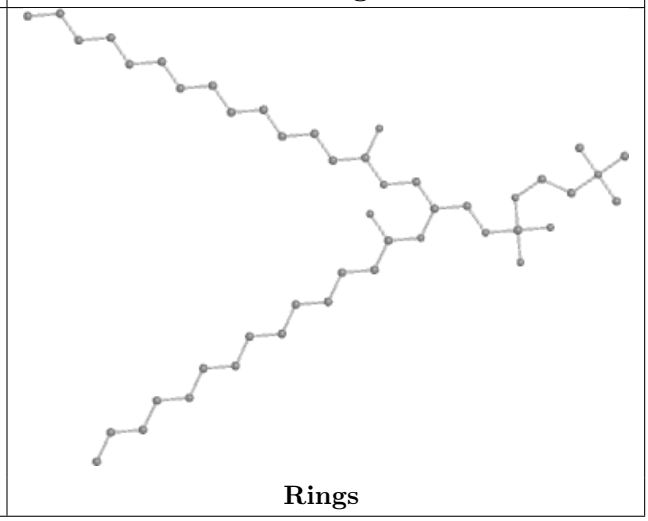
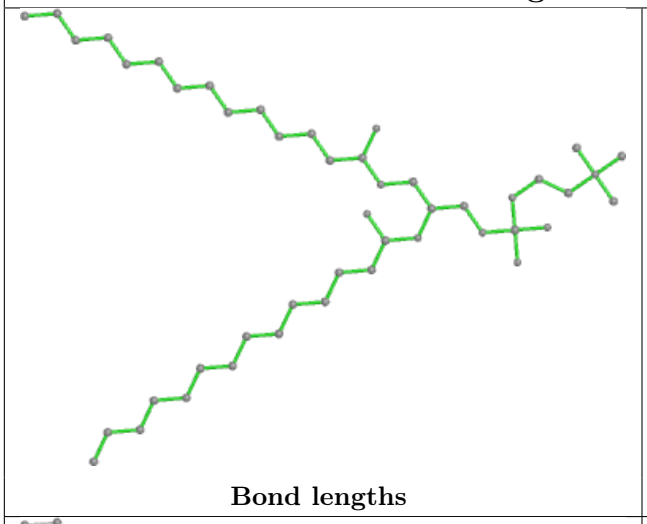


Rings

Ligand PX4 A 367



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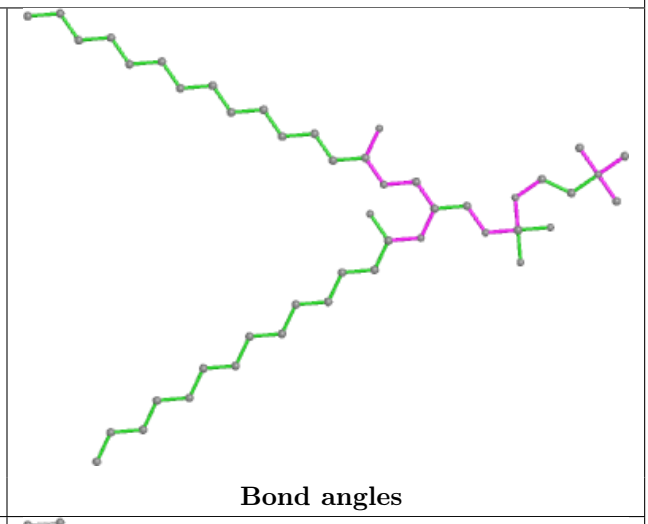
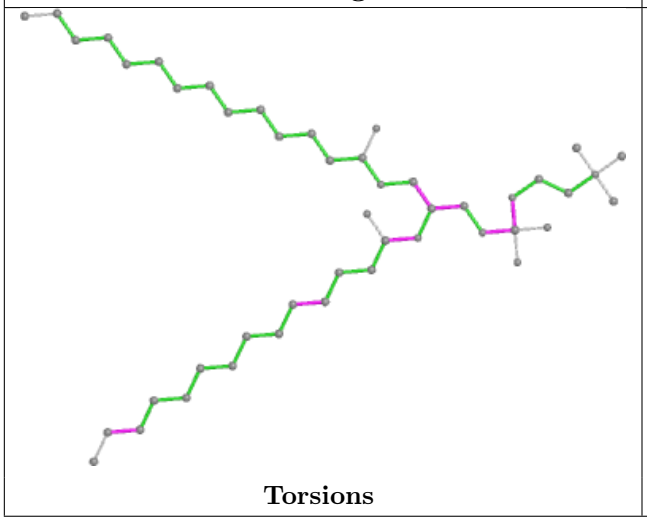


Bond angles



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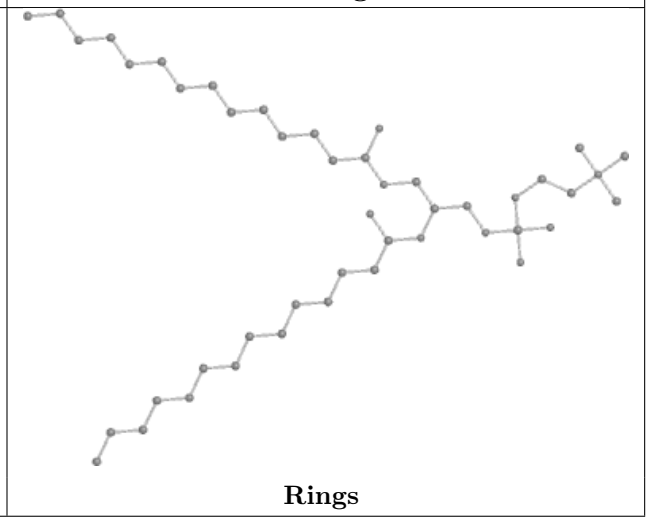
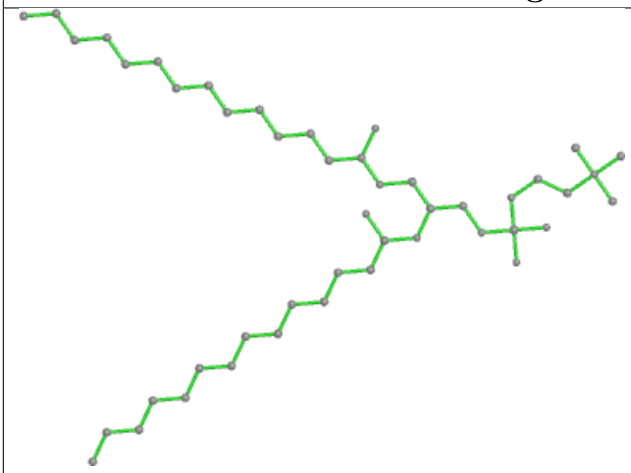


Rings

Ligand PX4 A 370



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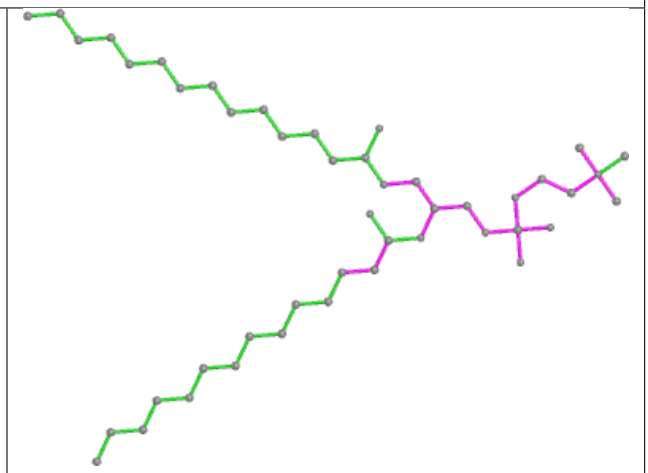

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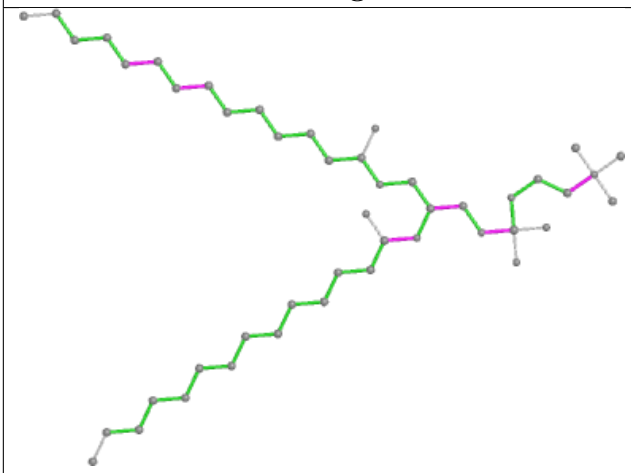
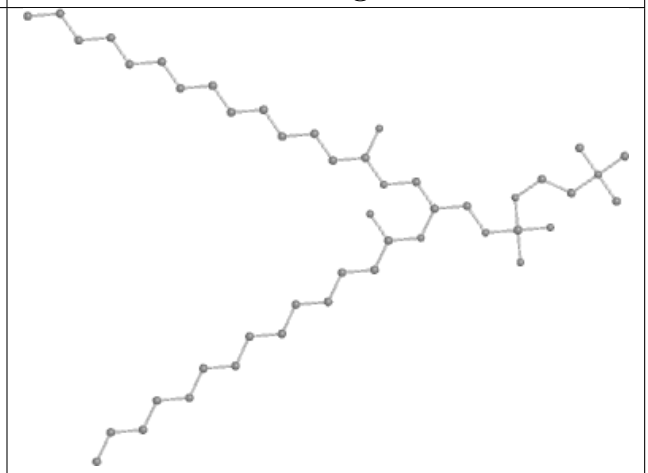
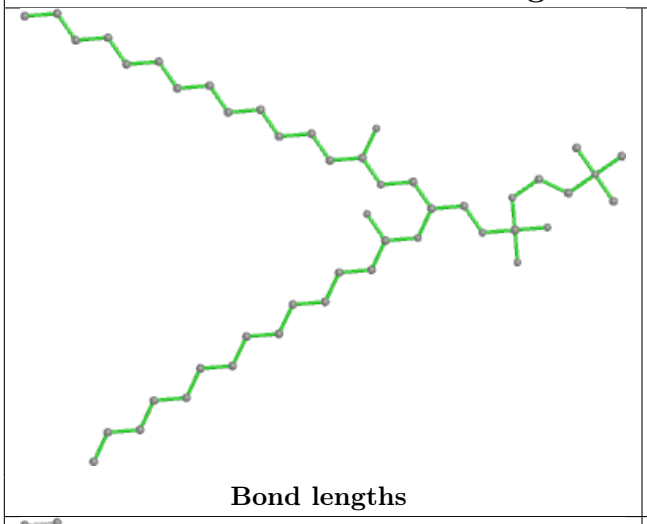


Torsions



Rings

Ligand PX4 A 336



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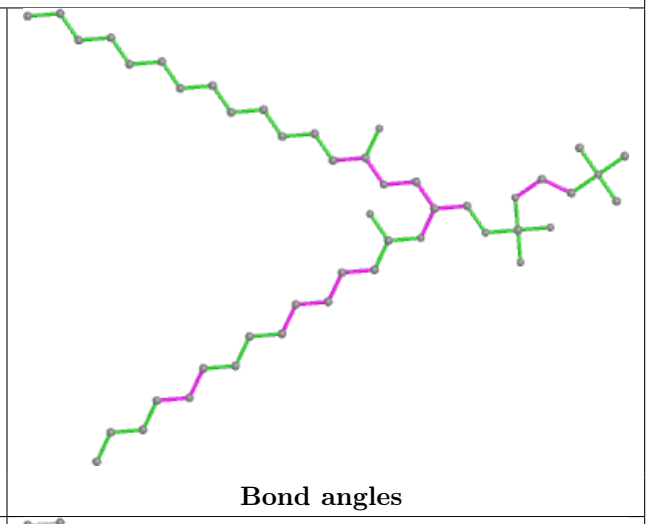
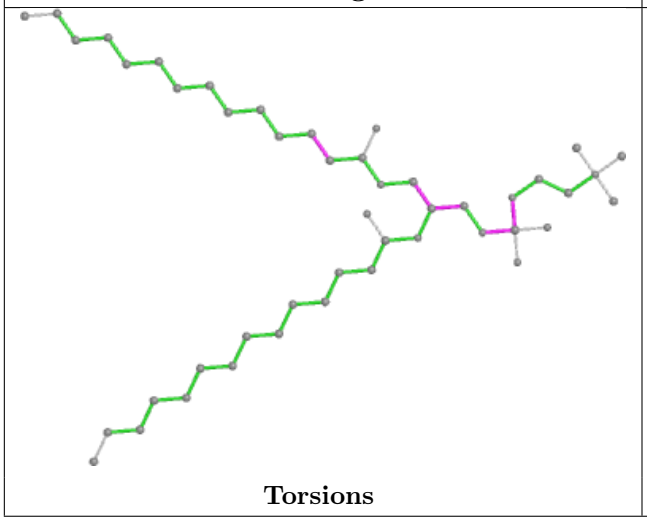
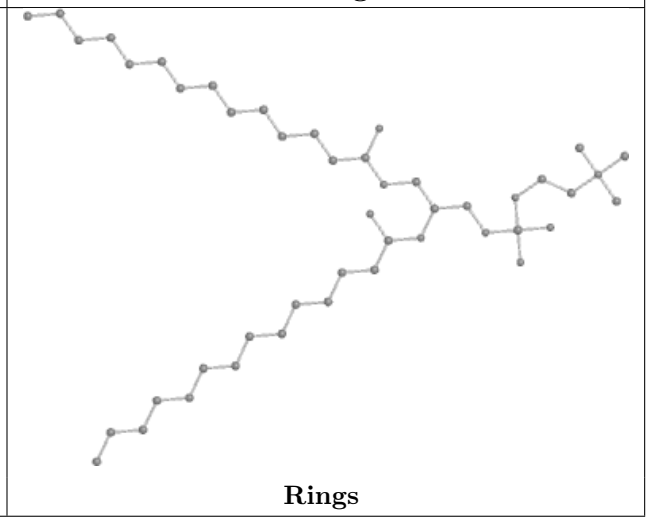


Bond angles

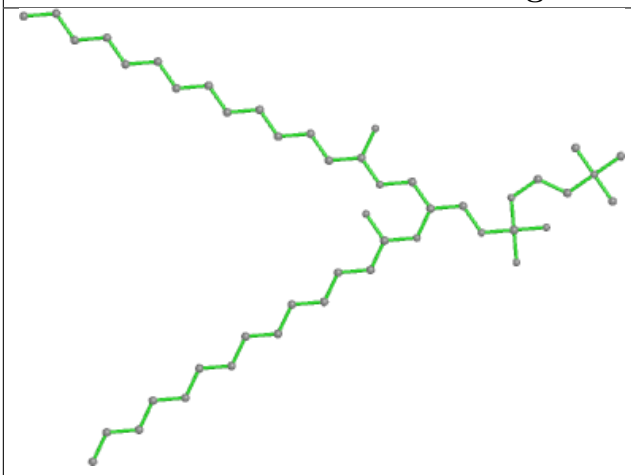


Torsions

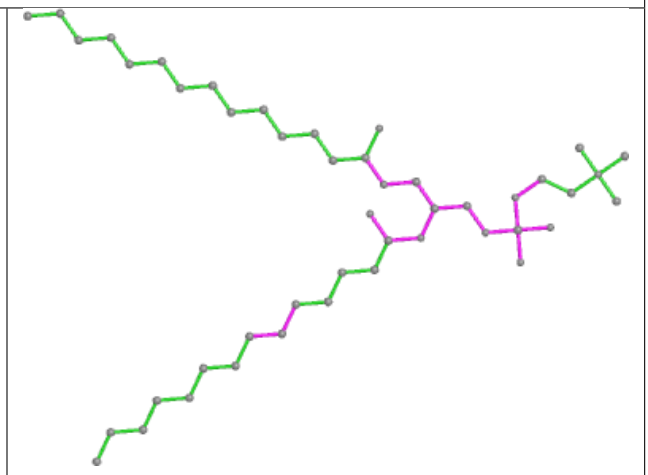


Rings

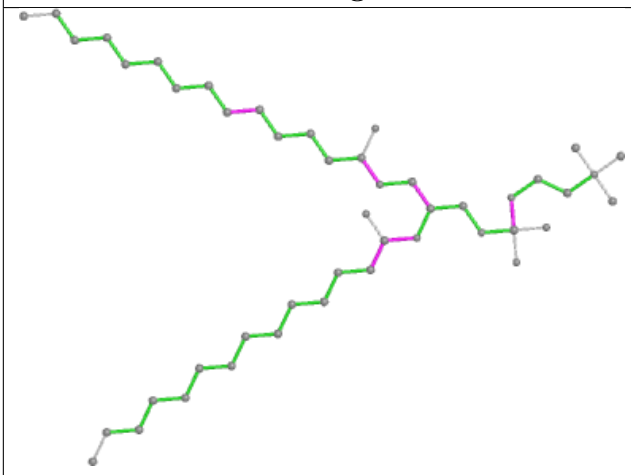
Ligand PX4 A 332



Bond lengths



Bond angles



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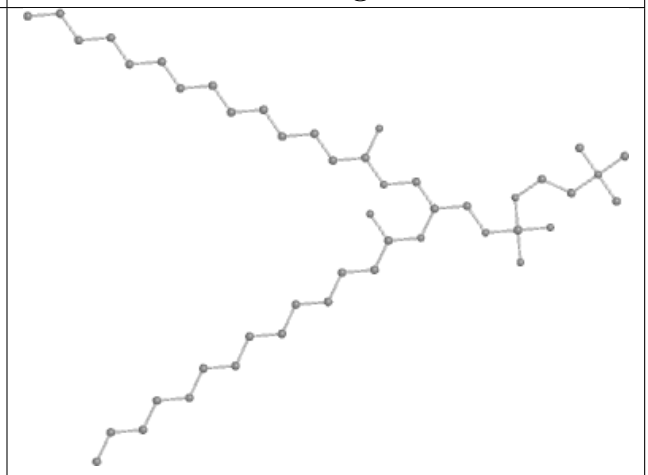
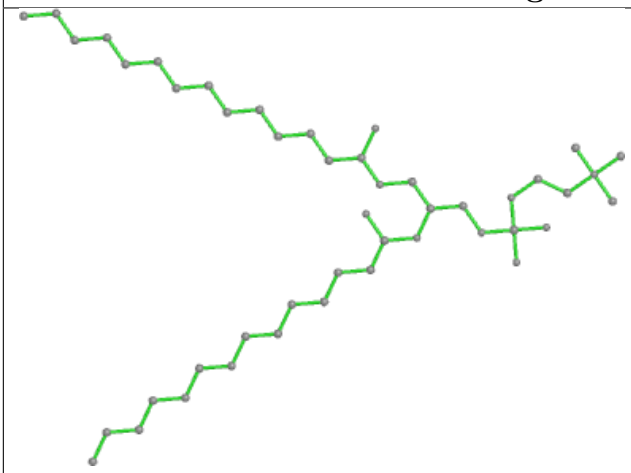


Rings

Ligand PX4 A 398



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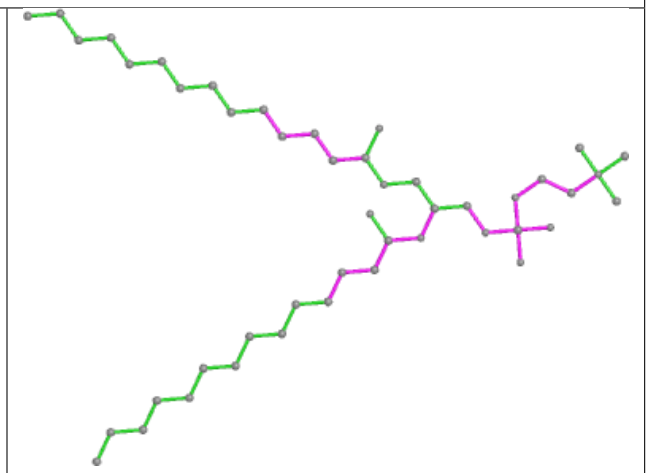
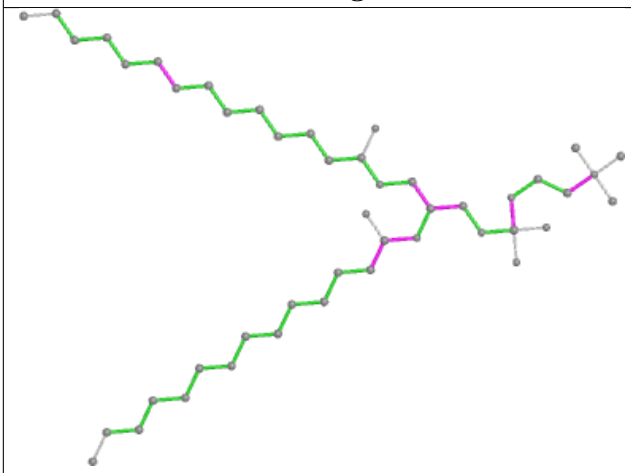


Bond angles



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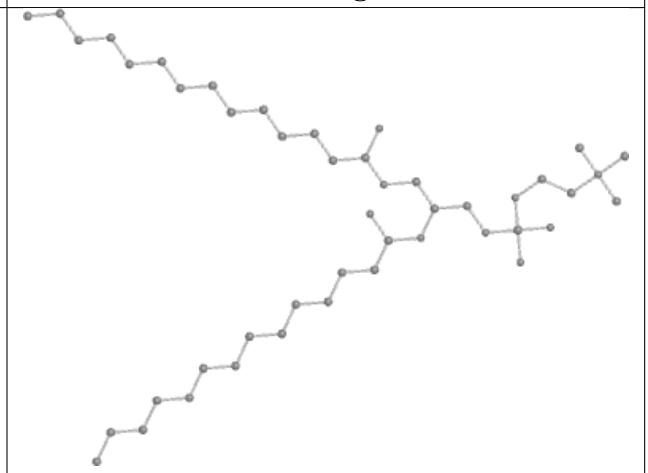
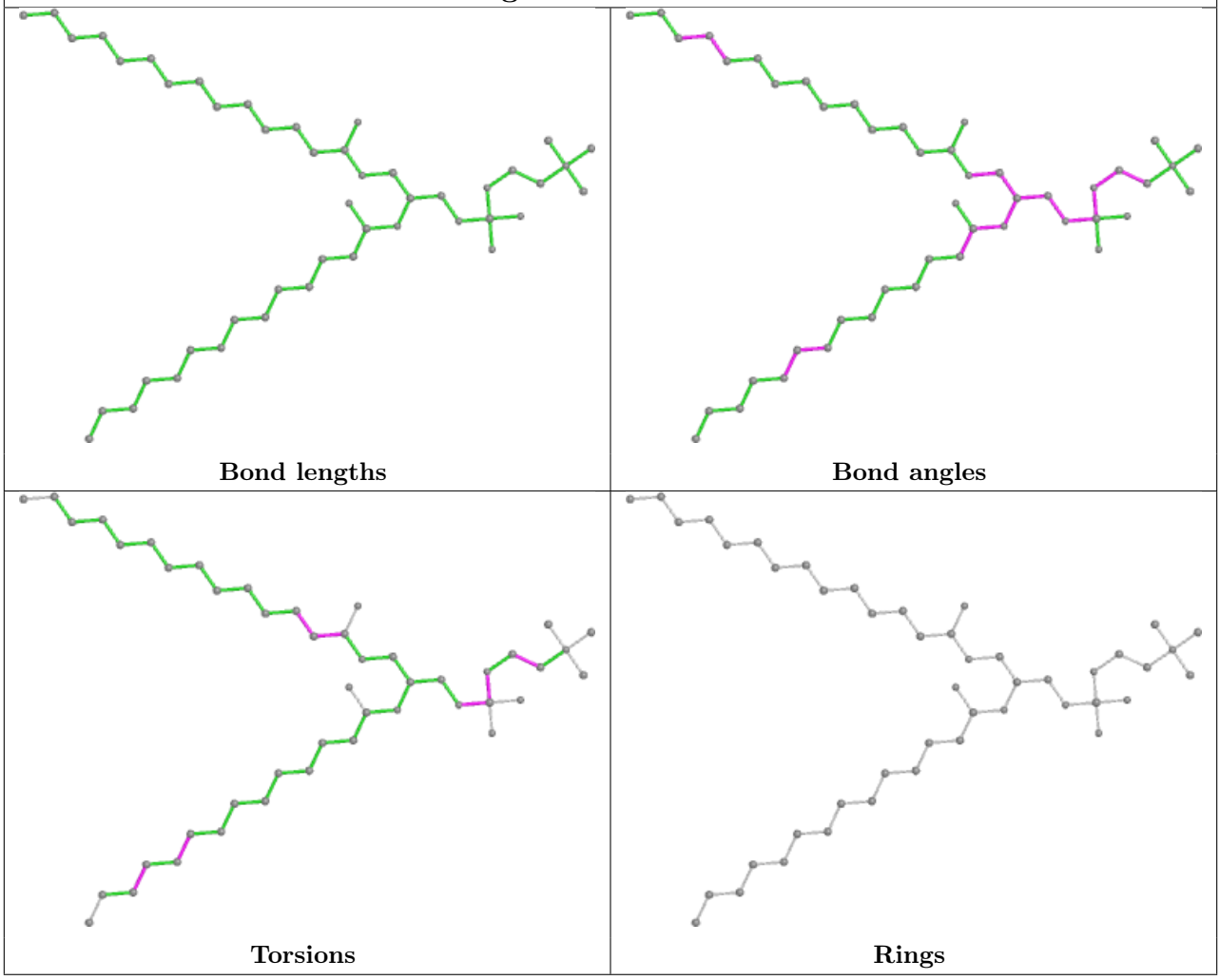
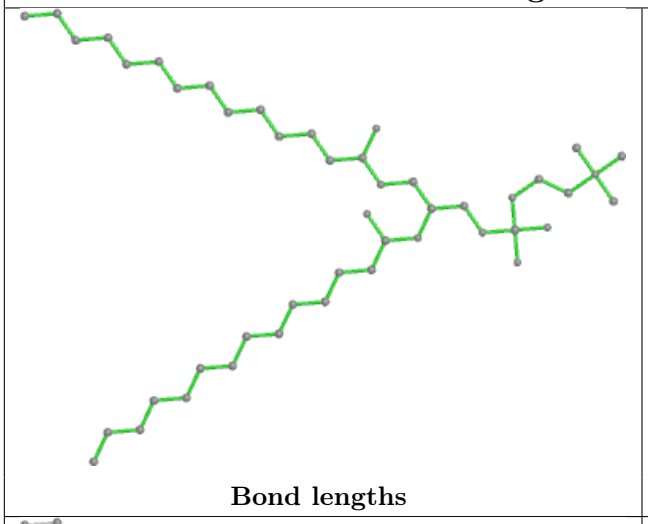


Rings

Ligand PX4 A 382



Ligand PX4 A 314



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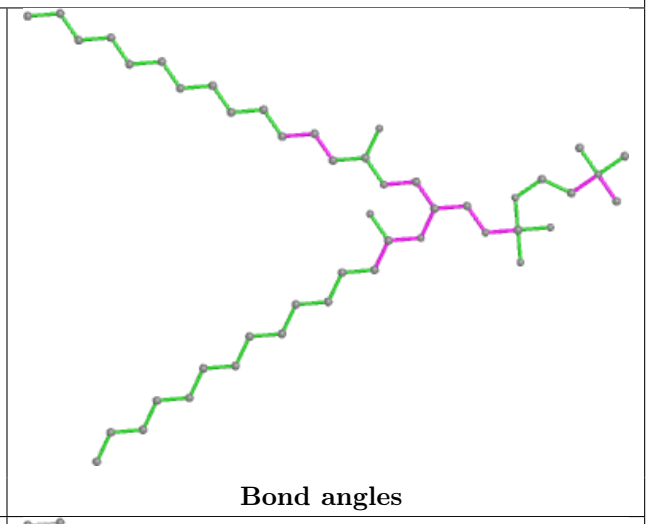
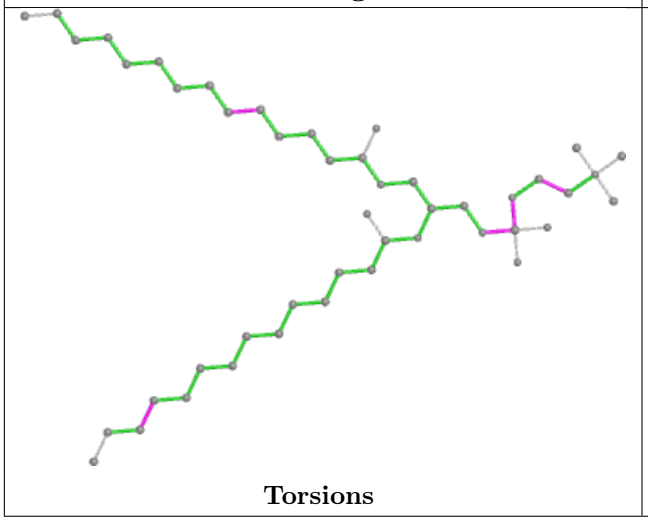


Bond angles



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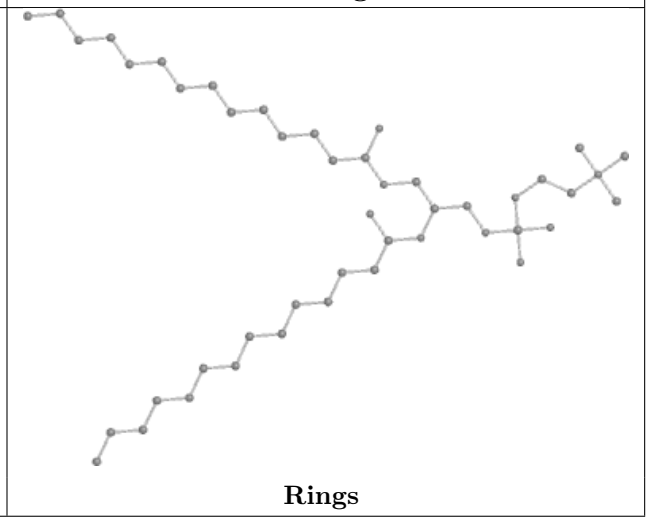
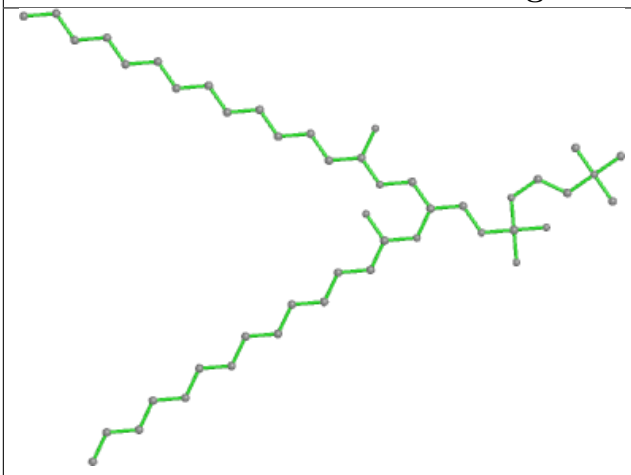


Rings

Ligand PX4 A 419



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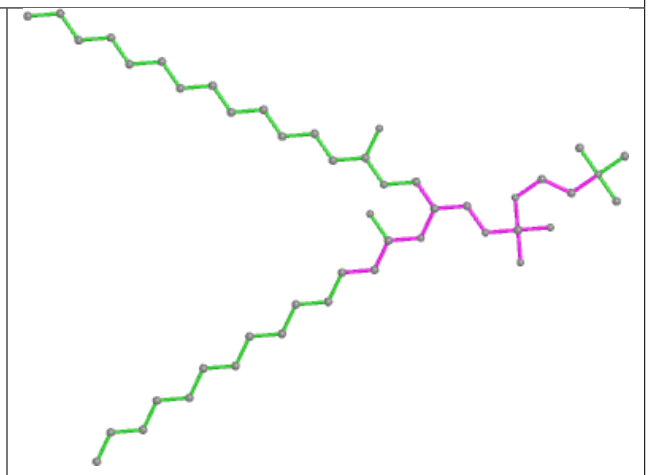
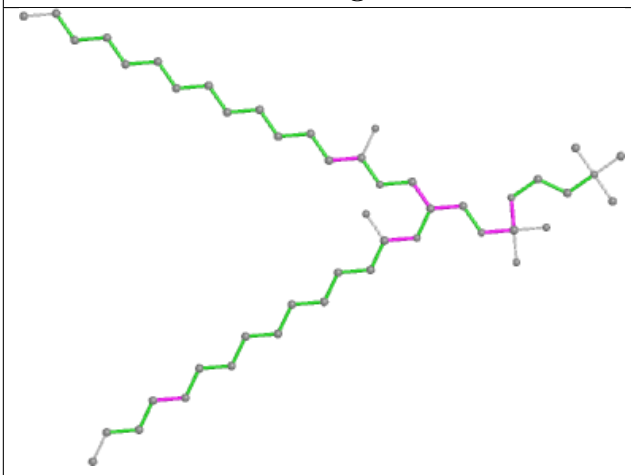


Bond angles



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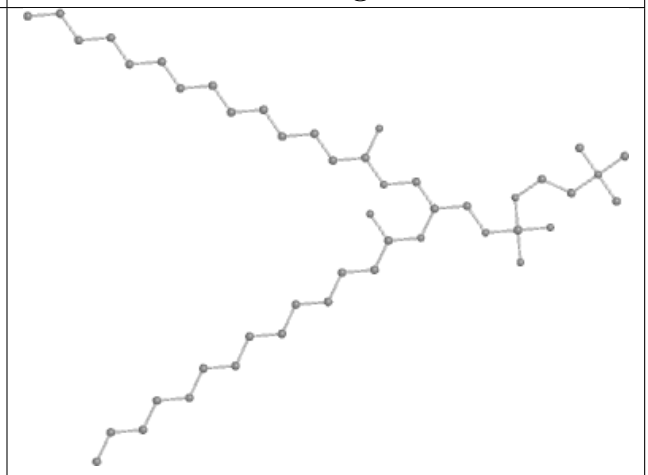
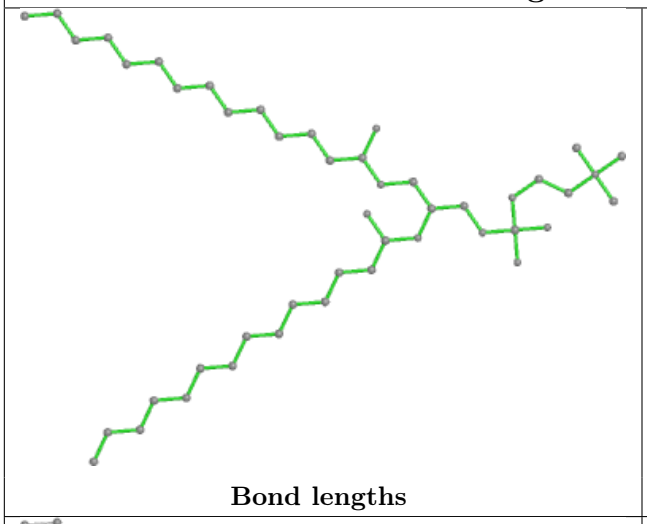


Rings

Ligand PX4 A 421



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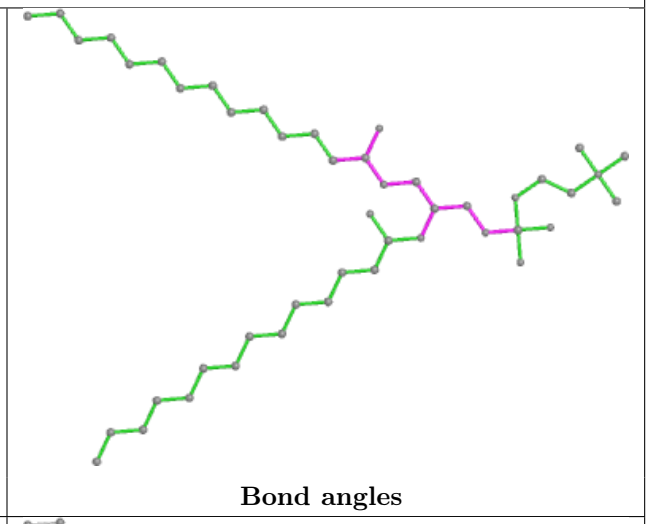
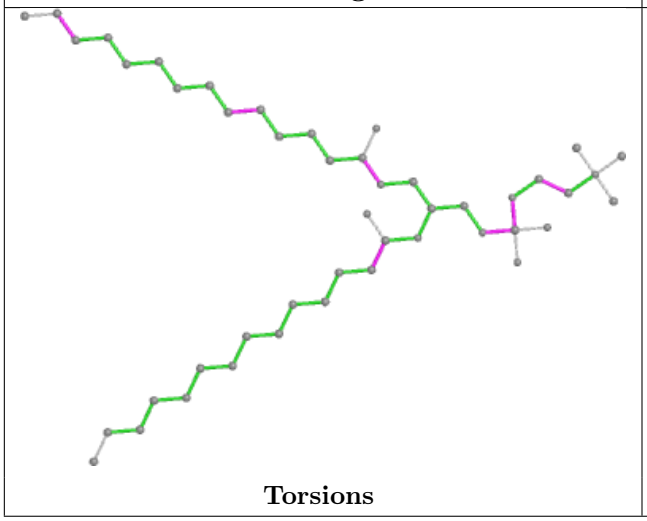


