Full wwPDB NMR Structure Validation Report (i)

Mar 24, 2026 – 09:21 AM UTC

PDB ID	:	6CLZ / pdb_00006clz
BMRB ID	:	30425
Title	:	MT1-MMP HPX domain with Blade 4 Loop Bound to Nanodiscs
Authors	:	Marcink, T.C.; Van Doren, S.R.
Deposited on	:	2018-03-02

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

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

The 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:

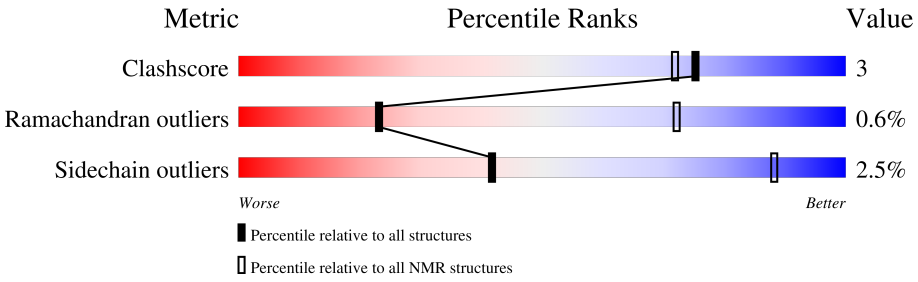
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 4%.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	196	44% 56%
2	B	211	33% 66%
2	C	211	30% 70%

2 Ensemble composition and analysis (i)

This entry contains 15 models. Model 9 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:316-A:511, B:55-B:265, C:55-C:265 (618)	1.59	9

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

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

The models can be grouped into 4 clusters. No single-model clusters were found.

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

3 Entry composition (i)

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

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

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

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

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

There are 44 discrepancies between the modelled and reference sequences:

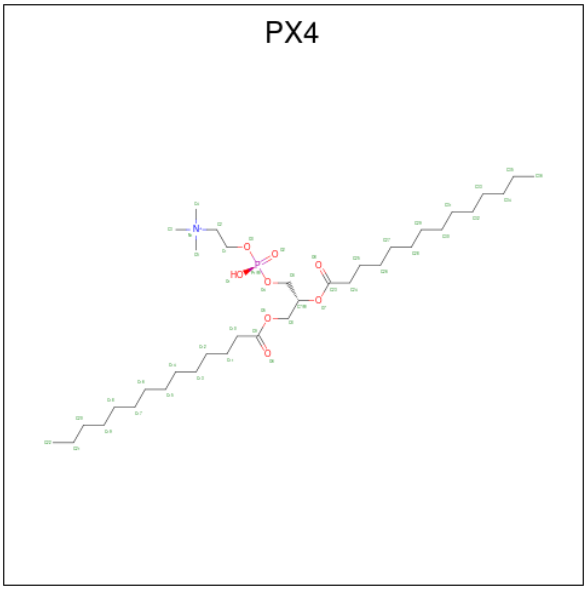
Chain	Residue	Modelled	Actual	Comment	Reference
B	99	PRO	-	insertion	UNP P02647
B	100	TYR	-	insertion	UNP P02647
B	101	LEU	-	insertion	UNP P02647
B	102	ASP	-	insertion	UNP P02647
B	103	ASP	-	insertion	UNP P02647
B	104	PHE	-	insertion	UNP P02647
B	105	GLN	-	insertion	UNP P02647
B	106	LYS	-	insertion	UNP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

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

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



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

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

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

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

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	
4	A	1	Total	Na
			1	1

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	
5	A	1	Total	Cl
			1	1

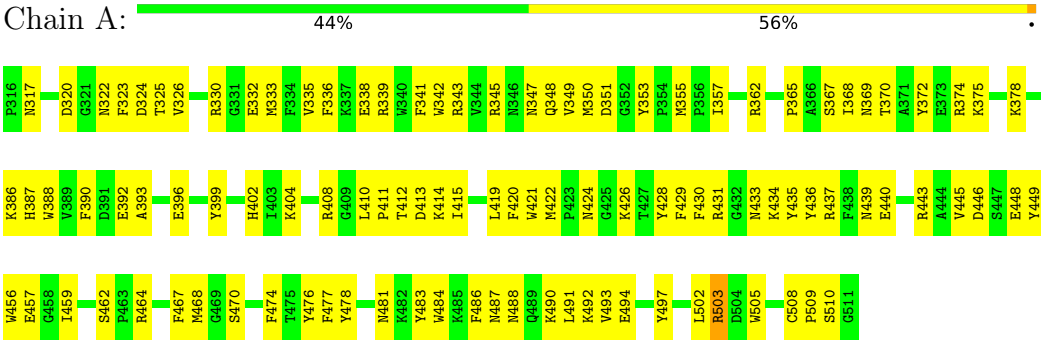
4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

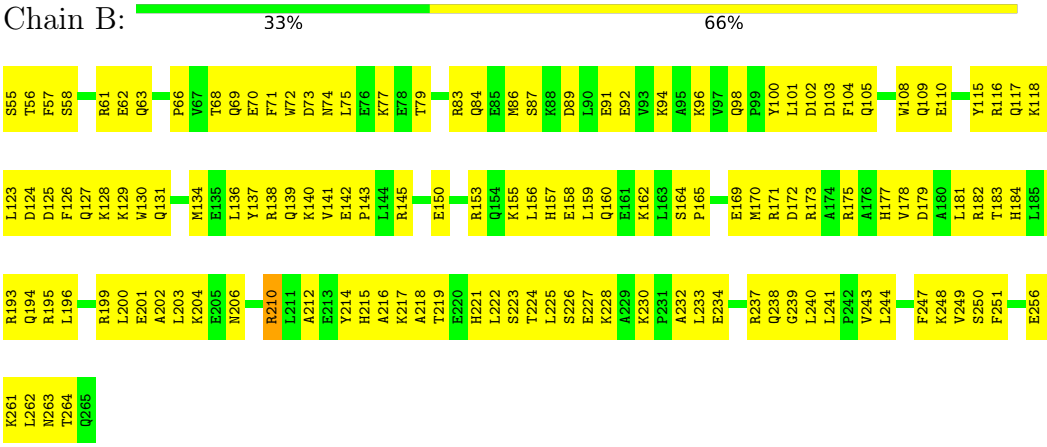
• Molecule 1: Matrix metalloproteinase-14

Chain A:



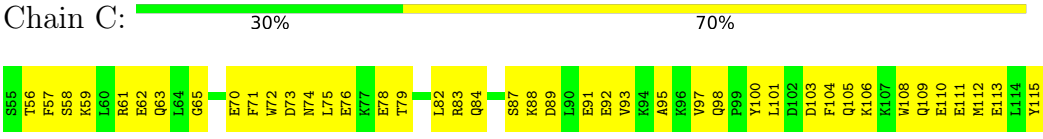
• Molecule 2: Apolipoprotein A-I

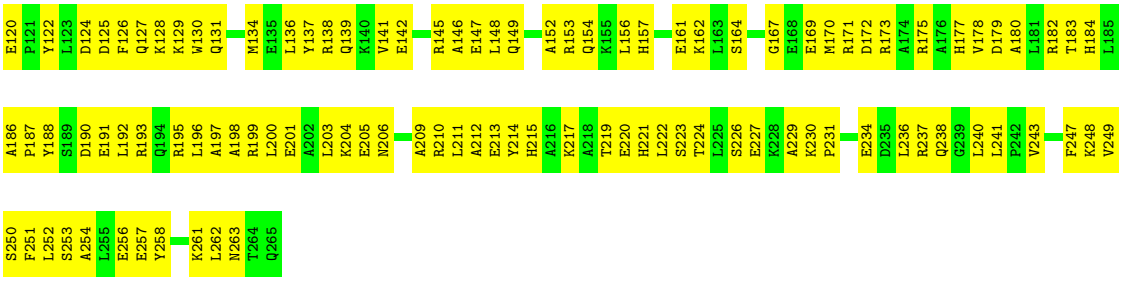
Chain B:



• Molecule 2: Apolipoprotein A-I

Chain C:





4.2 Scores per residue for each member of the ensemble

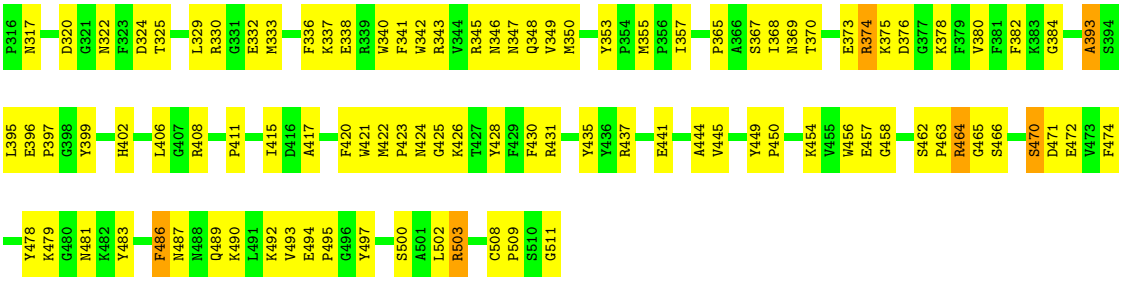
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Matrix metalloproteinase-14

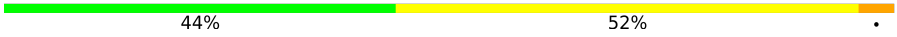
Chain A:

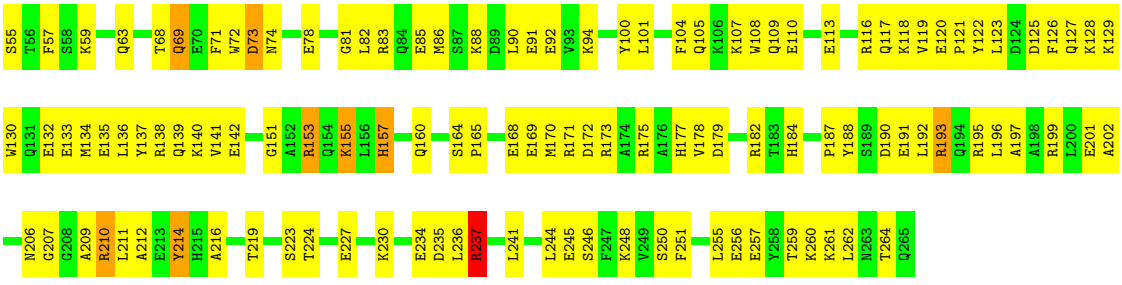




• Molecule 2: Apolipoprotein A-I

Chain B:

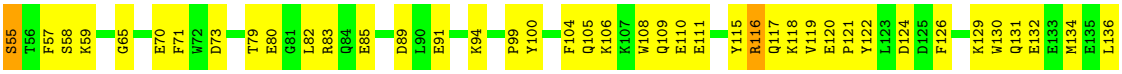


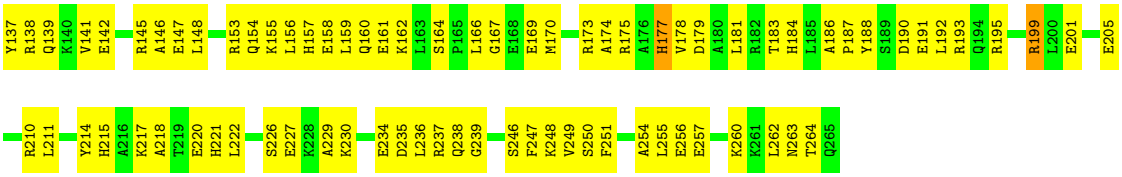


• Molecule 2: Apolipoprotein A-I

Chain C:





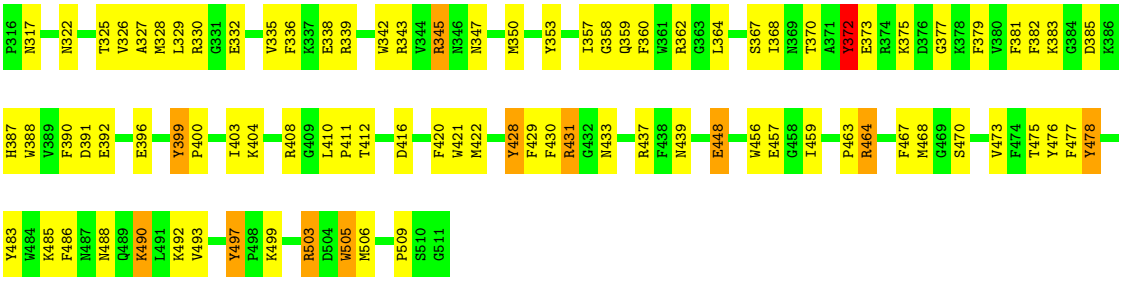


4.2.2 Score per residue for model 2

• Molecule 1: Matrix metalloproteinase-14

Chain A:





• Molecule 2: Apolipoprotein A-I

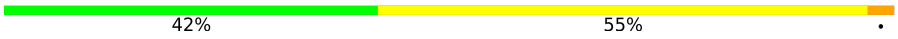
Chain B:

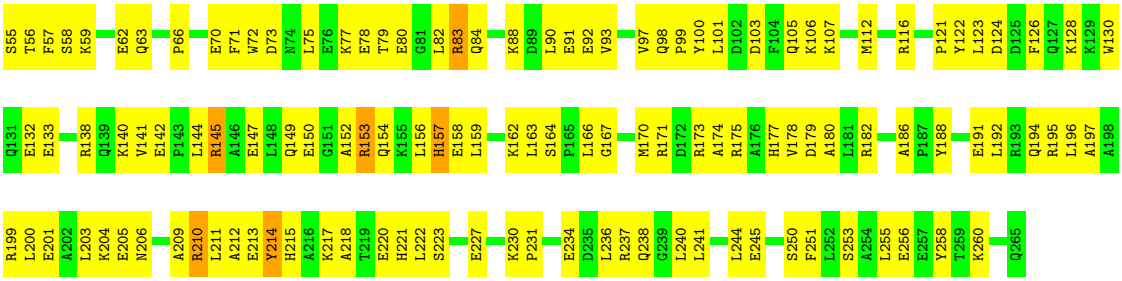




• Molecule 2: Apolipoprotein A-I

Chain C:

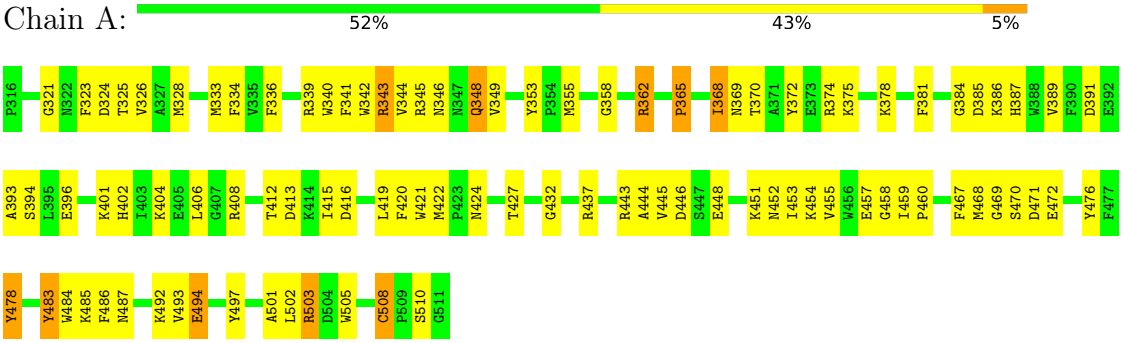




4.2.3 Score per residue for model 3

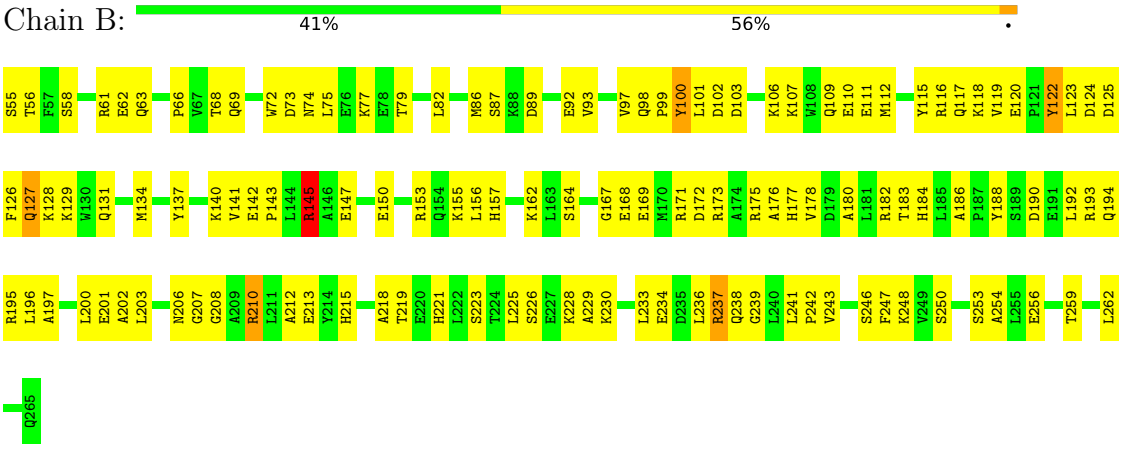
• Molecule 1: Matrix metalloproteinase-14

Chain A:



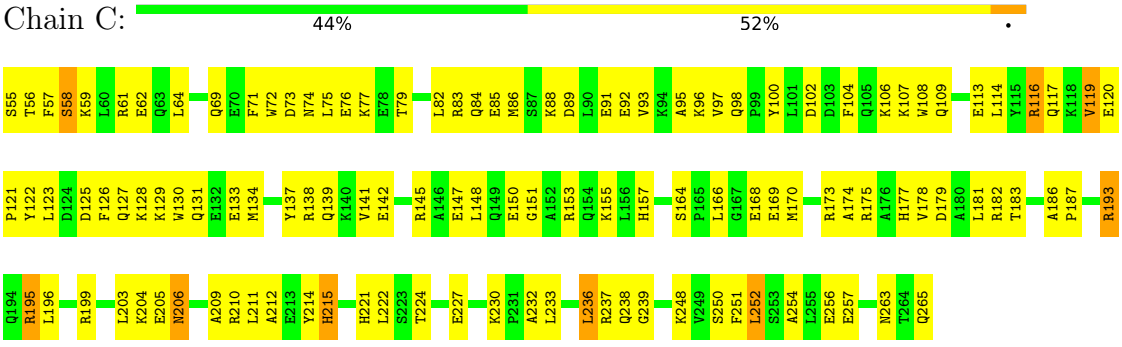
• Molecule 2: Apolipoprotein A-I

Chain B:



• Molecule 2: Apolipoprotein A-I

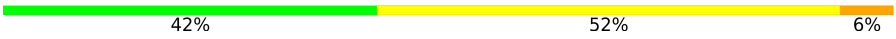
Chain C:

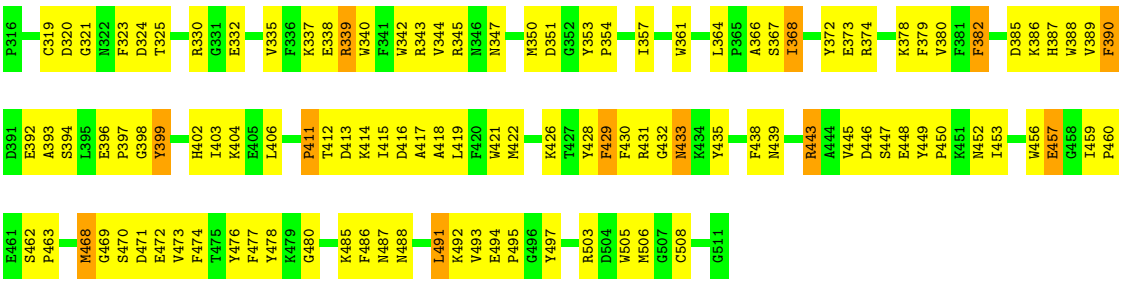


4.2.4 Score per residue for model 4

• Molecule 1: Matrix metalloproteinase-14

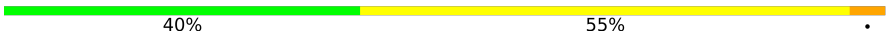
Chain A:

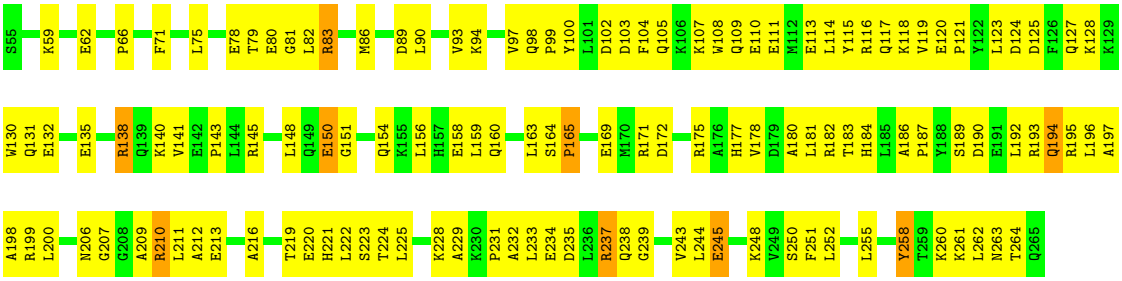




• Molecule 2: Apolipoprotein A-I

Chain B:

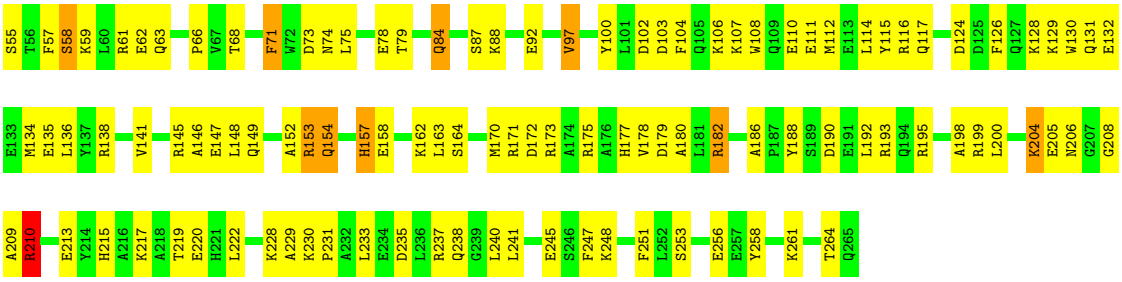




• Molecule 2: Apolipoprotein A-I

Chain C:



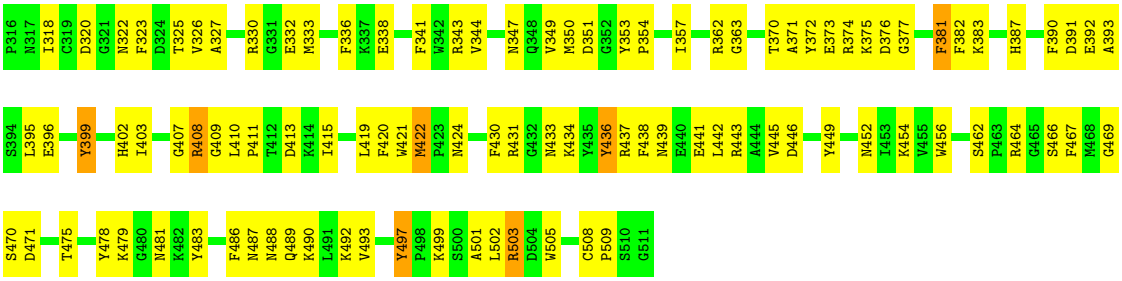


4.2.5 Score per residue for model 5

• Molecule 1: Matrix metalloproteinase-14

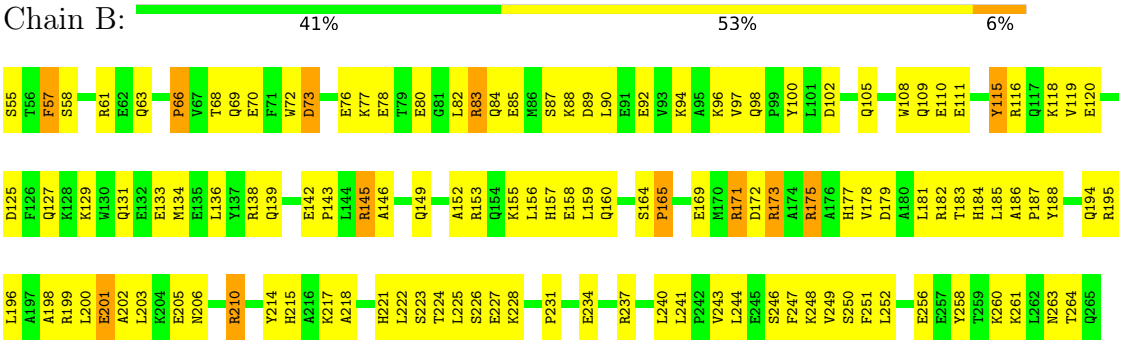
Chain A:





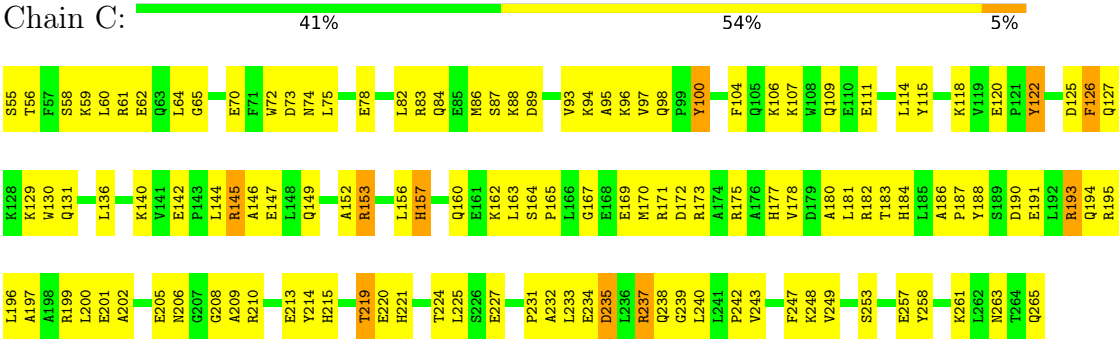
• Molecule 2: Apolipoprotein A-I

Chain B:



• Molecule 2: Apolipoprotein A-I

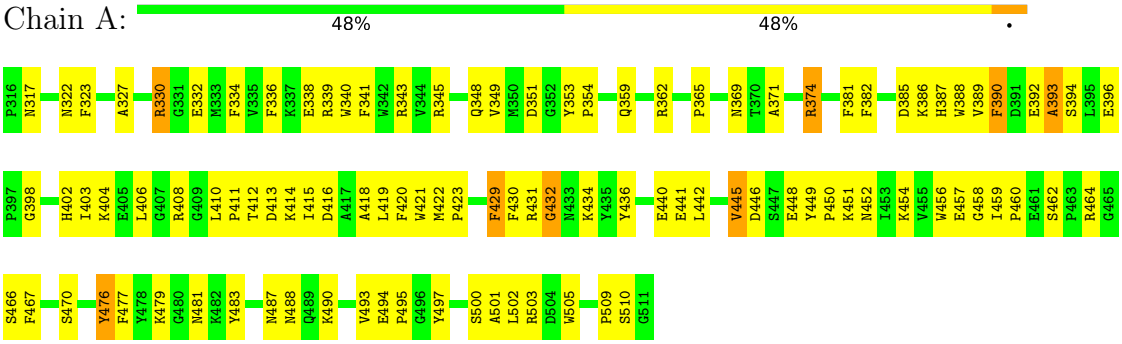
Chain C:



4.2.6 Score per residue for model 6

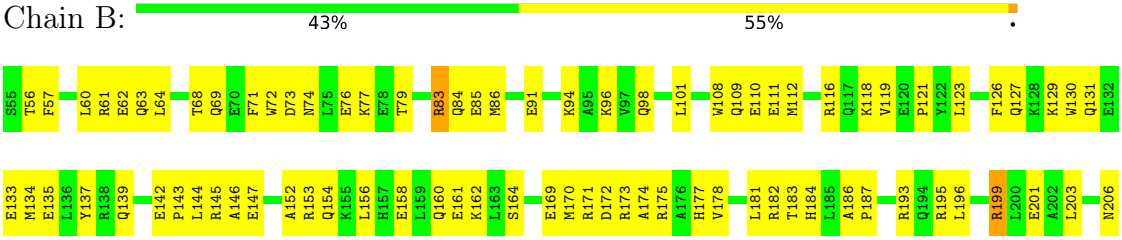
• Molecule 1: Matrix metalloproteinase-14

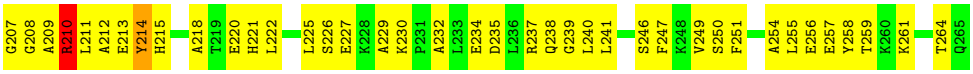
Chain A:



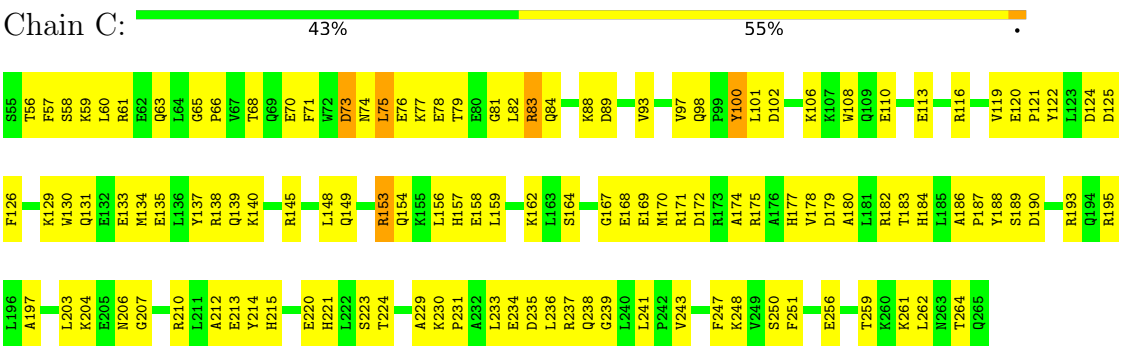
• Molecule 2: Apolipoprotein A-I

Chain B:



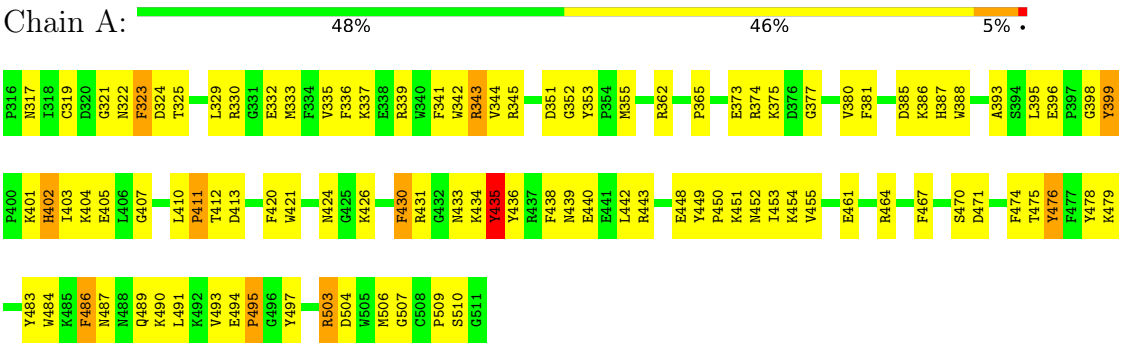


• Molecule 2: Apolipoprotein A-I



4.2.7 Score per residue for model 7

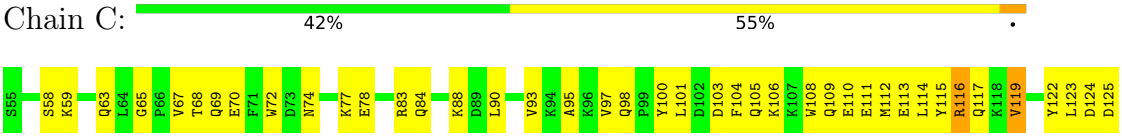
• Molecule 1: Matrix metalloproteinase-14

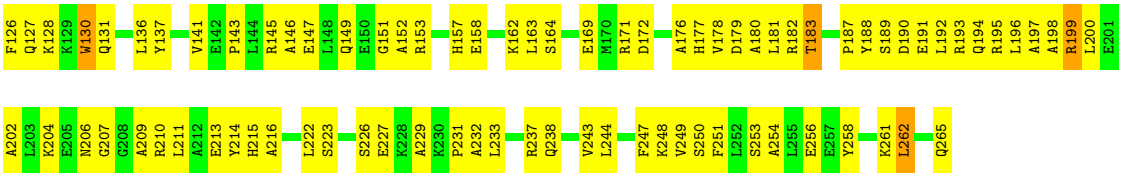


• Molecule 2: Apolipoprotein A-I



• Molecule 2: Apolipoprotein A-I



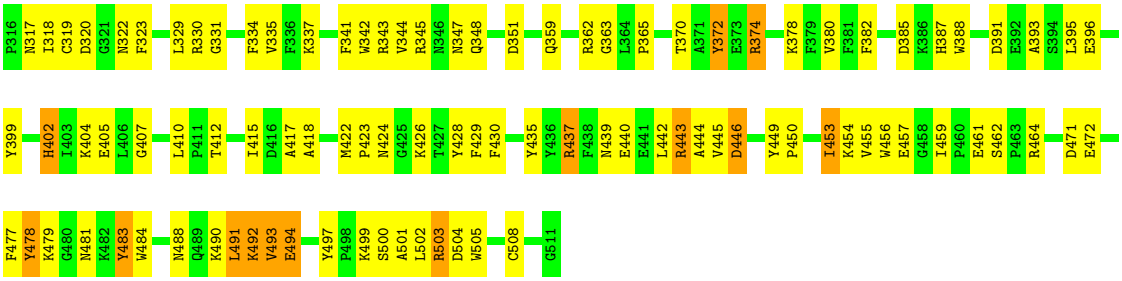


4.2.8 Score per residue for model 8

• Molecule 1: Matrix metalloproteinase-14

Chain A:





• Molecule 2: Apolipoprotein A-I

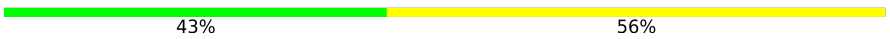
Chain B:





• Molecule 2: Apolipoprotein A-I

Chain C:

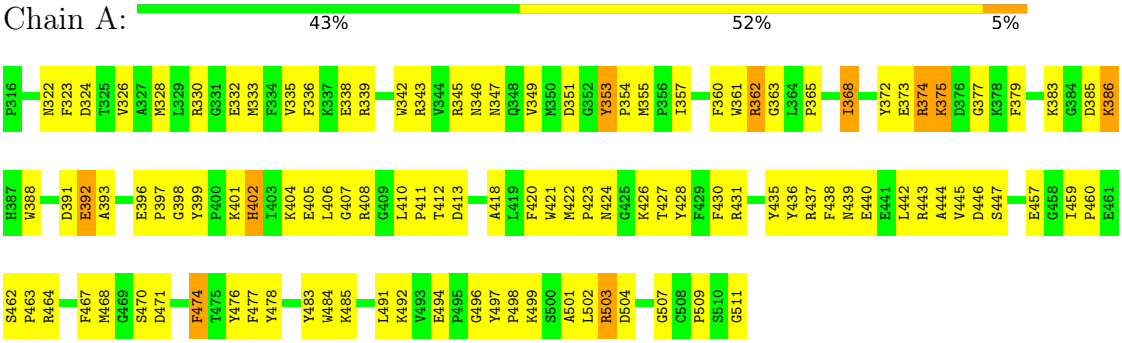




4.2.9 Score per residue for model 9 (medoid)

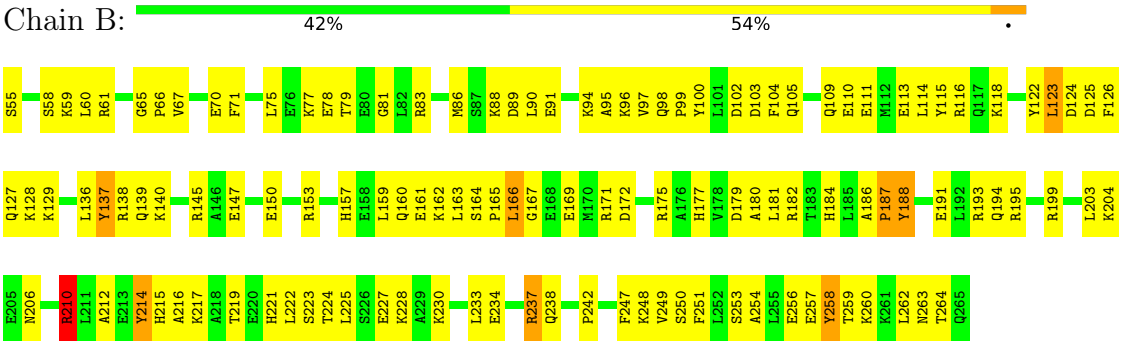
• Molecule 1: Matrix metalloproteinase-14

Chain A:



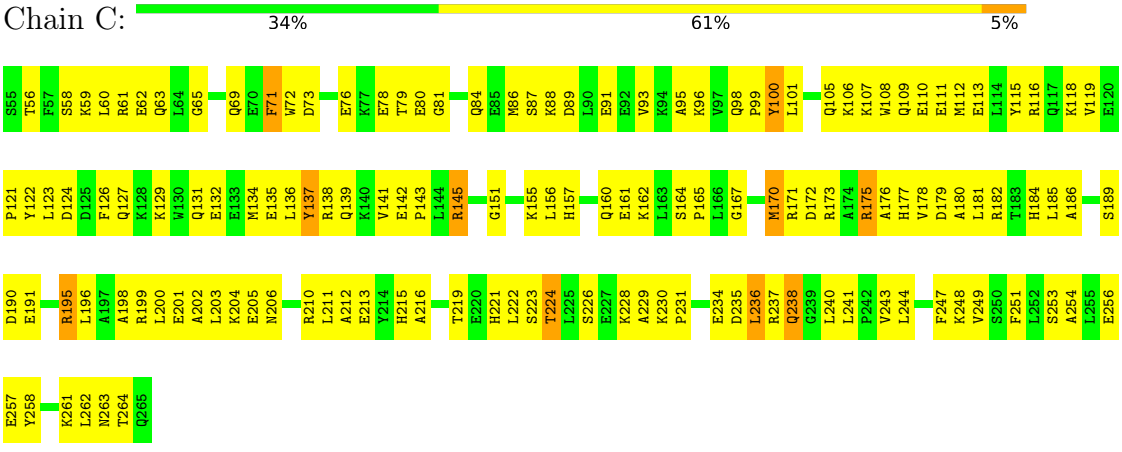
• Molecule 2: Apolipoprotein A-I

Chain B:



• Molecule 2: Apolipoprotein A-I

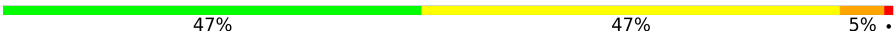
Chain C:

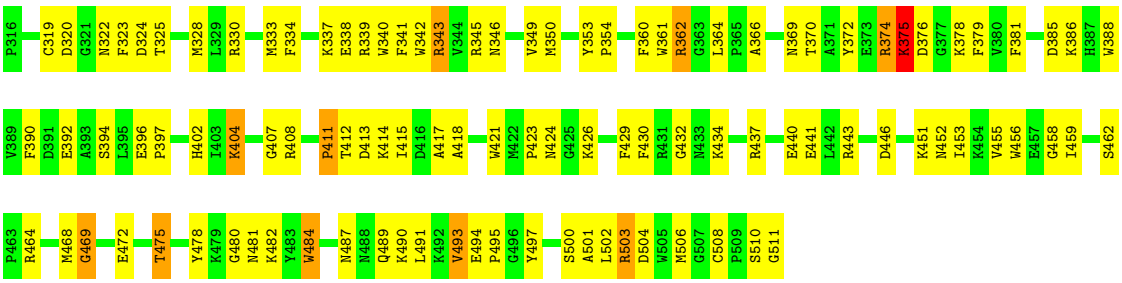


4.2.10 Score per residue for model 10

• Molecule 1: Matrix metalloproteinase-14

Chain A:

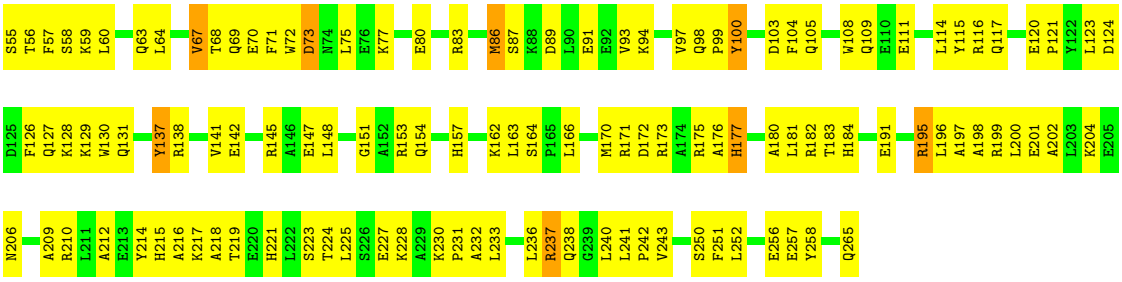




• Molecule 2: Apolipoprotein A-I

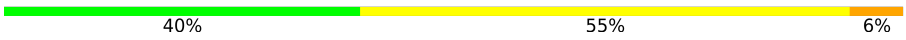
Chain B:

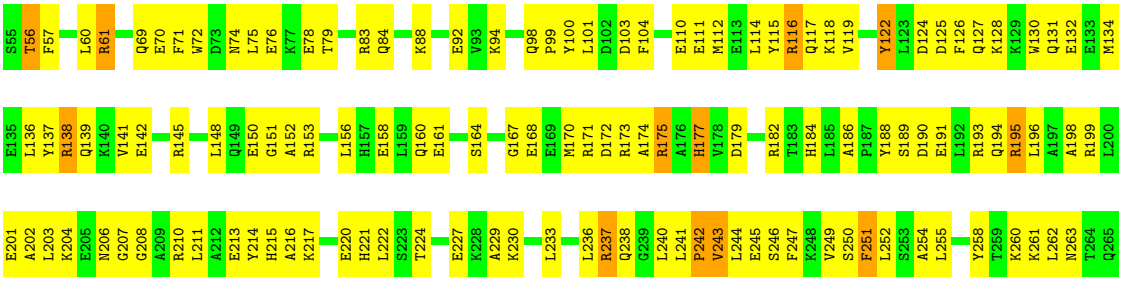




• Molecule 2: Apolipoprotein A-I

Chain C:

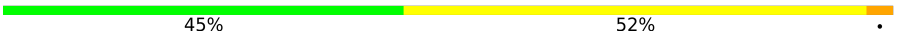


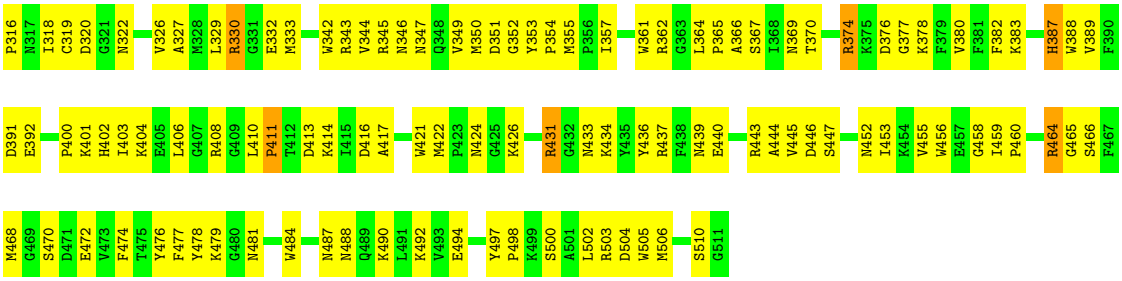


4.2.11 Score per residue for model 11

• Molecule 1: Matrix metalloproteinase-14

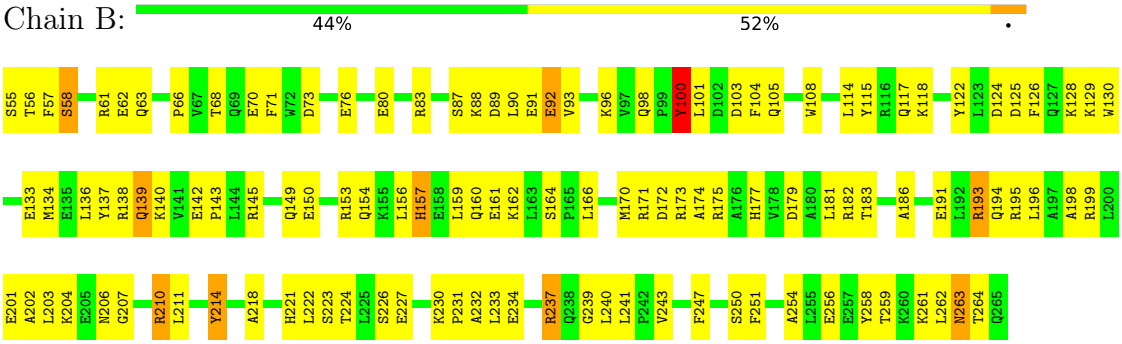
Chain A:





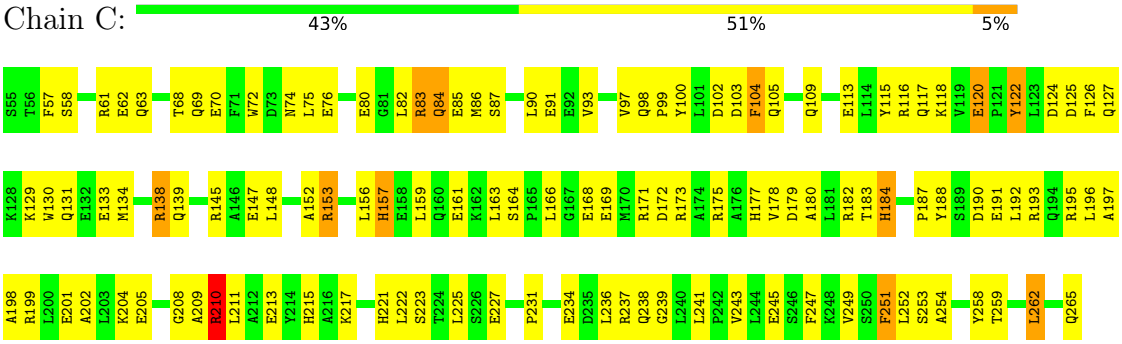
• Molecule 2: Apolipoprotein A-I

Chain B:



• Molecule 2: Apolipoprotein A-I

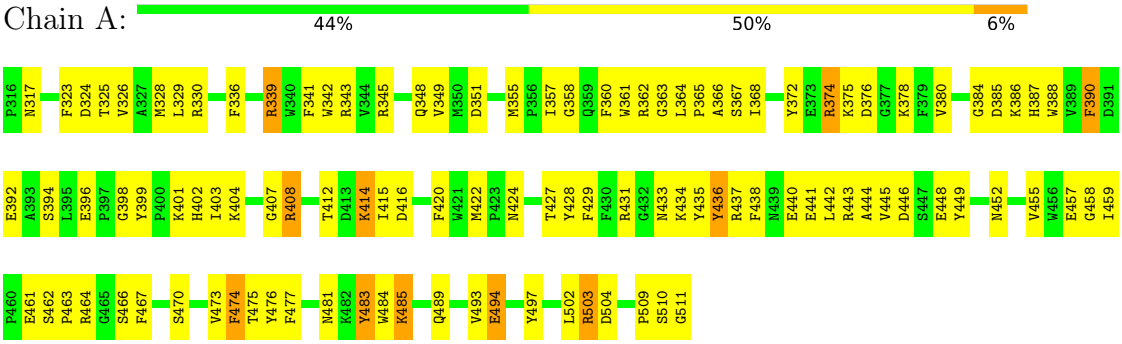
Chain C:



4.2.12 Score per residue for model 12

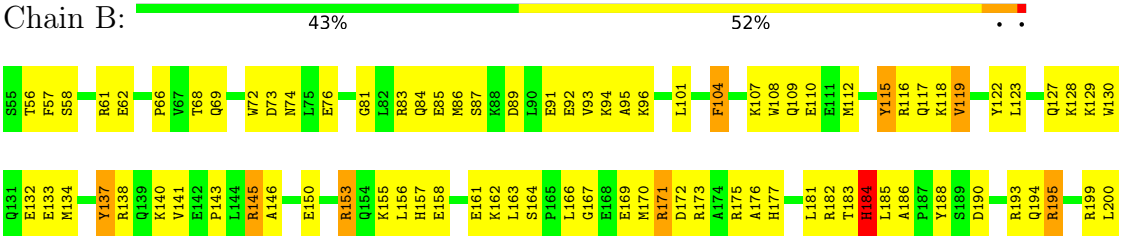
• Molecule 1: Matrix metalloproteinase-14

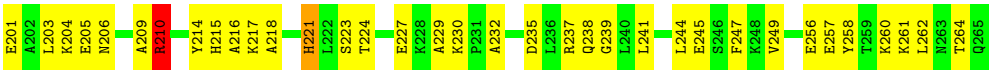
Chain A:



• Molecule 2: Apolipoprotein A-I

Chain B:

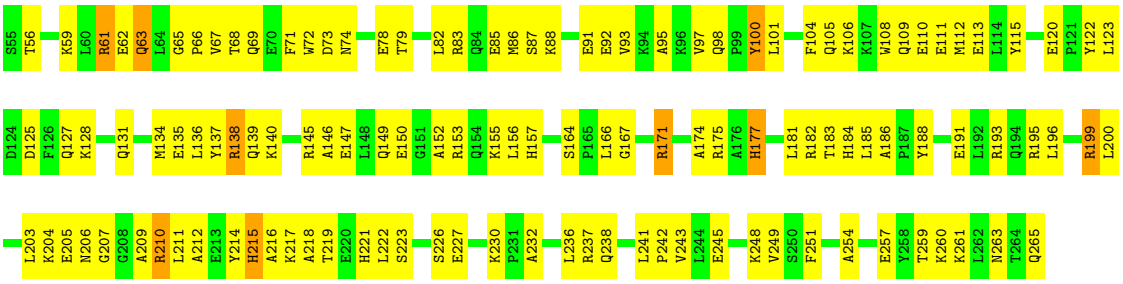




• Molecule 2: Apolipoprotein A-I

Chain C:



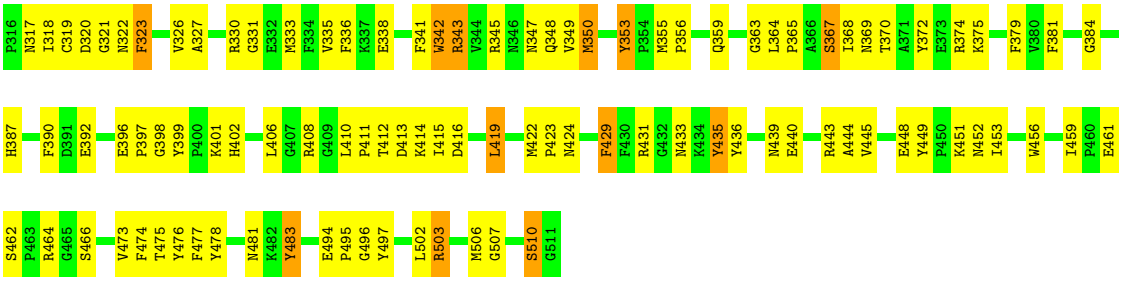


4.2.13 Score per residue for model 13

• Molecule 1: Matrix metalloproteinase-14

Chain A:

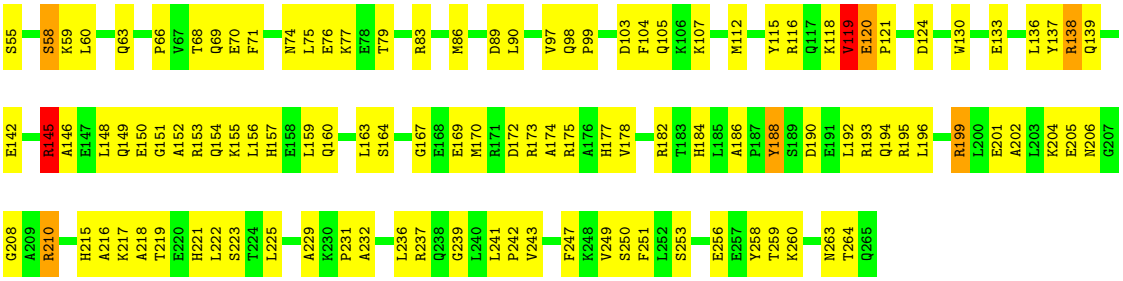




• Molecule 2: Apolipoprotein A-I

Chain B:



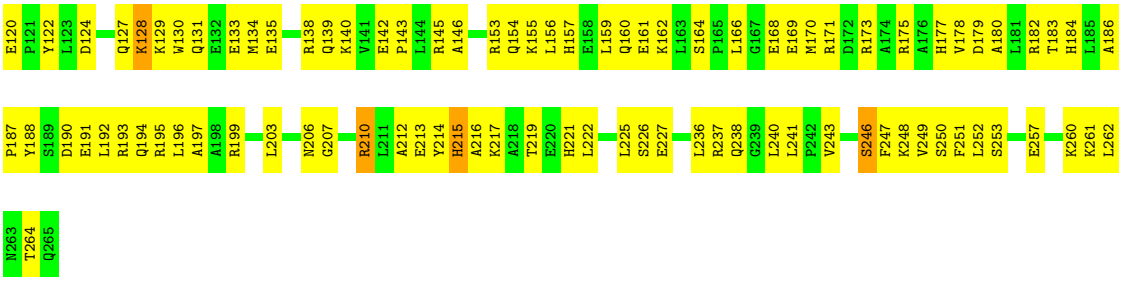


• Molecule 2: Apolipoprotein A-I

Chain C:





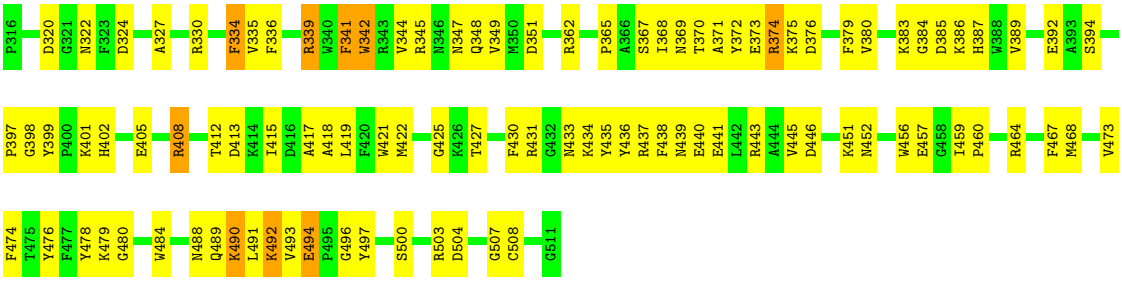


4.2.14 Score per residue for model 14

• Molecule 1: Matrix metalloproteinase-14

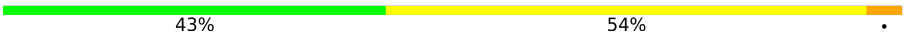
Chain A:

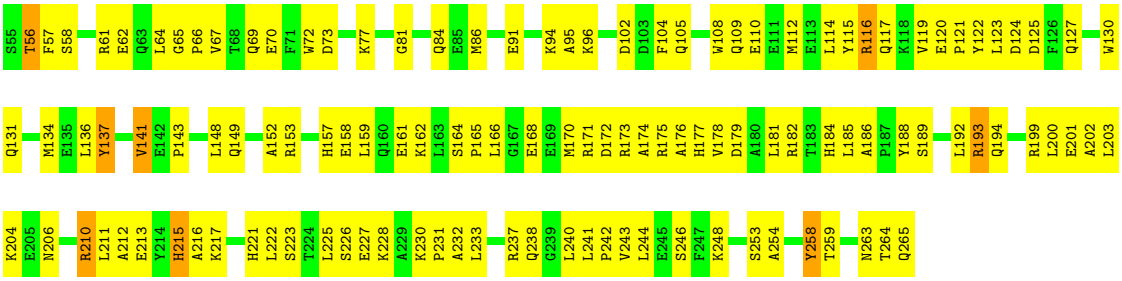




• Molecule 2: Apolipoprotein A-I

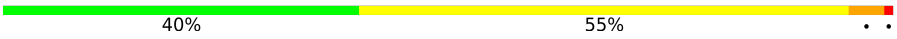
Chain B:

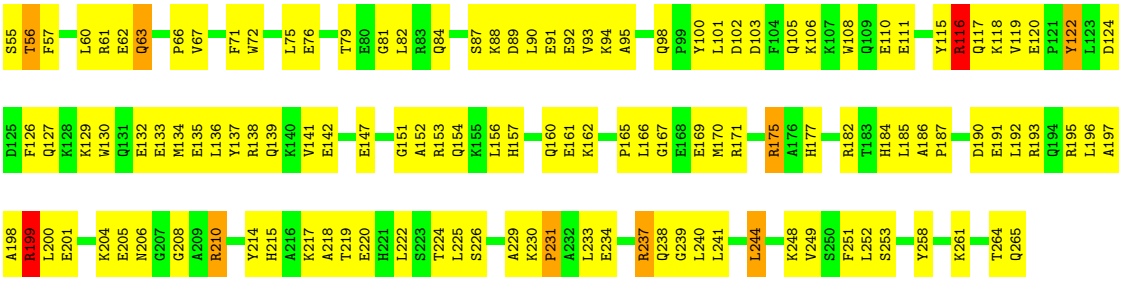




• Molecule 2: Apolipoprotein A-I

Chain C:





4.2.15 Score per residue for model 15

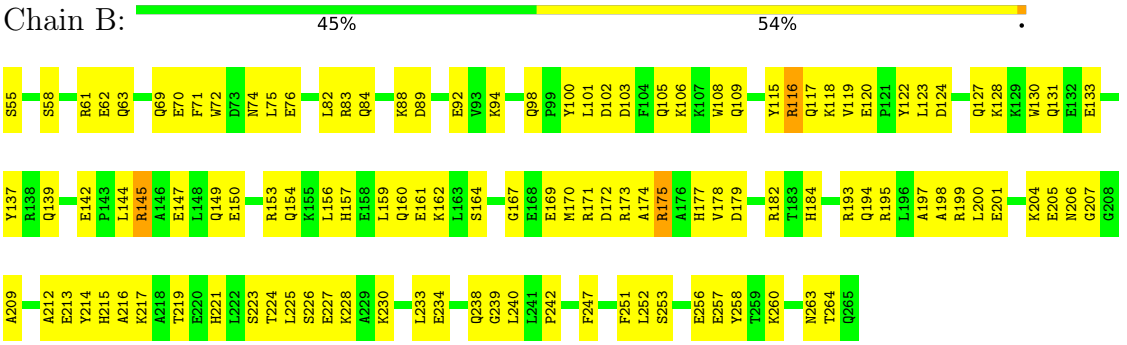
• Molecule 1: Matrix metalloproteinase-14

Chain A:



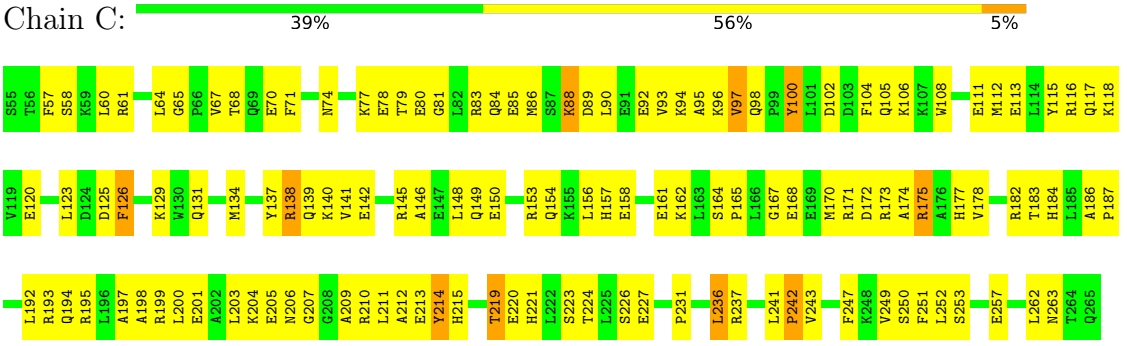
• Molecule 2: Apolipoprotein A-I

Chain B:



• Molecule 2: Apolipoprotein A-I

Chain C:



5 Refinement protocol and experimental data overview

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

Of the 500 calculated structures, 15 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
HADDOCK	structure calculation	HADDOCK2.1
NAMD	structure calculation	NAMD2.1 with CUDA GPU processing
NAMD	refinement	NAMD2.1 with CUDA GPU processing

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	324
Number of shifts mapped to atoms	324
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	4%

6 Model quality (i)

6.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	2.11±0.04	46±7/1696 (2.7± 0.4%)	2.39±0.05	102±13/2286 (4.5± 0.6%)
2	B	2.17±0.05	53±7/1784 (3.0± 0.4%)	2.63±0.04	153±11/2394 (6.4± 0.5%)
2	C	2.18±0.04	55±5/1784 (3.1± 0.3%)	2.63±0.05	157±14/2394 (6.5± 0.6%)
All	All	2.16	2309/78960 (2.9%)	2.56	6182/106110 (5.8%)