Bond angles



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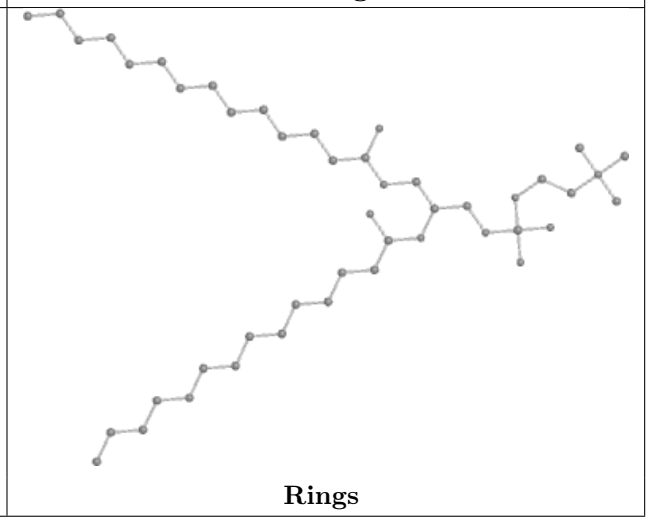
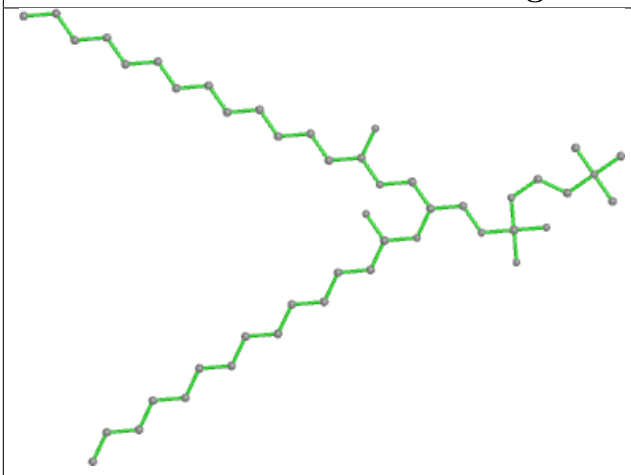


Rings

Ligand PX4 A 391



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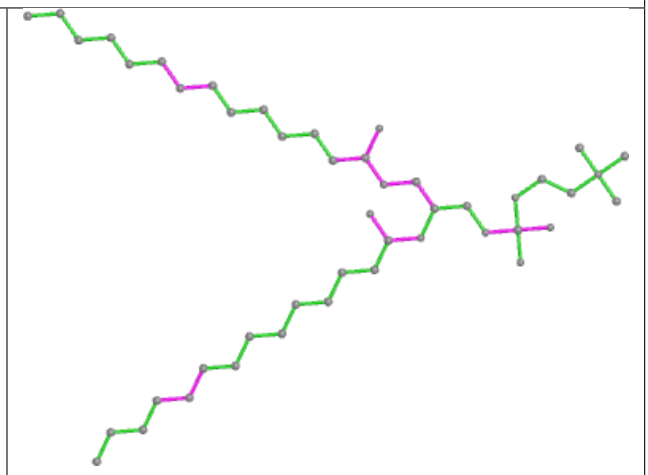
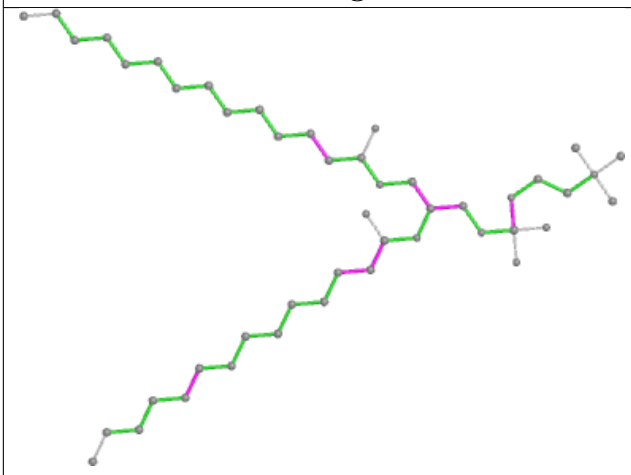


Bond angles



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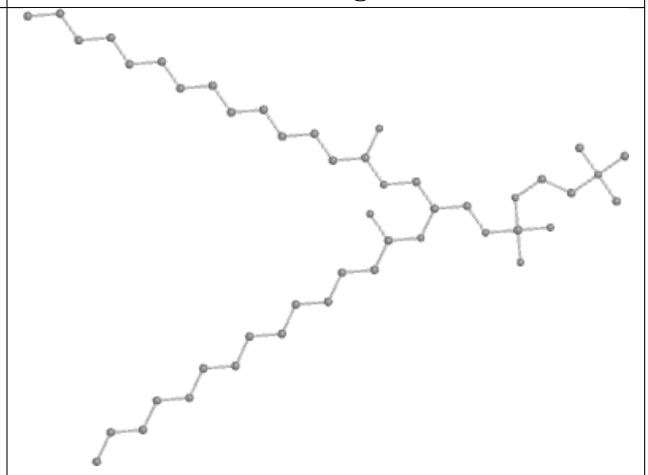
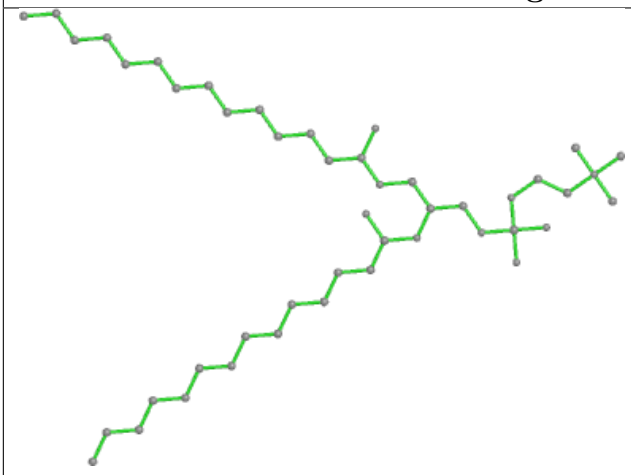


Rings

Ligand PX4 A 417



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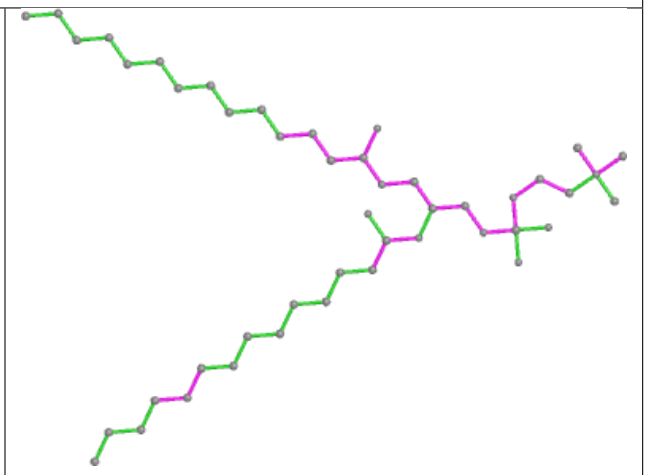
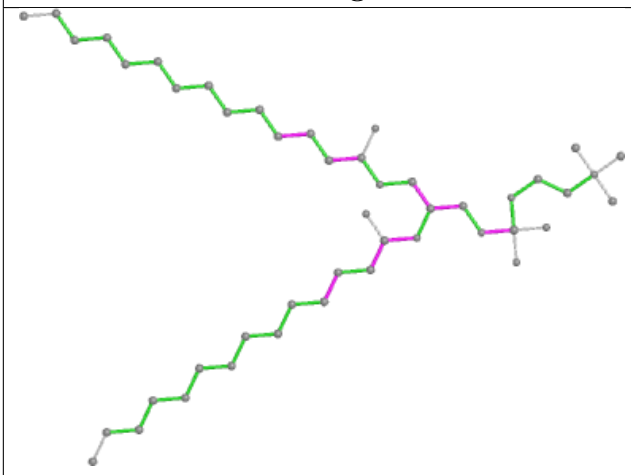


Bond angles



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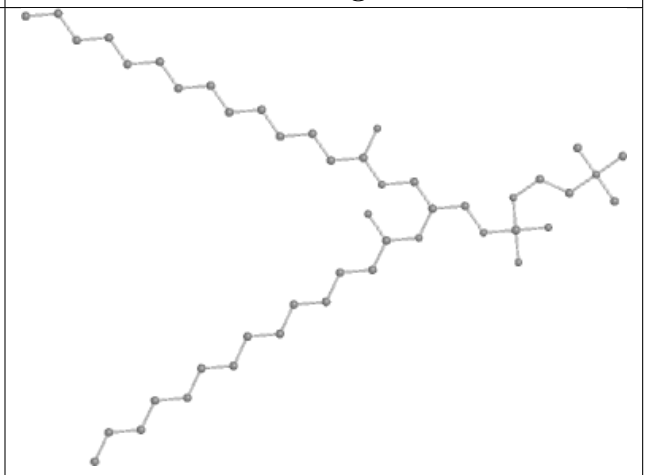
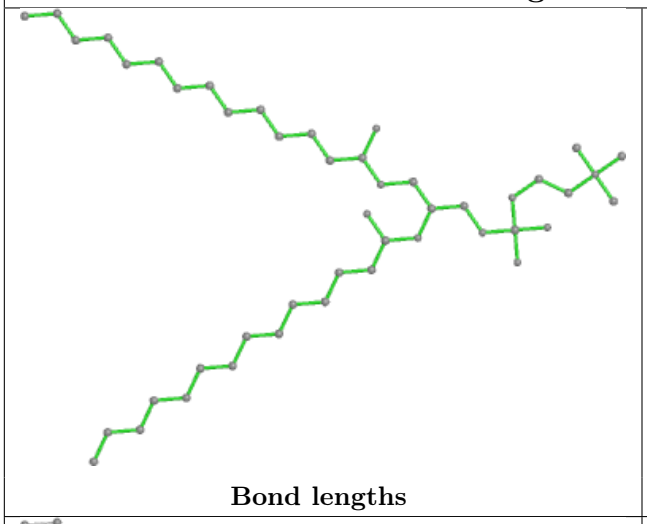


Rings

Ligand PX4 A 375



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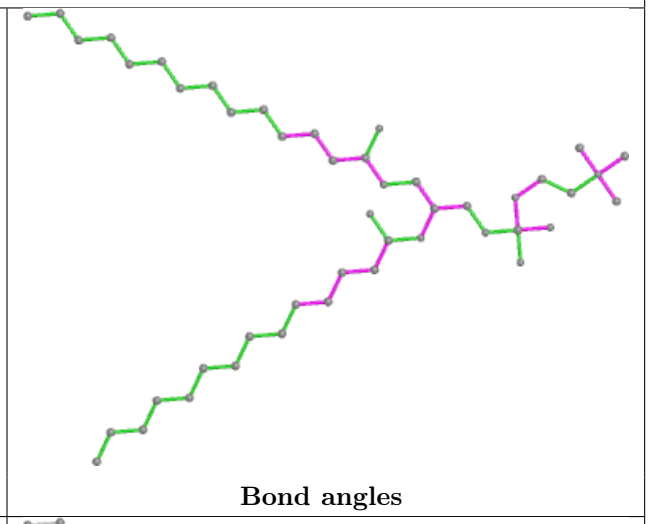

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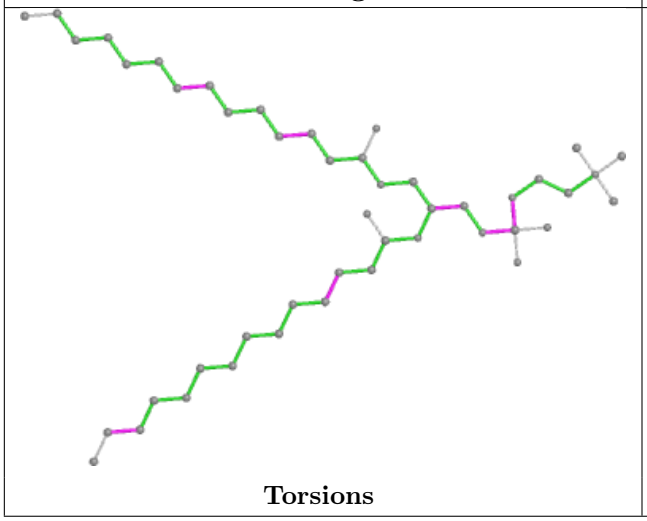

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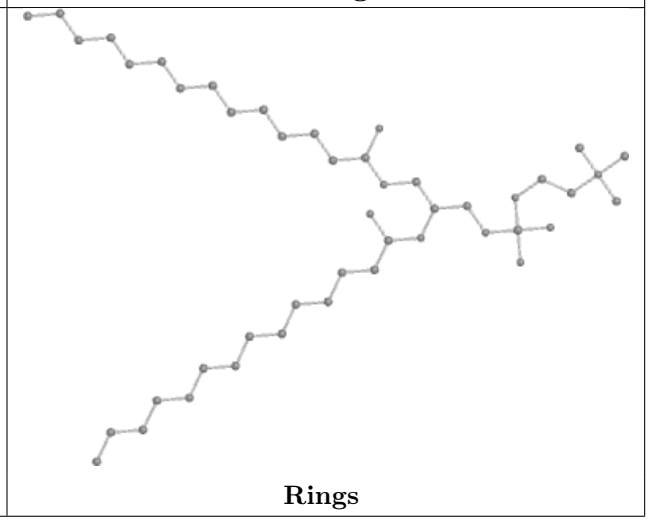
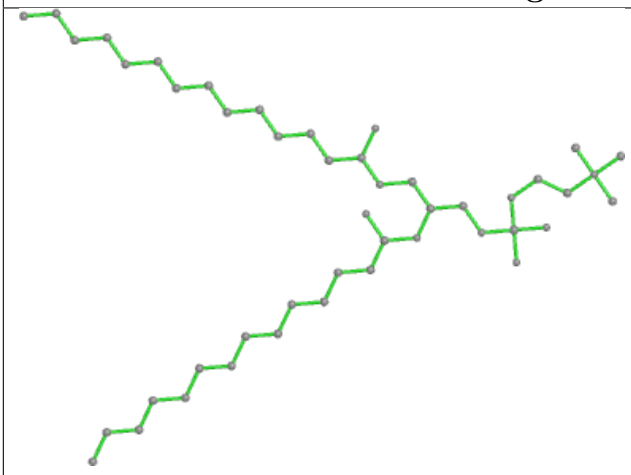


Rings

Ligand PX4 A 394



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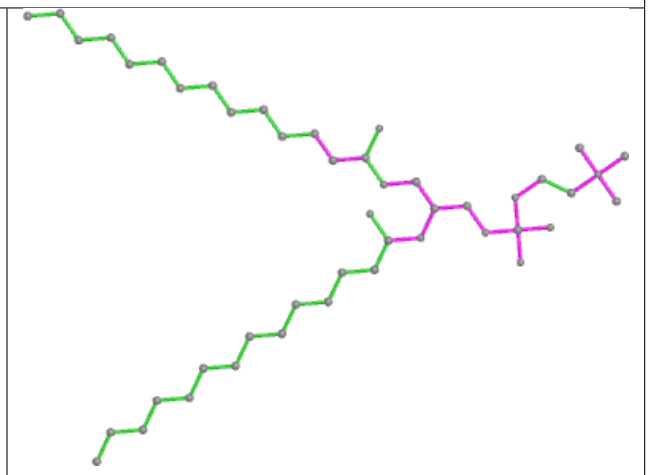
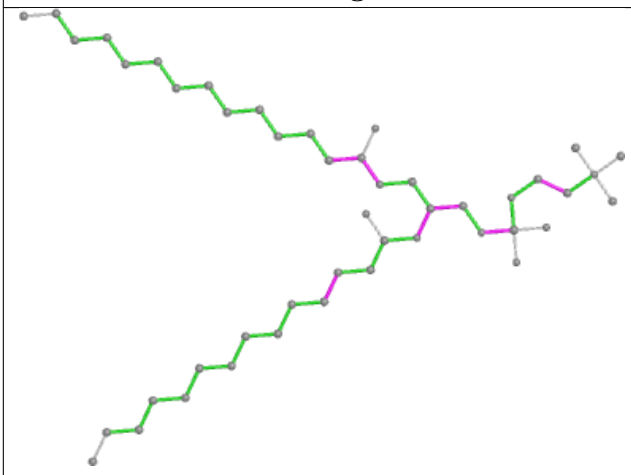


Bond angles



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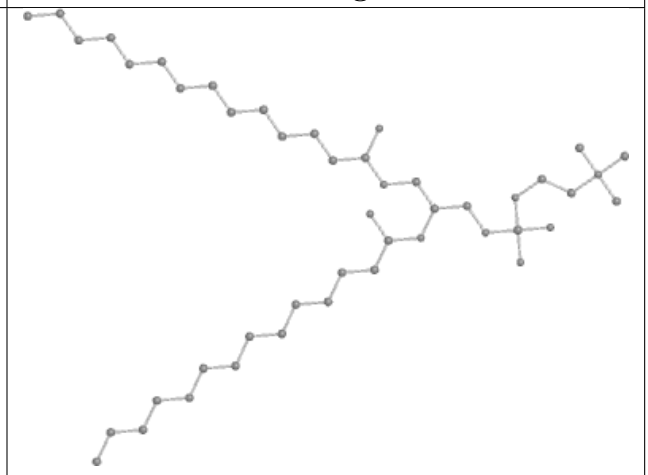
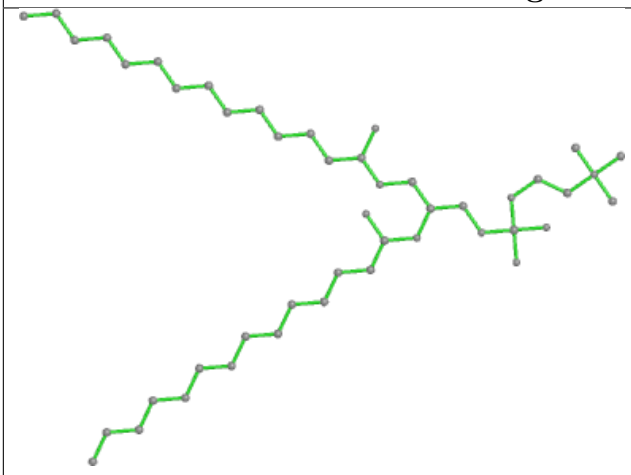


Rings

Ligand PX4 A 423



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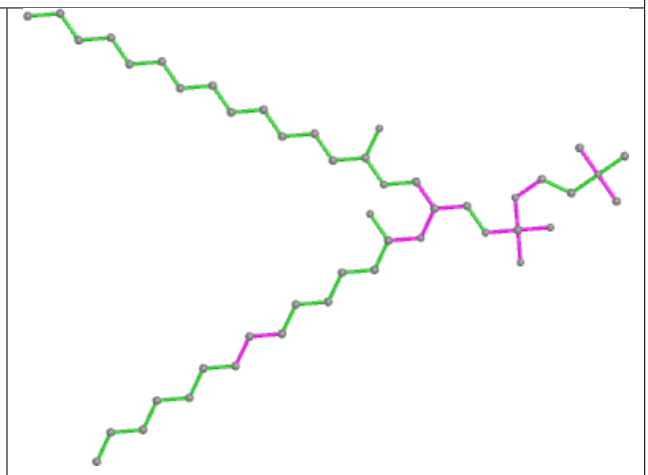
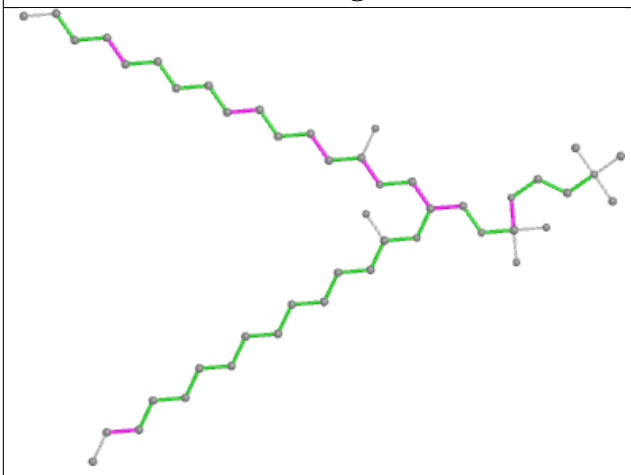


Bond angles



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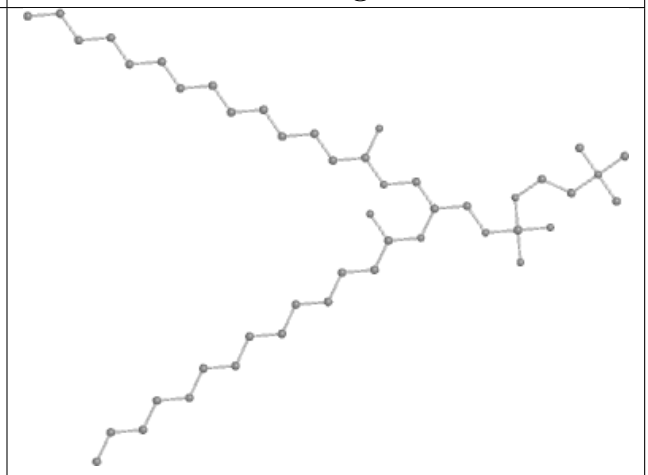
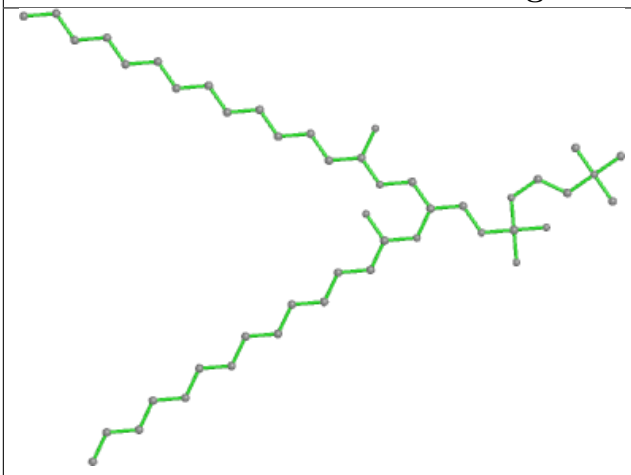


Rings

Ligand PX4 A 329



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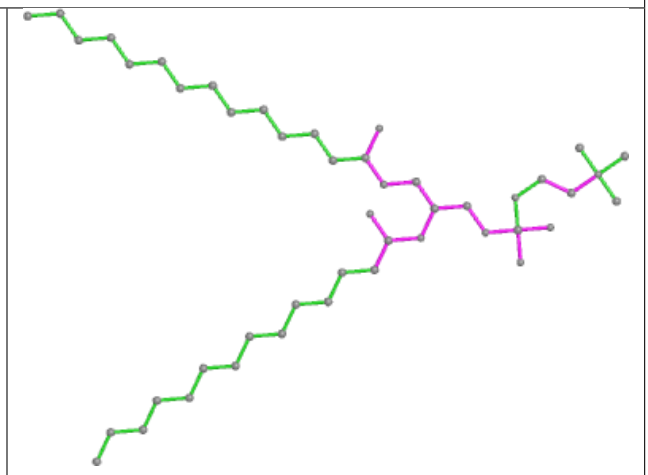
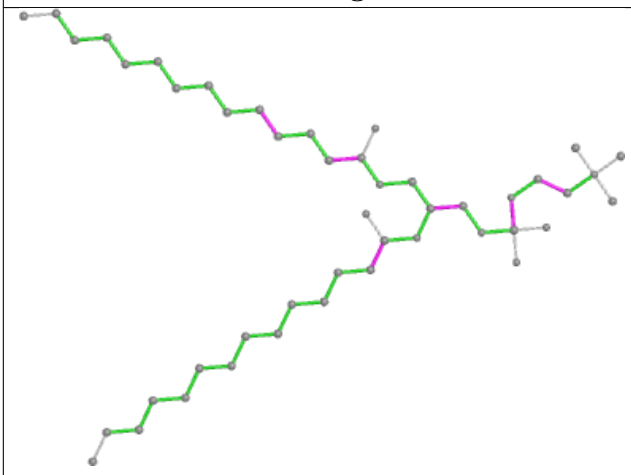


Bond angles



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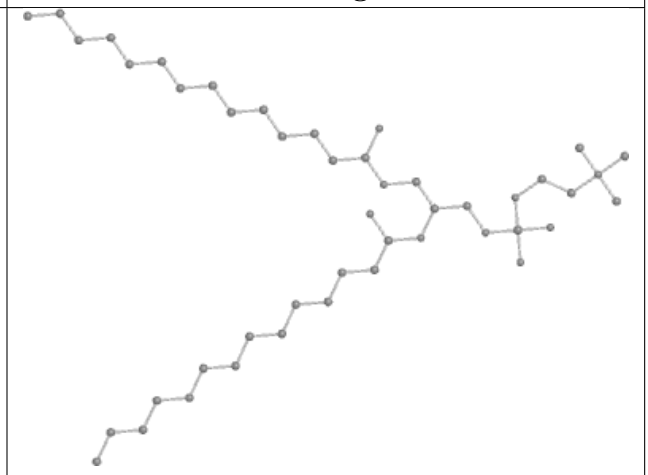
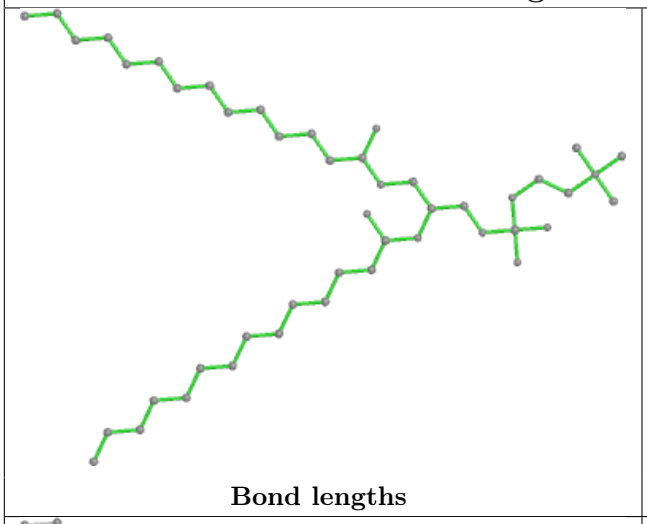


Rings

Ligand PX4 A 385



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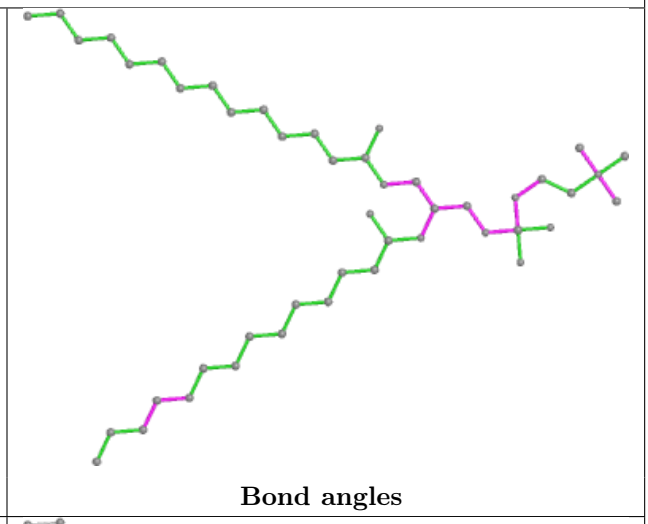
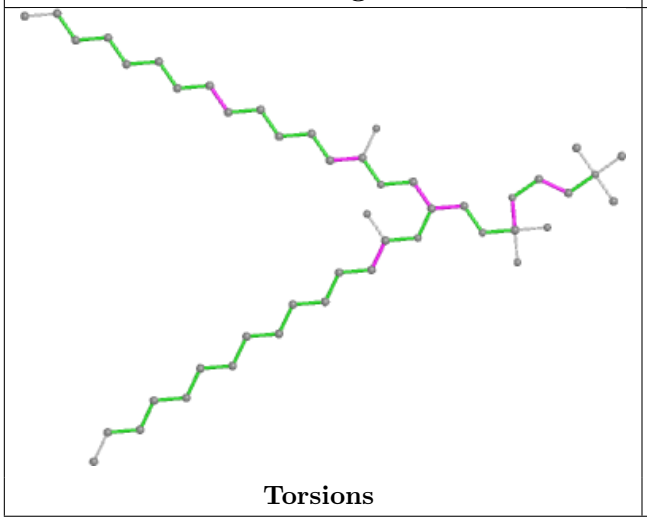


Bond angles



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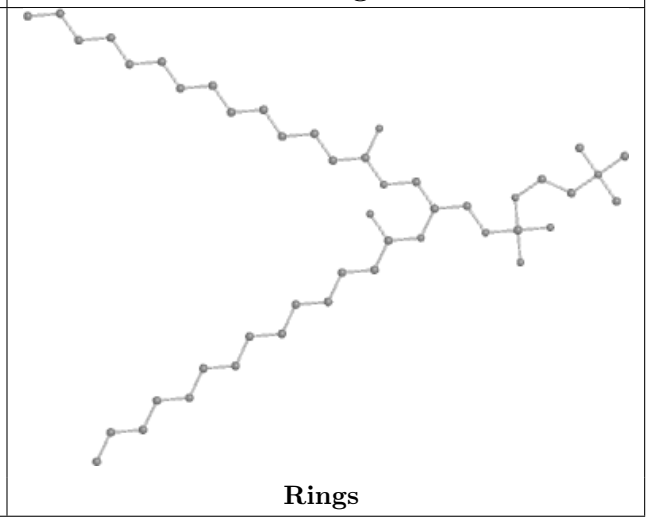
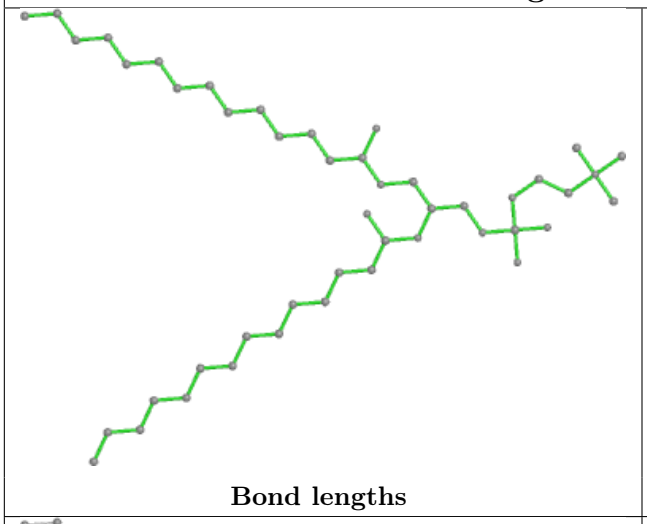
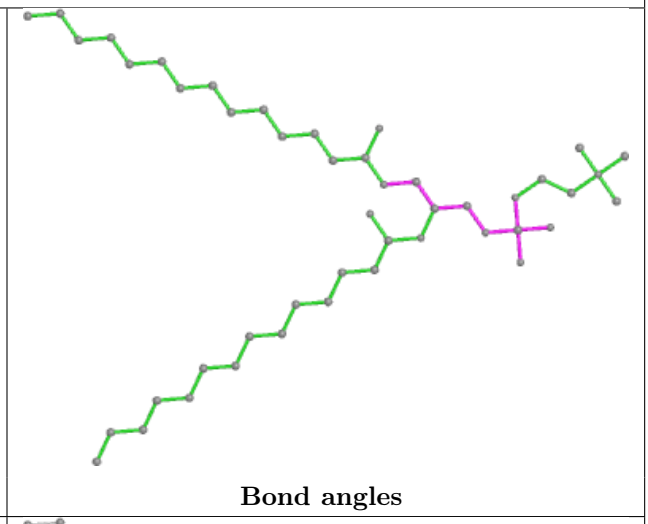


Rings

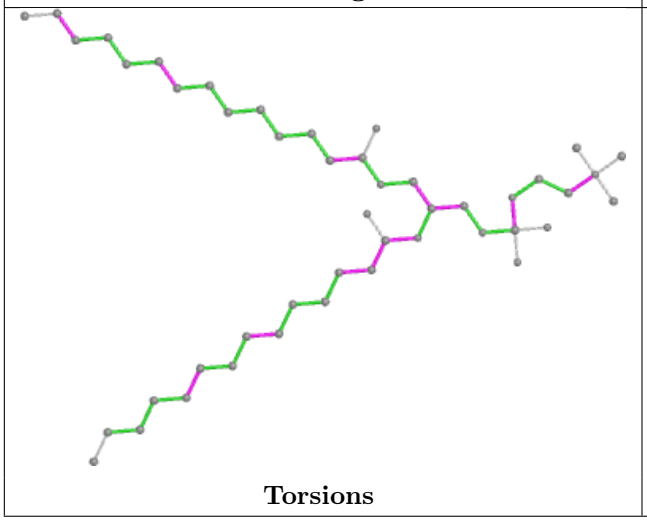
Ligand PX4 A 406



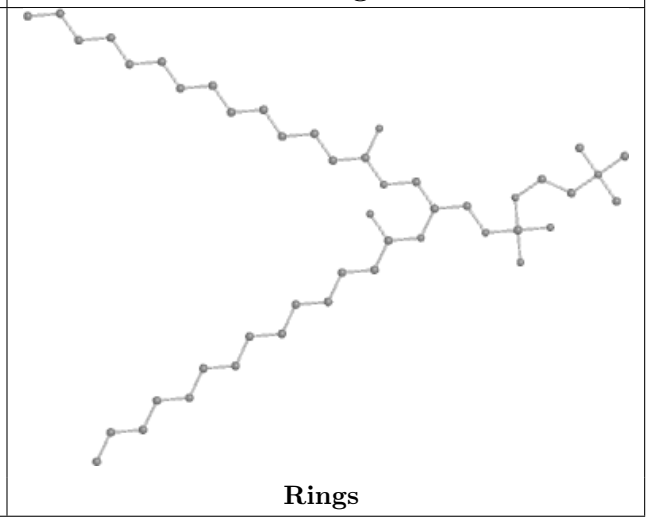
Bond lengths



Bond angles

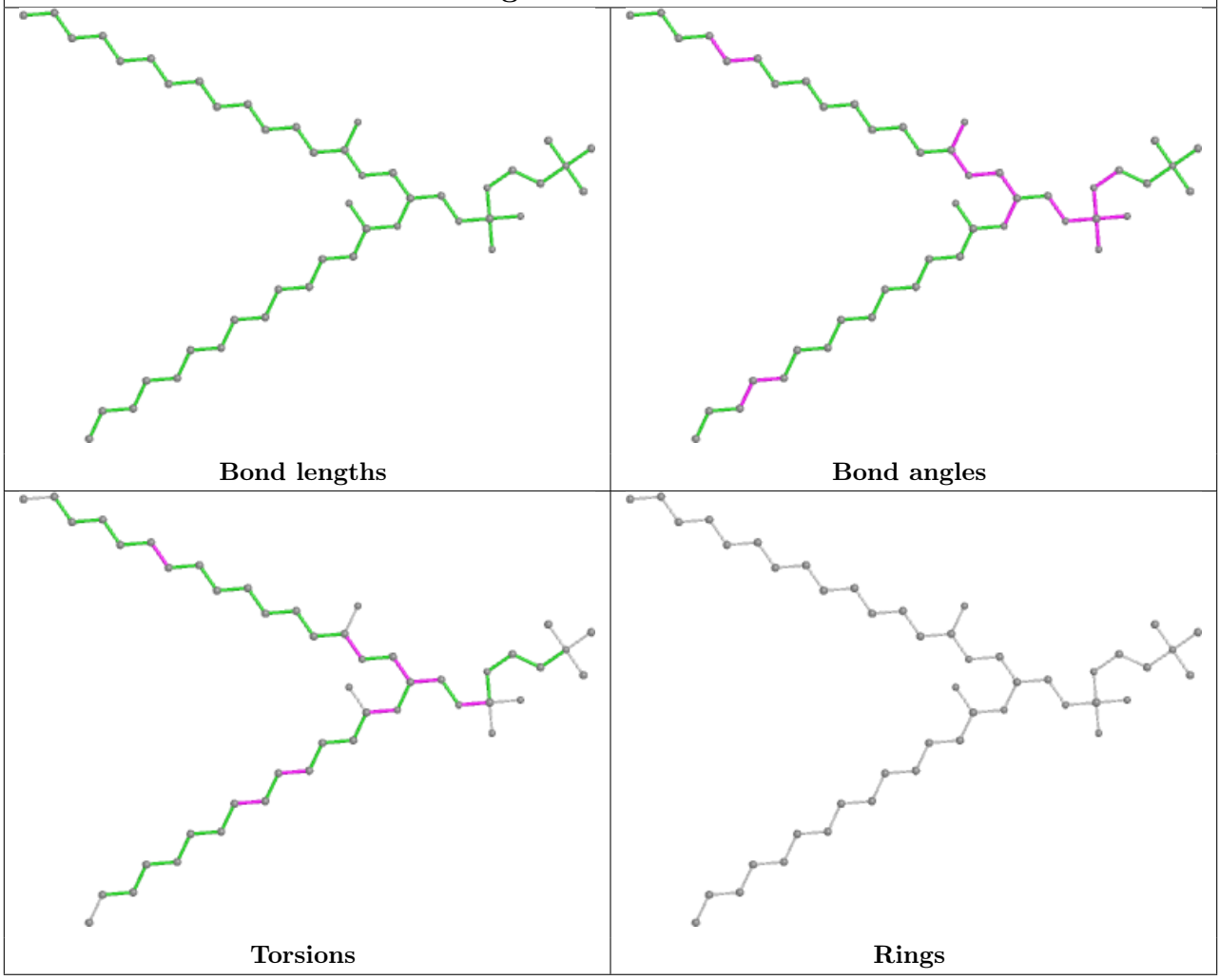


Torsions

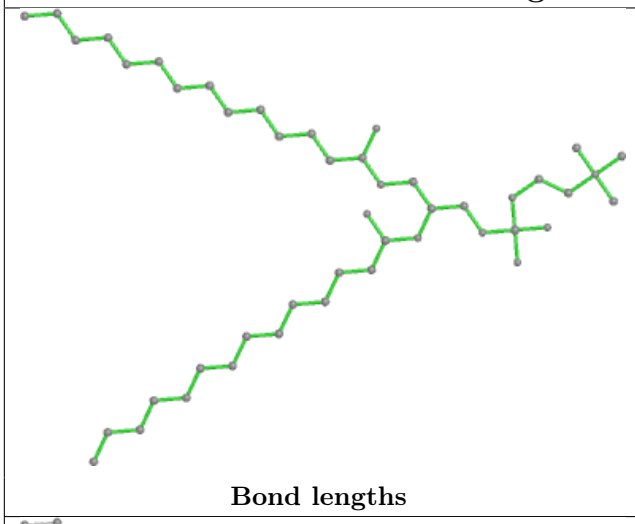


Rings

Ligand PX4 A 384



Ligand PX4 A 426



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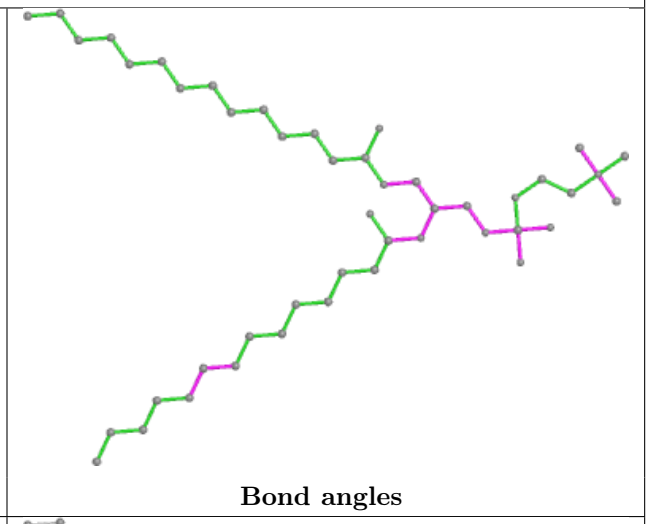
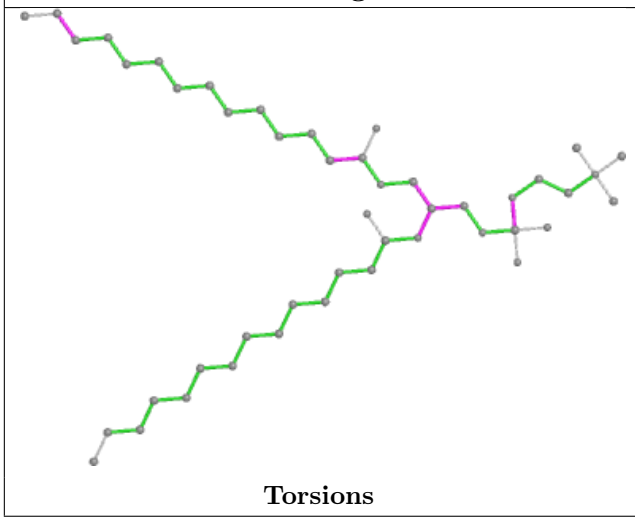


Bond angles



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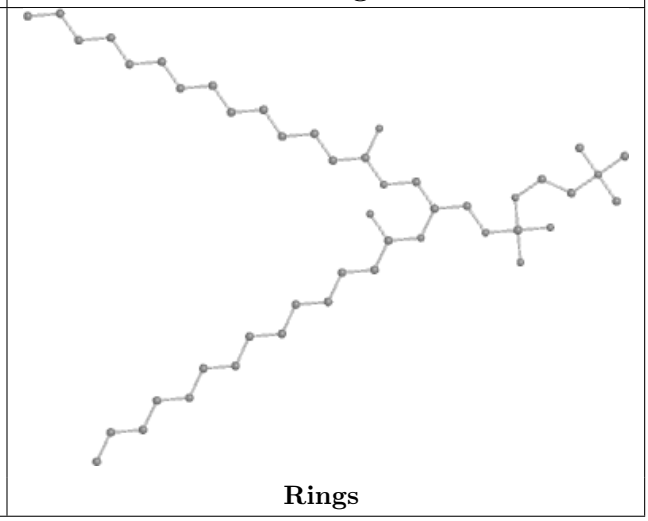
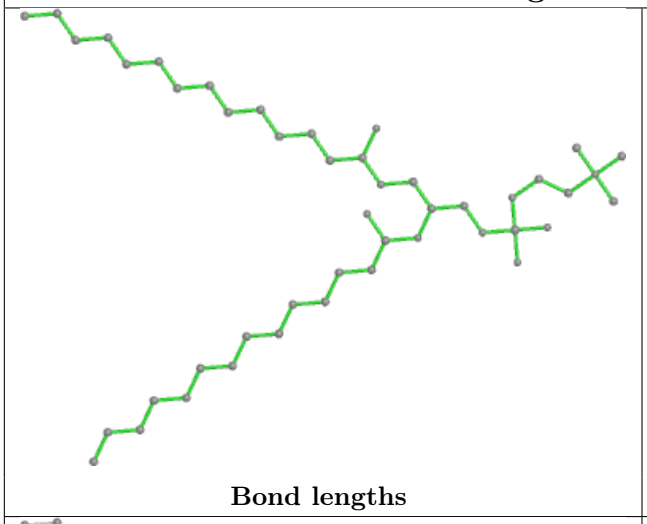


Rings

Ligand PX4 A 352



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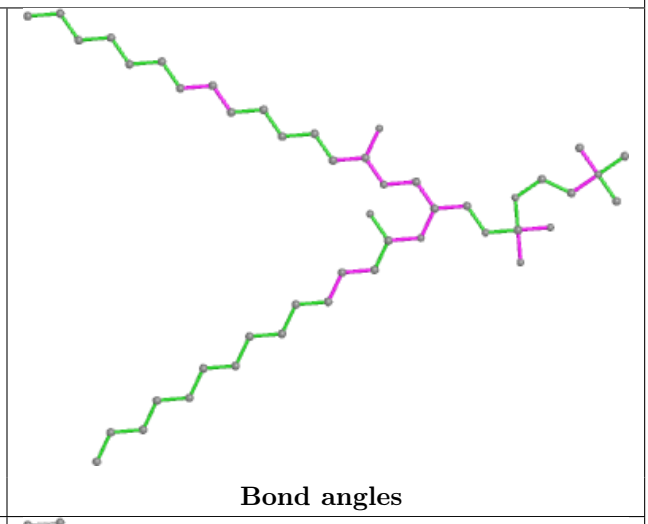

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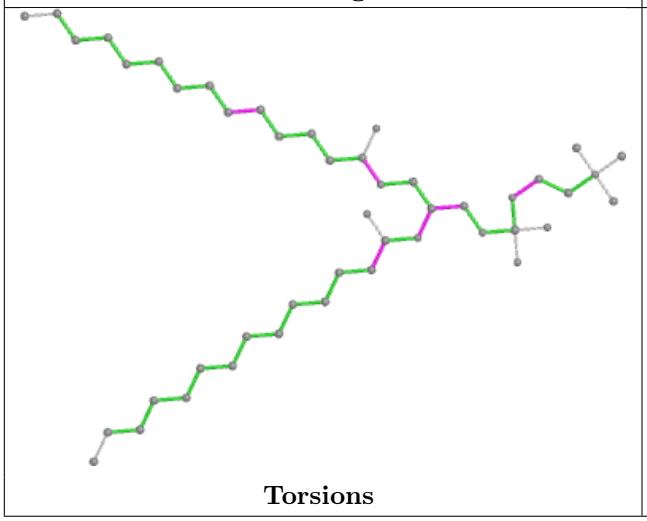

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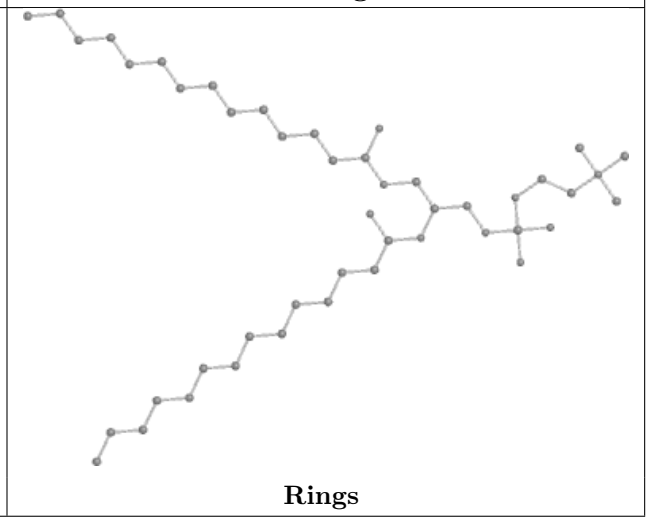
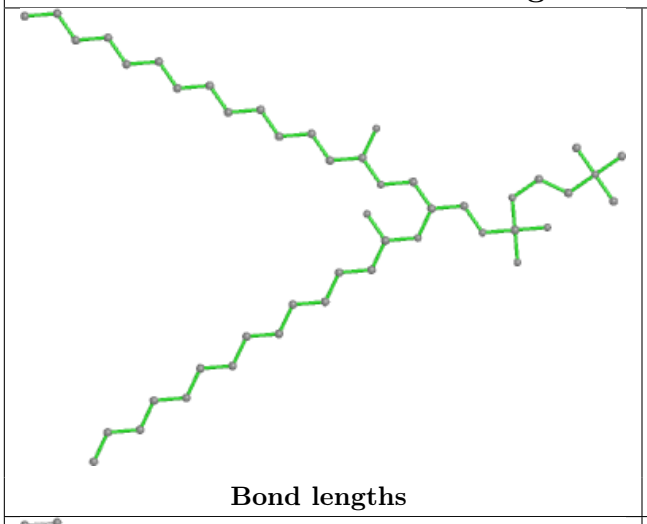


Rings

Ligand PX4 A 403



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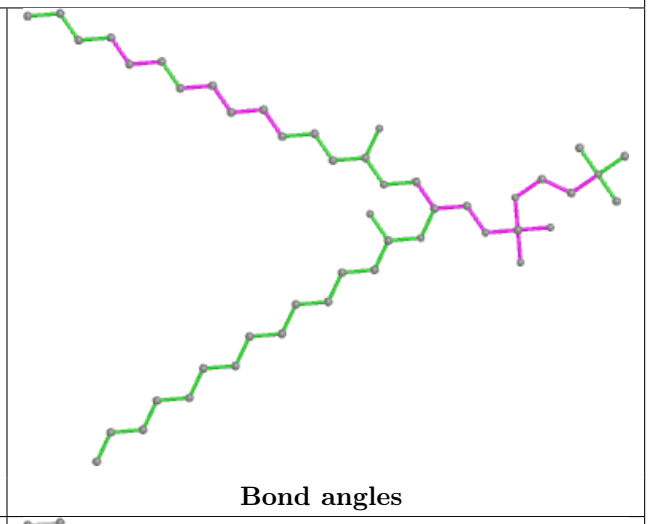
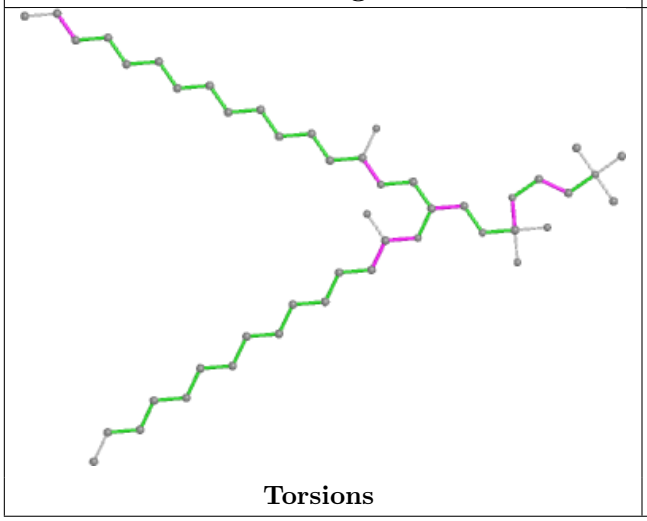


Bond angles



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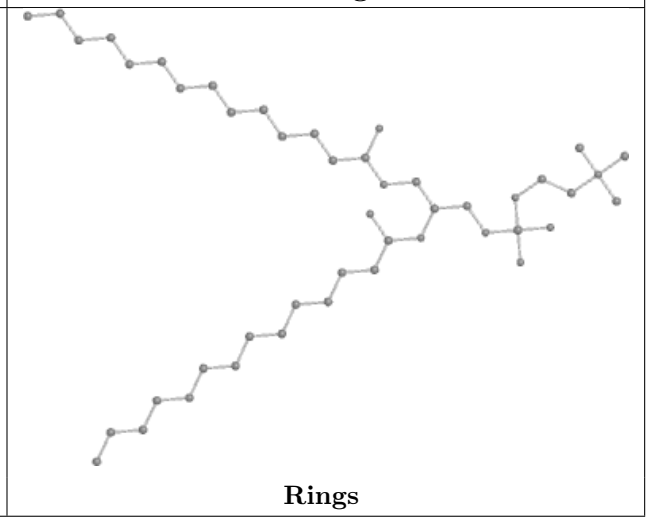
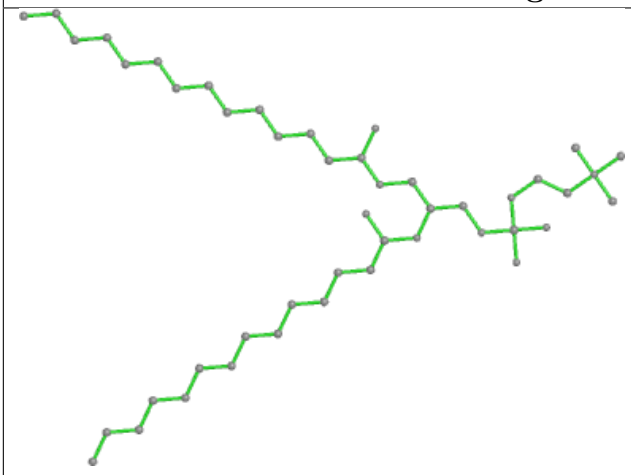


Rings

Ligand PX4 A 361



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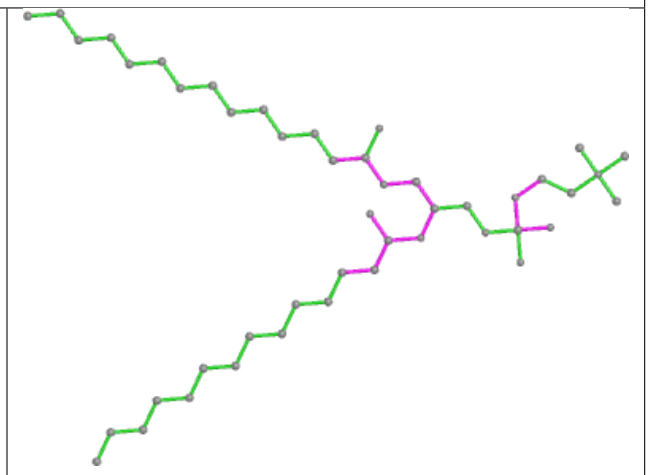

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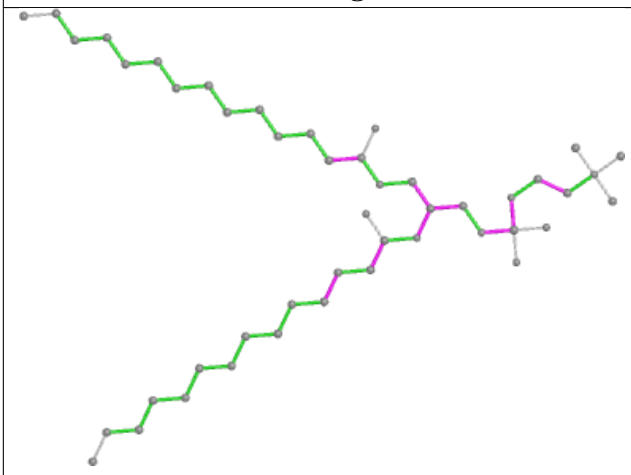

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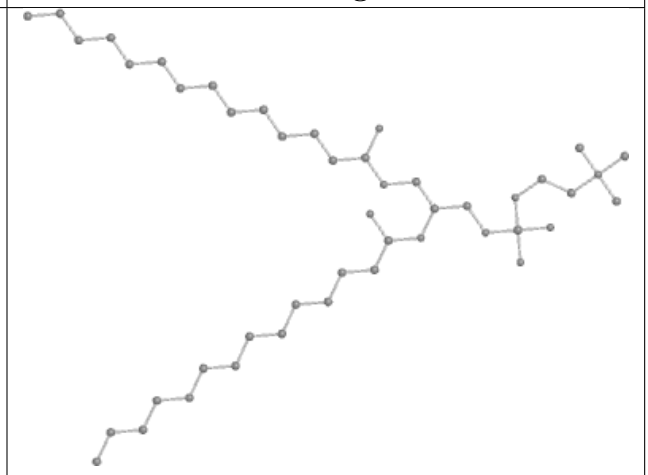
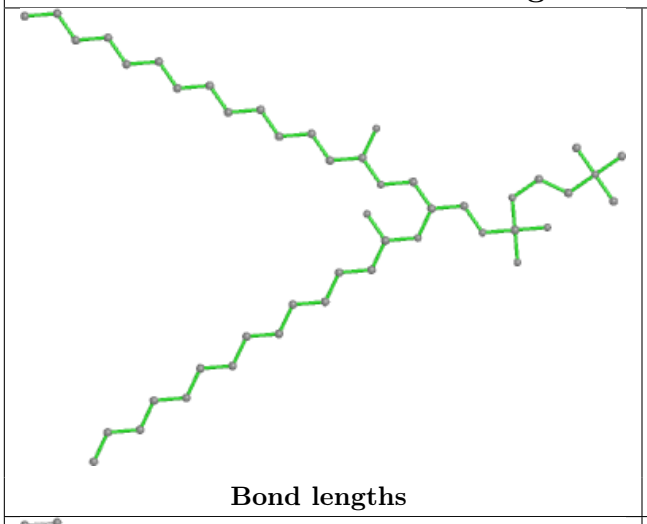


Rings

Ligand PX4 A 429



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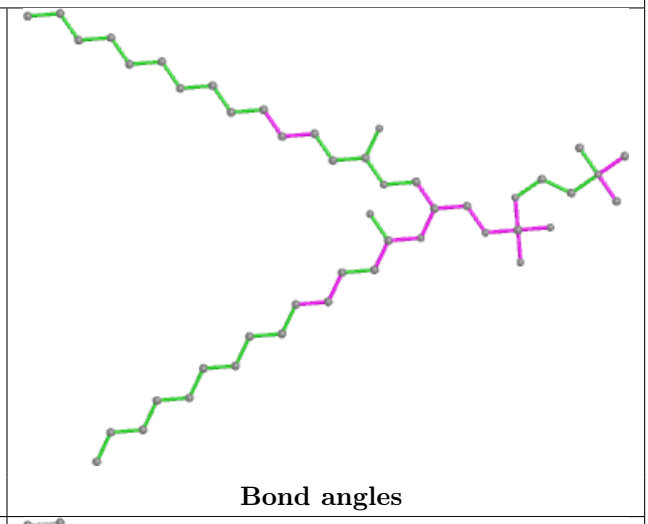
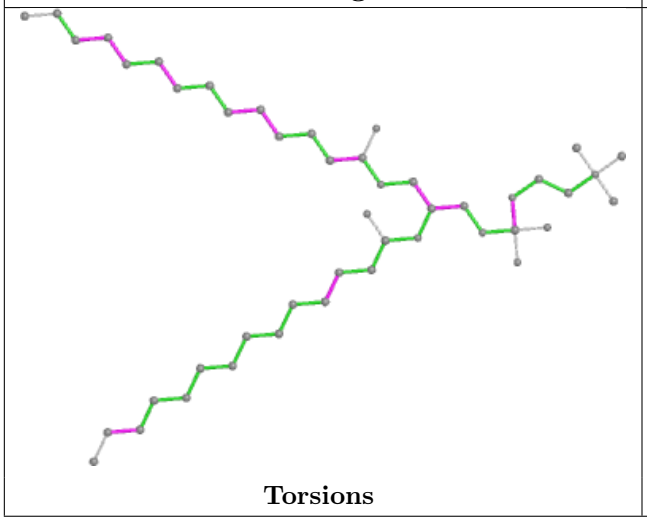


Bond angles



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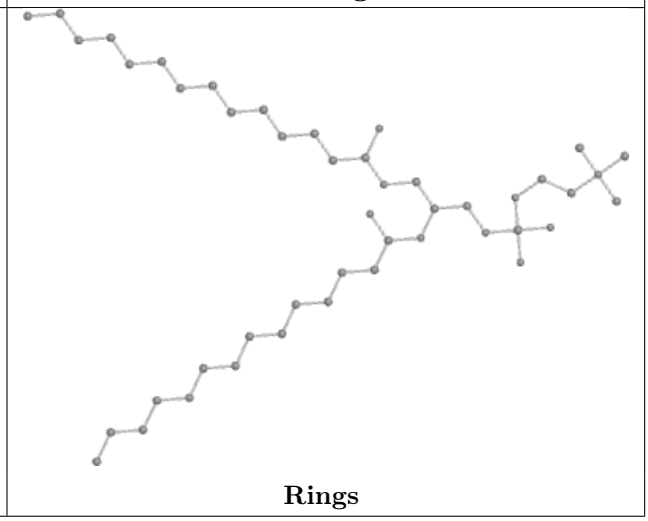
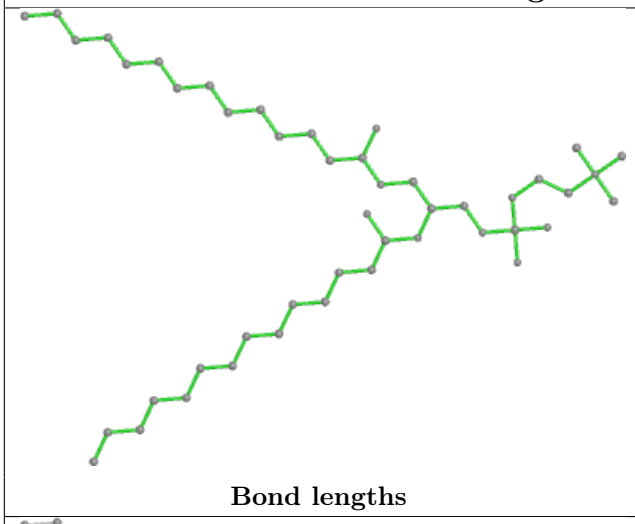


Rings

Ligand PX4 A 392



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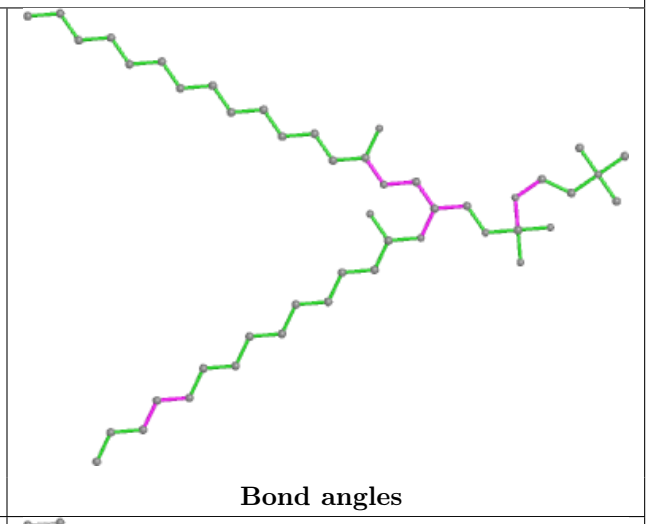
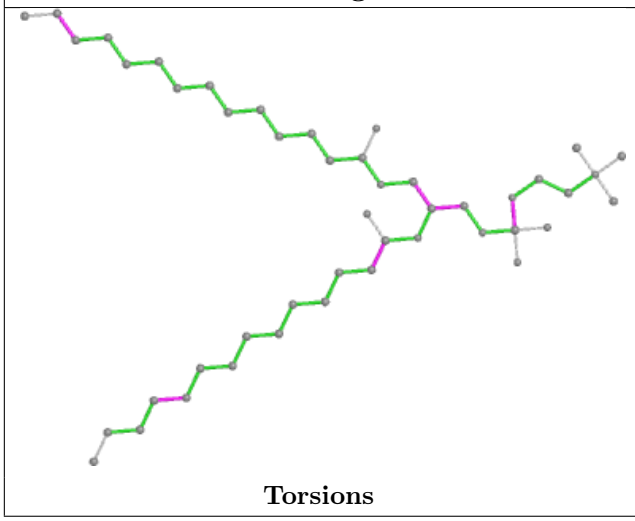


Bond angles



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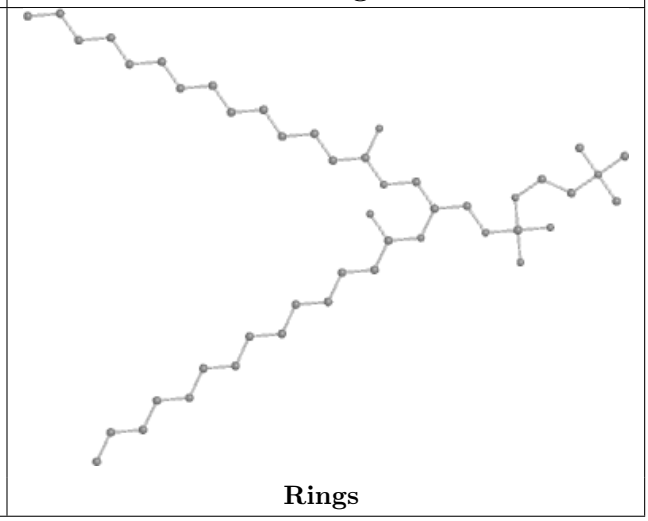
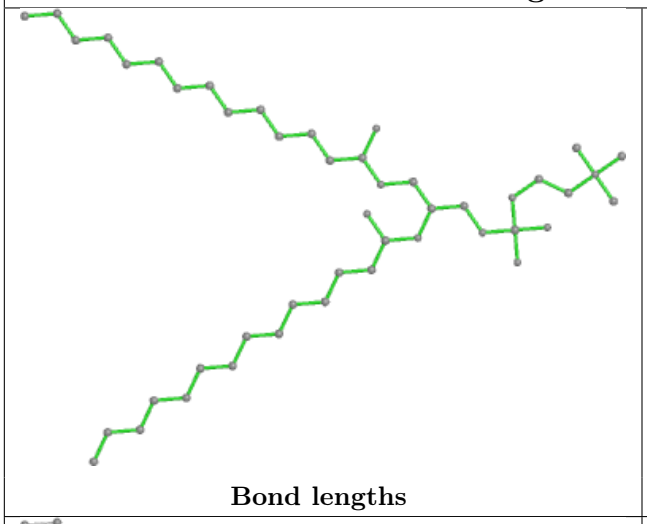


Rings

Ligand PX4 A 410



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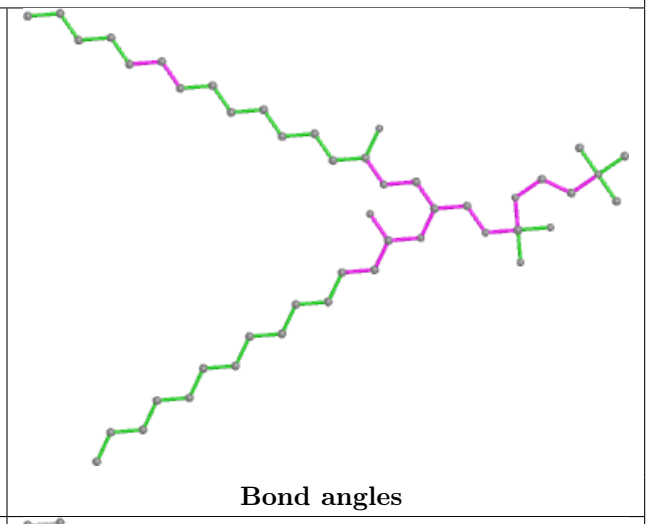
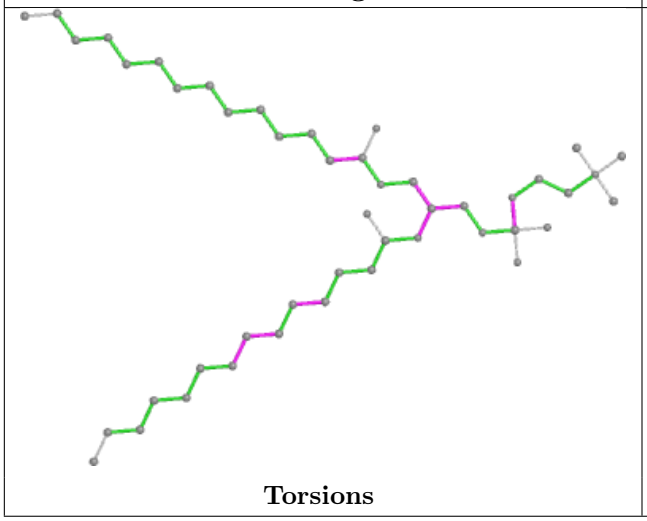


Bond angles



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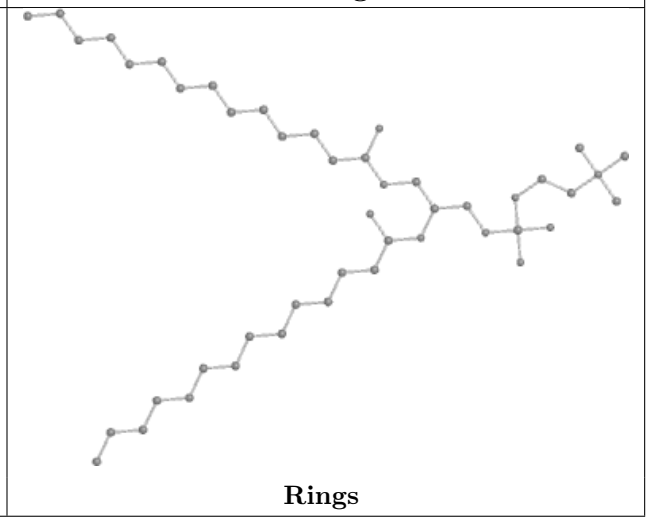
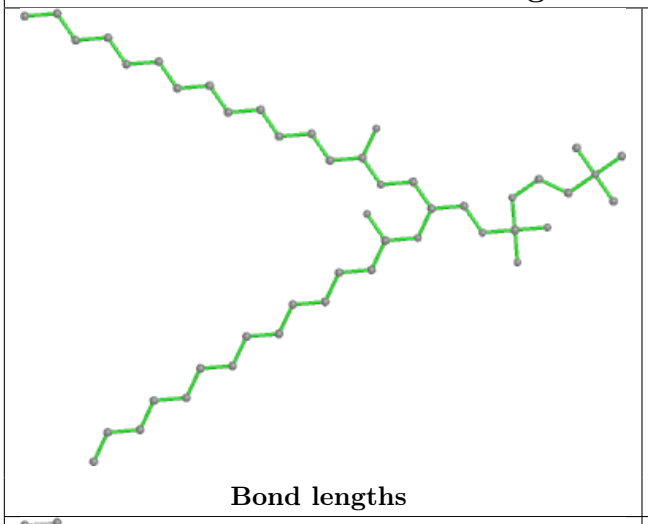


Rings

Ligand PX4 A 330



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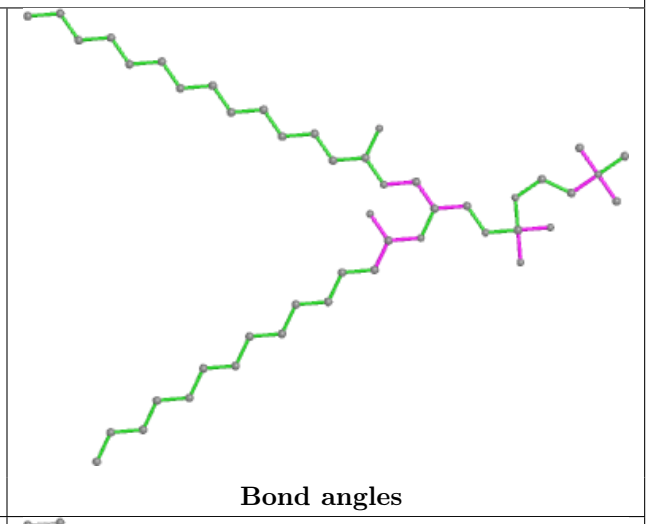
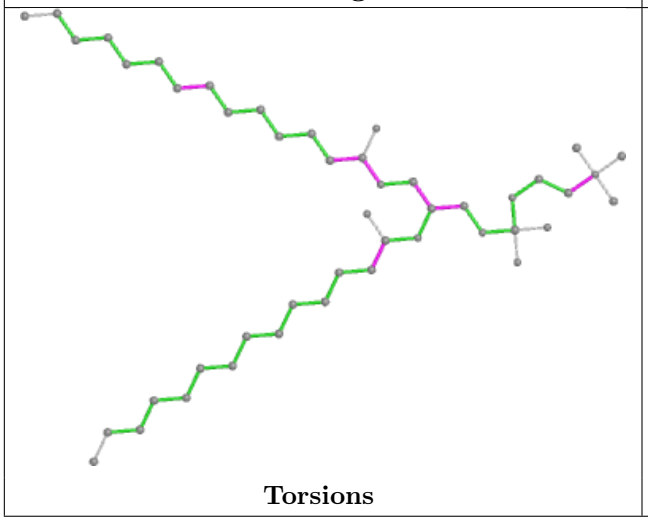