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

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	462	SER	CA-C	13.05	1.63	1.53	6	3
1	A	462	SER	N-CA	11.84	1.54	1.46	5	3
1	A	327	ALA	CA-C	-11.83	1.37	1.52	5	2
2	C	241	LEU	CA-C	11.57	1.64	1.52	6	3
1	A	459	ILE	CA-C	-11.50	1.42	1.52	10	4
2	B	118	LYS	N-CA	-11.46	1.33	1.47	9	3
2	C	236	LEU	CA-C	11.08	1.66	1.52	2	2
2	C	98	GLN	CA-CB	10.85	1.66	1.53	11	5
1	A	399	TYR	CA-C	10.69	1.62	1.52	4	3
1	A	445	VAL	CA-CB	-10.59	1.41	1.54	3	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	221	HIS	ND1-CE1	10.46	1.43	1.32	4	5
2	B	153	ARG	CA-CB	10.45	1.69	1.53	8	2
1	A	404	LYS	CA-C	10.24	1.66	1.52	9	4
1	A	458	GLY	C-N	10.21	1.44	1.33	1	2
2	C	98	GLN	C-N	-10.21	1.25	1.33	9	3
2	B	260	LYS	N-CA	-9.83	1.34	1.46	1	1
2	B	184	HIS	CA-C	9.78	1.65	1.52	10	2
2	B	109	GLN	CA-CB	9.76	1.68	1.53	4	4
2	C	236	LEU	CA-CB	9.49	1.68	1.53	8	3
1	A	476	TYR	C-N	9.45	1.47	1.33	6	2
1	A	338	GLU	CA-C	9.44	1.61	1.53	4	3
2	C	159	LEU	CA-C	9.44	1.66	1.52	1	1
2	B	63	GLN	CA-C	9.38	1.64	1.52	7	3
1	A	353	TYR	CA-C	9.33	1.61	1.52	10	2
1	A	421	TRP	NE1-CE2	-9.08	1.27	1.37	1	1
2	C	108	TRP	C-N	9.08	1.45	1.33	6	2
2	B	184	HIS	ND1-CE1	9.04	1.41	1.32	12	3
2	C	120	GLU	CA-CB	9.02	1.62	1.54	11	1
1	A	342	TRP	NE1-CE2	-8.90	1.27	1.37	3	2
2	C	157	HIS	ND1-CE1	8.89	1.41	1.32	15	4
2	B	177	HIS	ND1-CE1	8.86	1.41	1.32	9	3
2	B	197	ALA	N-CA	8.86	1.56	1.46	15	1
2	C	252	LEU	CA-CB	8.85	1.67	1.53	8	2
2	C	178	VAL	C-N	8.82	1.45	1.33	8	2
2	B	172	ASP	C-N	8.82	1.45	1.33	3	1
1	A	485	LYS	CA-CB	8.80	1.66	1.53	15	1
2	B	69	GLN	N-CA	-8.79	1.35	1.46	12	1
2	B	170	MET	CA-C	-8.74	1.41	1.52	13	1
2	C	140	LYS	CA-CB	8.69	1.68	1.53	6	1
2	C	145	ARG	C-N	8.67	1.44	1.33	15	1
2	B	134	MET	N-CA	-8.66	1.35	1.46	6	1
2	B	163	LEU	CA-C	-8.65	1.41	1.52	9	3
1	A	372	TYR	N-CA	8.63	1.56	1.45	8	1
2	C	177	HIS	ND1-CE1	8.59	1.41	1.32	9	5
2	C	125	ASP	CA-CB	8.56	1.66	1.53	11	4
2	B	237	ARG	CA-CB	8.52	1.66	1.53	1	1
2	B	230	LYS	N-CA	-8.51	1.38	1.46	8	1
2	B	211	LEU	CA-C	-8.47	1.41	1.52	14	4
1	A	401	LYS	CA-C	8.43	1.62	1.52	13	1
2	B	133	GLU	C-N	8.40	1.45	1.33	6	2
1	A	434	LYS	CA-C	8.40	1.63	1.52	11	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	C	243	VAL	CA-C	8.36	1.63	1.52	12	2
1	A	320	ASP	CA-C	8.34	1.64	1.52	1	3
2	B	147	GLU	CA-CB	8.34	1.66	1.53	9	1
2	B	241	LEU	CA-C	8.28	1.63	1.52	6	2
2	C	147	GLU	CA-C	8.23	1.63	1.52	8	1
2	B	223	SER	CA-C	8.23	1.63	1.52	13	2
2	B	158	GLU	CA-C	8.22	1.63	1.52	5	2
2	B	209	ALA	C-N	8.22	1.44	1.33	10	2
1	A	349	VAL	CA-CB	8.20	1.62	1.54	1	3
2	C	215	HIS	ND1-CE1	8.19	1.40	1.32	7	4
2	C	174	ALA	C-N	8.16	1.44	1.33	12	1
1	A	400	PRO	C-N	8.14	1.44	1.33	2	1
2	C	90	LEU	CA-C	8.14	1.63	1.52	8	1
2	C	184	HIS	CA-C	-8.13	1.42	1.52	12	3
2	C	197	ALA	CA-C	-8.12	1.42	1.52	2	1
2	B	200	LEU	N-CA	8.10	1.56	1.46	10	1
2	B	120	GLU	N-CA	-8.10	1.39	1.46	1	3
1	A	458	GLY	N-CA	8.09	1.57	1.45	6	1
2	C	130	TRP	CA-CB	8.08	1.66	1.53	6	1
1	A	449	TYR	N-CA	-8.07	1.39	1.45	4	2
1	A	443	ARG	CA-C	8.07	1.63	1.53	8	1
2	B	77	LYS	CA-CB	8.04	1.65	1.53	5	1
2	B	100	TYR	CA-CB	8.03	1.65	1.53	7	2
2	B	139	GLN	CA-CB	8.03	1.66	1.53	13	3
2	C	142	GLU	N-CA	8.02	1.53	1.46	2	2
2	C	207	GLY	C-N	8.01	1.44	1.33	10	1
2	C	157	HIS	CA-C	-8.01	1.42	1.52	3	3
2	B	129	LYS	N-CA	-8.00	1.35	1.46	1	2
1	A	418	ALA	CA-C	8.00	1.62	1.52	4	1
1	A	457	GLU	CA-C	7.99	1.62	1.52	15	1
2	C	85	GLU	C-N	7.99	1.44	1.33	13	1
2	C	164	SER	N-CA	7.98	1.53	1.46	12	3
1	A	464	ARG	CA-C	7.98	1.63	1.52	15	2
2	B	149	GLN	C-N	7.97	1.44	1.33	7	1
2	C	126	PHE	CA-CB	7.97	1.66	1.53	14	2
1	A	462	SER	CA-CB	7.95	1.58	1.52	4	3
2	B	215	HIS	ND1-CE1	7.95	1.40	1.32	10	4
2	C	181	LEU	C-N	7.95	1.43	1.33	12	1
2	B	71	PHE	CA-CB	7.94	1.65	1.53	2	2
1	A	431	ARG	N-CA	-7.94	1.35	1.46	5	2
2	C	224	THR	C-N	7.93	1.43	1.33	15	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	434	LYS	C-N	7.93	1.44	1.33	7	2
2	B	115	TYR	CA-C	-7.93	1.42	1.52	7	1
2	C	130	TRP	NE1-CE2	-7.93	1.28	1.37	4	1
2	B	138	ARG	CA-C	-7.92	1.42	1.52	7	1
2	B	161	GLU	N-CA	-7.92	1.36	1.46	9	2
2	C	127	GLN	N-CA	-7.92	1.36	1.46	14	1
2	B	172	ASP	CA-C	7.91	1.63	1.52	9	2
1	A	505	TRP	CA-C	7.90	1.61	1.52	3	2
2	C	174	ALA	CA-C	-7.90	1.42	1.52	1	1
1	A	323	PHE	CA-C	-7.88	1.42	1.52	10	2
2	C	99	PRO	C-N	7.88	1.44	1.33	10	1
2	C	263	ASN	C-N	7.86	1.44	1.33	12	3
2	B	164	SER	CA-CB	7.85	1.64	1.53	9	2
2	C	212	ALA	N-CA	-7.85	1.36	1.46	2	2
1	A	387	HIS	CA-C	-7.83	1.43	1.52	5	3
1	A	329	LEU	CA-C	7.83	1.61	1.52	12	1
1	A	387	HIS	CB-CG	7.80	1.61	1.50	5	2
2	B	198	ALA	CA-C	7.80	1.62	1.52	7	1
2	C	93	VAL	CA-C	-7.80	1.42	1.52	3	2
2	C	169	GLU	N-CA	-7.80	1.37	1.46	14	1
2	C	125	ASP	N-CA	-7.79	1.36	1.46	15	2
2	B	250	SER	N-CA	7.79	1.55	1.46	13	2
2	B	157	HIS	CA-CB	7.79	1.65	1.53	12	1
1	A	387	HIS	CE1-NE2	-7.78	1.24	1.32	4	2
2	C	138	ARG	C-N	7.78	1.44	1.33	15	2
2	C	188	TYR	CA-CB	7.77	1.65	1.53	12	1
2	B	122	TYR	CA-CB	7.76	1.65	1.53	3	3
2	B	197	ALA	CA-C	7.76	1.62	1.52	3	2
2	B	258	TYR	C-N	7.76	1.44	1.33	4	2
1	A	379	PHE	CA-C	7.76	1.62	1.52	14	1
2	B	177	HIS	CB-CG	7.74	1.60	1.50	14	1
1	A	433	ASN	CA-C	7.74	1.64	1.52	4	1
2	C	66	PRO	CA-CB	-7.74	1.41	1.53	14	2
1	A	345	ARG	CD-NE	7.72	1.57	1.46	7	4
2	C	230	LYS	C-O	-7.72	1.17	1.24	14	1
1	A	343	ARG	CA-C	-7.71	1.43	1.52	5	1
2	B	151	GLY	CA-C	-7.70	1.42	1.51	1	4
2	C	256	GLU	CA-C	7.69	1.62	1.52	9	1
2	B	71	PHE	C-N	7.69	1.43	1.33	10	1
2	C	222	LEU	CA-C	7.69	1.62	1.52	12	1
1	A	397	PRO	CA-CB	7.66	1.64	1.53	10	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	402	HIS	ND1-CE1	7.66	1.40	1.32	12	5
1	A	499	LYS	N-CA	7.64	1.55	1.45	8	1
2	B	58	SER	C-N	7.64	1.44	1.34	11	2
2	C	152	ALA	N-CA	-7.64	1.37	1.46	7	3
1	A	418	ALA	C-N	7.64	1.43	1.33	9	4
1	A	413	ASP	CA-C	-7.62	1.46	1.52	15	3
2	C	260	LYS	CA-C	7.62	1.62	1.52	13	2
1	A	407	GLY	N-CA	7.62	1.54	1.45	10	1
1	A	366	ALA	CA-CB	7.62	1.66	1.53	11	1
1	A	508	CYS	CA-CB	7.61	1.64	1.53	10	2
2	C	217	LYS	CA-C	-7.60	1.42	1.52	12	1
2	C	187	PRO	CA-C	-7.60	1.41	1.52	5	1
2	C	102	ASP	C-N	7.60	1.44	1.34	6	1
2	C	196	LEU	CA-C	7.60	1.62	1.52	9	2
2	B	193	ARG	CA-C	7.59	1.63	1.52	11	2
2	B	103	ASP	CA-CB	7.58	1.65	1.53	3	2
2	C	240	LEU	N-CA	-7.58	1.36	1.46	13	4
1	A	403	ILE	C-O	-7.58	1.15	1.24	2	1
1	A	427	THR	CA-C	-7.58	1.43	1.52	3	1
2	B	216	ALA	CA-C	7.57	1.62	1.52	1	2
1	A	446	ASP	CA-CB	7.56	1.64	1.53	12	2
2	B	152	ALA	CA-C	7.55	1.62	1.52	8	1
2	C	226	SER	N-CA	7.54	1.55	1.46	12	1
2	C	101	LEU	CA-CB	7.53	1.65	1.53	2	1
1	A	470	SER	CA-CB	7.52	1.65	1.53	3	2
1	A	369	ASN	CA-C	7.52	1.62	1.52	10	1
1	A	444	ALA	N-CA	-7.52	1.36	1.45	3	1
2	C	58	SER	CA-CB	7.51	1.65	1.53	13	2
2	C	261	LYS	CA-CB	7.51	1.65	1.53	9	5
2	B	137	TYR	CA-C	7.51	1.62	1.52	7	2
2	B	139	GLN	C-O	-7.50	1.15	1.24	9	1
2	C	135	GLU	N-CA	-7.50	1.37	1.46	13	1
2	B	127	GLN	CA-CB	7.49	1.65	1.53	14	1
2	C	214	TYR	CA-CB	7.49	1.65	1.53	7	3
2	C	209	ALA	C-N	7.48	1.43	1.33	7	2
2	C	81	GLY	CA-C	-7.48	1.41	1.51	15	3
2	C	120	GLU	N-CA	-7.47	1.39	1.46	15	1
1	A	476	TYR	N-CA	-7.47	1.37	1.46	6	1
2	C	147	GLU	C-N	7.47	1.43	1.33	1	1
1	A	340	TRP	NE1-CE2	-7.47	1.29	1.37	3	1
1	A	323	PHE	N-CA	7.46	1.55	1.45	12	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	70	GLU	N-CA	7.46	1.55	1.46	14	2
2	B	257	GLU	CA-CB	7.45	1.65	1.53	12	2
1	A	389	VAL	CA-C	-7.45	1.43	1.52	14	1
1	A	382	PHE	N-CA	7.44	1.54	1.46	5	1
2	C	178	VAL	N-CA	-7.44	1.37	1.46	5	1
2	C	153	ARG	N-CA	-7.43	1.36	1.46	10	1
2	B	221	HIS	CB-CG	7.43	1.60	1.50	10	2
2	B	109	GLN	CA-C	-7.43	1.43	1.52	3	1
2	C	154	GLN	CA-CB	7.42	1.64	1.53	6	4
2	C	248	LYS	C-N	7.42	1.42	1.33	4	1
1	A	330	ARG	CD-NE	7.41	1.56	1.46	8	2
2	C	221	HIS	CA-C	7.40	1.62	1.52	13	2
2	C	171	ARG	CD-NE	7.40	1.56	1.46	7	6
2	C	240	LEU	CA-CB	7.40	1.64	1.53	14	1
2	B	230	LYS	CA-CB	7.38	1.62	1.53	11	1
2	C	196	LEU	C-N	7.38	1.44	1.33	3	1
2	B	171	ARG	CD-NE	7.37	1.56	1.46	4	4
1	A	464	ARG	N-CA	-7.37	1.37	1.46	2	1
2	B	174	ALA	C-O	-7.37	1.15	1.24	11	1
2	C	241	LEU	CA-CB	7.37	1.64	1.53	11	2
1	A	369	ASN	CA-CB	7.36	1.65	1.53	15	2
1	A	502	LEU	C-O	-7.34	1.15	1.24	12	1
2	C	153	ARG	C-N	7.34	1.43	1.33	12	2
2	C	137	TYR	CA-CB	7.34	1.64	1.53	8	2
1	A	323	PHE	CA-CB	7.33	1.65	1.53	3	2
2	B	161	GLU	CA-CB	7.33	1.64	1.53	6	1
2	C	175	ARG	C-N	7.33	1.43	1.33	9	1
2	C	156	LEU	C-N	7.33	1.44	1.34	2	1
2	C	253	SER	CA-CB	7.32	1.64	1.53	9	3
2	B	169	GLU	N-CA	-7.32	1.37	1.46	9	2
2	B	186	ALA	C-N	-7.32	1.25	1.34	12	2
2	B	156	LEU	CA-C	7.32	1.62	1.52	4	3
2	C	210	ARG	CD-NE	7.32	1.56	1.46	11	1
2	C	58	SER	C-N	7.32	1.43	1.33	15	1
2	C	196	LEU	N-CA	-7.31	1.37	1.46	9	1
2	C	172	ASP	C-N	7.31	1.44	1.34	5	2
2	B	214	TYR	N-CA	-7.30	1.37	1.46	1	3
2	B	146	ALA	N-CA	-7.30	1.37	1.46	8	1
2	B	82	LEU	CA-C	7.28	1.62	1.52	1	2
1	A	483	TYR	C-N	7.28	1.43	1.33	6	1
1	A	410	LEU	CA-C	7.28	1.61	1.52	5	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	479	LYS	CA-C	-7.26	1.43	1.52	6	1
2	B	92	GLU	CA-CB	7.26	1.64	1.53	12	1
2	C	262	LEU	N-CA	-7.26	1.37	1.46	7	2
2	C	110	GLU	CA-CB	7.25	1.65	1.53	9	3
2	C	119	VAL	N-CA	7.25	1.56	1.46	10	2
1	A	325	THR	C-N	7.24	1.42	1.33	10	1
1	A	344	VAL	CA-CB	-7.24	1.45	1.54	3	2
2	B	237	ARG	CD-NE	7.23	1.56	1.46	11	5
1	A	503	ARG	CZ-NH2	-7.22	1.24	1.33	11	1
1	A	387	HIS	ND1-CE1	7.22	1.39	1.32	5	4
2	C	63	GLN	CA-CB	7.22	1.64	1.53	11	3
1	A	433	ASN	CA-CB	7.20	1.63	1.53	5	3
2	B	177	HIS	N-CA	-7.20	1.37	1.46	1	2
2	C	103	ASP	C-N	7.20	1.42	1.33	13	2
2	C	138	ARG	CD-NE	7.19	1.56	1.46	1	5
2	C	83	ARG	CA-C	7.18	1.62	1.52	5	2
1	A	462	SER	C-O	-7.17	1.20	1.23	4	1
2	B	85	GLU	CA-C	7.16	1.62	1.52	12	2
2	B	206	ASN	CA-CB	7.16	1.64	1.53	5	3
2	B	258	TYR	CA-C	7.16	1.61	1.52	7	2
2	B	196	LEU	C-O	-7.15	1.15	1.24	3	2
1	A	374	ARG	CA-CB	7.15	1.64	1.53	13	1
1	A	386	LYS	CA-C	7.13	1.61	1.52	3	2
2	B	193	ARG	CD-NE	7.13	1.56	1.46	11	2
1	A	374	ARG	N-CA	7.13	1.54	1.45	6	1
1	A	422	MET	CA-CB	7.13	1.63	1.53	13	3
2	C	58	SER	N-CA	-7.12	1.37	1.46	6	2
2	B	149	GLN	N-CA	-7.12	1.37	1.46	15	1
2	C	95	ALA	CA-C	7.12	1.62	1.52	9	5
2	C	257	GLU	CA-CB	7.12	1.64	1.53	9	2
2	C	97	VAL	CA-C	7.11	1.61	1.52	3	1
1	A	478	TYR	CA-C	7.11	1.61	1.52	3	2
2	C	79	THR	C-N	7.11	1.43	1.33	6	1
2	C	172	ASP	N-CA	-7.10	1.38	1.46	9	2
2	C	146	ALA	C-N	7.10	1.42	1.33	8	1