Bond angles



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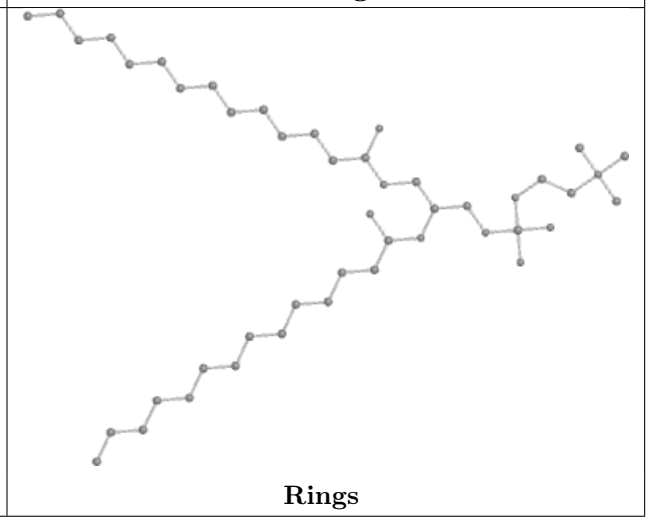
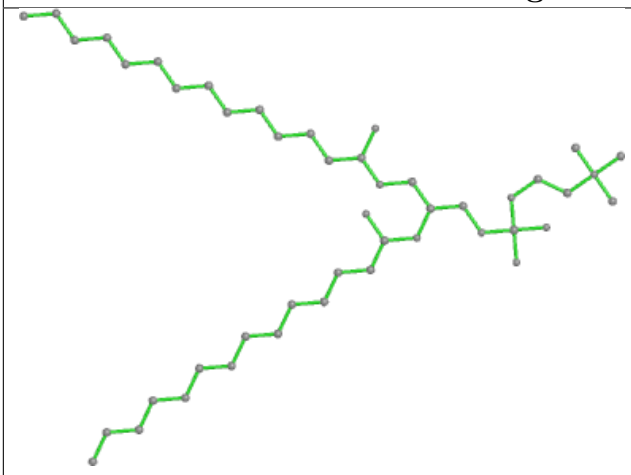


Rings

Ligand PX4 A 405



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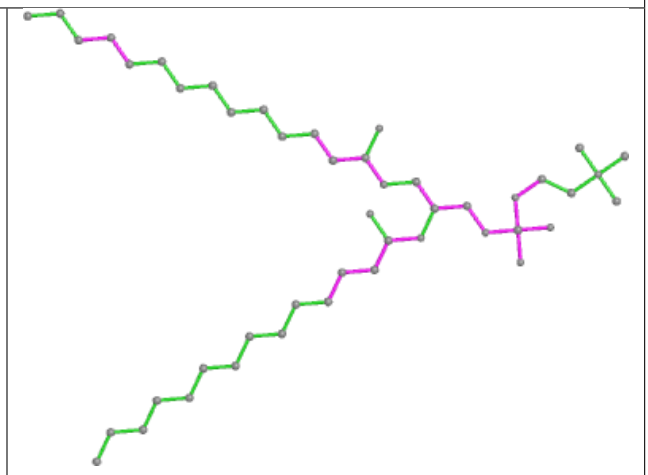

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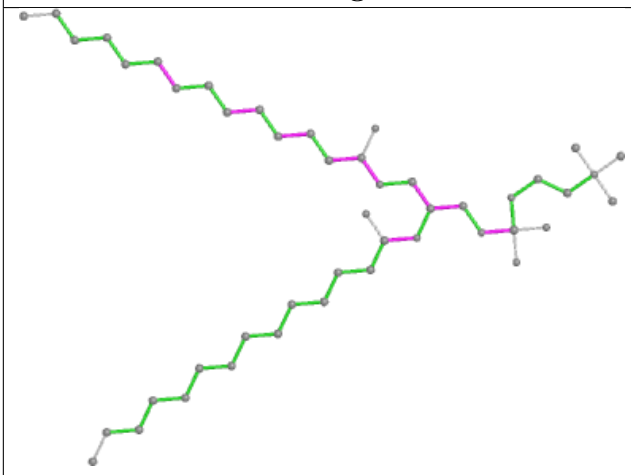

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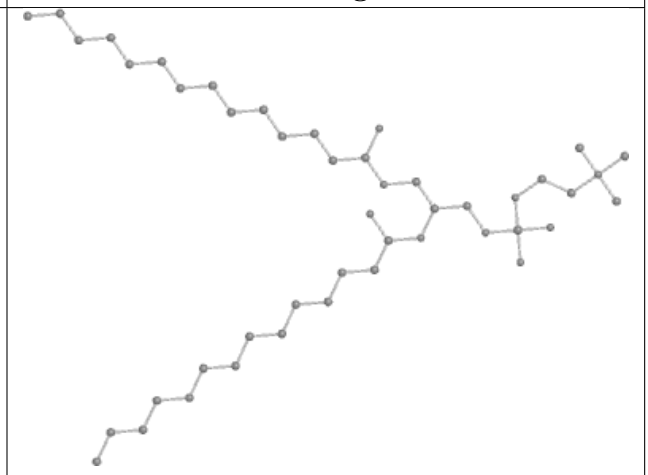
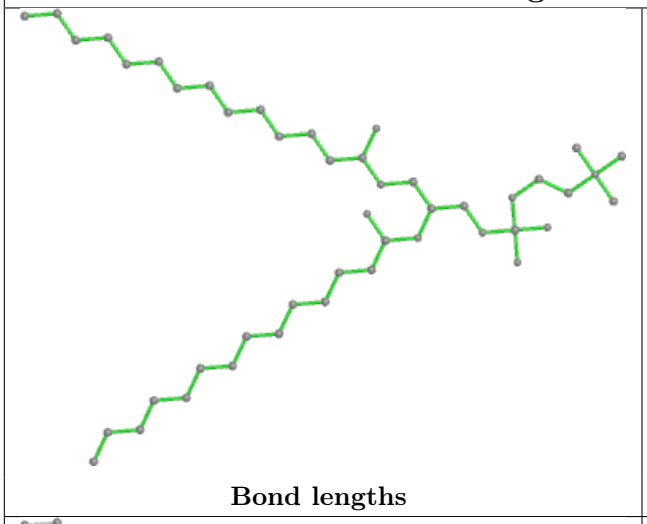


Rings

Ligand PX4 A 425



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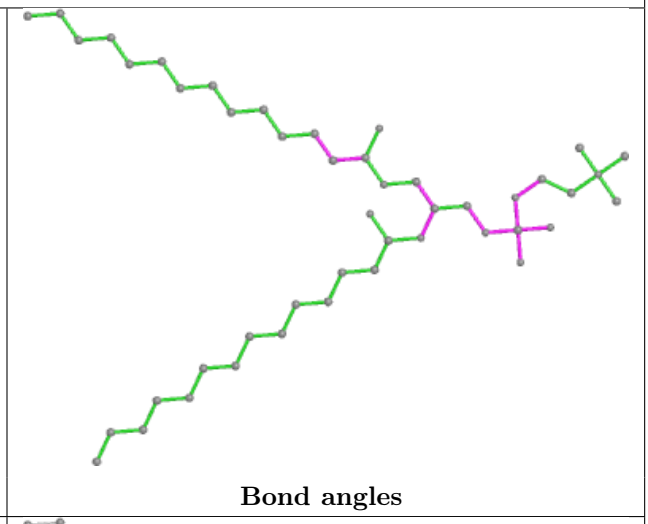
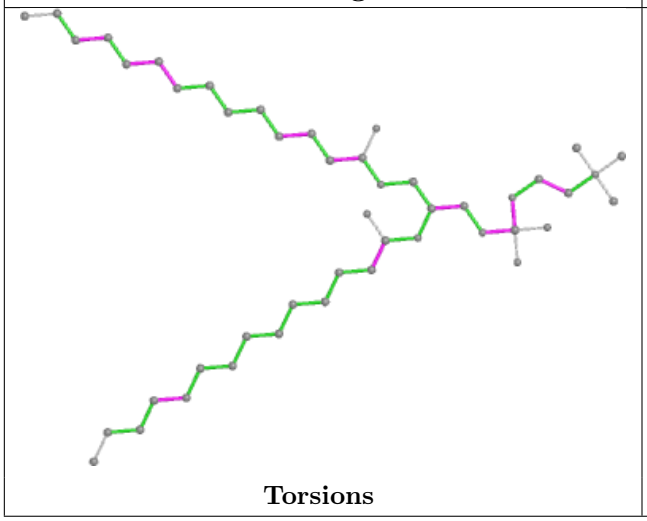


Bond angles



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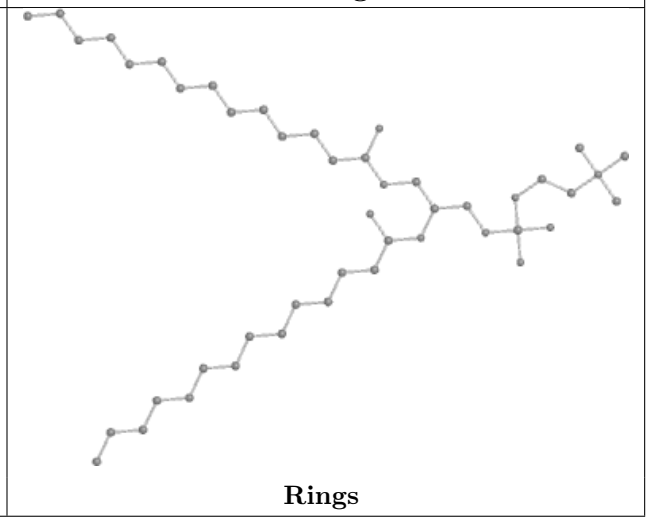
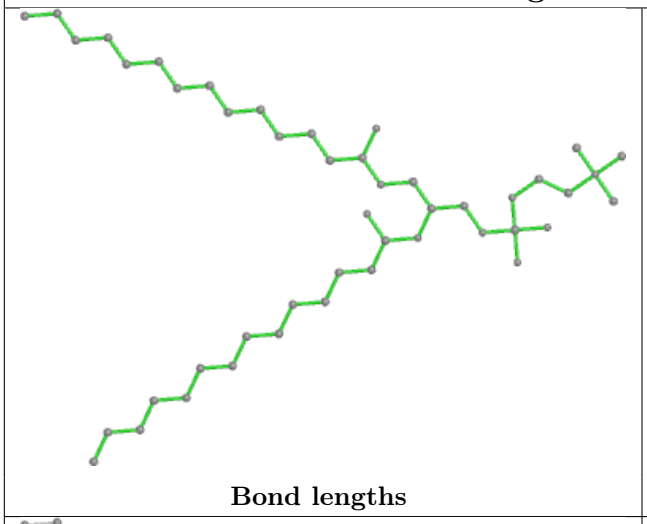
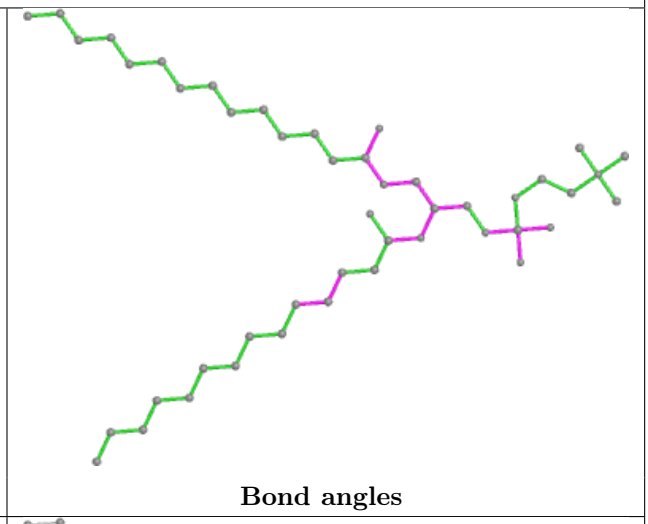


Rings

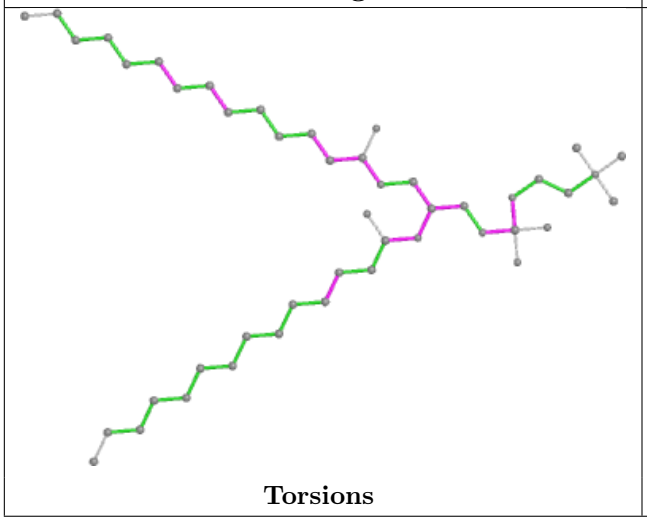
Ligand PX4 A 350



Bond lengths



Bond angles



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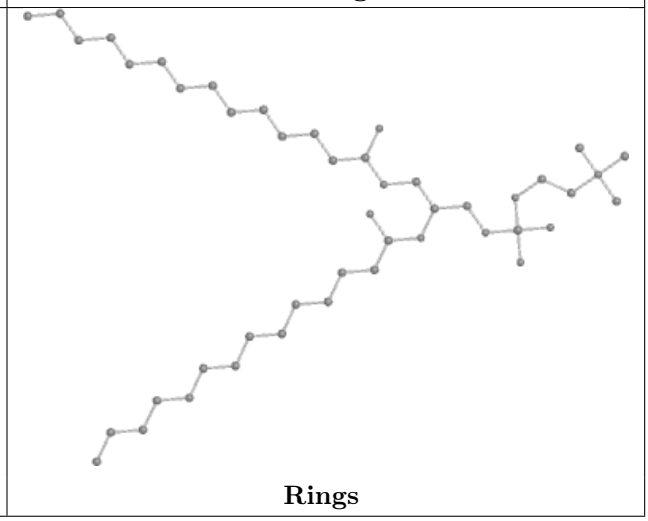
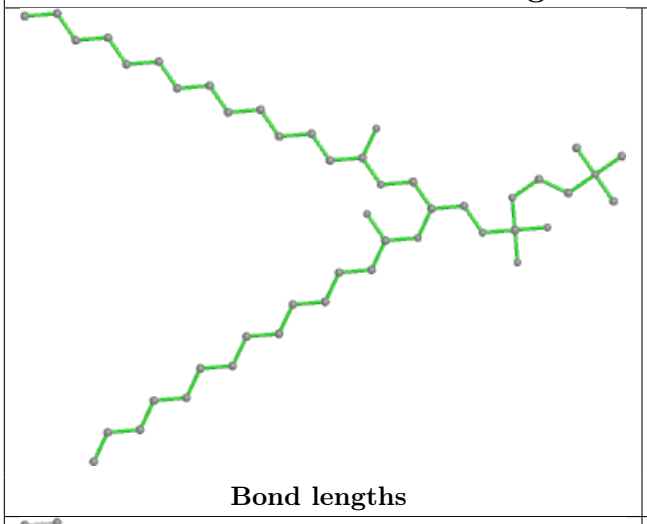
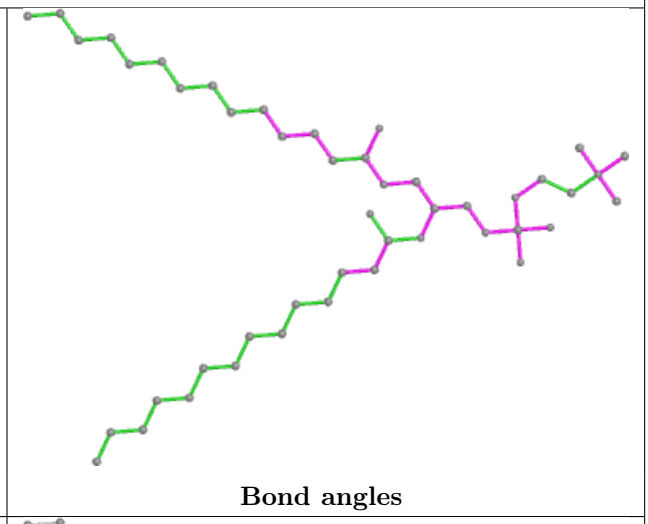


Rings

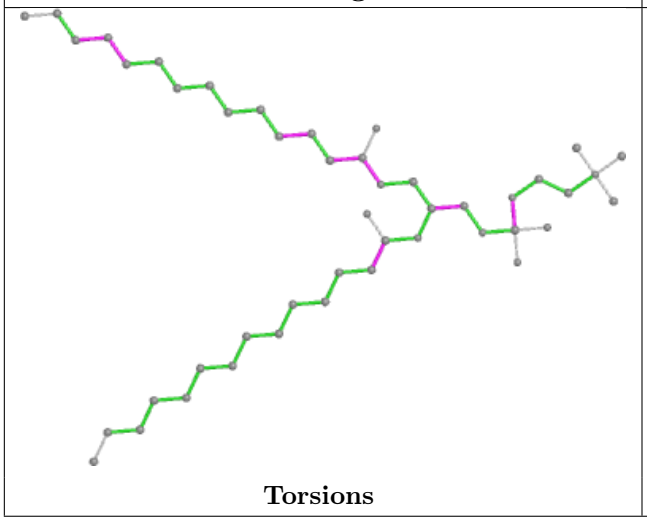
Ligand PX4 A 381



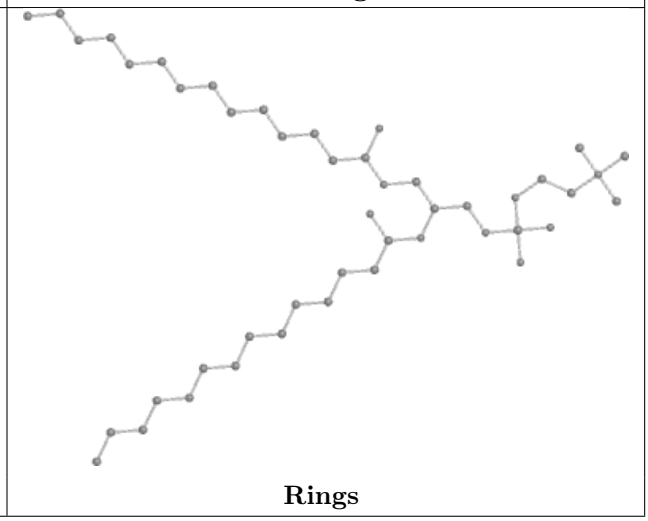
Bond lengths



Bond angles

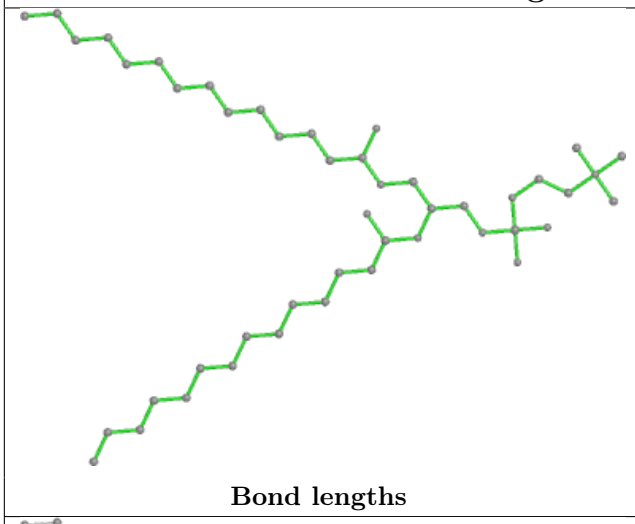


Torsions

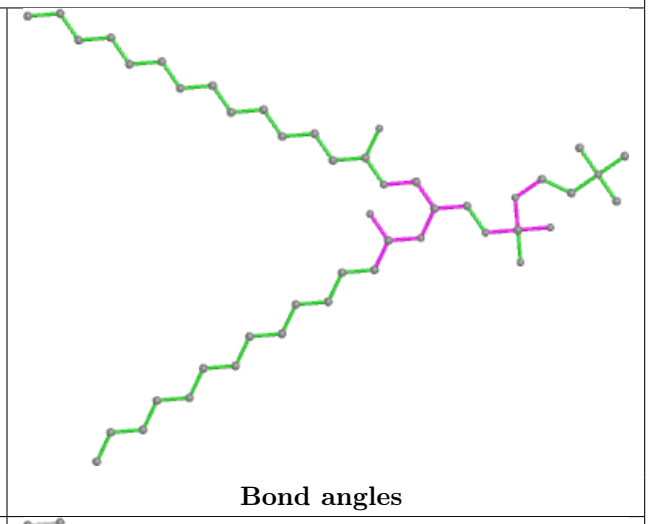


Rings

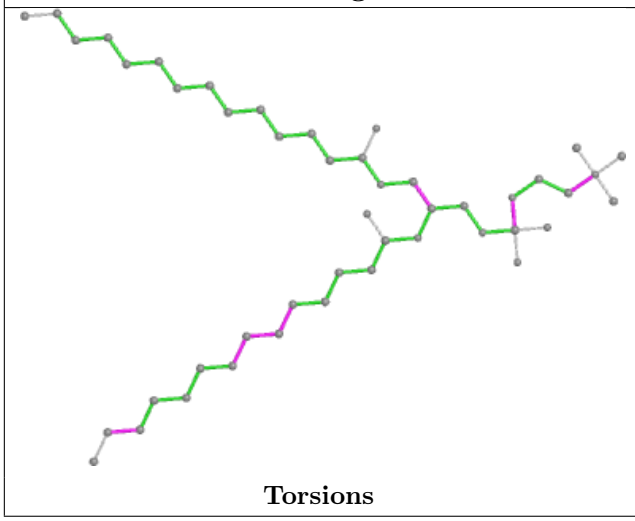
Ligand PX4 A 322



Bond lengths



Bond angles



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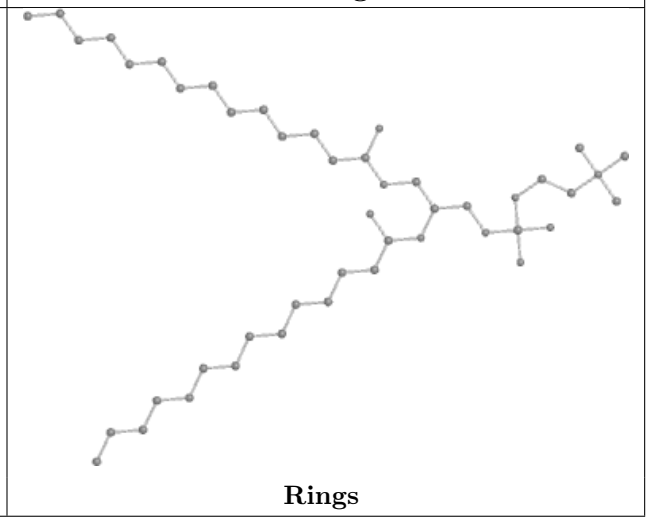
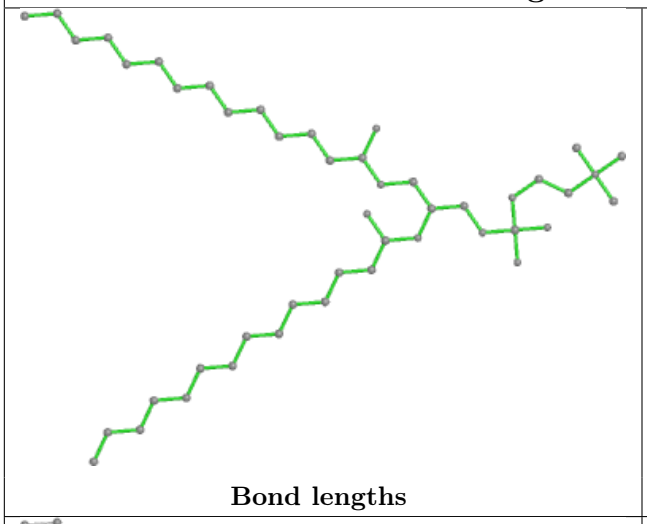


Rings

Ligand PX4 A 415



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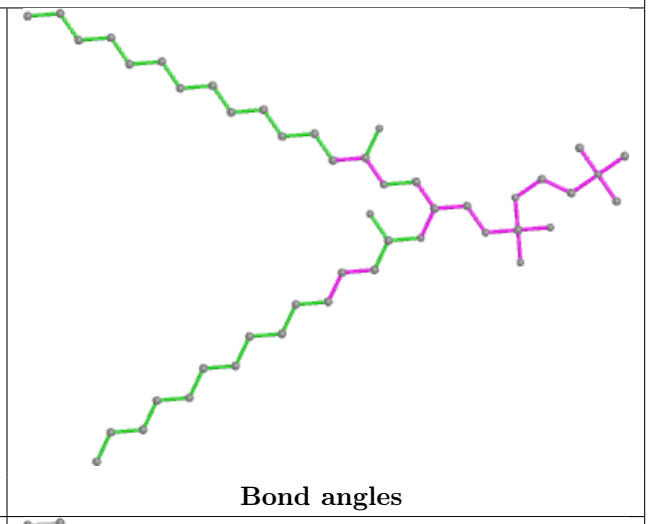
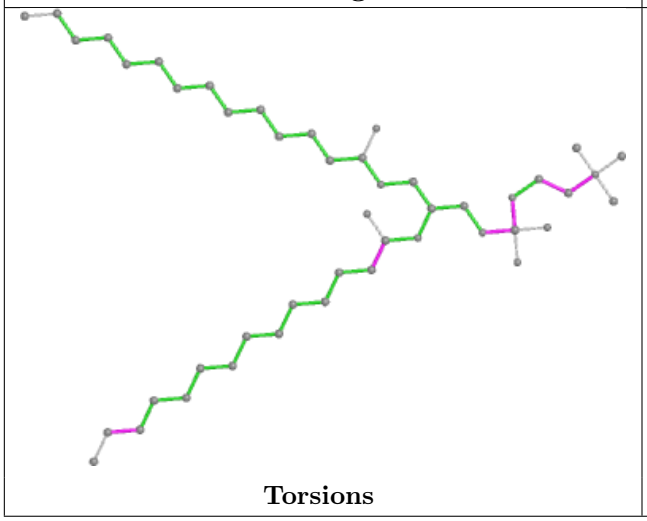


Bond angles



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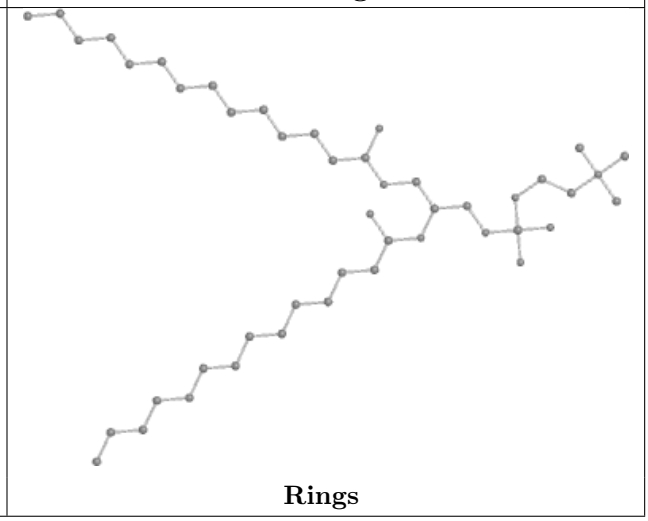
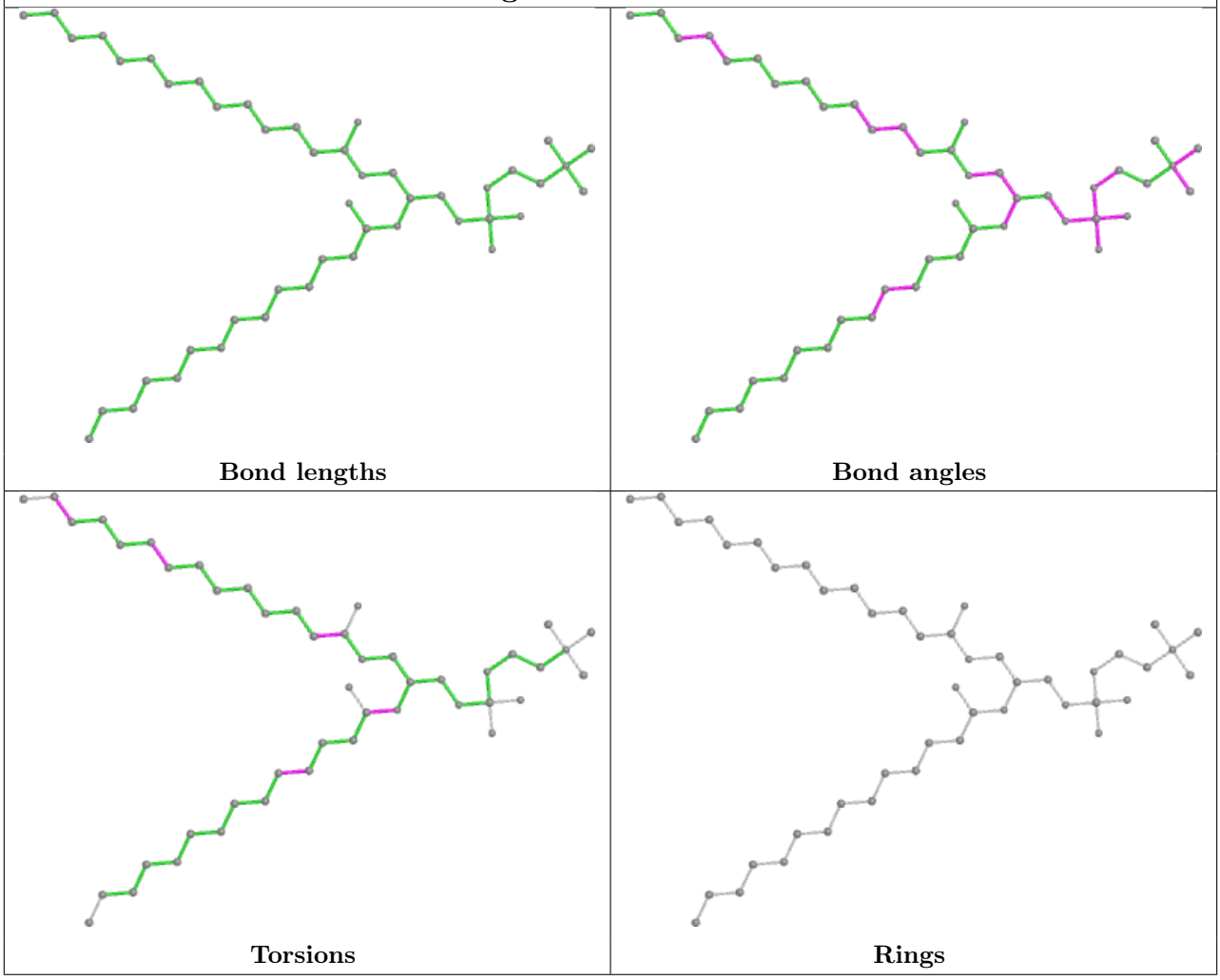
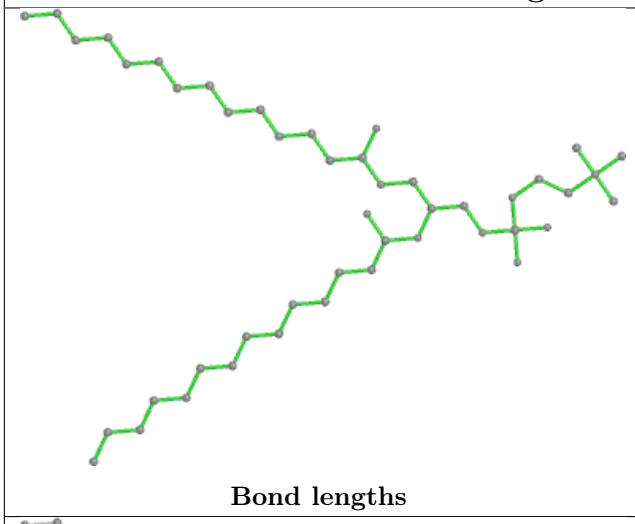


Rings

Ligand PX4 A 351



Ligand PX4 A 393



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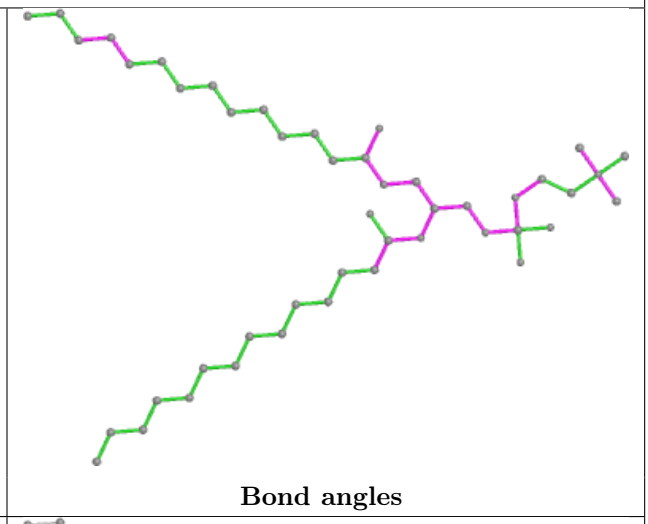
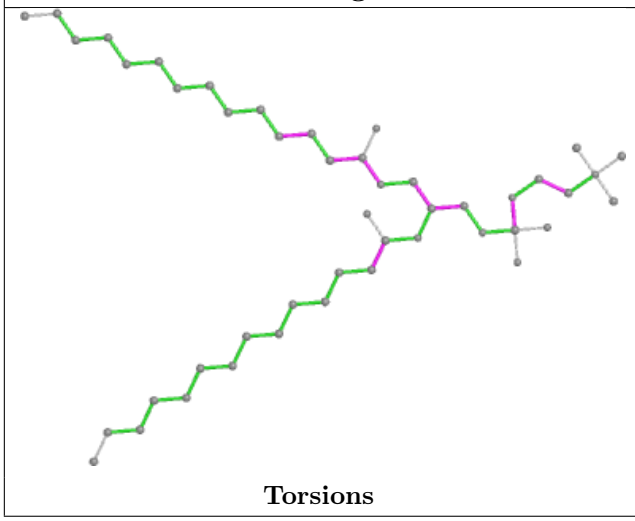


Bond angles



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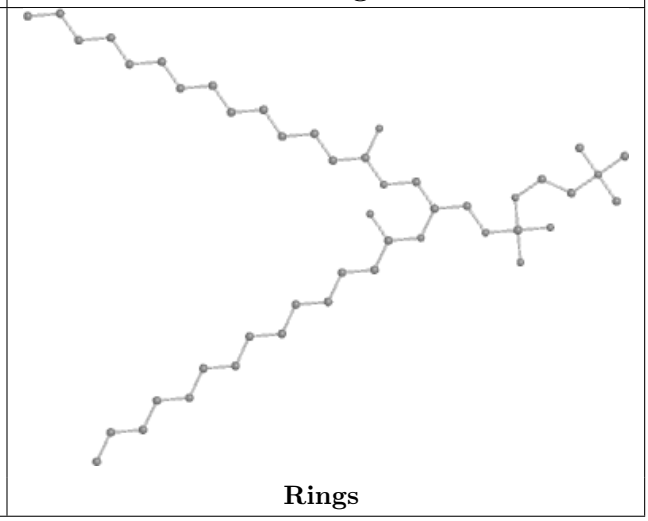
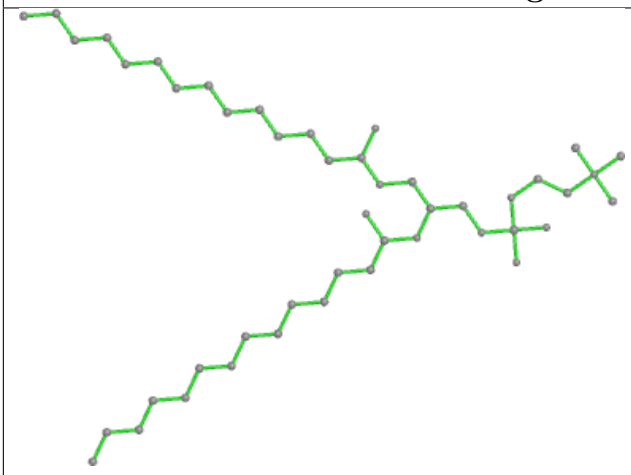


Rings

Ligand PX4 A 334



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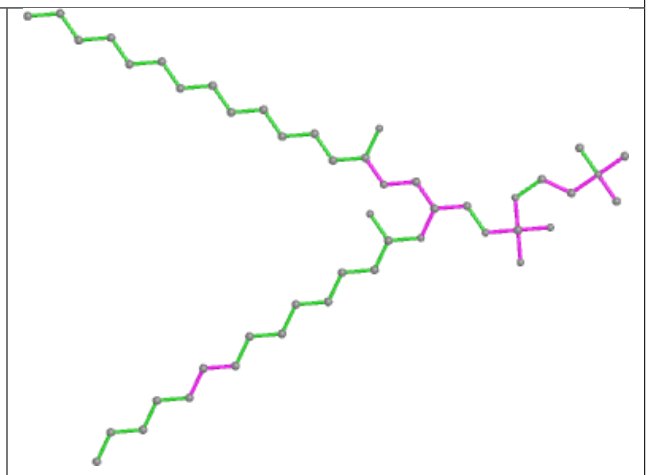
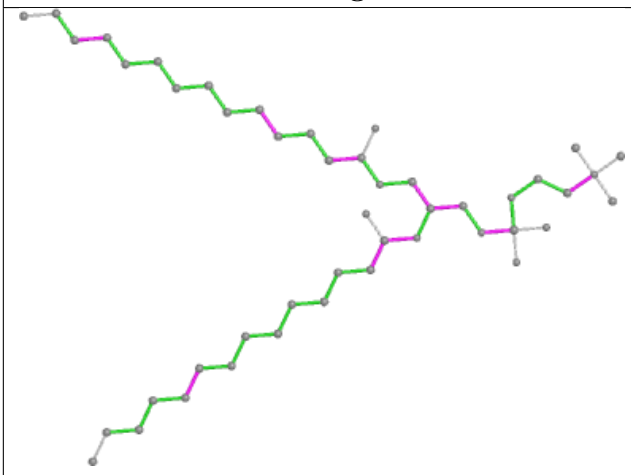


Bond angles



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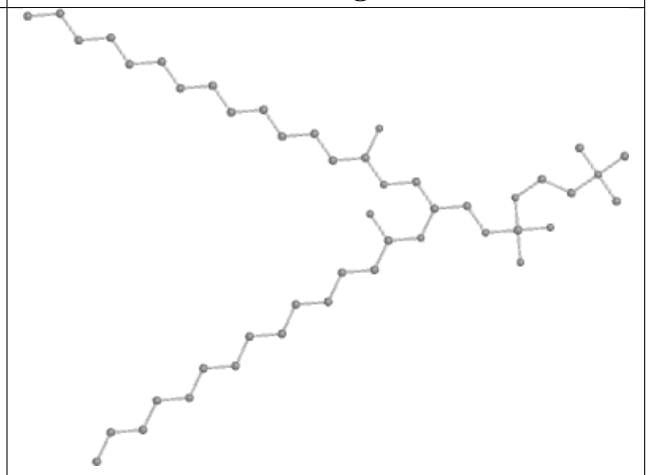
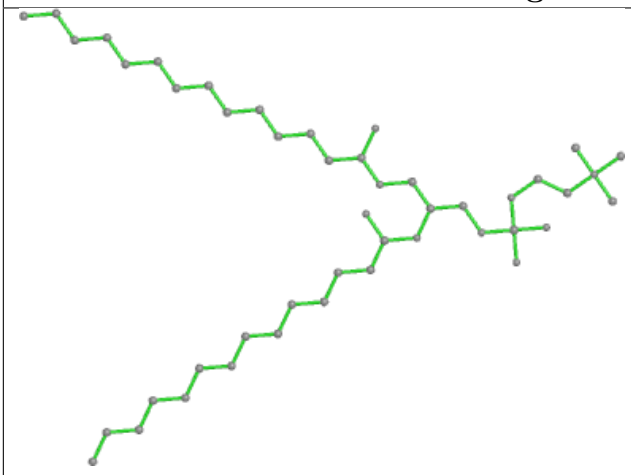
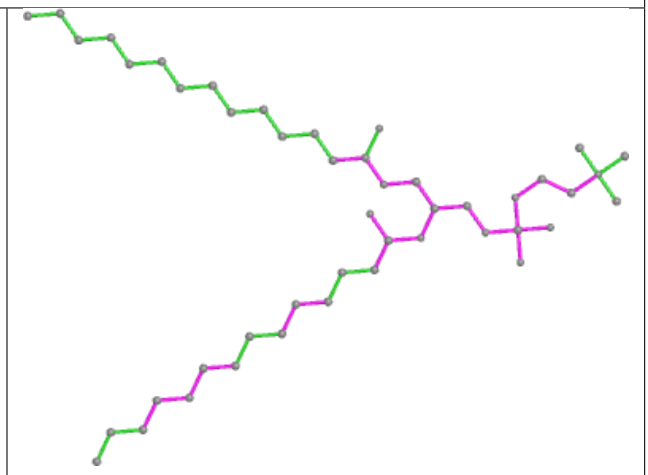


Rings

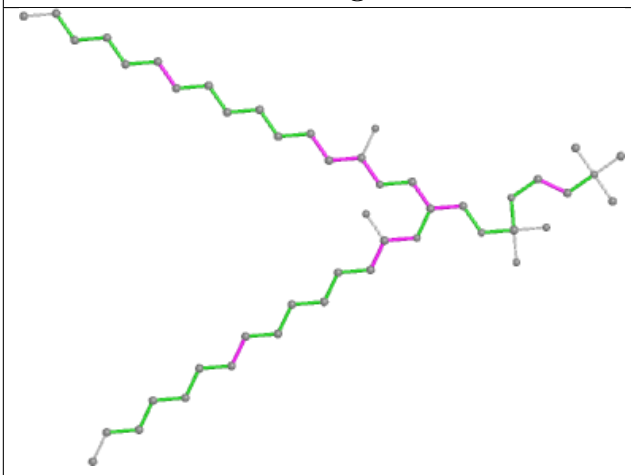
Ligand PX4 A 407



Bond lengths



Bond angles



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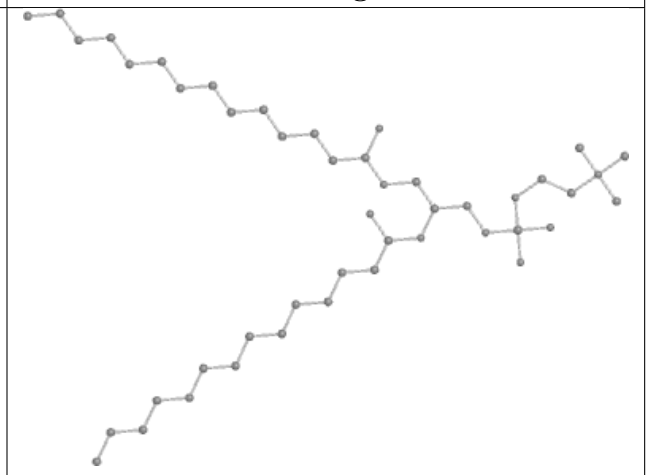
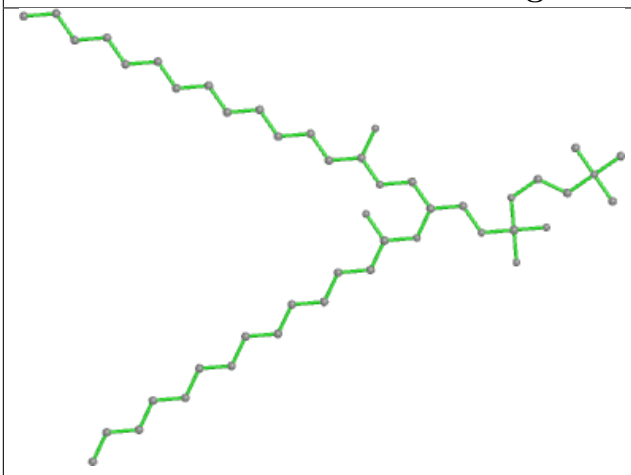


Rings

Ligand PX4 A 416



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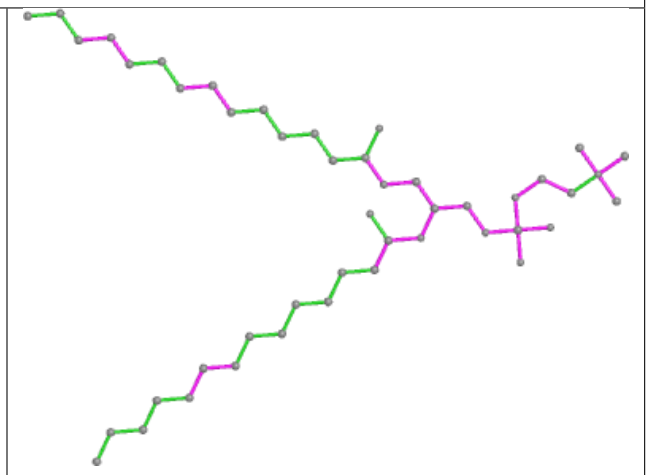
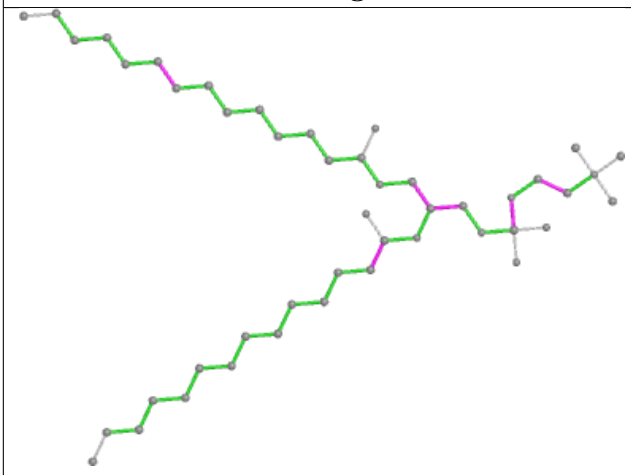


Bond angles



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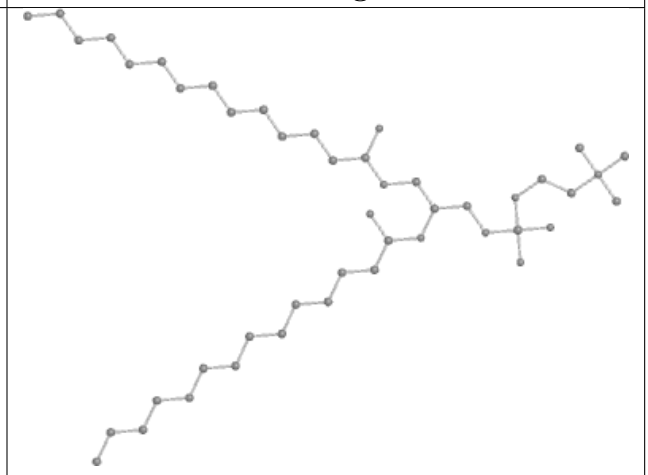
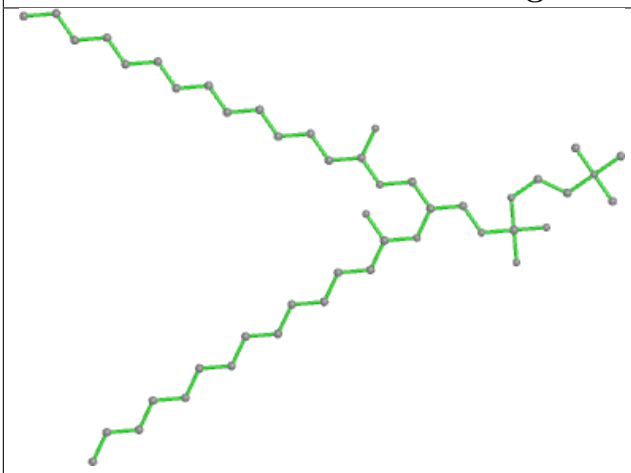


Rings

Ligand PX4 A 402



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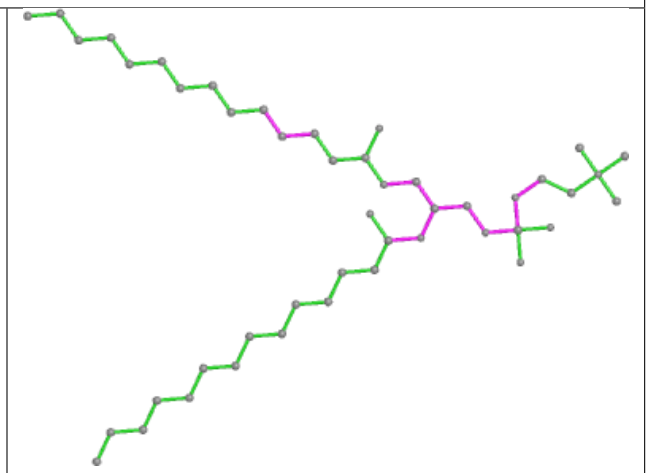
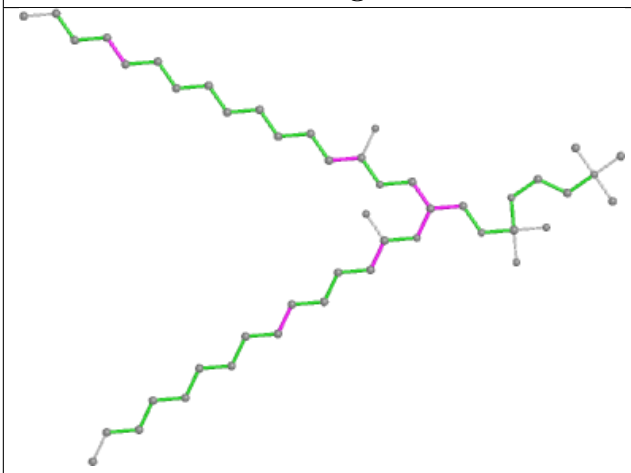


Bond angles



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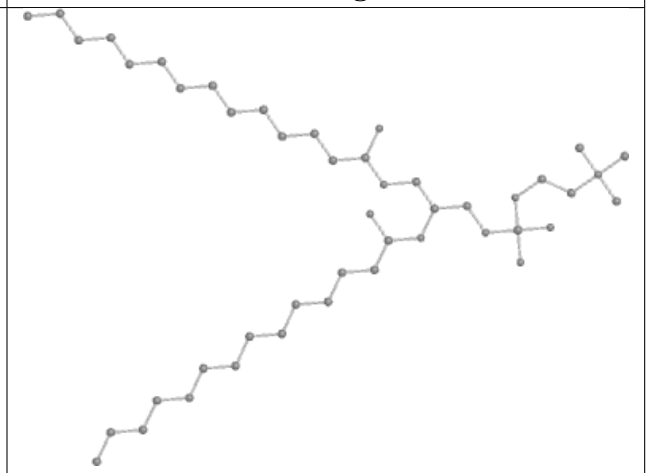
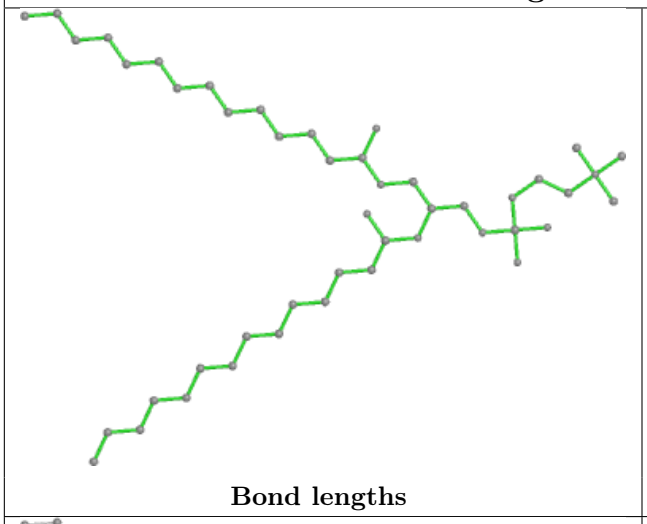


Rings

Ligand PX4 A 343



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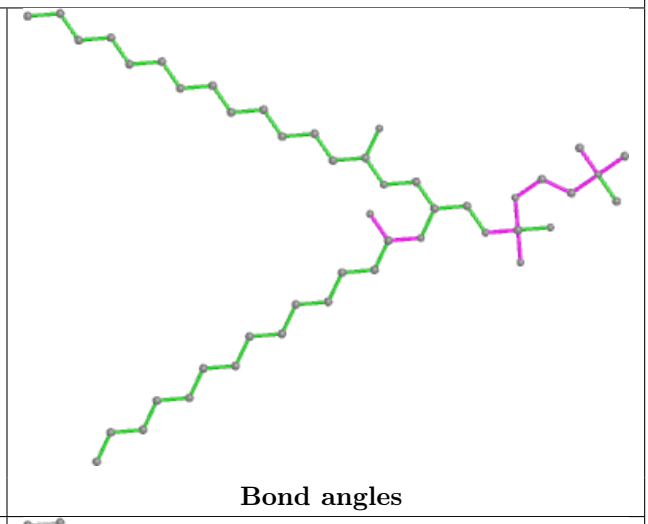
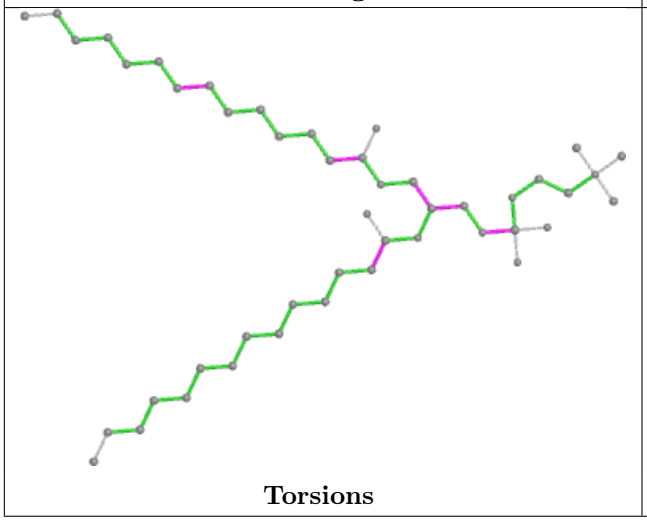


Bond angles



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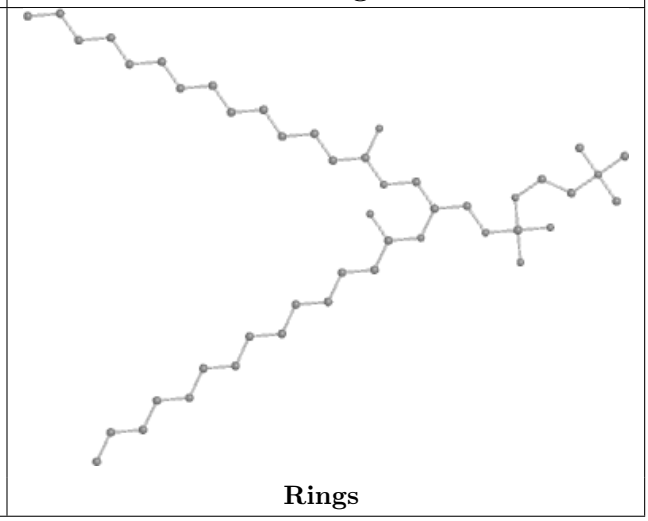
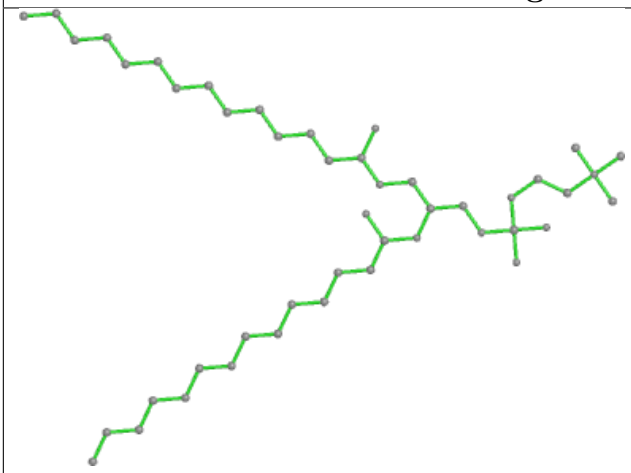


Rings

Ligand PX4 A 309



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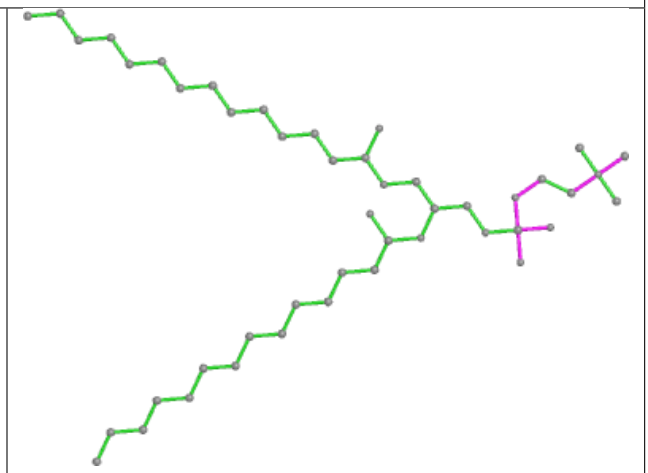
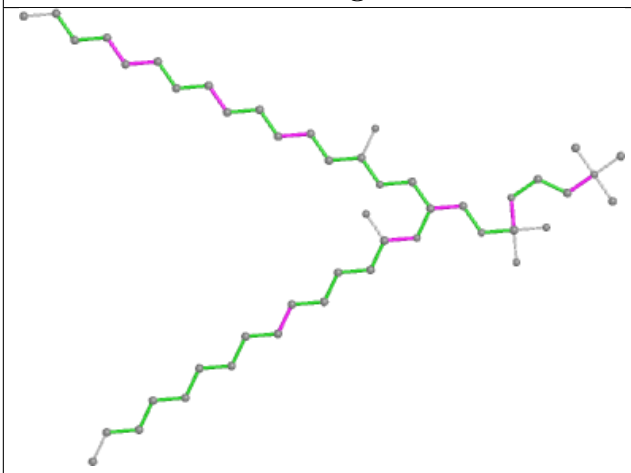


Bond angles



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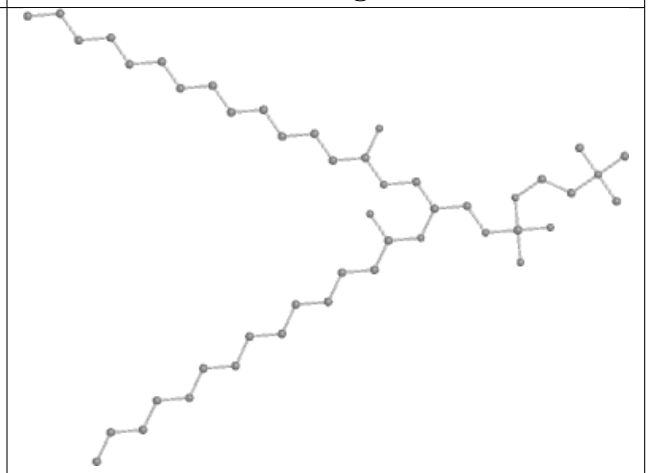
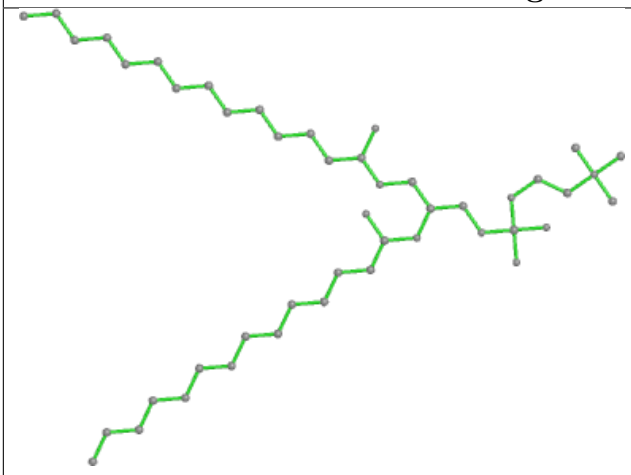
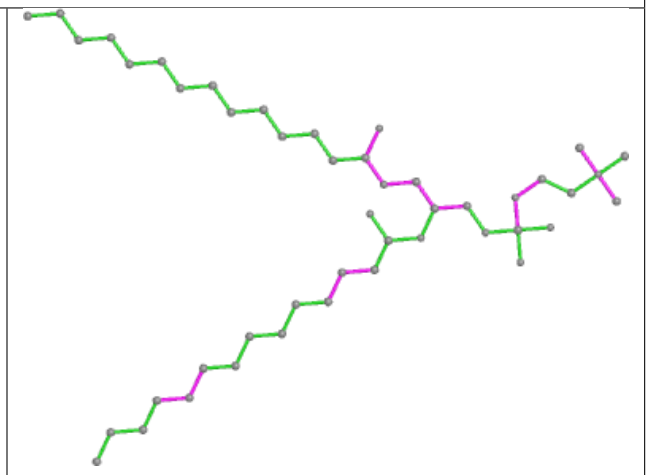


Rings

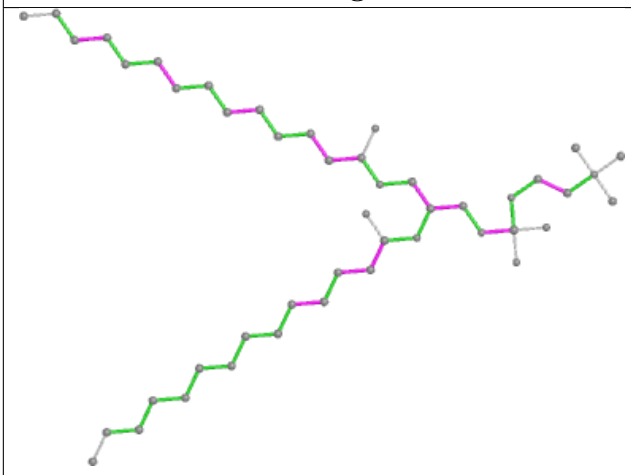
Ligand PX4 A 428



Bond lengths



Bond angles



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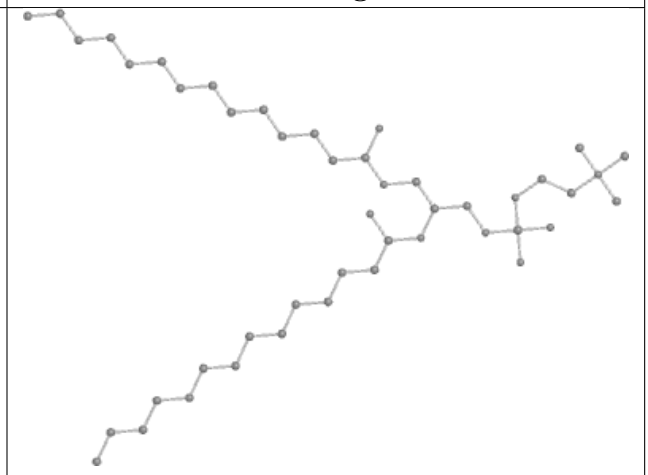
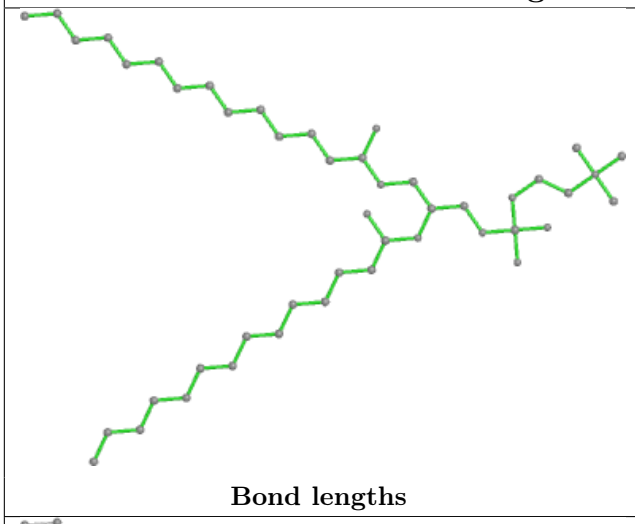


Rings

Ligand PX4 A 399



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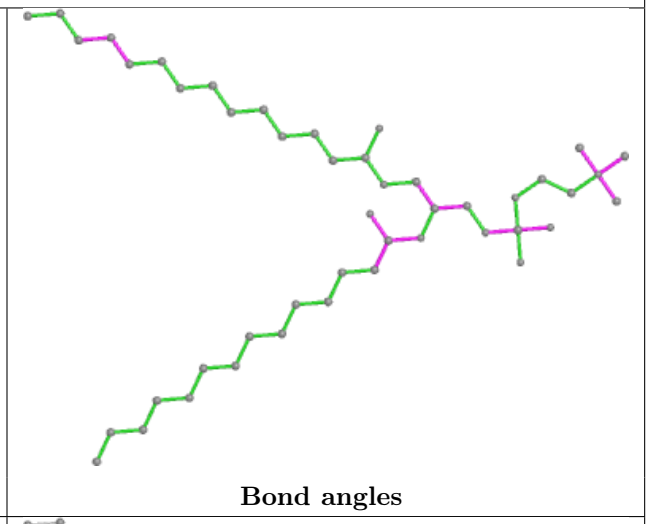
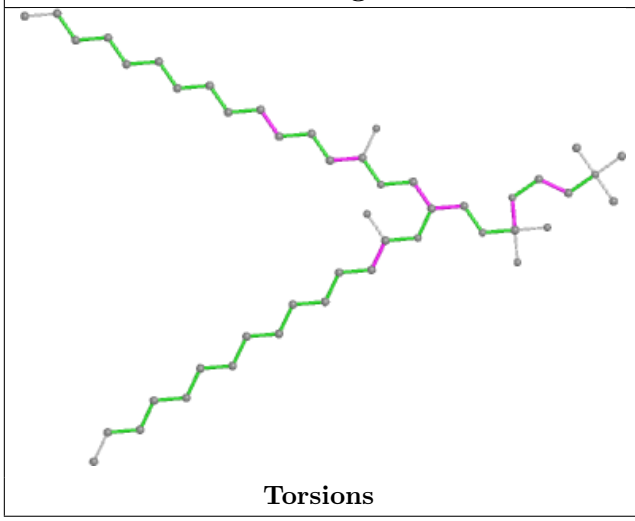


Bond angles



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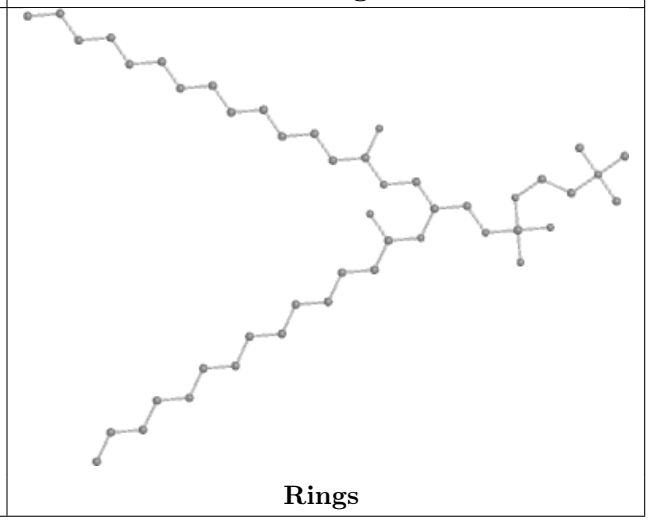
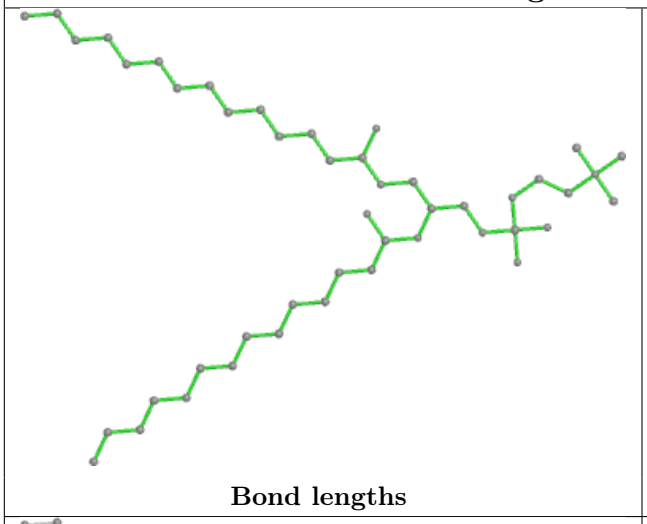


Rings

Ligand PX4 A 413



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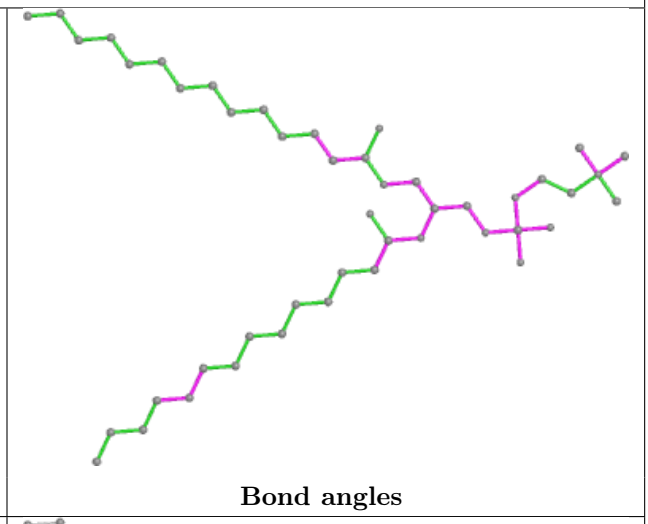
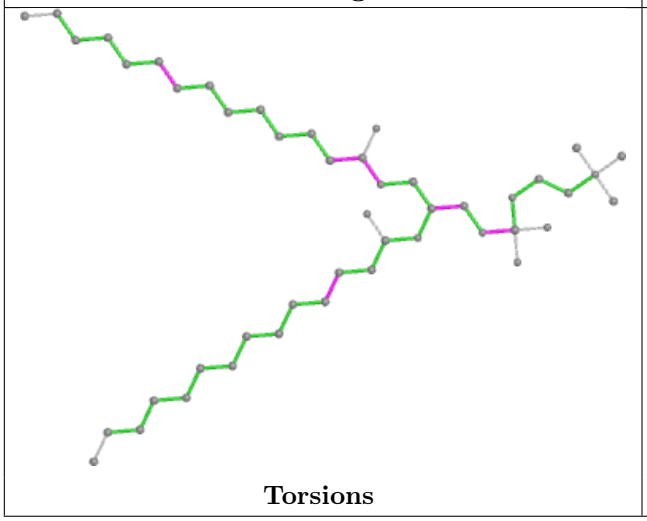
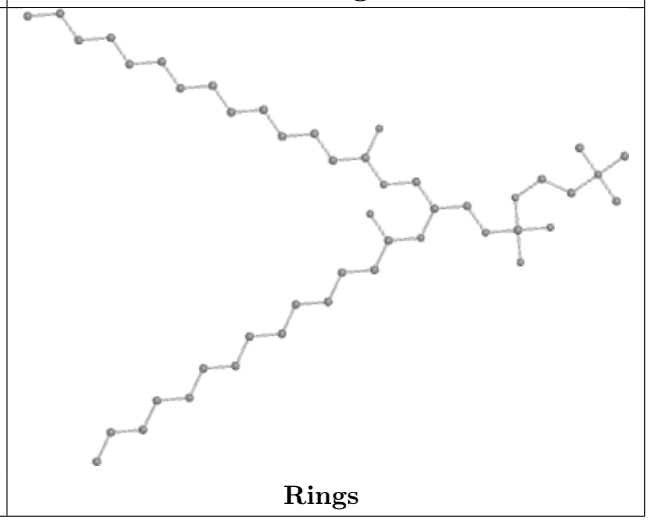