1	A	402	HIS	N-CA	7.09	1.54	1.46	1	1
1	A	471	ASP	CA-CB	7.09	1.64	1.53	1	1
2	B	184	HIS	C-N	7.09	1.44	1.33	5	1
2	C	221	HIS	ND1-CE1	7.09	1.39	1.32	5	3
2	C	165	PRO	N-CD	-7.09	1.37	1.47	9	1
2	B	76	GLU	N-CA	-7.08	1.37	1.46	12	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	94	LYS	N-CA	7.08	1.55	1.46	1	1
2	C	174	ALA	CA-CB	7.08	1.64	1.53	3	2
2	B	188	TYR	N-CA	-7.08	1.37	1.46	7	3
2	B	153	ARG	N-CA	-7.07	1.37	1.46	9	1
2	C	204	LYS	CA-CB	7.07	1.64	1.53	14	1
2	B	238	GLN	CA-C	7.06	1.62	1.52	8	2
1	A	504	ASP	CA-CB	7.05	1.64	1.53	11	1
2	C	152	ALA	C-N	7.05	1.43	1.33	12	1
2	B	240	LEU	CA-C	-7.05	1.43	1.52	2	2
1	A	423	PRO	CA-C	7.05	1.59	1.52	8	1
2	C	129	LYS	C-O	-7.05	1.15	1.24	13	2
2	B	187	PRO	C-N	7.04	1.43	1.33	5	1
2	C	213	GLU	CA-CB	7.04	1.65	1.53	8	4
1	A	342	TRP	CA-CB	7.04	1.64	1.53	15	2
1	A	345	ARG	C-N	7.04	1.43	1.33	4	1
1	A	335	VAL	CA-CB	-7.04	1.45	1.54	13	2
2	C	75	LEU	CA-C	7.04	1.62	1.52	10	3
2	B	232	ALA	N-CA	7.04	1.54	1.46	12	2
2	C	77	LYS	CA-C	-7.03	1.44	1.52	6	1
2	C	262	LEU	CA-CB	7.03	1.64	1.53	13	2
2	B	203	LEU	CA-CB	7.03	1.65	1.53	3	3
1	A	453	ILE	CA-CB	-7.03	1.44	1.54	7	2
2	C	97	VAL	CA-CB	-7.02	1.45	1.54	4	1
1	A	391	ASP	CA-CB	7.02	1.63	1.53	3	2
2	C	169	GLU	CA-CB	-7.02	1.42	1.53	3	1
2	C	223	SER	CA-CB	7.01	1.65	1.53	11	3
2	B	226	SER	CA-CB	7.00	1.64	1.53	11	2
2	C	135	GLU	CA-CB	-7.00	1.42	1.53	4	1
1	A	324	ASP	CA-CB	7.00	1.64	1.53	15	1
1	A	493	VAL	CA-CB	-7.00	1.47	1.54	15	1
2	C	220	GLU	CA-C	-7.00	1.43	1.52	10	1
2	B	251	PHE	CA-C	7.00	1.62	1.52	11	1
1	A	493	VAL	C-N	6.99	1.43	1.33	14	1
2	C	253	SER	C-N	6.99	1.43	1.33	7	2
2	B	254	ALA	C-N	6.99	1.42	1.33	7	2
2	B	193	ARG	CA-CB	6.99	1.64	1.53	7	1
2	B	56	THR	C-N	6.99	1.42	1.33	11	1
2	B	109	GLN	N-CA	-6.97	1.38	1.46	3	1
2	C	61	ARG	CA-C	6.97	1.61	1.52	14	1
2	C	118	LYS	N-CA	-6.97	1.37	1.46	15	1
2	C	180	ALA	CA-CB	6.97	1.64	1.53	4	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	250	SER	C-N	6.97	1.43	1.33	7	1
1	A	387	HIS	N-CA	-6.97	1.37	1.46	4	2
1	A	505	TRP	N-CA	-6.96	1.36	1.46	4	1
1	A	390	PHE	CA-C	-6.95	1.44	1.52	2	1
2	C	68	THR	CA-CB	6.95	1.64	1.53	6	1
2	B	57	PHE	CA-CB	6.94	1.64	1.53	7	1
2	B	179	ASP	N-CA	-6.93	1.37	1.46	9	1
2	B	74	ASN	CA-C	6.93	1.61	1.52	1	3
2	C	100	TYR	C-N	6.92	1.42	1.33	2	1
2	B	160	GLN	N-CA	6.92	1.54	1.46	6	2
2	C	118	LYS	C-N	6.92	1.43	1.34	5	5
1	A	471	ASP	N-CA	-6.91	1.37	1.46	1	2
2	C	145	ARG	CA-CB	6.91	1.64	1.53	3	1
2	C	136	LEU	CA-C	6.91	1.61	1.52	4	1
2	C	71	PHE	N-CA	-6.91	1.38	1.46	15	2
2	C	188	TYR	N-CA	-6.90	1.36	1.46	2	1
2	B	63	GLN	CA-CB	6.90	1.64	1.53	15	2
2	C	89	ASP	CA-CB	6.90	1.64	1.53	6	1
2	C	148	LEU	CA-C	-6.90	1.44	1.52	10	1
2	C	74	ASN	CA-CB	6.90	1.64	1.53	8	2
2	B	133	GLU	N-CA	-6.90	1.38	1.46	12	1
2	B	251	PHE	CA-CB	6.89	1.64	1.53	9	1
2	B	184	HIS	CB-CG	6.88	1.59	1.50	3	2
2	B	109	GLN	C-N	6.88	1.43	1.33	4	1
2	C	62	GLU	N-CA	-6.88	1.37	1.46	11	1
1	A	484	TRP	CA-CB	6.88	1.62	1.53	12	1
1	A	427	THR	N-CA	-6.88	1.37	1.46	14	1
1	A	454	LYS	N-CA	-6.88	1.36	1.46	7	4
2	B	201	GLU	N-CA	-6.87	1.38	1.46	3	1
1	A	395	LEU	CA-C	-6.87	1.43	1.52	8	1
2	C	210	ARG	C-O	-6.87	1.16	1.24	9	2
2	C	127	GLN	CA-C	-6.86	1.44	1.52	13	2
1	A	368	ILE	CA-CB	6.86	1.61	1.54	14	1
2	C	170	MET	CA-CB	6.86	1.64	1.53	14	2
2	B	122	TYR	N-CA	-6.85	1.38	1.46	1	2
2	C	106	LYS	CA-C	6.85	1.61	1.52	13	1
2	B	66	PRO	CA-CB	6.85	1.63	1.53	12	2
1	A	505	TRP	NE1-CE2	-6.84	1.29	1.37	8	2
2	B	108	TRP	CA-C	-6.84	1.44	1.52	6	4
2	C	196	LEU	CB-CG	6.84	1.67	1.53	11	1
2	C	121	PRO	N-CA	6.83	1.56	1.47	2	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	396	GLU	CA-C	6.83	1.61	1.52	7	2
1	A	432	GLY	C-N	6.83	1.42	1.33	6	1
1	A	484	TRP	N-CA	-6.82	1.38	1.46	9	3
2	C	179	ASP	N-CA	-6.82	1.38	1.46	8	3
2	C	215	HIS	CG-ND1	-6.82	1.30	1.38	1	1
1	A	391	ASP	N-CA	-6.81	1.37	1.46	15	2
1	A	337	LYS	CA-C	6.81	1.60	1.52	8	4
1	A	339	ARG	CD-NE	6.81	1.55	1.46	7	3
2	B	72	TRP	C-N	6.81	1.42	1.33	10	2
1	A	383	LYS	CA-C	-6.80	1.44	1.52	2	1
1	A	384	GLY	CA-C	6.80	1.61	1.51	3	2
2	B	241	LEU	CA-CB	6.79	1.62	1.53	7	4
2	C	236	LEU	C-N	6.79	1.43	1.34	12	2
1	A	410	LEU	C-N	6.79	1.41	1.33	9	1
2	B	239	GLY	C-N	-6.79	1.24	1.33	8	1
2	C	164	SER	CA-C	6.78	1.61	1.52	6	4
1	A	492	LYS	C-N	6.78	1.41	1.33	15	1
2	B	234	GLU	CA-CB	6.77	1.64	1.53	2	2
1	A	364	LEU	CA-C	-6.77	1.45	1.52	13	1
1	A	430	PHE	CA-C	-6.76	1.44	1.52	7	1
1	A	459	ILE	C-N	6.76	1.42	1.33	9	1
2	C	155	LYS	C-N	6.76	1.42	1.33	8	1
2	B	147	GLU	CA-C	6.76	1.62	1.52	15	2
2	B	188	TYR	CA-C	6.76	1.61	1.52	9	1
2	B	169	GLU	CA-CB	6.75	1.63	1.53	1	1
1	A	511	GLY	CA-C	6.75	1.64	1.52	12	1
2	B	231	PRO	N-CA	6.74	1.55	1.47	13	1
1	A	322	ASN	C-N	6.74	1.42	1.33	15	1
2	C	103	ASP	CA-C	-6.74	1.43	1.52	11	1
1	A	397	PRO	CA-C	-6.74	1.42	1.52	1	2
2	B	117	GLN	C-O	6.74	1.32	1.24	10	1
1	A	322	ASN	CA-C	-6.74	1.46	1.53	2	1
2	B	192	LEU	C-N	6.73	1.42	1.33	1	2
2	B	155	LYS	C-N	6.73	1.42	1.33	1	1
2	B	88	LYS	N-CA	-6.72	1.38	1.46	11	3
2	B	120	GLU	CA-C	6.72	1.60	1.52	5	1
1	A	481	ASN	CA-CB	6.72	1.64	1.53	6	3
1	A	317	ASN	CA-CB	6.72	1.63	1.53	8	1
2	B	243	VAL	CA-CB	-6.72	1.46	1.54	13	2
2	B	153	ARG	CD-NE	6.71	1.55	1.46	10	3
2	B	117	GLN	CA-CB	6.71	1.63	1.53	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	343	ARG	CA-CB	6.70	1.62	1.53	11	1
2	C	111	GLU	C-N	6.70	1.42	1.33	9	2
2	C	59	LYS	CA-C	6.70	1.61	1.52	5	1
2	B	253	SER	CA-C	-6.69	1.44	1.52	2	1
2	C	141	VAL	C-N	6.69	1.42	1.33	10	1
2	B	238	GLN	C-N	6.69	1.42	1.33	9	3
2	C	170	MET	N-CA	-6.69	1.38	1.46	15	1
1	A	406	LEU	N-CA	6.68	1.54	1.46	1	2
2	C	158	GLU	CA-C	6.68	1.61	1.52	1	1
2	C	236	LEU	CB-CG	6.68	1.66	1.53	1	1
2	B	72	TRP	CA-CB	6.68	1.63	1.53	12	3
2	C	215	HIS	CE1-NE2	-6.68	1.25	1.32	5	1
2	B	228	LYS	N-CA	-6.68	1.38	1.46	15	1
1	A	496	GLY	N-CA	6.68	1.54	1.45	9	1
2	B	81	GLY	CA-C	-6.67	1.44	1.52	4	1
1	A	362	ARG	C-N	6.67	1.40	1.33	8	3
2	C	80	GLU	C-N	6.66	1.42	1.33	9	3
1	A	466	SER	N-CA	-6.65	1.37	1.46	1	2
1	A	437	ARG	CD-NE	6.65	1.55	1.46	10	3
2	B	236	LEU	N-CA	-6.64	1.38	1.46	13	2
2	B	244	LEU	C-N	6.64	1.42	1.33	7	1
2	B	128	LYS	C-N	6.63	1.43	1.34	4	2
2	C	145	ARG	CD-NE	6.63	1.55	1.46	5	5
2	C	114	LEU	C-N	6.63	1.43	1.33	4	2
1	A	362	ARG	CA-CB	6.63	1.61	1.53	9	2
2	B	196	LEU	C-N	6.62	1.42	1.33	13	1
1	A	463	PRO	CA-C	-6.62	1.45	1.52	9	2
2	C	250	SER	C-N	6.62	1.42	1.33	3	1
2	C	63	GLN	N-CA	6.62	1.54	1.46	13	2
2	B	92	GLU	C-N	-6.62	1.25	1.33	12	2
1	A	371	ALA	CA-C	-6.61	1.44	1.52	14	2
2	C	175	ARG	CA-CB	6.61	1.64	1.53	5	1
2	B	104	PHE	CA-CB	6.61	1.64	1.53	1	2
2	C	100	TYR	CA-C	-6.61	1.44	1.52	7	1
2	C	74	ASN	N-CA	6.61	1.54	1.46	11	2
2	C	98	GLN	N-CA	6.61	1.52	1.46	10	2
2	B	219	THR	CA-C	-6.60	1.43	1.52	8	1
2	B	215	HIS	C-N	6.60	1.42	1.33	15	1
2	B	219	THR	C-N	6.59	1.42	1.33	9	1
2	B	66	PRO	C-N	6.59	1.42	1.33	7	2
2	C	132	GLU	C-O	-6.59	1.16	1.24	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	178	VAL	N-CA	-6.58	1.38	1.46	7	1
1	A	398	GLY	C-N	6.58	1.40	1.33	14	2
2	B	98	GLN	CA-C	6.58	1.61	1.52	8	1
2	B	243	VAL	C-N	6.58	1.42	1.33	3	1
2	C	210	ARG	C-N	6.57	1.42	1.33	4	1
2	C	81	GLY	N-CA	-6.56	1.37	1.45	6	1
1	A	461	GLU	CA-C	6.56	1.61	1.52	8	1
1	A	500	SER	CA-CB	6.56	1.62	1.53	14	3
2	C	124	ASP	N-CA	6.56	1.54	1.46	1	2
1	A	361	TRP	CA-CB	6.56	1.61	1.52	12	1
2	C	94	LYS	C-O	-6.55	1.16	1.24	14	1
1	A	333	MET	CA-CB	6.55	1.61	1.53	10	1
2	C	94	LYS	N-CA	6.55	1.54	1.46	5	1
1	A	392	GLU	C-N	6.54	1.42	1.33	11	2
2	B	116	ARG	CA-C	6.54	1.61	1.52	13	2
2	B	112	MET	N-CA	-6.54	1.38	1.46	14	1
2	C	132	GLU	N-CA	6.54	1.54	1.46	9	1
2	C	192	LEU	N-CA	-6.53	1.38	1.46	2	3
1	A	496	GLY	C-N	-6.53	1.24	1.33	14	2
1	A	408	ARG	CD-NE	6.53	1.55	1.46	10	4
1	A	485	LYS	CA-C	-6.53	1.44	1.52	12	3
1	A	423	PRO	N-CA	-6.53	1.39	1.47	1	1
1	A	342	TRP	CA-C	-6.53	1.44	1.52	4	2
2	B	249	VAL	C-N	6.53	1.42	1.33	13	1
2	C	204	LYS	N-CA	-6.52	1.38	1.46	10	1
1	A	509	PRO	CA-C	6.52	1.60	1.52	1	2
1	A	322	ASN	CA-CB	6.52	1.64	1.53	15	2
1	A	373	GLU	C-N	6.52	1.43	1.33	4	3
2	C	224	THR	CB-OG1	-6.50	1.33	1.43	8	1
2	B	67	VAL	CA-CB	6.50	1.61	1.54	9	1
2	B	215	HIS	CA-C	6.50	1.61	1.52	10	1
2	B	61	ARG	CD-NE	6.50	1.55	1.46	9	1
2	B	217	LYS	CA-CB	6.49	1.63	1.53	2	2
2	C	259	THR	CA-CB	6.49	1.63	1.53	6	1
1	A	483	TYR	CA-C	-6.49	1.44	1.52	7	1
2	B	196	LEU	CA-C	-6.48	1.44	1.52	2	3
2	B	204	LYS	N-CA	-6.47	1.38	1.46	11	2
2	B	145	ARG	CD-NE	6.47	1.55	1.46	13	1
2	B	119	VAL	CA-CB	-6.47	1.46	1.54	4	1
2	B	127	GLN	C-N	6.47	1.42	1.33	3	2
2	B	129	LYS	CA-CB	6.47	1.63	1.53	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	102	ASP	N-CA	-6.46	1.38	1.46	5	1
2	C	193	ARG	C-O	-6.46	1.16	1.24	8	1
2	B	154	GLN	N-CA	-6.46	1.38	1.46	13	1
2	C	193	ARG	CD-NE	6.45	1.55	1.46	12	5
2	B	186	ALA	CA-C	6.45	1.60	1.52	13	1
2	C	199	ARG	CA-C	6.45	1.61	1.52	13	2
1	A	344	VAL	N-CA	-6.45	1.38	1.46	4	1
2	B	195	ARG	N-CA	6.45	1.54	1.46	15	1
1	A	486	PHE	CA-CB	6.45	1.63	1.53	3	2
2	C	122	TYR	CA-C	6.44	1.61	1.52	14	3
2	B	133	GLU	CA-CB	6.44	1.63	1.53	11	1
1	A	486	PHE	N-CA	-6.44	1.38	1.46	3	2
1	A	344	VAL	CA-C	-6.43	1.45	1.52	7	3
2	B	118	LYS	CA-CB	6.43	1.63	1.53	7	3
1	A	345	ARG	CA-C	6.43	1.60	1.52	12	4
2	C	133	GLU	N-CA	-6.43	1.38	1.46	2	2
2	B	166	LEU	C-N	6.43	1.41	1.33	14	1
2	B	181	LEU	CA-C	6.43	1.60	1.52	5	1
2	B	123	LEU	CA-C	-6.43	1.44	1.52	6	2
2	C	128	LYS	C-O	-6.43	1.16	1.24	7	1
1	A	329	LEU	CA-CB	6.43	1.63	1.53	2	1
2	C	55	SER	N-CA	6.43	1.58	1.46	3	2
2	B	173	ARG	CA-C	6.43	1.61	1.52	10	3
2	B	108	TRP	C-O	-6.42	1.16	1.24	5	1
2	C	182	ARG	CA-CB	6.42	1.63	1.53	6	1
2	B	70	GLU	C-N	6.42	1.41	1.33	13	1
1	A	367	SER	CA-CB	6.41	1.63	1.53	1	1
2	C	163	LEU	CA-C	-6.41	1.44	1.52	5	3
2	B	222	LEU	CA-C	6.41	1.61	1.52	2	2
2	C	193	ARG	N-CA	6.41	1.54	1.46	14	2
2	C	150	GLU	C-N	6.41	1.42	1.33	15	1
2	B	212	ALA	N-CA	-6.41	1.38	1.46	7	1
2	C	212	ALA	CA-C	6.41	1.61	1.52	2	1
1	A	415	ILE	CA-C	6.40	1.60	1.52	12	5
1	A	431	ARG	CD-NE	6.40	1.55	1.46	5	3
2	C	215	HIS	CA-C	-6.40	1.44	1.52	14	1
2	B	110	GLU	N-CA	-6.40	1.38	1.46	6	3
1	A	414	LYS	CA-C	-6.40	1.44	1.52	12	2
2	C	138	ARG	CA-CB	6.40	1.63	1.53	13	1
2	C	243	VAL	CA-CB	-6.39	1.46	1.54	9	2
1	A	448	GLU	N-CA	-6.39	1.37	1.46	4	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	61	ARG	CA-C	6.39	1.61	1.52	3	2