Bond angles

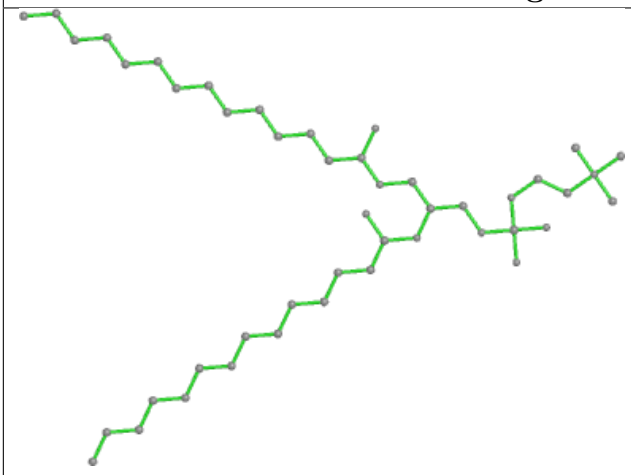


Torsions

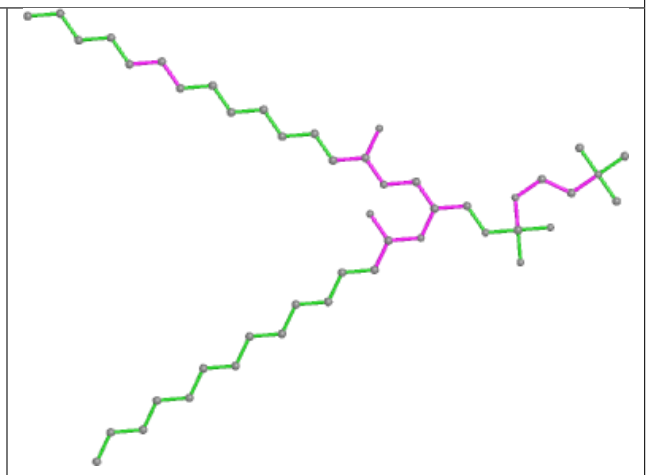


Rings

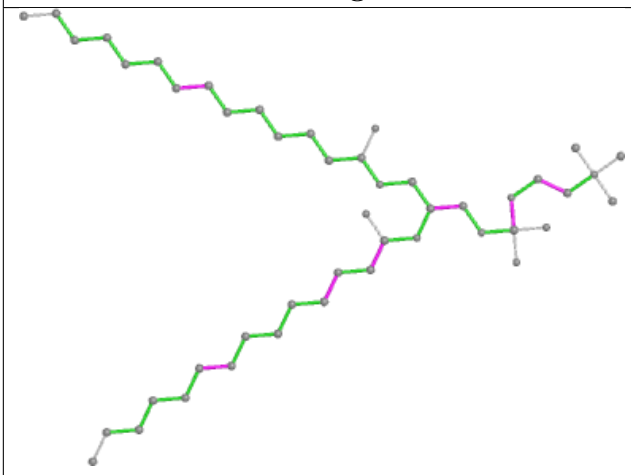
Ligand PX4 A 409



Bond lengths



Bond angles



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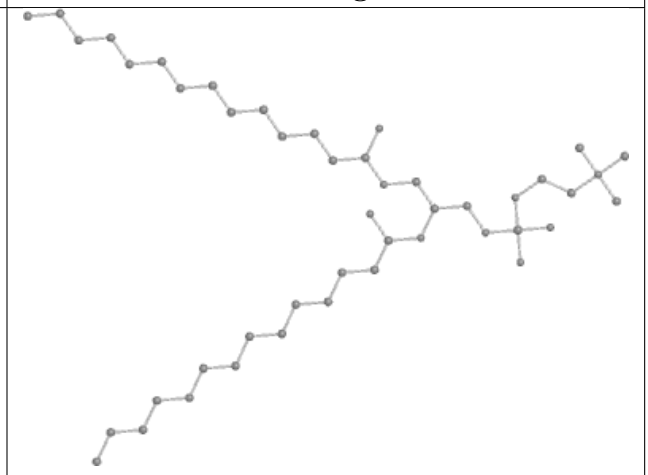
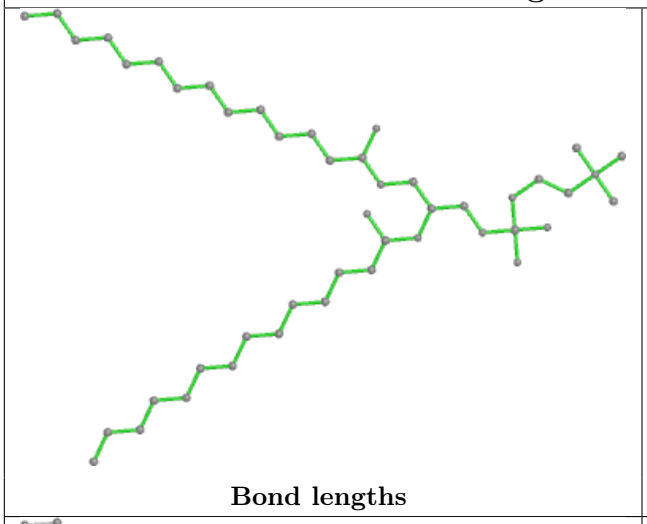


Rings

Ligand PX4 A 373



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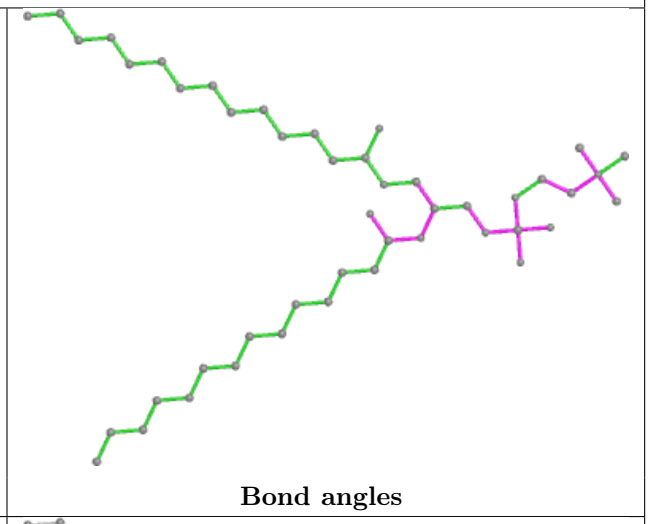
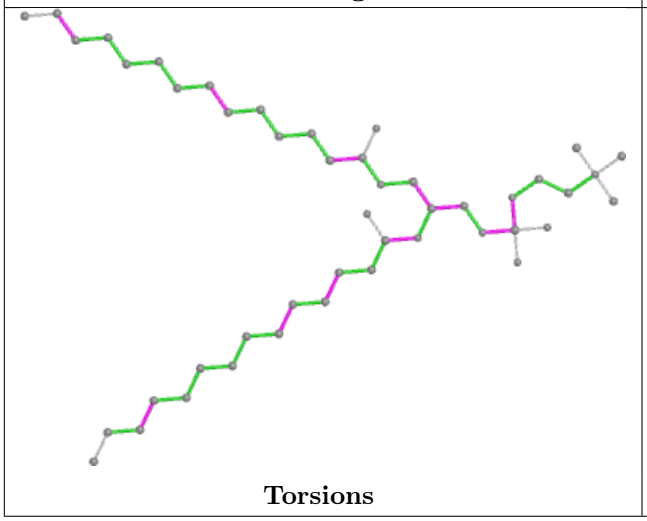


Bond angles



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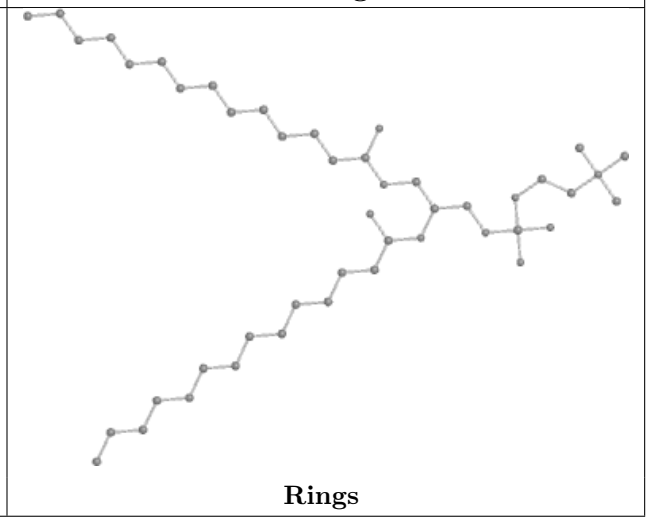
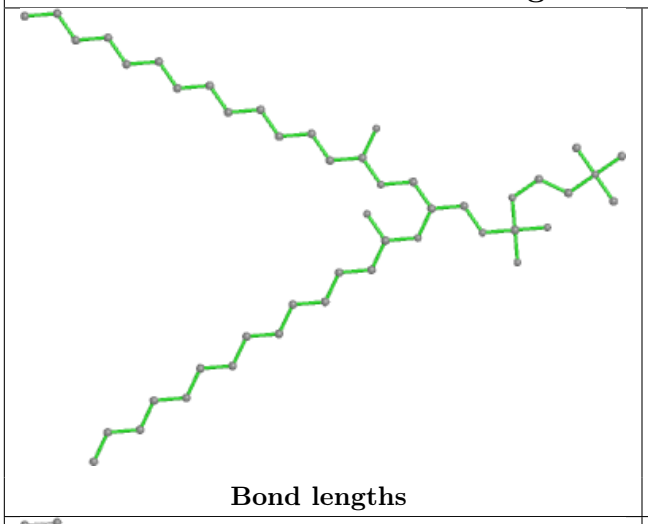


Rings

Ligand PX4 A 312



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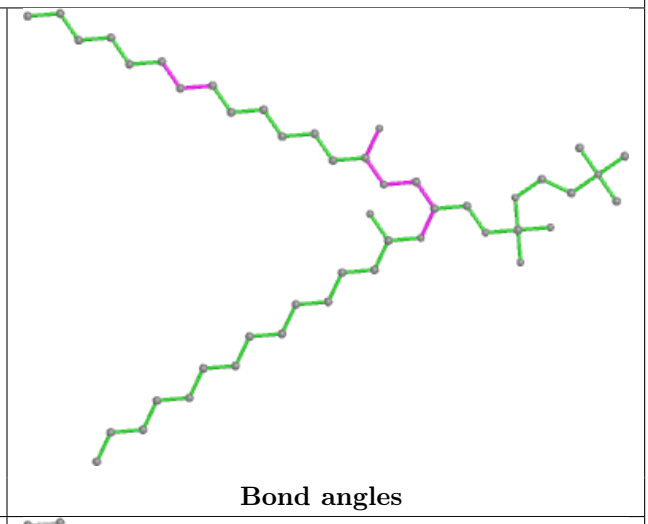

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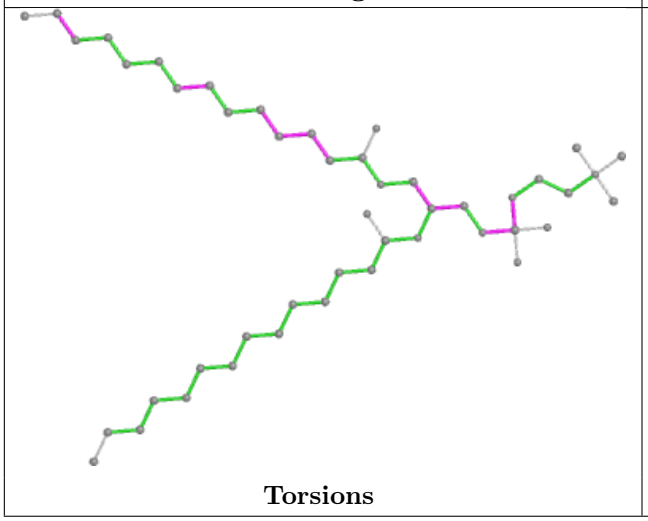

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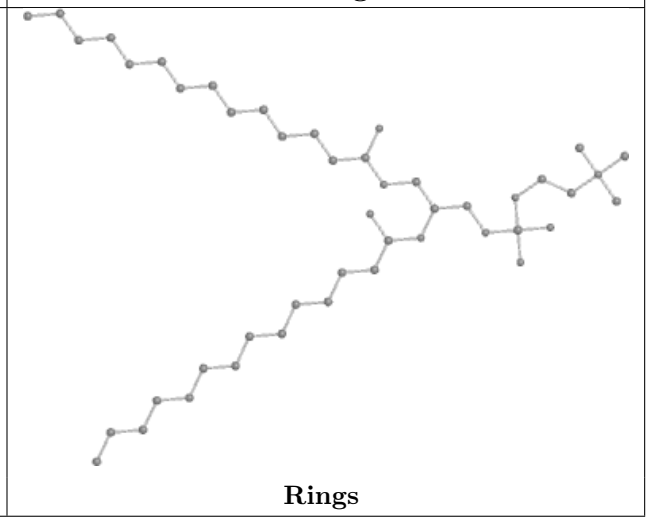
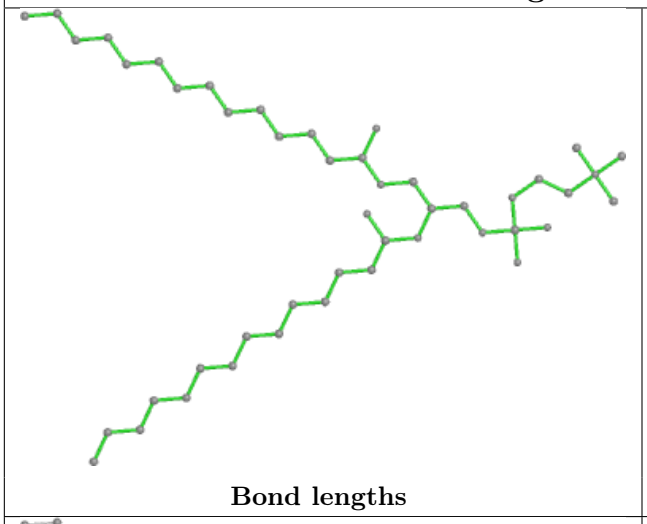


Rings

Ligand PX4 A 313



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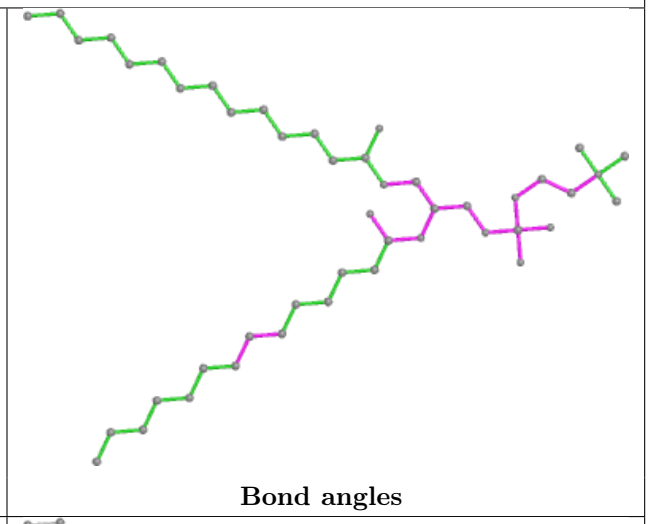

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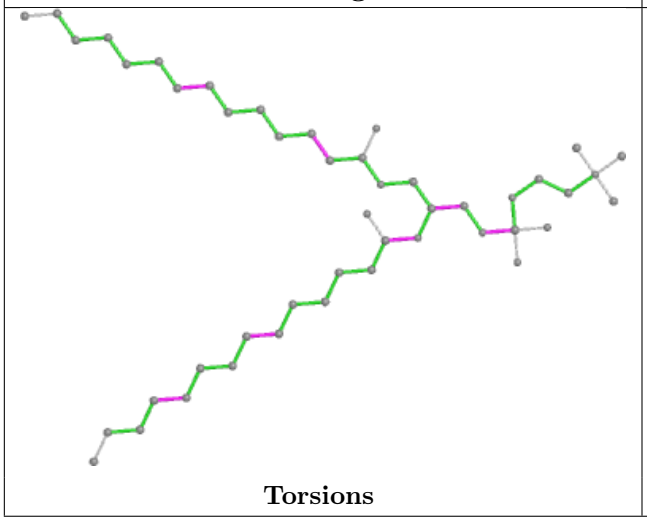

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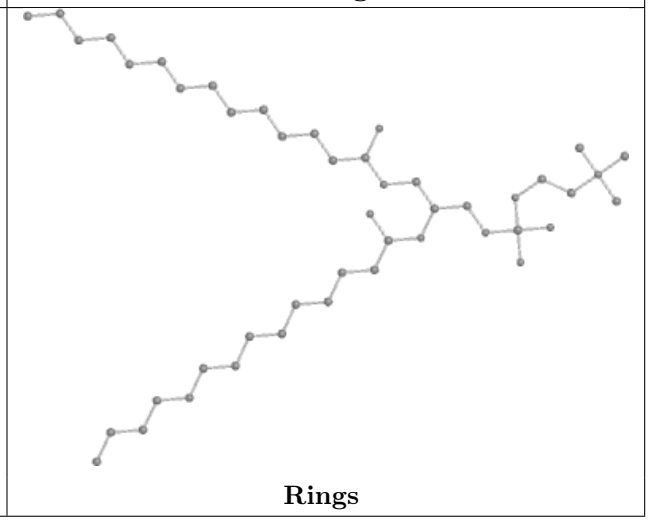
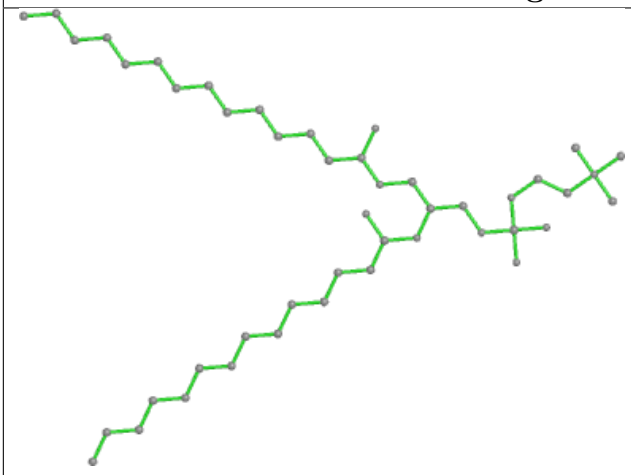


Rings

Ligand PX4 A 319



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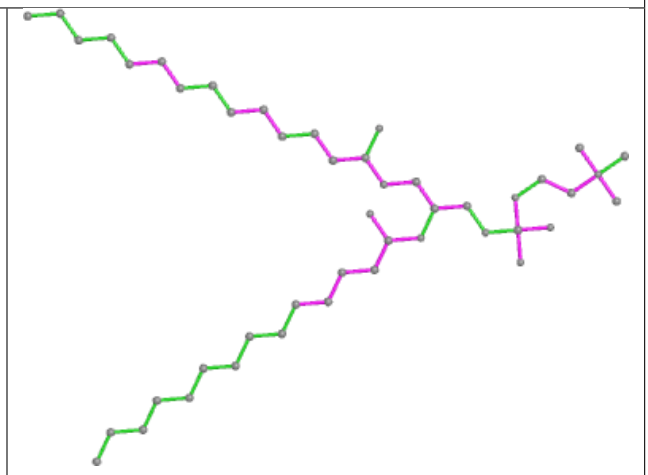
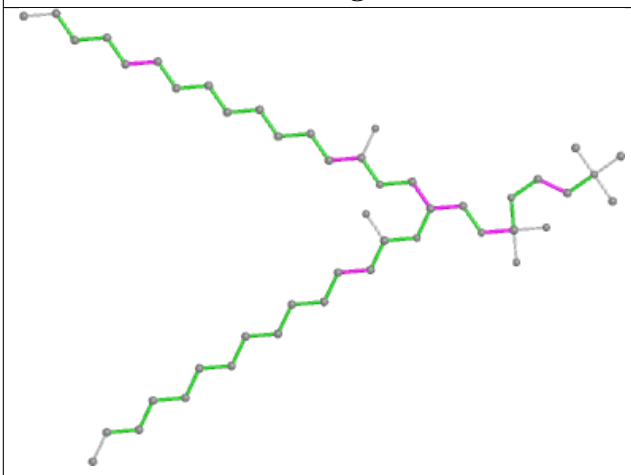


Bond angles



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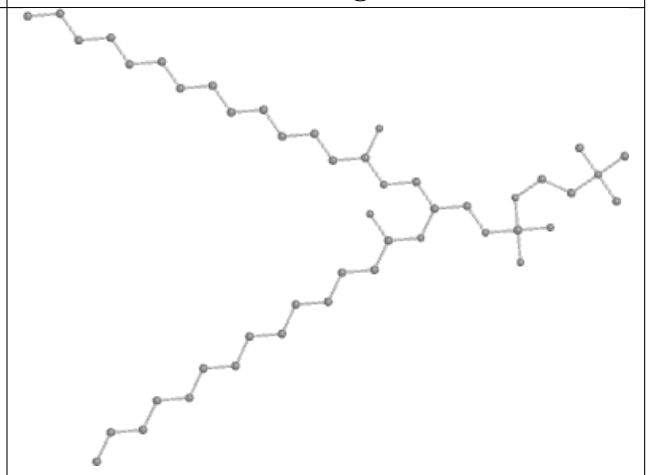
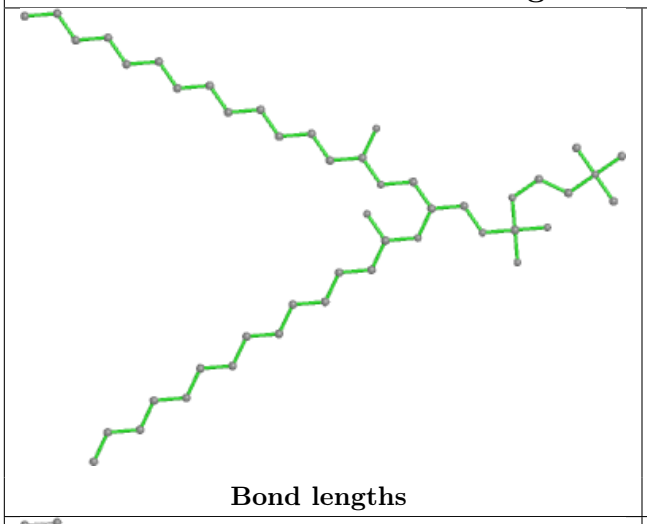


Rings

Ligand PX4 A 331



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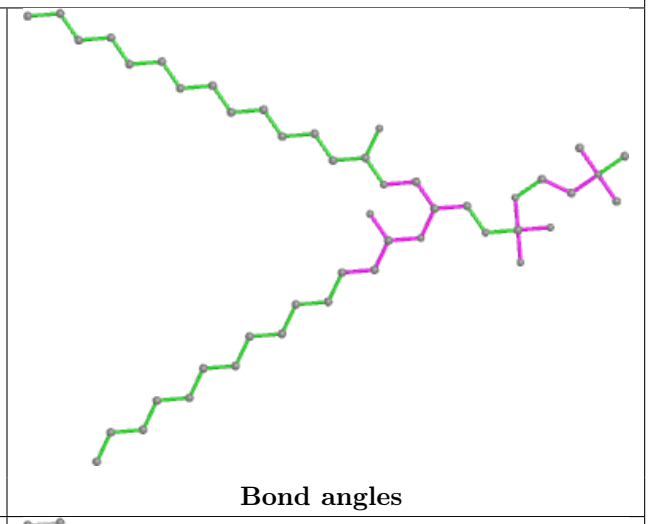
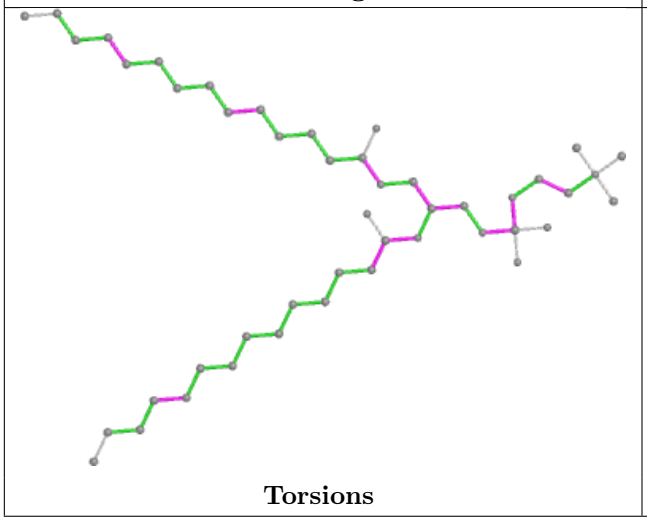


Bond angles



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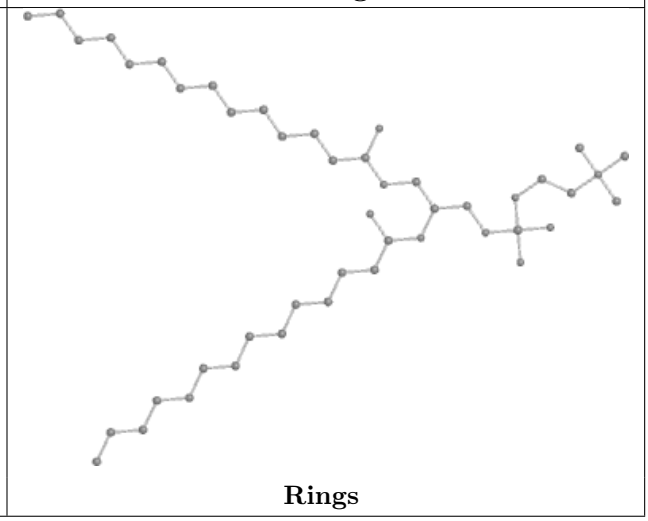
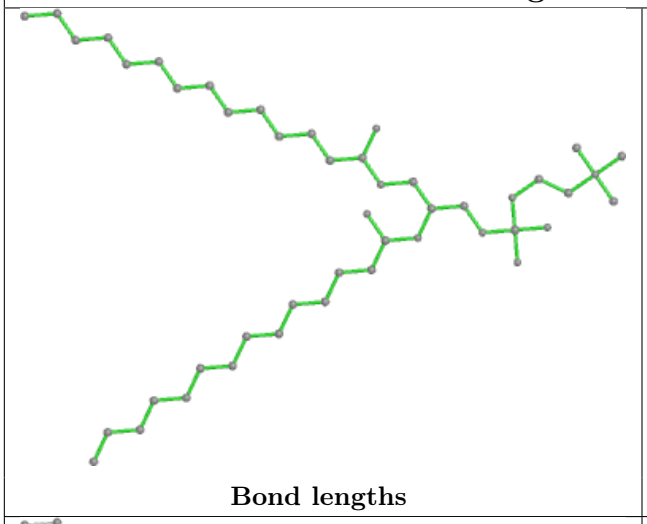


Rings

Ligand PX4 A 353



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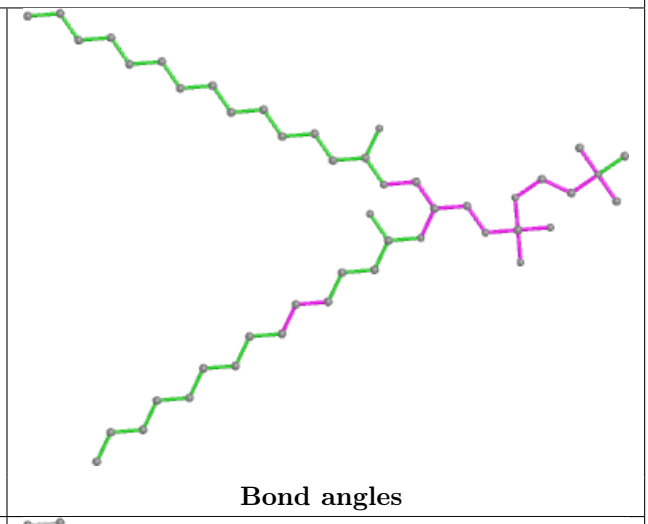
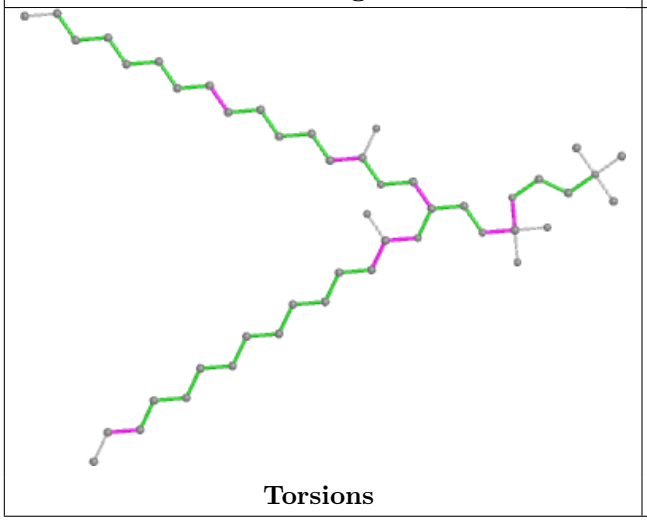


Bond angles



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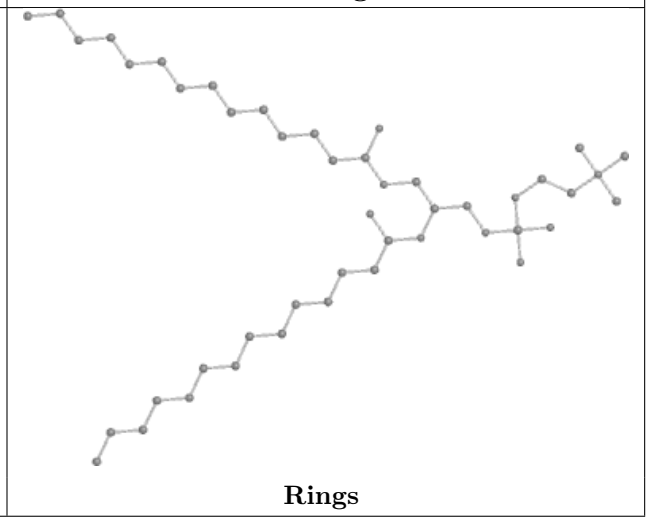
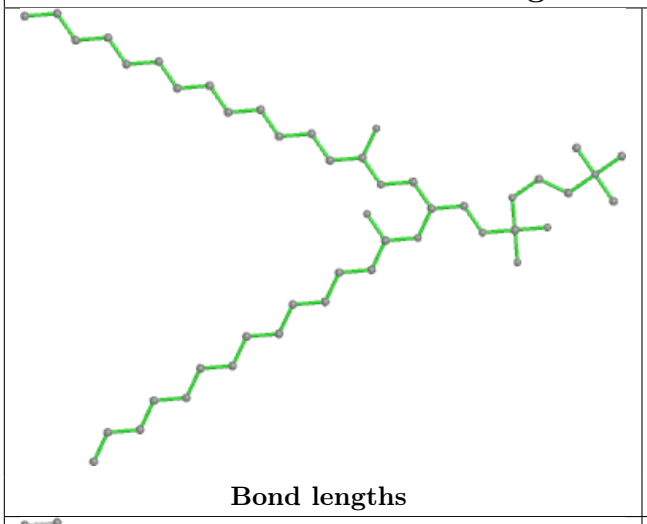


Rings

Ligand PX4 A 318



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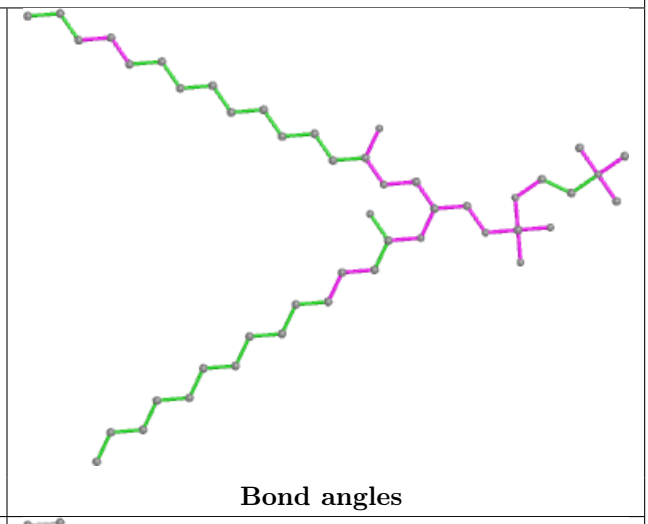

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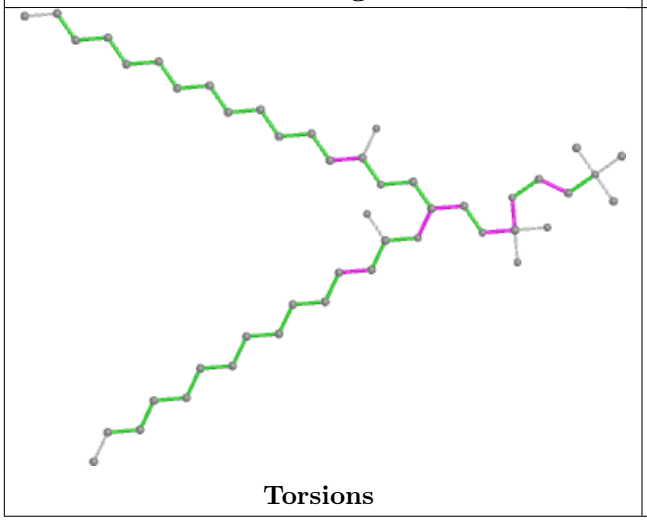

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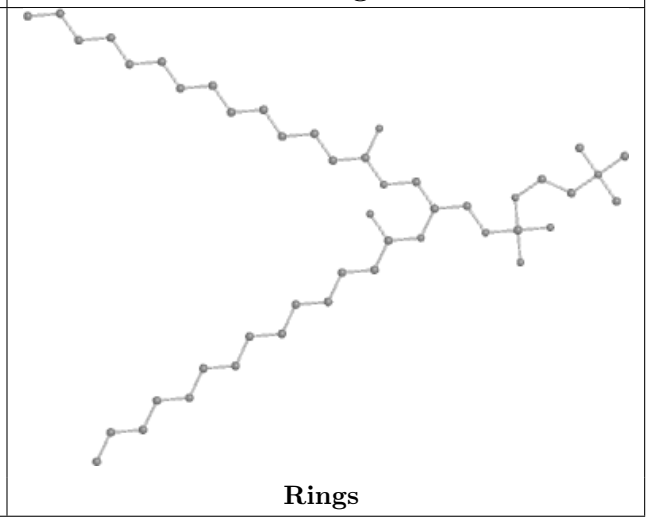
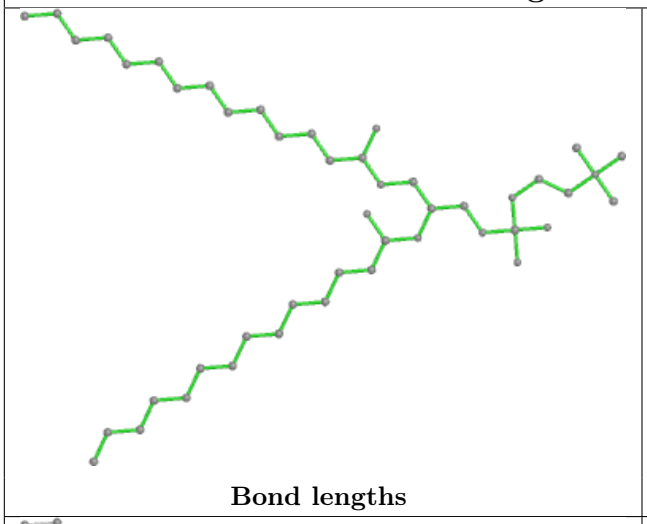


Rings

Ligand PX4 A 395



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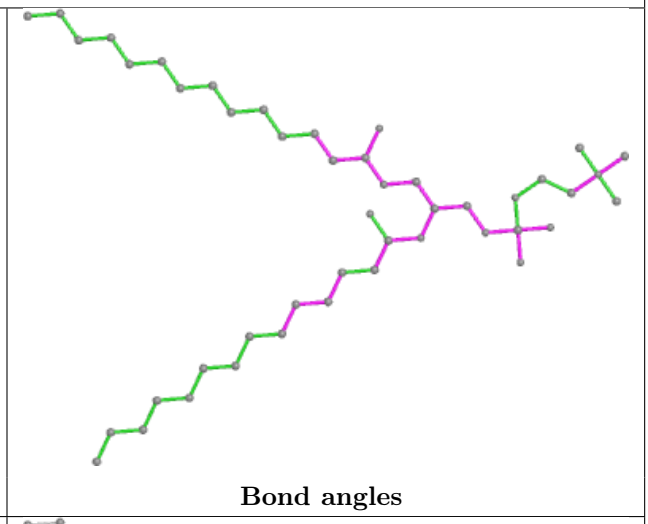
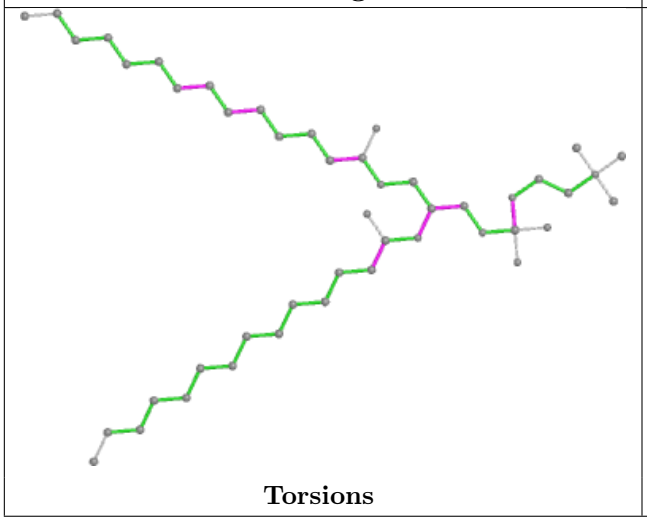


Bond angles



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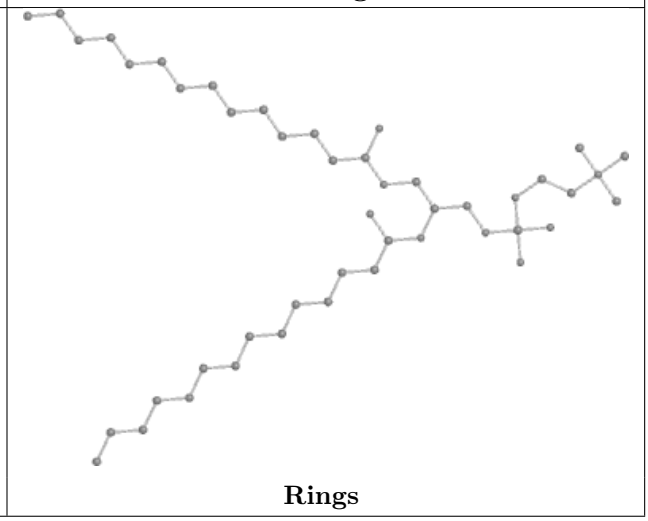
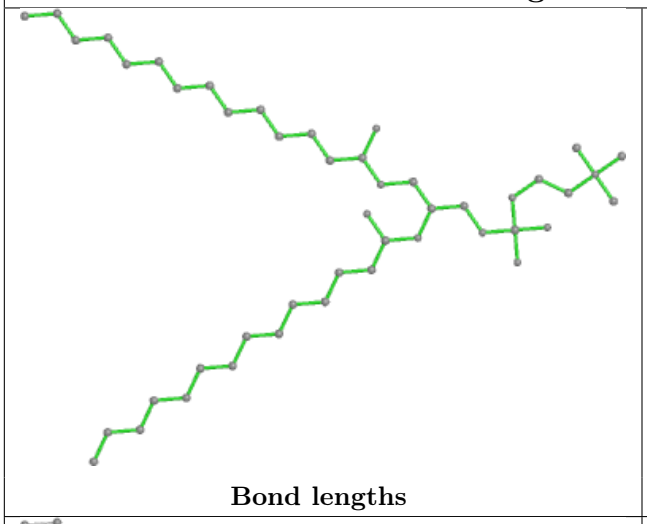


Rings

Ligand PX4 A 374



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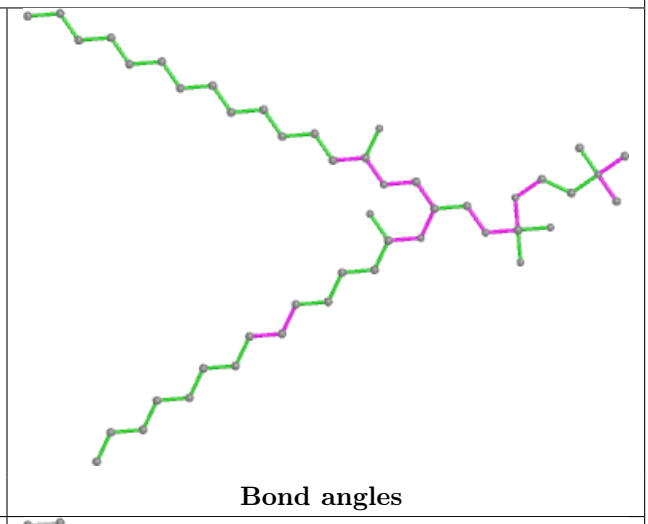
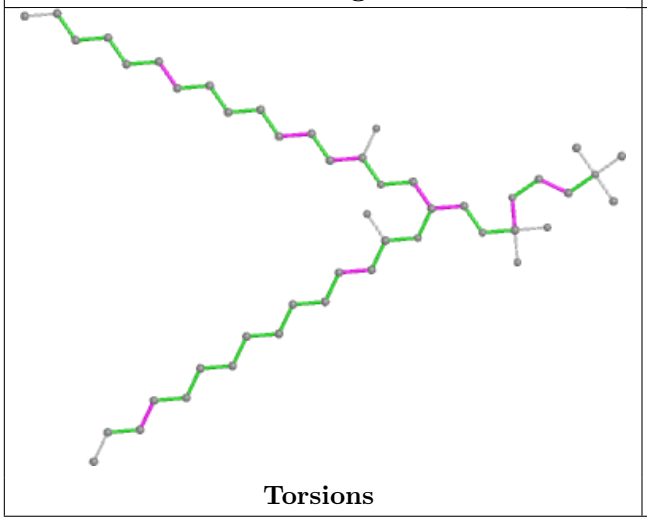


Bond angles



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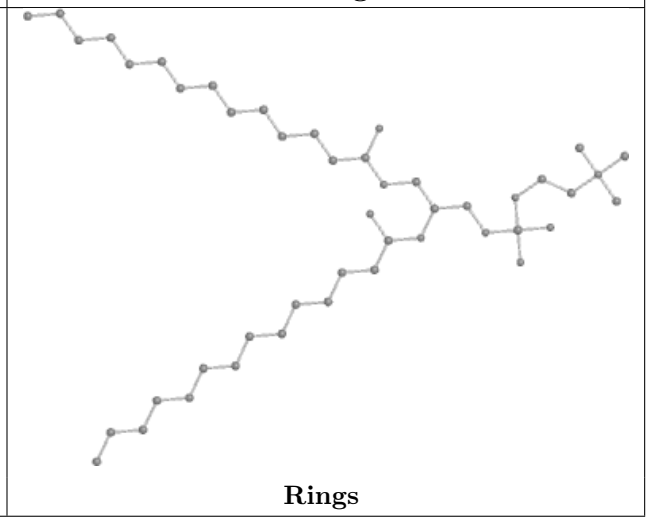
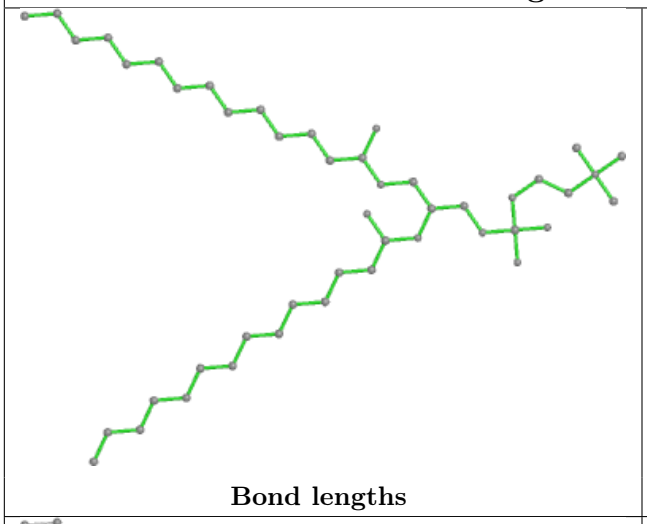


Rings

Ligand PX4 A 340



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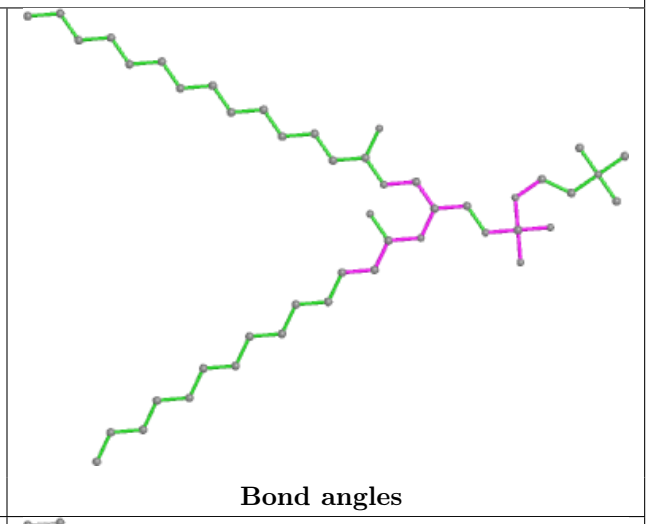
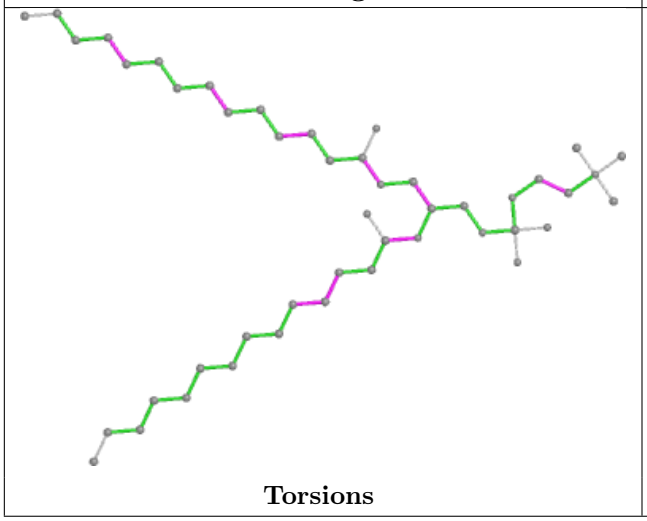


Bond angles



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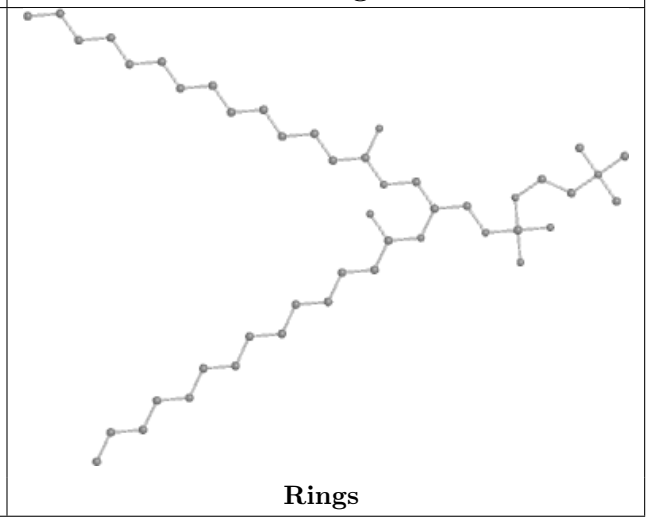
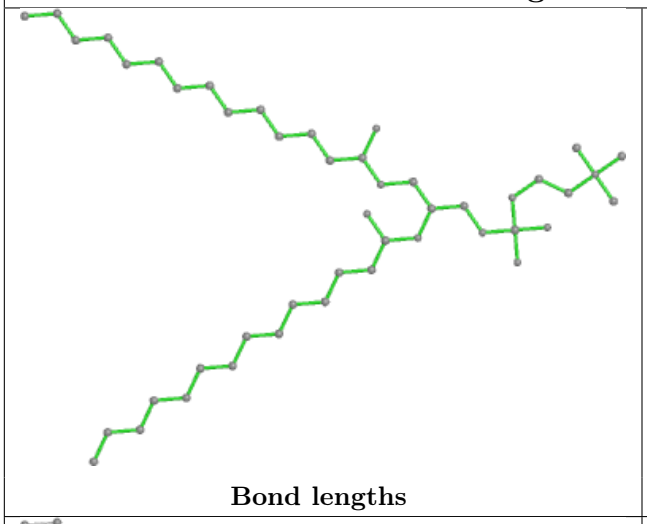


Rings

Ligand PX4 A 388



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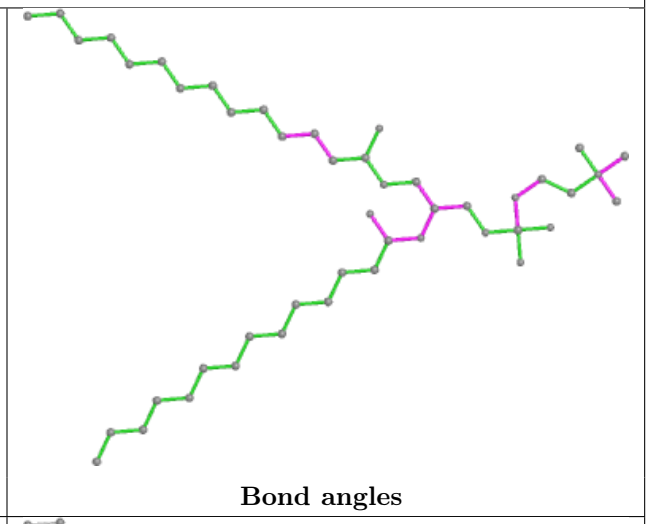
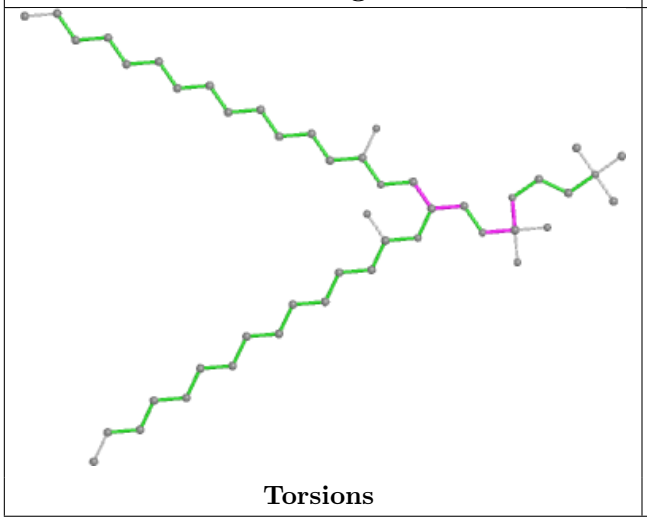


Bond angles



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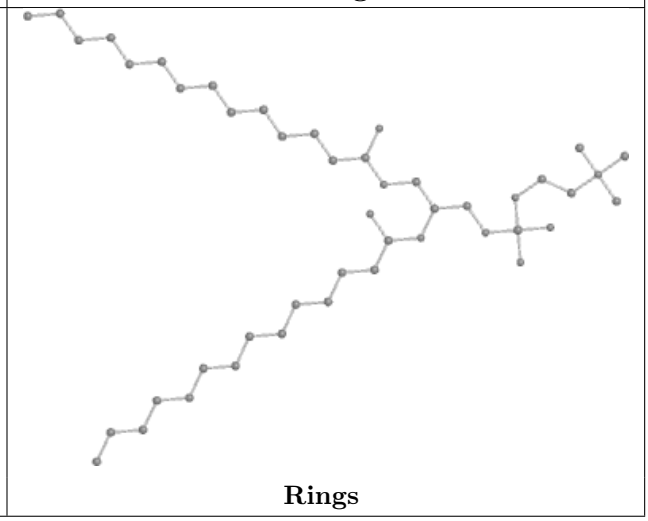
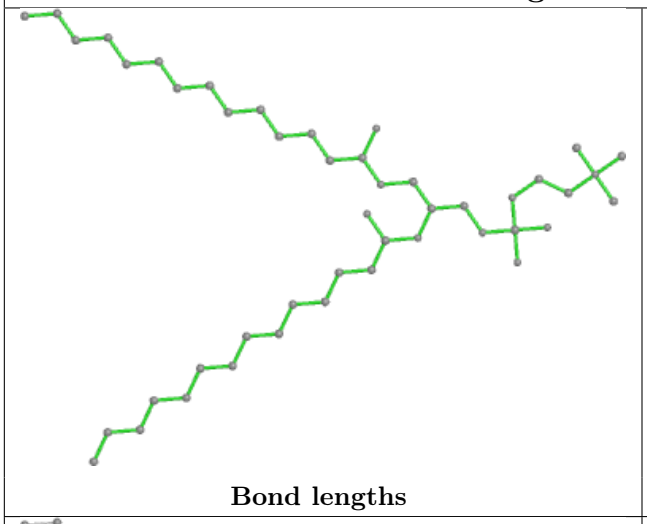
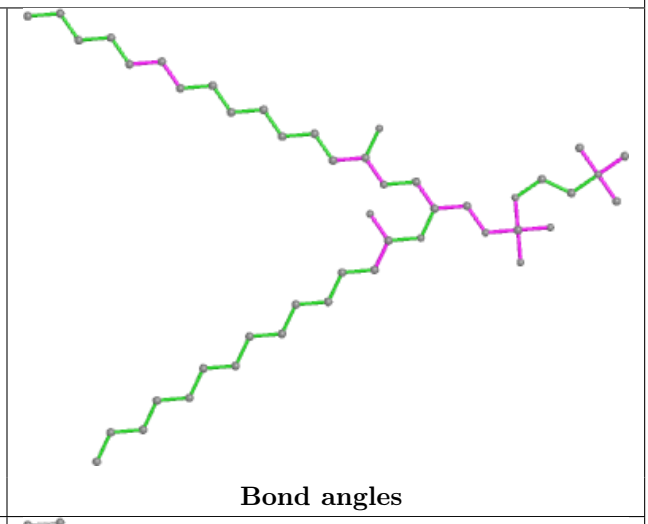


Rings

Ligand PX4 A 311



Bond lengths



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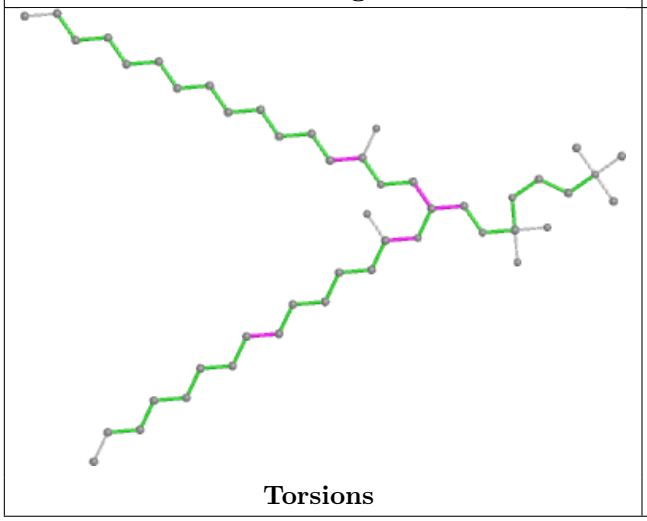

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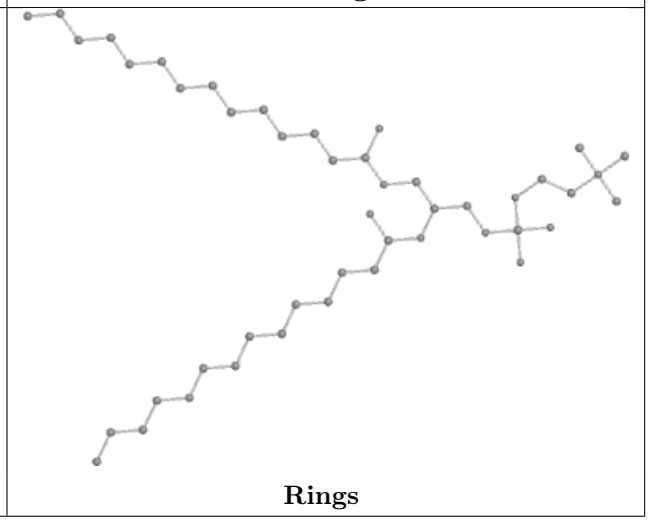
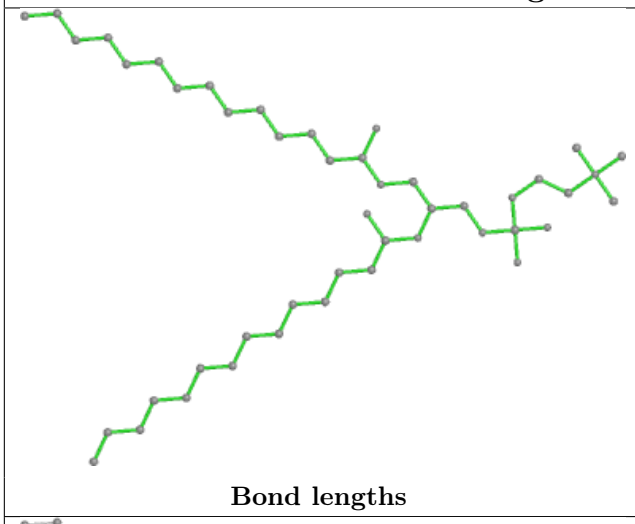


Rings

Ligand PX4 A 377



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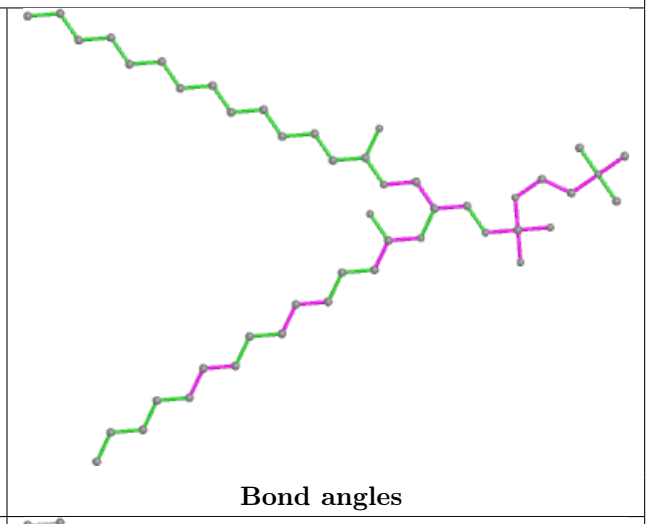

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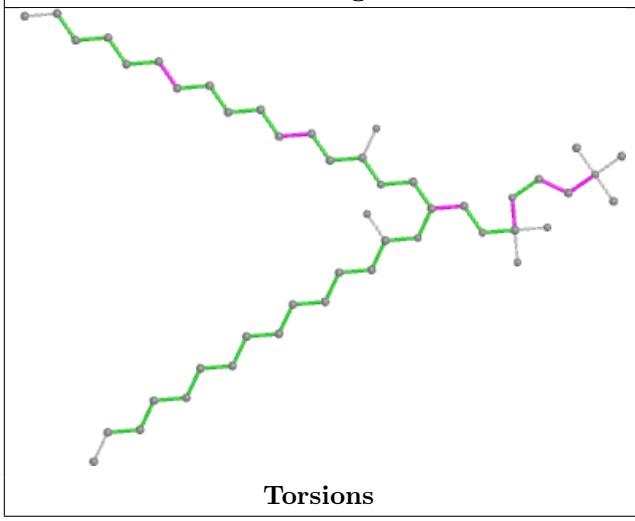

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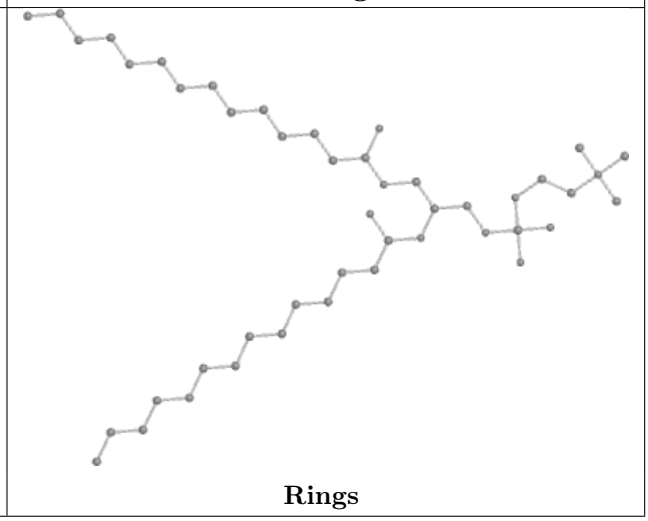
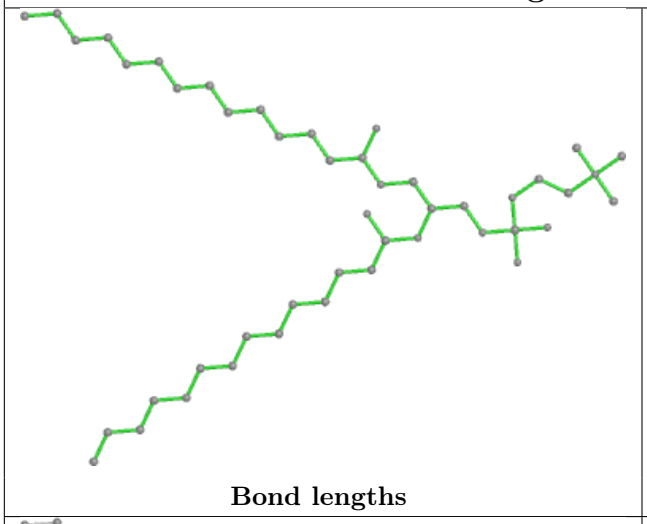


Rings

Ligand PX4 A 360



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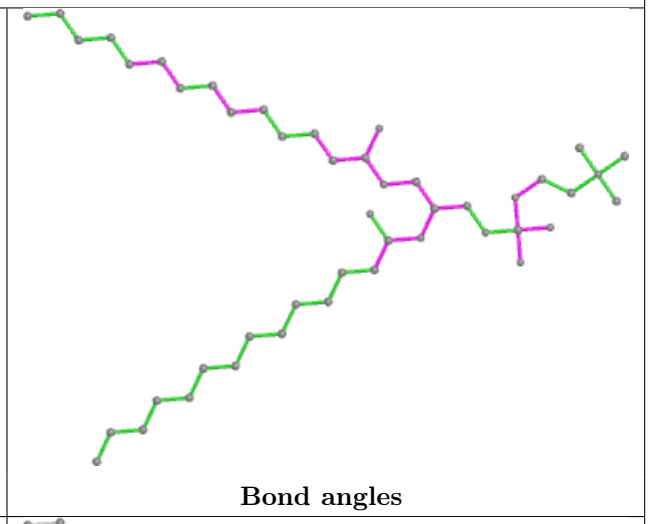

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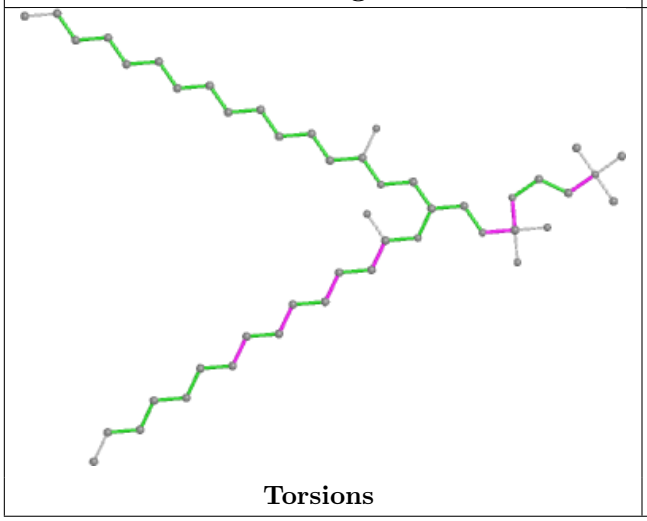

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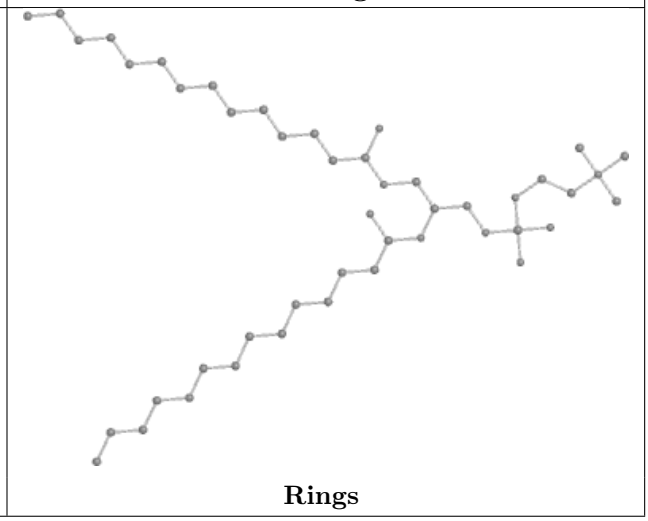
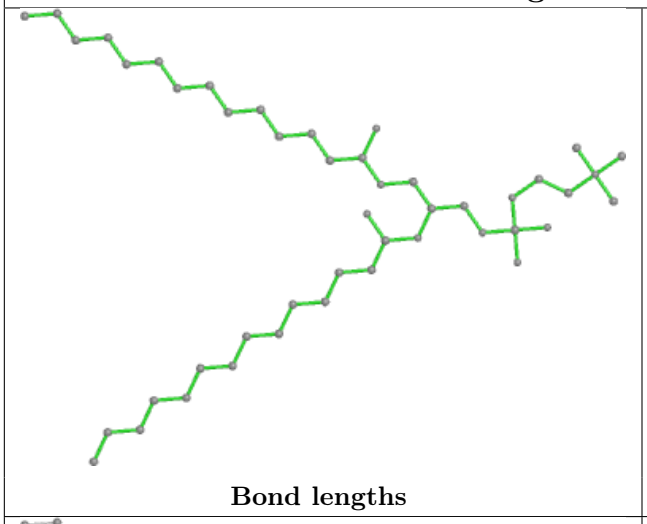


Rings

Ligand PX4 A 308



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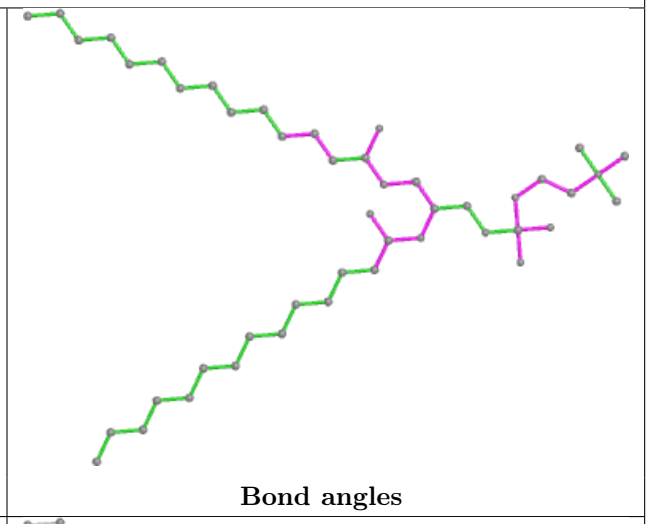

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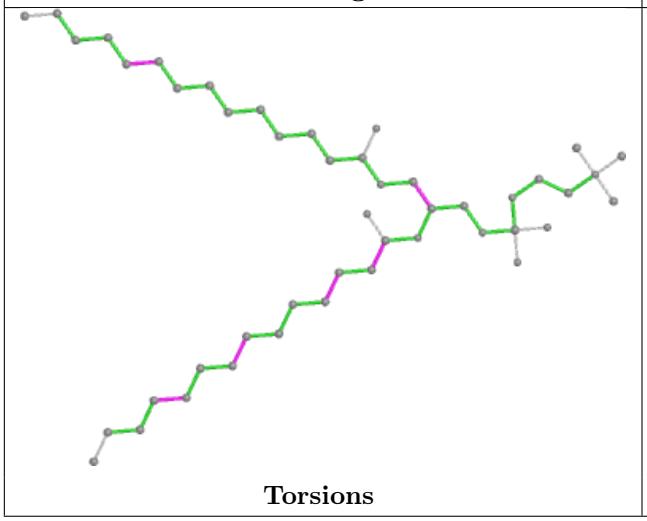

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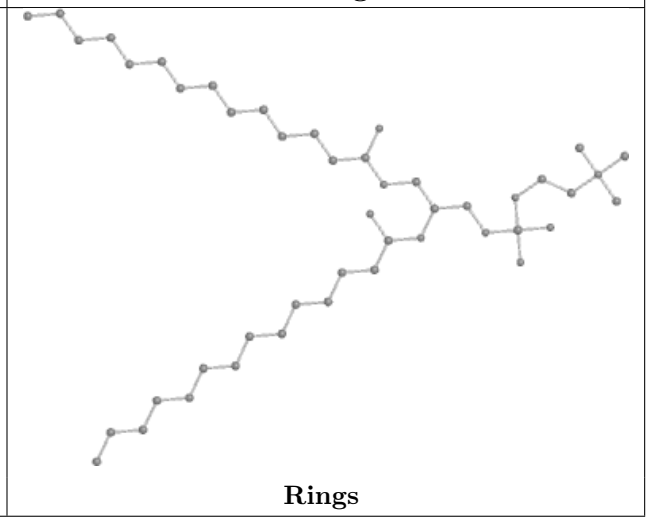
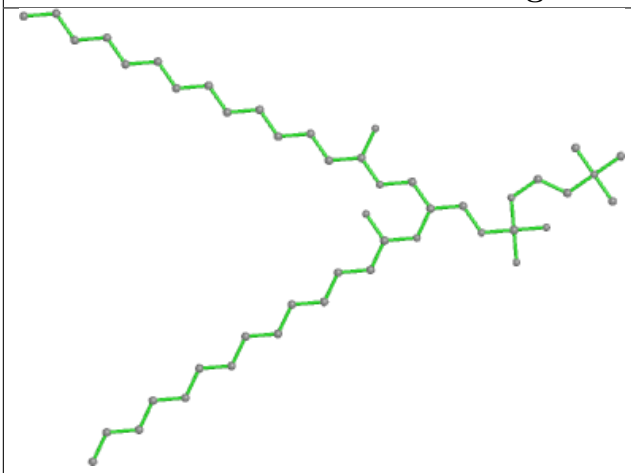


Rings

Ligand PX4 A 326



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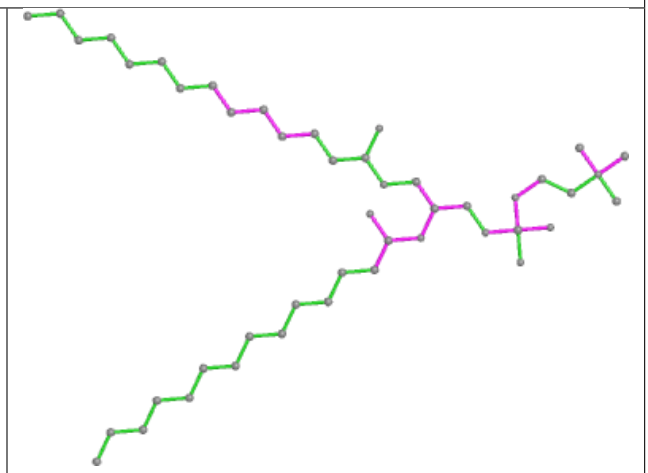

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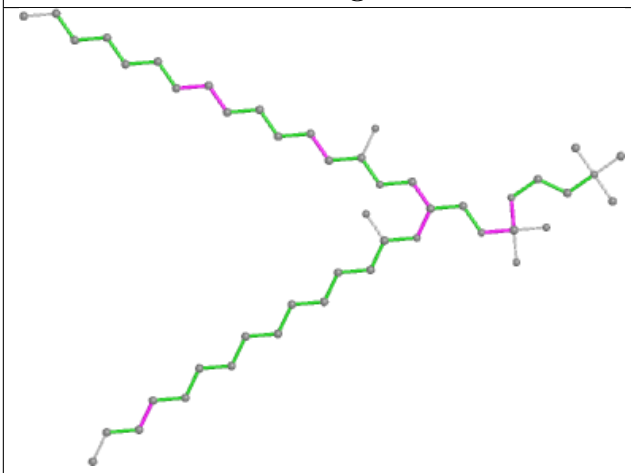

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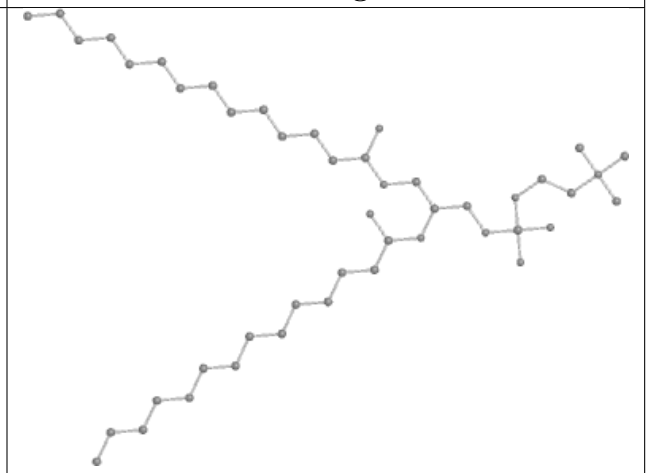
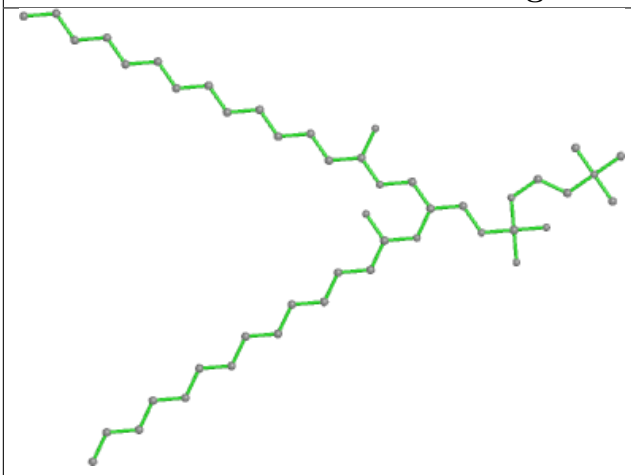