2	C	187	PRO	N-CD	6.39	1.56	1.47	6	3
2	B	180	ALA	C-N	6.39	1.42	1.33	4	1
2	B	123	LEU	CA-CB	6.38	1.63	1.53	12	2
2	B	164	SER	C-N	6.38	1.41	1.34	4	2
1	A	477	PHE	C-N	6.38	1.42	1.33	11	1
2	B	163	LEU	N-CA	6.38	1.54	1.46	13	2
2	C	94	LYS	C-N	6.38	1.42	1.33	13	1
2	C	77	LYS	C-N	6.38	1.41	1.33	2	2
1	A	360	PHE	CA-C	6.37	1.58	1.52	2	2
2	B	89	ASP	CA-CB	6.37	1.63	1.53	3	3
2	B	175	ARG	N-CA	-6.37	1.38	1.46	8	2
2	C	217	LYS	CA-CB	6.37	1.63	1.53	12	1
2	C	74	ASN	C-O	-6.37	1.16	1.24	5	1
2	C	191	GLU	CA-CB	6.37	1.63	1.53	13	2
2	B	261	LYS	CA-C	6.37	1.61	1.52	8	1
1	A	495	PRO	N-CA	-6.37	1.39	1.47	1	2
2	C	186	ALA	CA-C	6.36	1.59	1.52	2	4
1	A	391	ASP	CA-C	6.36	1.60	1.52	8	1
2	B	96	LYS	CA-CB	6.35	1.63	1.53	14	2
2	B	141	VAL	CA-C	-6.35	1.45	1.52	14	1
2	B	124	ASP	N-CA	-6.35	1.39	1.46	7	2
2	B	91	GLU	N-CA	-6.34	1.38	1.46	11	1
2	C	217	LYS	N-CA	-6.34	1.38	1.46	1	2
1	A	402	HIS	CG-ND1	-6.34	1.31	1.38	11	2
2	B	128	LYS	CA-CB	6.34	1.63	1.53	7	1
2	C	256	GLU	CA-CB	6.34	1.63	1.53	4	2
2	C	108	TRP	NE1-CE2	-6.34	1.30	1.37	4	3
1	A	443	ARG	CD-NE	6.34	1.55	1.46	3	2
2	C	92	GLU	CA-CB	6.34	1.63	1.53	14	2
1	A	343	ARG	CD-NE	6.34	1.55	1.46	5	2
2	B	184	HIS	CE1-NE2	-6.33	1.26	1.32	5	1
2	C	247	PHE	CA-CB	6.33	1.63	1.53	6	2
1	A	351	ASP	CA-CB	6.32	1.64	1.53	5	2
1	A	336	PHE	CA-C	-6.32	1.45	1.52	12	3
1	A	376	ASP	CA-CB	6.32	1.63	1.53	10	4
2	B	135	GLU	CA-C	6.32	1.61	1.52	8	1
2	B	72	TRP	N-CA	-6.31	1.38	1.46	1	1
2	C	237	ARG	CD-NE	6.31	1.55	1.46	14	4
1	A	332	GLU	CA-CB	6.31	1.65	1.53	1	1
2	B	193	ARG	CZ-NH2	-6.31	1.25	1.33	8	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	194	GLN	C-N	6.31	1.42	1.33	12	1
2	B	66	PRO	CA-C	-6.30	1.43	1.52	9	2
2	B	131	GLN	C-N	6.30	1.42	1.33	5	2
1	A	380	VAL	CA-CB	-6.30	1.46	1.54	7	1
1	A	402	HIS	CD2-NE2	6.30	1.44	1.37	5	2
2	C	258	TYR	C-N	6.30	1.41	1.33	2	1
2	C	167	GLY	CA-C	-6.30	1.45	1.52	10	4
1	A	506	MET	C-N	6.30	1.41	1.33	13	1
2	B	134	MET	C-N	6.29	1.41	1.33	1	1
2	C	238	GLN	C-N	6.29	1.42	1.33	4	1
2	B	248	LYS	CA-C	6.29	1.60	1.52	7	1
2	C	62	GLU	CA-C	-6.28	1.44	1.52	3	2
1	A	367	SER	CA-C	6.28	1.59	1.53	12	1
1	A	358	GLY	CA-C	-6.28	1.43	1.51	2	1
2	C	170	MET	CA-C	6.28	1.60	1.52	5	2
2	B	151	GLY	N-CA	6.28	1.53	1.45	13	2
2	B	59	LYS	C-N	6.28	1.42	1.33	4	2
1	A	442	LEU	C-N	6.28	1.42	1.33	5	2
2	C	93	VAL	N-CA	-6.27	1.39	1.46	2	1
1	A	357	ILE	C-O	-6.27	1.16	1.24	4	1
2	C	90	LEU	CA-CB	6.27	1.63	1.53	7	2
2	B	237	ARG	N-CA	-6.26	1.38	1.46	3	1
2	B	214	TYR	C-N	6.26	1.42	1.33	6	2
1	A	375	LYS	N-CA	6.26	1.54	1.46	14	1
1	A	484	TRP	CD2-CE3	6.26	1.50	1.40	10	1
2	C	190	ASP	N-CA	6.26	1.53	1.46	5	1
2	B	119	VAL	N-CA	-6.26	1.39	1.46	12	1
2	B	56	THR	N-CA	6.25	1.53	1.46	3	1
1	A	472	GLU	C-N	6.25	1.41	1.33	8	2
2	B	182	ARG	CD-NE	6.24	1.54	1.46	9	3
2	B	210	ARG	CA-C	-6.24	1.44	1.52	14	1
1	A	428	TYR	CA-CB	6.24	1.62	1.53	2	1
2	C	200	LEU	CA-C	6.24	1.60	1.52	12	1
2	B	227	GLU	N-CA	-6.24	1.38	1.46	8	1
2	B	186	ALA	N-CA	-6.24	1.39	1.46	2	2
2	C	129	LYS	C-N	6.24	1.41	1.33	8	1
2	C	145	ARG	C-O	-6.24	1.17	1.24	9	2
1	A	401	LYS	N-CA	-6.24	1.38	1.46	12	1
2	B	259	THR	CA-C	-6.23	1.44	1.52	2	1
2	C	173	ARG	CA-C	6.23	1.61	1.52	9	2
2	B	258	TYR	CA-CB	6.23	1.63	1.53	10	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	74	ASN	N-CA	-6.23	1.38	1.46	13	1
1	A	452	ASN	N-CA	6.23	1.53	1.45	5	2
2	B	62	GLU	CA-CB	6.22	1.63	1.53	11	1
2	B	95	ALA	C-N	6.22	1.42	1.33	14	1
2	B	257	GLU	N-CA	6.21	1.53	1.46	2	1
1	A	424	ASN	CA-CB	6.21	1.62	1.54	3	2
2	B	261	LYS	C-N	-6.21	1.24	1.33	12	1
1	A	406	LEU	C-N	6.21	1.42	1.33	3	3
2	B	130	TRP	NE1-CE2	6.21	1.44	1.37	6	1
2	B	172	ASP	CA-CB	6.21	1.63	1.53	13	3
2	C	90	LEU	N-CA	-6.21	1.38	1.46	15	1
2	B	88	LYS	C-N	6.21	1.42	1.33	9	1
2	B	72	TRP	NE1-CE2	-6.21	1.30	1.37	10	2
2	C	237	ARG	CA-CB	6.20	1.63	1.53	12	1
2	B	150	GLU	CA-CB	6.20	1.62	1.53	9	2
2	B	239	GLY	N-CA	6.20	1.53	1.45	6	1
1	A	320	ASP	C-N	6.20	1.41	1.33	8	2
2	C	203	LEU	CA-C	-6.20	1.44	1.52	15	1
2	B	159	LEU	CA-CB	6.18	1.63	1.53	2	4
2	B	200	LEU	CA-CB	6.18	1.62	1.53	2	3
1	A	374	ARG	CD-NE	6.18	1.54	1.46	12	3
1	A	419	LEU	CA-C	-6.18	1.45	1.52	15	1
2	C	138	ARG	NE-CZ	6.18	1.39	1.33	1	1
2	C	238	GLN	CA-C	-6.18	1.44	1.52	1	1
1	A	445	VAL	N-CA	-6.18	1.38	1.46	11	1
2	C	112	MET	CA-CB	6.18	1.63	1.53	12	1
2	C	114	LEU	CA-CB	6.18	1.63	1.53	5	2
2	B	264	THR	CA-C	6.18	1.60	1.52	6	1
1	A	326	VAL	CA-C	-6.17	1.45	1.52	3	2
2	B	87	SER	N-CA	6.17	1.53	1.46	3	1
2	B	87	SER	C-N	6.17	1.42	1.34	5	1
1	A	452	ASN	CA-C	6.17	1.60	1.52	14	4
2	C	119	VAL	CA-CB	-6.17	1.46	1.54	9	2
2	B	233	LEU	C-N	6.17	1.41	1.33	15	1
2	C	195	ARG	C-N	6.17	1.42	1.33	3	2
2	B	220	GLU	N-CA	-6.17	1.39	1.46	6	3
2	C	158	GLU	CA-CB	6.17	1.63	1.53	2	1
1	A	347	ASN	CA-CB	6.17	1.63	1.53	5	1
2	B	90	LEU	CA-C	6.16	1.60	1.52	1	2
2	C	221	HIS	CE1-NE2	6.16	1.38	1.32	1	1
2	C	91	GLU	CA-C	6.16	1.61	1.52	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	341	PHE	CA-C	6.16	1.60	1.52	7	1
2	B	252	LEU	N-CA	-6.16	1.38	1.46	4	2
1	A	482	LYS	CA-C	6.15	1.60	1.52	10	1
2	C	100	TYR	CB-CG	6.15	1.65	1.51	9	1
1	A	481	ASN	N-CA	6.15	1.54	1.46	13	1
2	C	210	ARG	CA-CB	6.15	1.62	1.53	5	2
1	A	488	ASN	C-N	6.15	1.41	1.33	14	1
1	A	388	TRP	C-N	6.14	1.41	1.33	6	1
1	A	349	VAL	N-CA	-6.14	1.38	1.46	1	2
2	B	221	HIS	CG-CD2	6.14	1.42	1.35	5	4
2	C	173	ARG	CA-CB	6.14	1.63	1.53	5	2
2	C	76	GLU	CA-CB	6.14	1.62	1.53	9	2
2	B	89	ASP	CA-C	6.14	1.60	1.52	10	2
2	B	225	LEU	CA-C	-6.14	1.44	1.52	4	1
2	B	145	ARG	CA-C	-6.14	1.44	1.52	2	1
1	A	328	MET	CA-C	-6.14	1.45	1.52	3	1
2	C	173	ARG	N-CA	-6.13	1.39	1.46	4	1
2	B	118	LYS	CA-C	6.13	1.58	1.53	9	1
2	C	97	VAL	C-N	6.13	1.42	1.33	11	1
2	B	160	GLN	CA-C	6.13	1.60	1.52	15	2
2	C	177	HIS	C-N	6.12	1.41	1.33	8	1
2	B	102	ASP	C-N	6.12	1.41	1.33	3	2
2	C	109	GLN	C-N	6.12	1.42	1.33	8	2
1	A	502	LEU	CA-CB	-6.12	1.43	1.53	8	1
2	C	231	PRO	CA-CB	6.12	1.62	1.53	2	2
2	C	79	THR	N-CA	6.12	1.53	1.46	4	1
2	B	157	HIS	ND1-CE1	6.11	1.38	1.32	7	5
1	A	491	LEU	C-N	6.11	1.41	1.33	10	1
1	A	355	MET	CA-C	6.11	1.59	1.52	3	2
2	B	138	ARG	CD-NE	6.11	1.54	1.46	5	3
1	A	446	ASP	CA-C	6.11	1.60	1.52	10	1
2	C	228	LYS	N-CA	6.11	1.53	1.46	4	1
1	A	467	PHE	CA-C	6.11	1.60	1.52	2	2
2	B	104	PHE	C-N	6.11	1.41	1.33	11	1
2	B	225	LEU	C-N	6.10	1.41	1.33	14	3
2	C	186	ALA	C-O	6.10	1.30	1.24	14	2
2	C	249	VAL	CA-C	6.10	1.60	1.52	1	1
2	B	108	TRP	N-CA	-6.10	1.39	1.46	15	1
2	C	142	GLU	CA-CB	6.09	1.61	1.53	1	3
2	B	216	ALA	N-CA	-6.09	1.39	1.46	7	1
2	B	182	ARG	N-CA	-6.09	1.39	1.46	10	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	371	ALA	N-CA	-6.09	1.38	1.45	15	1
2	B	125	ASP	CA-C	-6.09	1.44	1.52	1	1
2	C	241	LEU	N-CA	6.09	1.52	1.46	4	2
1	A	401	LYS	C-N	6.09	1.41	1.33	9	2
1	A	430	PHE	C-O	-6.09	1.16	1.23	1	1
2	B	175	ARG	CA-C	6.08	1.60	1.52	5	5
1	A	379	PHE	CA-CB	6.08	1.61	1.53	9	1
2	B	221	HIS	CA-CB	6.08	1.62	1.53	5	2
2	C	89	ASP	CA-C	6.08	1.60	1.52	14	2
2	C	216	ALA	CA-C	6.07	1.60	1.52	8	1
2	C	149	GLN	CA-CB	6.07	1.62	1.53	12	1
2	B	101	LEU	CA-C	6.07	1.60	1.52	1	1
2	B	175	ARG	CD-NE	6.07	1.54	1.46	11	1
1	A	320	ASP	N-CA	-6.06	1.38	1.46	14	1
2	C	56	THR	N-CA	-6.05	1.39	1.46	5	1
2	B	67	VAL	N-CA	6.05	1.53	1.46	10	2
2	C	206	ASN	CA-CB	6.05	1.61	1.53	7	1
2	B	144	LEU	CA-C	6.05	1.61	1.52	15	1
2	C	182	ARG	C-O	-6.05	1.17	1.24	13	2
2	B	260	LYS	CA-CB	6.04	1.63	1.53	5	2
2	C	157	HIS	CD2-NE2	6.04	1.44	1.37	6	1
2	C	237	ARG	CA-C	6.04	1.60	1.52	8	1
2	C	95	ALA	C-N	-6.04	1.26	1.33	15	1
2	C	134	MET	C-N	6.04	1.41	1.33	6	1
2	B	116	ARG	CD-NE	6.04	1.54	1.46	8	2
1	A	420	PHE	CA-C	6.03	1.60	1.52	9	1
2	C	216	ALA	N-CA	-6.03	1.39	1.46	10	1
2	C	209	ALA	CA-C	6.03	1.60	1.52	2	1
1	A	351	ASP	CA-C	6.03	1.60	1.52	14	1
2	C	57	PHE	CA-C	-6.03	1.45	1.52	3	1
1	A	470	SER	CA-C	-6.03	1.45	1.52	3	1
2	C	93	VAL	CA-CB	-6.02	1.47	1.54	6	2
2	B	247	PHE	CA-CB	6.02	1.63	1.53	3	1
2	B	108	TRP	C-N	6.02	1.41	1.33	5	3
1	A	386	LYS	CA-CB	6.02	1.65	1.53	4	1
2	B	156	LEU	N-CA	-6.02	1.39	1.46	13	1
1	A	348	GLN	C-N	6.02	1.41	1.33	3	1
2	C	202	ALA	N-CA	-6.02	1.39	1.46	7	1
1	A	459	ILE	N-CA	-6.01	1.39	1.47	13	2
1	A	368	ILE	C-O	-6.01	1.16	1.24	1	1
1	A	444	ALA	CA-C	-6.01	1.45	1.52	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	497	TYR	CA-C	-6.01	1.47	1.52	2	1
2	B	177	HIS	CD2-NE2	6.01	1.44	1.37	15	1
2	B	223	SER	N-CA	6.01	1.53	1.46	11	2
2	B	99	PRO	N-CD	-6.00	1.39	1.47	7	1
2	C	184	HIS	CG-ND1	6.00	1.44	1.38	9	1
2	C	163	LEU	CA-CB	6.00	1.62	1.53	2	3
2	C	251	PHE	CA-C	6.00	1.60	1.52	12	3
2	B	84	GLN	C-N	6.00	1.42	1.33	8	1
1	A	426	LYS	CA-CB	6.00	1.62	1.53	10	1
2	C	165	PRO	C-O	-6.00	1.17	1.24	15	1
2	B	233	LEU	N-CA	-5.99	1.39	1.46	11	1
2	C	177	HIS	CA-CB	5.99	1.62	1.53	2	2
2	C	122	TYR	CA-CB	5.99	1.62	1.53	3	1
2	C	254	ALA	C-N	5.98	1.41	1.33	1	1
1	A	328	MET	CA-CB	5.98	1.60	1.53	9	1
2	C	135	GLU	CA-C	5.98	1.60	1.52	6	2
2	B	68	THR	C-N	5.98	1.41	1.33	10	1
2	C	116	ARG	CA-CB	5.98	1.62	1.53	7	1
2	B	179	ASP	CA-CB	5.98	1.62	1.53	15	1
1	A	423	PRO	N-CD	-5.98	1.39	1.47	8	2
2	C	161	GLU	N-CA	5.98	1.53	1.46	8	1
2	C	76	GLU	CA-C	5.97	1.60	1.52	14	1
1	A	439	ASN	CA-CB	5.97	1.63	1.53	7	2
2	B	153	ARG	CA-C	5.97	1.60	1.52	6	3
2	B	238	GLN	CA-CB	5.97	1.62	1.53	9	3
2	B	250	SER	CA-CB	5.97	1.62	1.53	3	2
2	C	197	ALA	N-CA	-5.97	1.39	1.46	5	1
2	B	99	PRO	CA-C	5.96	1.61	1.52	3	1
2	B	177	HIS	CA-C	5.96	1.60	1.52	5	1
2	C	218	ALA	CA-C	-5.96	1.47	1.52	12	2
2	C	59	LYS	N-CA	5.96	1.53	1.46	3	1
2	B	108	TRP	CA-CB	5.96	1.62	1.53	6	3
2	C	131	GLN	CA-C	5.96	1.60	1.52	5	2
2	B	96	LYS	C-N	5.96	1.41	1.33	7	2
2	C	152	ALA	CA-C	5.96	1.60	1.52	11	2
1	A	348	GLN	CA-C	5.95	1.59	1.52	3	1
2	C	88	LYS	CA-C	5.95	1.60	1.52	6	2
1	A	352	GLY	N-CA	5.95	1.53	1.45	15	2
2	C	214	TYR	CA-C	-5.95	1.44	1.52	3	1
1	A	332	GLU	N-CA	5.95	1.53	1.45	9	1
1	A	505	TRP	CA-CB	5.94	1.62	1.53	15	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	69	GLN	CA-CB	5.94	1.62	1.53	1	3
2	C	97	VAL	N-CA	-5.94	1.39	1.46	6	1
2	B	84	GLN	CA-C	5.94	1.60	1.52	7	1
2	C	113	GLU	CA-C	-5.94	1.45	1.52	9	1
2	C	191	GLU	C-O	-5.94	1.17	1.24	13	1
2	B	80	GLU	CA-CB	5.94	1.62	1.53	2	1
2	B	89	ASP	C-N	5.94	1.41	1.33	7	1
2	B	213	GLU	CA-CB	-5.94	1.44	1.53	15	1
1	A	336	PHE	N-CA	5.93	1.53	1.46	3	2
2	C	132	GLU	CA-C	-5.93	1.45	1.52	8	1