Rings

Ligand PX4 A 345



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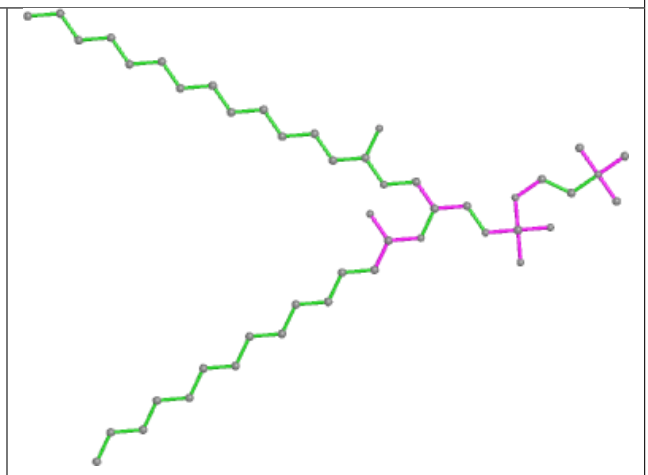

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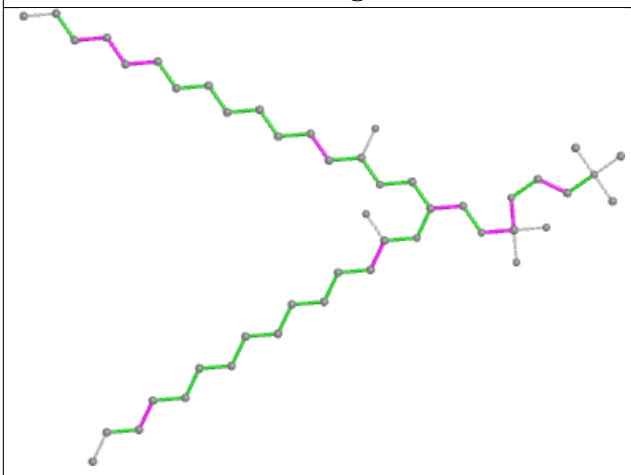

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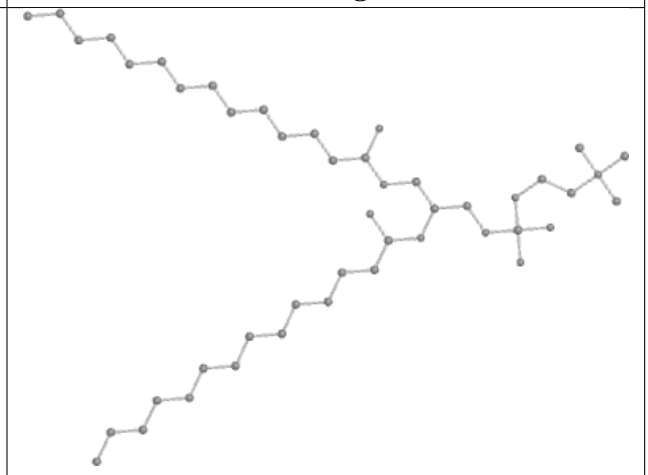
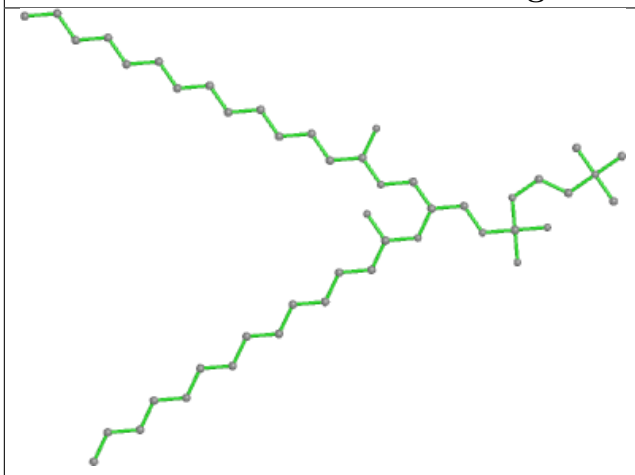


Rings

Ligand PX4 A 320



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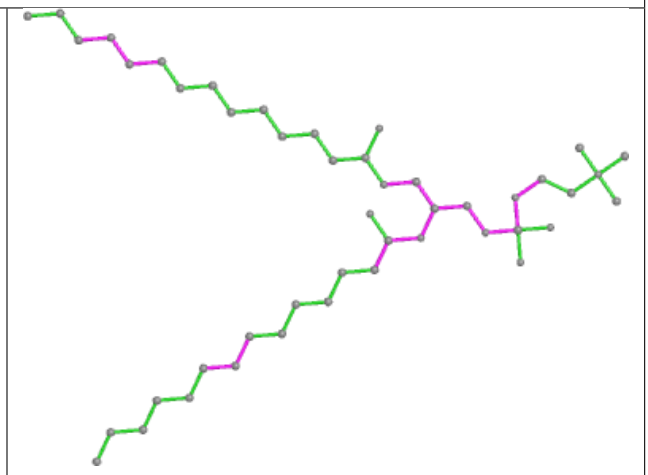
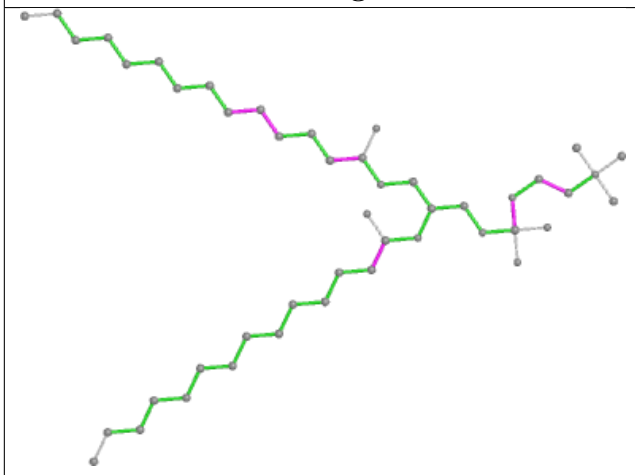


Bond angles



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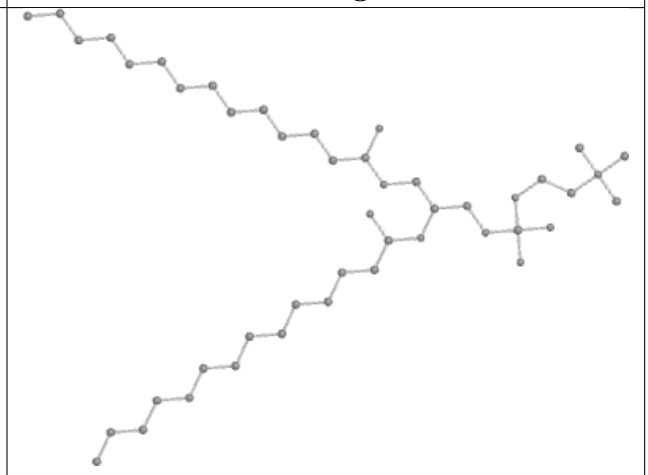
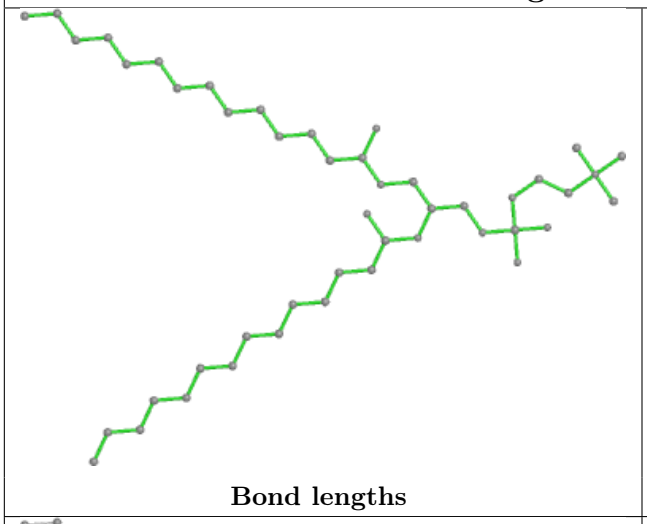


Rings

Ligand PX4 A 347



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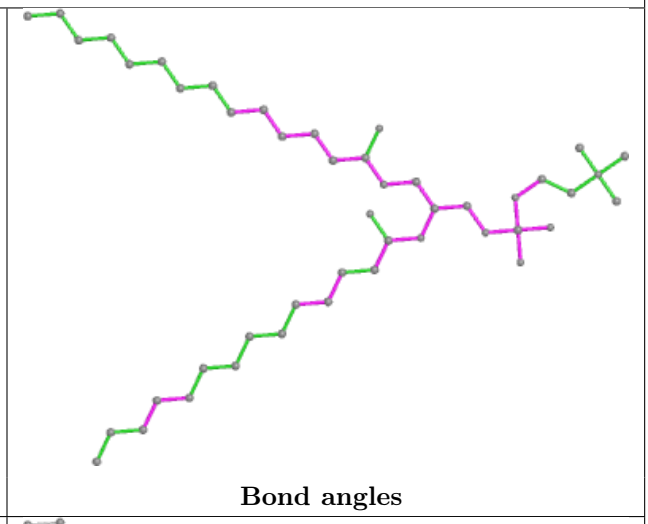

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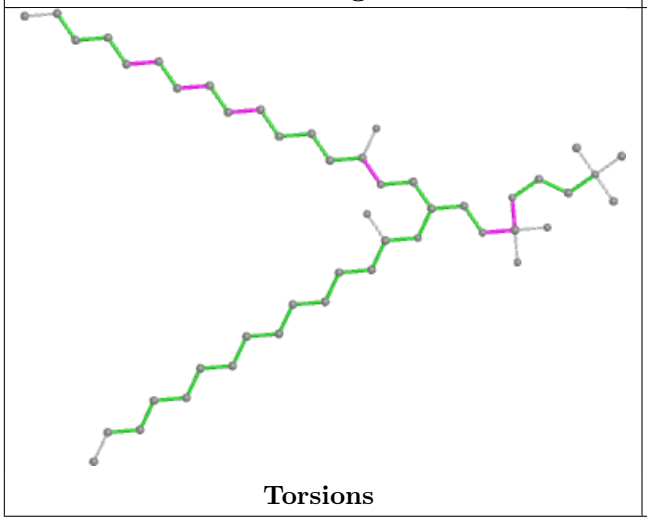

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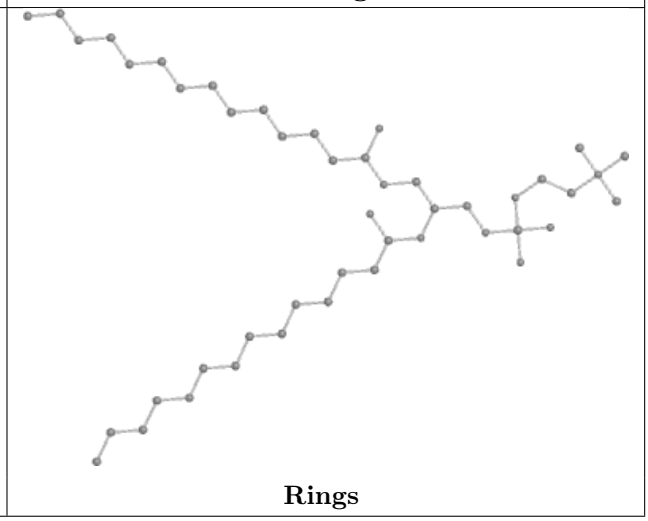
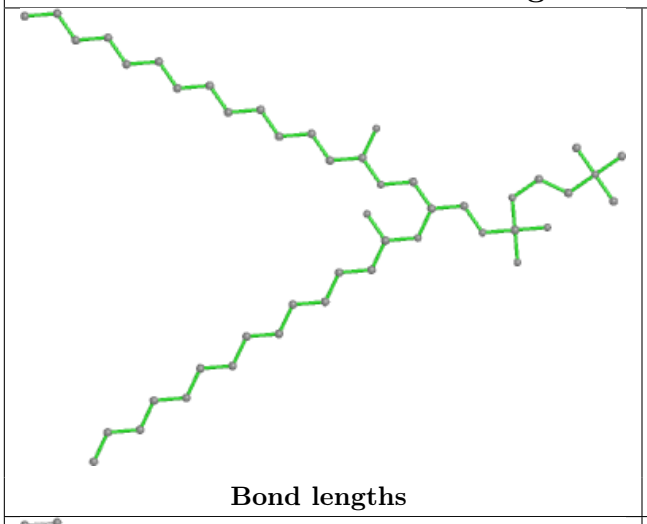


Rings

Ligand PX4 A 387



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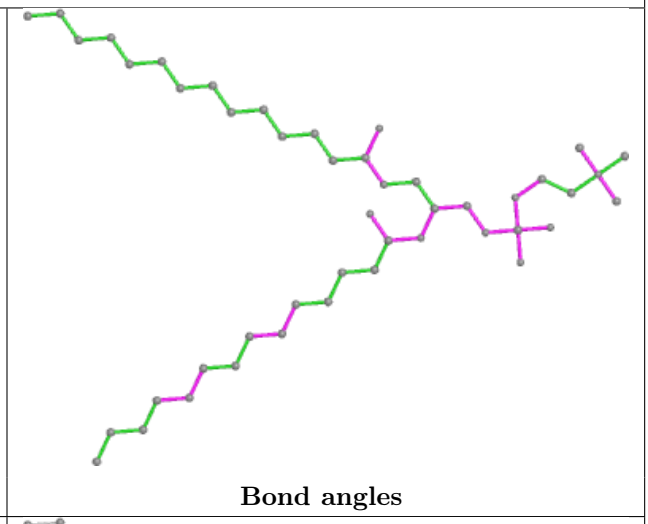

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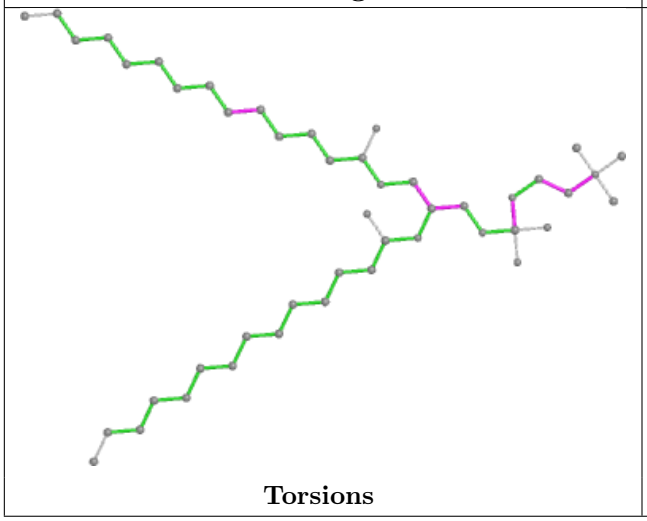

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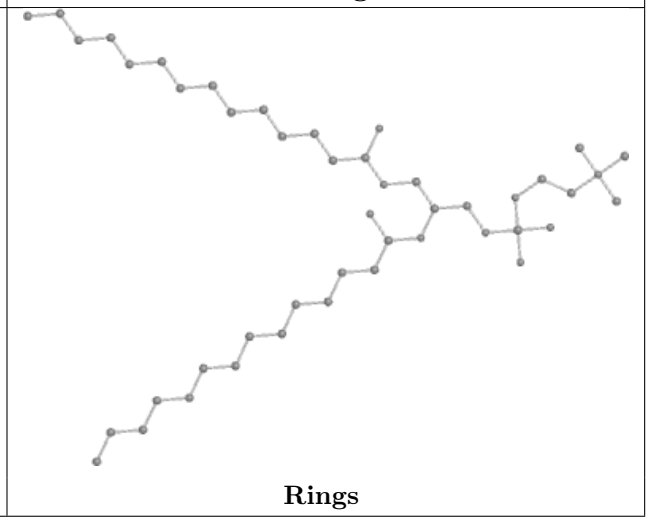
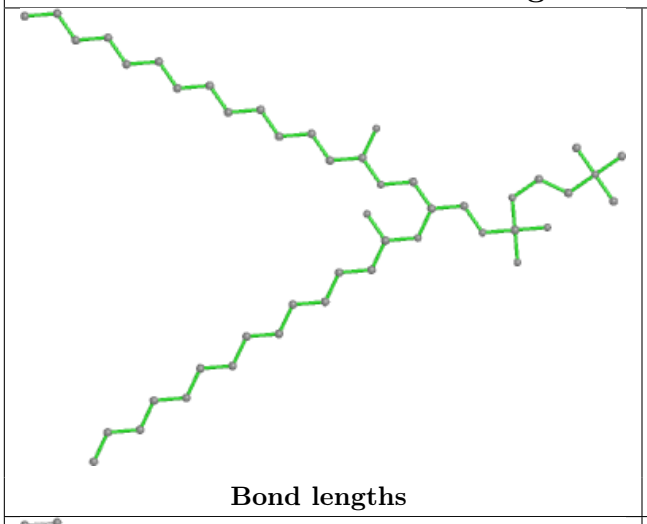


Rings

Ligand PX4 A 358



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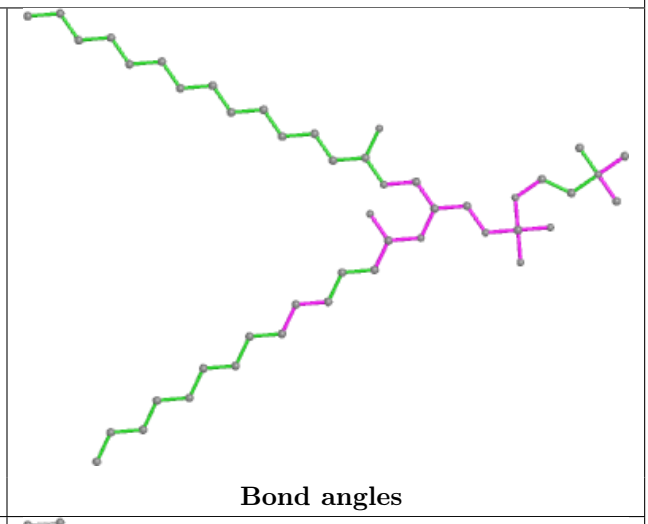

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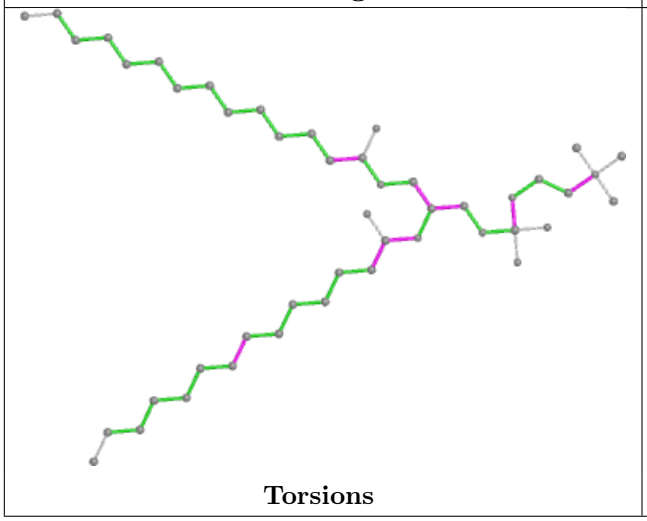

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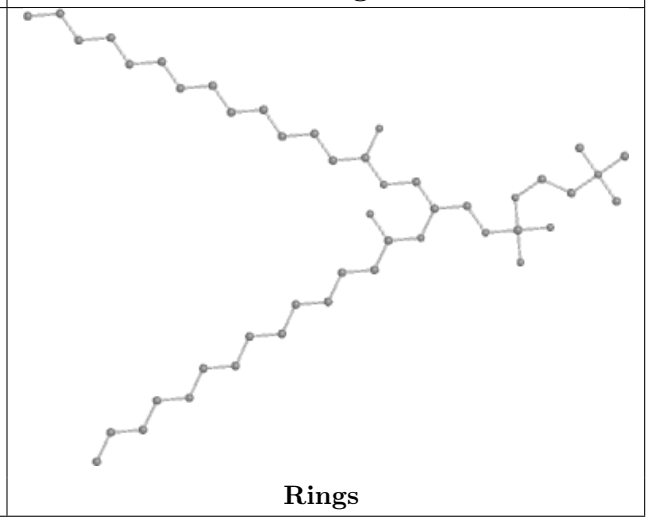
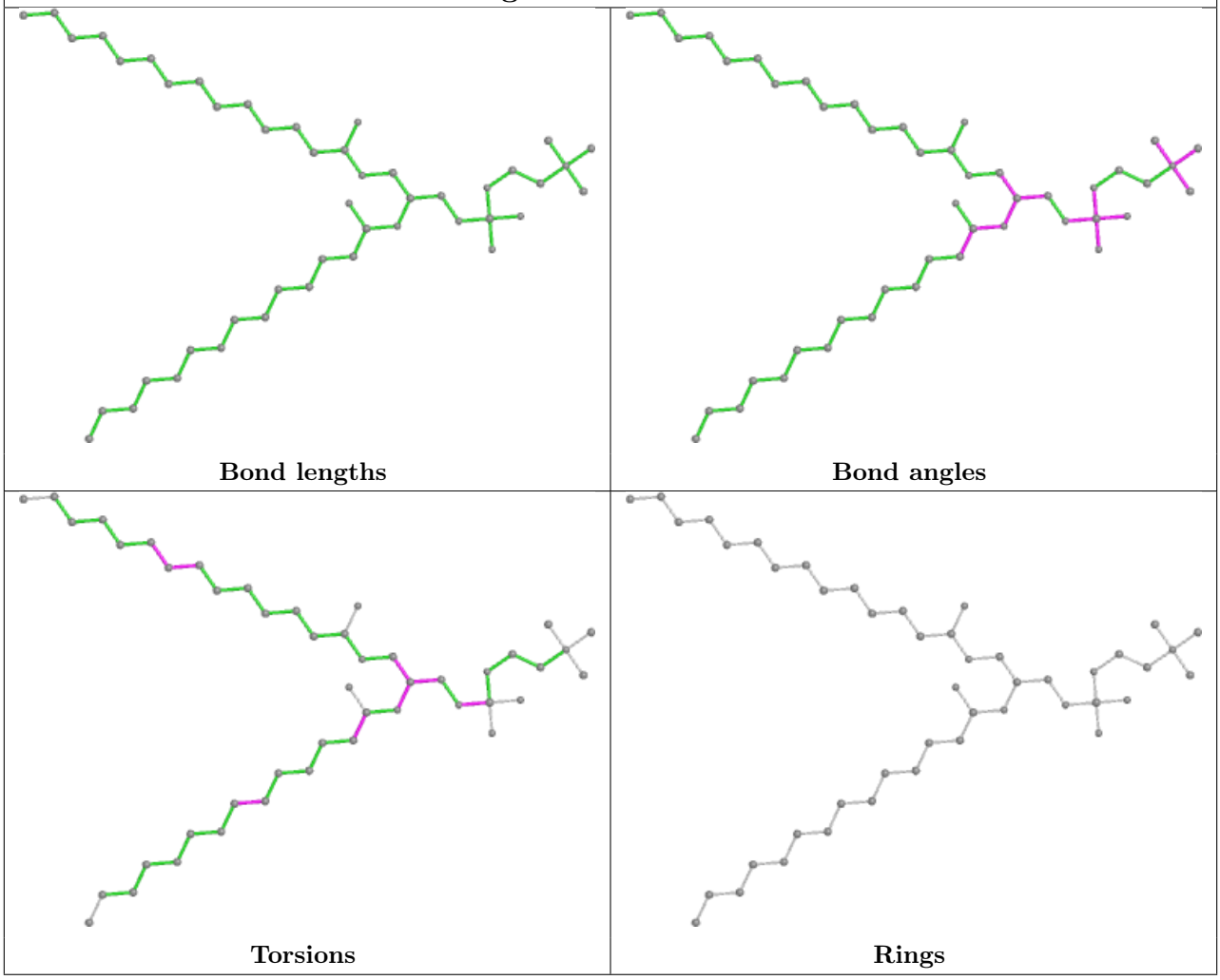
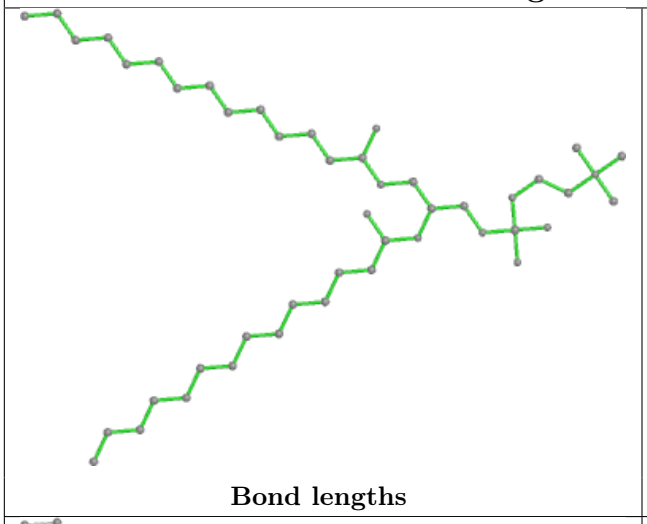


Rings

Ligand PX4 A 396



Ligand PX4 A 401



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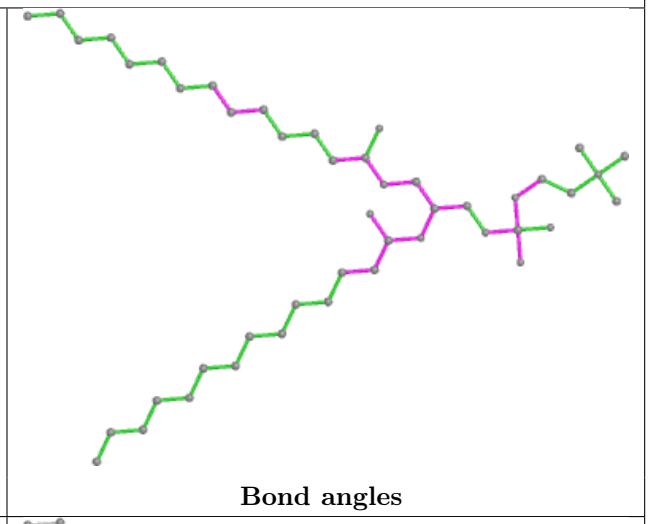
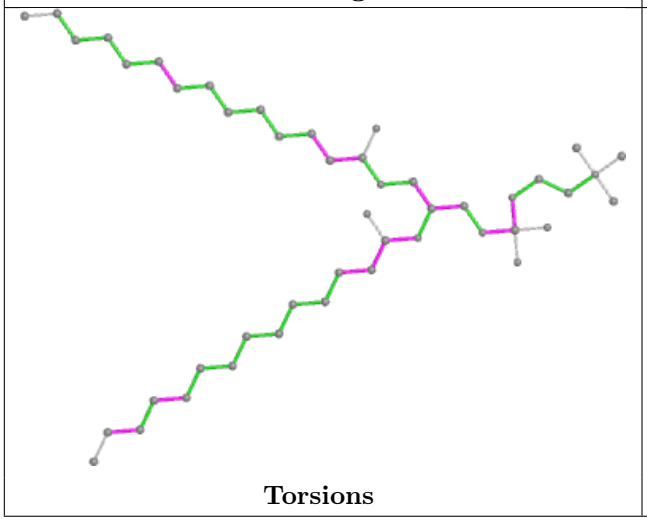


Bond angles



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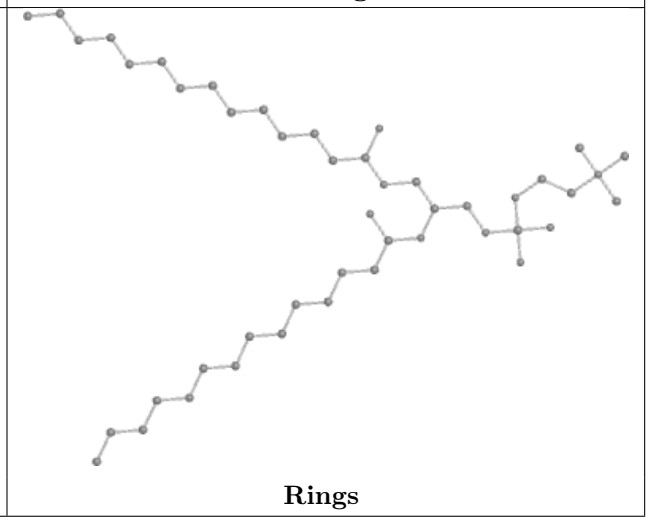
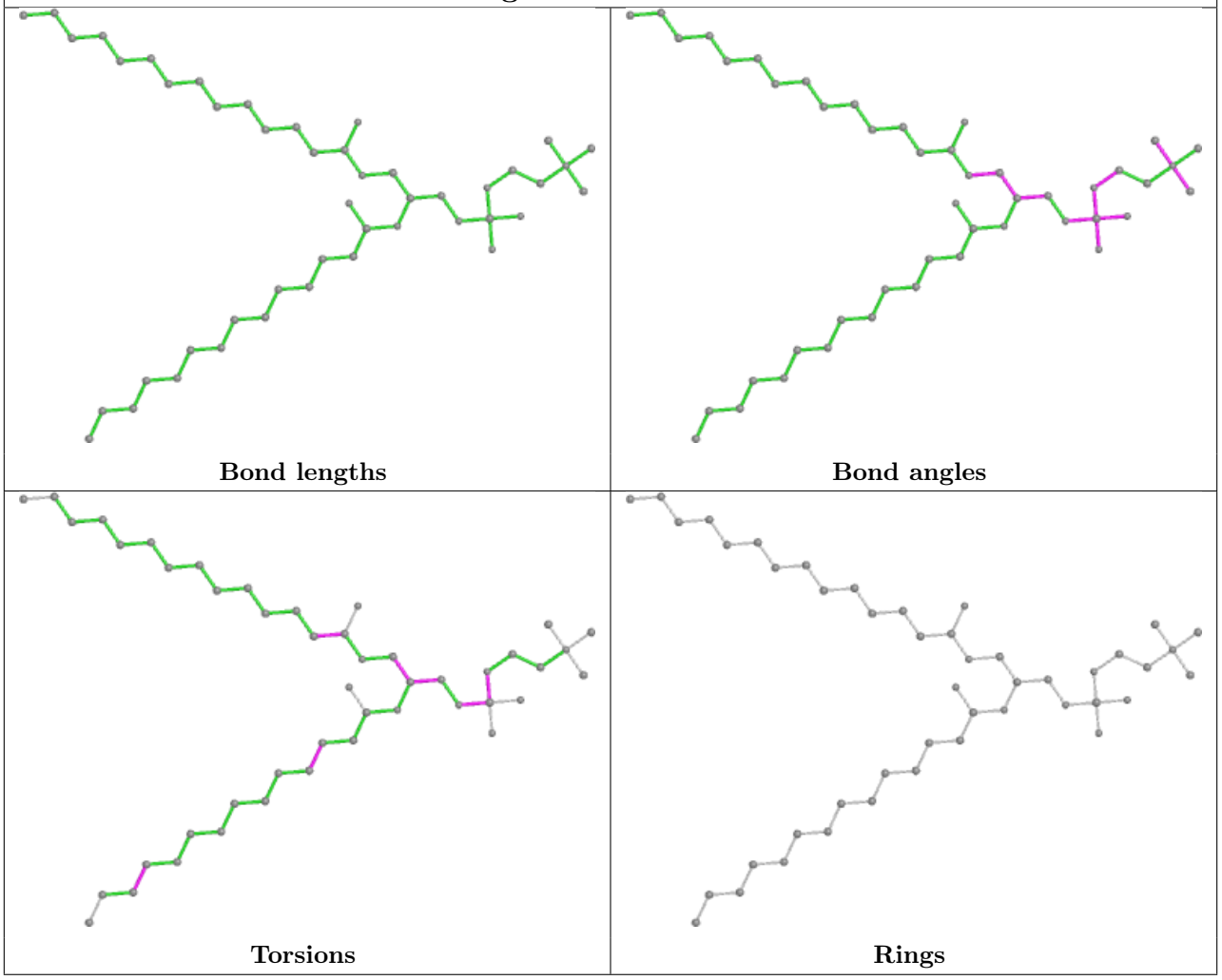


Rings

Ligand PX4 A 344



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 81% for the well-defined parts and 81% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	1762
Number of shifts mapped to atoms	1762
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	160	-0.25 ± 0.12	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	138	0.12 ± 0.15	None needed (< 0.5 ppm)
$^{13}C'$	129	-0.17 ± 0.12	None needed (< 0.5 ppm)
^{15}N	154	-0.67 ± 0.35	None needed (imprecise)

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 81%, i.e. 1729 atoms were assigned a chemical shift out of a possible 2139. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	757/804 (94%)	323/331 (98%)	284/320 (89%)	150/153 (98%)
Sidechain	814/1053 (77%)	537/687 (78%)	268/326 (82%)	9/40 (22%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	158/282 (56%)	79/142 (56%)	76/128 (59%)	3/12 (25%)
Overall	1729/2139 (81%)	939/1160 (81%)	628/774 (81%)	162/205 (79%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 81%, i.e. 1762 atoms were assigned a chemical shift out of a possible 2177. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	775/826 (94%)	332/341 (97%)	289/328 (88%)	154/157 (98%)
Sidechain	829/1069 (78%)	547/698 (78%)	273/331 (82%)	9/40 (22%)
Aromatic	158/282 (56%)	79/142 (56%)	76/128 (59%)	3/12 (25%)
Overall	1762/2177 (81%)	958/1181 (81%)	638/787 (81%)	166/209 (79%)

7.1.4 Statistically unusual chemical shifts (i)

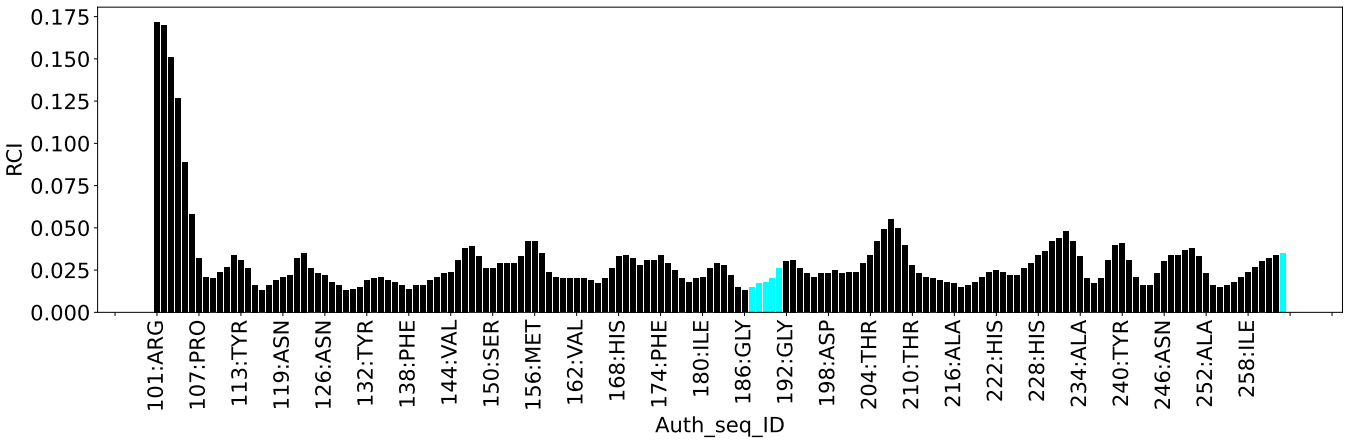
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	214	LEU	CG	33.00	21.37 – 32.19	5.8
1	A	226	LEU	CG	33.00	21.37 – 32.19	5.8
1	A	224	LEU	CG	32.30	21.37 – 32.19	5.1

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:


RCI
0.175
0.150
0.125
0.100
0.075
0.050
0.025
0.000
101:ARG
107:PRO
113:TYR
119:ASN
126:ASN
132:TYR
138:PHE
144:VAL
150:SER
156:MET
162:VAL
168:HIS
174:PHE
180:ILE
186:GLY
192:GLY
198:ASP
204:THR
210:THR
216:ALA
222:HIS
228:HIS
234:ALA
240:TYR
246:ASN
252:ALA
258:ILE
Auth_seq_ID