1	A	460	PRO	CA-CB	5.93	1.61	1.53	9	1
2	C	199	ARG	C-N	5.93	1.41	1.33	7	1
2	B	199	ARG	CD-NE	5.93	1.54	1.46	1	3
2	B	246	SER	CA-C	-5.93	1.45	1.52	8	1
1	A	350	MET	C-N	5.93	1.41	1.33	15	1
1	A	454	LYS	C-N	5.92	1.41	1.33	3	1
2	C	242	PRO	N-CA	-5.92	1.39	1.47	10	1
2	C	104	PHE	N-CA	-5.92	1.39	1.46	13	1
1	A	459	ILE	CA-CB	-5.92	1.49	1.54	11	1
2	C	201	GLU	C-N	5.92	1.41	1.33	5	1
2	B	69	GLN	CA-C	-5.92	1.45	1.52	8	1
2	C	104	PHE	CA-CB	5.91	1.62	1.53	3	1
2	B	79	THR	CA-CB	-5.91	1.44	1.53	13	1
2	C	139	GLN	C-N	5.91	1.41	1.33	11	1
1	A	467	PHE	N-CA	-5.91	1.39	1.46	12	1
2	B	113	GLU	CA-C	5.91	1.60	1.52	9	1
2	B	237	ARG	CA-C	-5.91	1.44	1.52	2	1
2	C	170	MET	C-N	5.91	1.42	1.33	3	1
2	C	233	LEU	CA-CB	5.91	1.62	1.53	6	2
2	B	206	ASN	CA-C	5.91	1.60	1.52	11	1
1	A	378	LYS	CA-C	5.91	1.60	1.52	8	3
2	C	60	LEU	N-CA	5.91	1.53	1.46	8	1
2	C	115	TYR	C-N	5.90	1.42	1.34	1	1
2	B	114	LEU	C-O	-5.90	1.17	1.24	2	1
2	C	88	LYS	C-N	5.90	1.41	1.33	2	3
1	A	421	TRP	CD2-CE2	5.90	1.51	1.41	7	1
2	B	232	ALA	CA-CB	5.90	1.62	1.53	8	1
2	B	245	GLU	N-CA	5.89	1.53	1.46	12	1
2	C	148	LEU	N-CA	-5.89	1.39	1.46	6	1
2	C	225	LEU	CA-CB	5.89	1.62	1.53	11	2
2	B	60	LEU	N-CA	5.89	1.53	1.46	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	C	57	PHE	N-CA	5.89	1.53	1.46	14	1
2	B	230	LYS	CA-C	5.88	1.59	1.52	1	1
2	C	260	LYS	CA-CB	-5.88	1.44	1.53	1	1
1	A	389	VAL	C-N	5.88	1.41	1.33	3	1
2	C	218	ALA	CA-CB	5.88	1.62	1.53	1	1
2	C	211	LEU	CA-C	5.88	1.60	1.52	10	2
2	C	222	LEU	CA-CB	5.88	1.62	1.53	2	1
2	B	91	GLU	CA-C	5.87	1.60	1.52	8	2
1	A	494	GLU	CA-C	5.87	1.59	1.53	12	1
1	A	425	GLY	CA-C	-5.87	1.43	1.51	14	2
2	B	130	TRP	N-CA	-5.87	1.39	1.46	11	2
2	C	65	GLY	N-CA	5.87	1.50	1.44	8	2
2	B	233	LEU	CA-CB	-5.87	1.44	1.53	14	2
2	C	180	ALA	N-CA	5.87	1.53	1.46	6	1
2	C	61	ARG	N-CA	-5.87	1.39	1.46	11	2
2	B	115	TYR	CZ-OH	5.87	1.50	1.38	11	1
2	B	103	ASP	C-N	5.86	1.41	1.33	2	1
1	A	319	CYS	C-N	5.86	1.42	1.33	8	1
2	C	82	LEU	CA-CB	5.86	1.62	1.53	1	2
2	C	218	ALA	N-CA	-5.86	1.38	1.46	2	1
1	A	432	GLY	CA-C	5.86	1.60	1.51	6	1
1	A	335	VAL	N-CA	5.86	1.53	1.46	8	1
2	C	243	VAL	C-N	5.86	1.41	1.33	6	2
1	A	440	GLU	N-CA	-5.86	1.38	1.46	7	1
2	C	177	HIS	N-CA	5.85	1.53	1.46	11	1
2	C	245	GLU	N-CA	-5.85	1.39	1.46	11	1
2	C	226	SER	C-N	5.85	1.41	1.33	13	1
1	A	347	ASN	CA-C	5.85	1.61	1.52	2	3
2	C	223	SER	N-CA	-5.85	1.39	1.46	15	1
2	C	227	GLU	N-CA	-5.85	1.39	1.46	1	3
2	B	82	LEU	C-N	5.85	1.41	1.33	4	1
2	C	110	GLU	CA-C	-5.85	1.45	1.52	12	2
1	A	394	SER	CA-CB	5.85	1.61	1.53	10	1
1	A	319	CYS	N-CA	-5.84	1.38	1.46	11	1
2	B	99	PRO	N-CA	-5.84	1.39	1.47	3	2
2	C	162	LYS	CA-CB	5.84	1.62	1.53	14	2
1	A	411	PRO	CA-C	5.84	1.60	1.52	13	1
2	C	88	LYS	N-CA	-5.84	1.39	1.46	5	1
1	A	434	LYS	CA-CB	5.83	1.62	1.53	7	1
2	C	219	THR	CA-C	5.83	1.60	1.52	15	1
2	C	234	GLU	N-CA	-5.83	1.39	1.46	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	431	ARG	CA-CB	5.83	1.64	1.53	1	2
2	B	262	LEU	N-CA	5.83	1.53	1.46	1	2
2	B	136	LEU	CA-C	5.83	1.60	1.52	7	1
2	C	80	GLU	CA-C	5.83	1.60	1.52	9	1
2	C	186	ALA	C-N	5.82	1.41	1.34	9	3
1	A	505	TRP	CZ2-CH2	5.82	1.48	1.37	4	1
2	C	109	GLN	N-CA	-5.82	1.39	1.46	12	2
1	A	324	ASP	N-CA	-5.82	1.38	1.46	12	2
2	C	199	ARG	CZ-NH2	-5.82	1.25	1.33	14	1
2	B	92	GLU	C-O	5.82	1.30	1.24	3	2
2	C	252	LEU	N-CA	5.82	1.53	1.46	15	2
2	C	258	TYR	CA-C	5.81	1.60	1.52	14	1
2	C	73	ASP	CA-CB	5.81	1.62	1.53	12	1
2	C	153	ARG	CD-NE	5.81	1.54	1.46	11	3
1	A	441	GLU	CA-CB	5.80	1.62	1.53	14	1
2	C	190	ASP	CA-C	5.80	1.60	1.52	7	1
2	B	75	LEU	CB-CG	5.80	1.65	1.53	4	1
1	A	326	VAL	C-N	5.80	1.41	1.33	2	1
1	A	317	ASN	C-N	5.80	1.41	1.33	13	2
2	C	251	PHE	C-N	5.80	1.41	1.33	13	2
2	C	134	MET	C-O	-5.80	1.17	1.24	13	1
2	B	181	LEU	N-CA	-5.79	1.39	1.46	5	1
2	B	223	SER	C-N	5.79	1.41	1.33	3	1
2	B	202	ALA	C-N	5.79	1.41	1.33	14	1
1	A	447	SER	CA-CB	5.79	1.62	1.53	11	2
2	C	136	LEU	C-N	5.79	1.41	1.33	1	1
2	B	153	ARG	C-N	5.79	1.40	1.33	1	1
2	C	256	GLU	C-N	5.78	1.41	1.33	9	1
1	A	489	GLN	N-CA	-5.78	1.39	1.46	7	1
2	C	132	GLU	CA-CB	5.78	1.62	1.53	14	1
1	A	325	THR	CA-C	-5.78	1.45	1.52	1	1
2	B	157	HIS	CE1-NE2	5.78	1.38	1.32	11	2
2	B	180	ALA	C-O	5.78	1.30	1.24	10	1
2	C	210	ARG	CA-C	5.78	1.60	1.52	13	1
2	B	169	GLU	CA-C	-5.78	1.45	1.52	15	1
2	C	156	LEU	CA-CB	5.78	1.62	1.53	15	2
2	C	148	LEU	CA-CB	5.77	1.62	1.53	11	1
2	B	59	LYS	N-CA	-5.77	1.39	1.46	4	1
1	A	447	SER	C-N	5.77	1.41	1.33	15	1
2	B	140	LYS	C-N	5.76	1.41	1.33	1	1
2	B	71	PHE	N-CA	-5.76	1.39	1.46	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	317	ASN	N-CA	5.76	1.53	1.46	7	1
2	B	177	HIS	CE1-NE2	5.76	1.38	1.32	15	1
2	B	206	ASN	C-O	5.76	1.30	1.24	12	1
1	A	411	PRO	N-CA	5.76	1.54	1.47	10	2
2	C	182	ARG	CD-NE	5.76	1.54	1.46	3	1
2	B	155	LYS	CA-C	5.76	1.60	1.52	8	1
2	B	120	GLU	C-O	-5.76	1.18	1.24	13	1
2	B	61	ARG	CA-CB	5.76	1.62	1.53	14	2
2	B	117	GLN	N-CA	-5.76	1.39	1.46	3	1
1	A	441	GLU	C-N	5.76	1.41	1.33	6	1
1	A	449	TYR	CA-CB	5.76	1.61	1.54	6	2
2	C	182	ARG	CZ-NH1	-5.75	1.24	1.32	12	1
1	A	348	GLN	N-CA	-5.75	1.38	1.45	14	2
2	B	264	THR	C-N	5.75	1.41	1.33	14	1
2	C	184	HIS	CA-CB	5.75	1.62	1.53	11	2
2	C	171	ARG	CA-CB	5.75	1.62	1.53	14	1
2	B	88	LYS	CA-C	-5.75	1.44	1.52	2	1
1	A	385	ASP	CA-C	-5.75	1.44	1.52	8	1
2	B	187	PRO	N-CD	-5.75	1.39	1.47	1	1
2	B	209	ALA	CA-CB	5.75	1.62	1.53	15	1
2	C	137	TYR	C-N	5.75	1.41	1.33	7	1
1	A	500	SER	CA-C	-5.74	1.44	1.52	8	1
2	C	86	MET	N-CA	-5.74	1.39	1.46	12	1
2	B	183	THR	CA-C	5.74	1.60	1.52	10	1
2	B	207	GLY	C-N	5.74	1.40	1.33	15	1
1	A	388	TRP	NE1-CE2	-5.74	1.31	1.37	6	1
1	A	355	MET	C-N	5.74	1.40	1.33	13	2
2	B	129	LYS	CA-C	5.73	1.60	1.52	10	2
2	B	90	LEU	N-CA	-5.73	1.39	1.46	11	1
1	A	422	MET	N-CA	-5.73	1.40	1.46	14	2
1	A	431	ARG	C-N	5.73	1.42	1.33	2	1
2	C	186	ALA	CA-CB	5.73	1.60	1.53	10	2
1	A	370	THR	CA-C	-5.73	1.45	1.52	2	3
1	A	455	VAL	N-CA	5.73	1.54	1.46	12	1
2	C	128	LYS	CA-CB	5.73	1.62	1.53	10	2
1	A	464	ARG	CZ-NH2	-5.73	1.26	1.33	7	1
2	B	168	GLU	CA-CB	5.72	1.62	1.53	1	3
2	B	130	TRP	C-O	-5.72	1.17	1.24	13	2
2	B	205	GLU	CA-CB	5.72	1.62	1.53	15	2
2	B	137	TYR	C-O	-5.72	1.17	1.24	10	2
2	C	221	HIS	CG-ND1	-5.71	1.31	1.38	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	404	LYS	CA-CB	5.71	1.62	1.53	7	1
1	A	456	TRP	NE1-CE2	-5.71	1.31	1.37	2	1
2	B	264	THR	CA-CB	-5.71	1.43	1.53	8	1
1	A	464	ARG	C-N	5.71	1.41	1.33	6	2
2	B	182	ARG	CA-CB	-5.70	1.44	1.53	15	1
2	C	139	GLN	CA-CB	5.70	1.62	1.53	12	1
1	A	456	TRP	CZ2-CH2	5.70	1.48	1.37	14	1
1	A	341	PHE	N-CA	-5.70	1.38	1.45	12	1
2	B	61	ARG	N-CA	-5.69	1.39	1.46	3	2
2	C	64	LEU	CA-C	-5.69	1.44	1.52	8	1
2	C	206	ASN	N-CA	5.69	1.52	1.46	15	1
2	B	187	PRO	C-O	5.69	1.31	1.24	6	1
1	A	385	ASP	C-N	5.69	1.41	1.33	7	2
2	C	238	GLN	N-CA	5.69	1.53	1.46	11	2
1	A	510	SER	N-CA	-5.69	1.39	1.46	7	1
2	B	178	VAL	CA-CB	-5.69	1.47	1.54	14	3
2	C	199	ARG	C-O	-5.69	1.17	1.24	8	1
2	C	141	VAL	CA-CB	-5.69	1.47	1.54	4	4
2	B	139	GLN	N-CA	5.69	1.53	1.46	11	1
2	C	192	LEU	CA-CB	5.69	1.62	1.53	15	2
2	C	79	THR	CA-C	5.68	1.60	1.52	12	3
2	B	94	LYS	CA-C	-5.68	1.45	1.52	5	1
2	B	96	LYS	N-CA	5.68	1.53	1.46	9	1
2	C	246	SER	CA-C	-5.68	1.45	1.52	1	1
2	B	80	GLU	C-N	5.68	1.42	1.33	10	2
2	C	254	ALA	CA-C	5.68	1.60	1.52	10	1
2	C	73	ASP	N-CA	-5.68	1.39	1.46	13	1
1	A	422	MET	CA-C	5.68	1.59	1.52	3	1
1	A	325	THR	N-CA	-5.68	1.38	1.45	4	1
2	C	129	LYS	N-CA	-5.68	1.39	1.46	1	1
2	B	139	GLN	C-N	5.68	1.41	1.33	5	1
2	B	87	SER	CA-CB	5.68	1.62	1.53	12	1
1	A	457	GLU	C-N	5.68	1.41	1.33	14	1
2	B	208	GLY	N-CA	5.67	1.52	1.45	3	2
2	C	83	ARG	CD-NE	5.67	1.54	1.46	3	2
2	C	139	GLN	CA-C	5.67	1.60	1.52	11	1
2	B	231	PRO	CA-C	-5.67	1.44	1.52	14	1
2	C	186	ALA	N-CA	5.67	1.51	1.46	15	1
2	C	224	THR	CA-C	-5.67	1.45	1.52	9	2
2	B	143	PRO	CA-CB	-5.67	1.45	1.53	8	2
2	B	73	ASP	CA-CB	5.67	1.62	1.53	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	C	194	GLN	C-N	5.67	1.41	1.33	13	1
2	B	254	ALA	CA-C	5.66	1.60	1.52	6	1
2	C	198	ALA	C-N	5.66	1.41	1.33	7	1
1	A	368	ILE	CB-CG1	5.66	1.64	1.53	12	1
2	B	113	GLU	CA-CB	5.66	1.62	1.53	2	1
2	B	260	LYS	CA-C	-5.65	1.44	1.52	13	3
2	B	167	GLY	N-CA	5.65	1.52	1.45	8	1
2	B	205	GLU	CA-C	-5.65	1.45	1.52	2	1
2	B	86	MET	CA-CB	5.65	1.62	1.53	3	1
2	B	252	LEU	C-N	5.65	1.41	1.33	4	1
2	B	119	VAL	CA-C	5.65	1.59	1.52	15	2
1	A	473	VAL	CA-C	-5.65	1.45	1.53	13	1
2	B	253	SER	CA-CB	5.65	1.62	1.53	2	1
2	C	175	ARG	C-O	-5.65	1.17	1.24	9	1
1	A	404	LYS	C-N	5.65	1.42	1.33	12	1
2	C	227	GLU	C-N	5.64	1.41	1.33	15	1
2	B	194	GLN	N-CA	-5.64	1.39	1.46	9	3
2	B	193	ARG	C-N	5.64	1.40	1.33	11	1
2	B	156	LEU	C-N	5.64	1.41	1.33	8	2
2	B	62	GLU	N-CA	-5.64	1.39	1.46	8	1
1	A	480	GLY	CA-C	-5.63	1.44	1.51	4	2
2	C	230	LYS	CA-CB	5.63	1.60	1.53	4	2
2	C	237	ARG	N-CA	5.63	1.53	1.46	7	2
1	A	497	TYR	CA-CB	5.63	1.60	1.53	8	2
2	C	212	ALA	C-N	5.63	1.41	1.34	8	1
1	A	363	GLY	C-N	5.63	1.40	1.33	13	1
2	C	215	HIS	C-N	5.62	1.41	1.33	12	2
2	C	124	ASP	CA-C	5.62	1.60	1.52	13	1
2	C	183	THR	N-CA	5.62	1.53	1.46	1	2
2	B	215	HIS	C-O	-5.62	1.17	1.24	13	1
1	A	468	MET	C-N	5.62	1.41	1.33	14	1
2	B	111	GLU	CA-C	5.61	1.60	1.52	7	1
1	A	339	ARG	NE-CZ	-5.61	1.26	1.33	3	2
2	B	143	PRO	CA-C	5.61	1.60	1.52	11	1
2	C	211	LEU	CA-CB	5.61	1.62	1.53	1	1
1	A	334	PHE	CA-C	-5.61	1.46	1.52	14	3
2	C	215	HIS	N-CA	5.61	1.53	1.46	10	1
2	C	71	PHE	CA-CB	5.61	1.62	1.53	12	1
2	C	86	MET	CA-CB	5.61	1.62	1.53	15	2
1	A	456	TRP	N-CA	5.60	1.53	1.46	1	1
2	B	135	GLU	CA-CB	5.60	1.62	1.53	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	C	57	PHE	CA-CB	5.60	1.62	1.53	11	2
2	C	83	ARG	CZ-NH2	-5.60	1.26	1.33	3	1
1	A	439	ASN	CA-C	-5.60	1.46	1.52	15	2
2	C	73	ASP	CA-C	-5.60	1.45	1.52	8	2
2	B	224	THR	C-N	5.60	1.41	1.33	7	2
2	B	100	TYR	CA-C	-5.60	1.45	1.52	11	1
2	C	117	GLN	CA-C	5.60	1.60	1.52	1	1
1	A	414	LYS	C-N	5.59	1.39	1.33	4	1
1	A	416	ASP	CA-C	-5.59	1.45	1.53	12	1
1	A	498	PRO	CA-C	-5.59	1.41	1.52	11	1
2	C	203	LEU	C-O	-5.59	1.17	1.24	12	1
1	A	422	MET	C-N	-5.59	1.29	1.33	8	1
2	C	107	LYS	CA-C	-5.59	1.45	1.52	4	1
2	C	191	GLU	CA-C	-5.59	1.45	1.52	8	1
1	A	470	SER	C-O	5.58	1.30	1.24	5	1
2	C	252	LEU	C-N	5.58	1.41	1.33	15	1
2	B	203	LEU	C-N	5.58	1.41	1.33	8	1
2	B	176	ALA	C-N	5.57	1.41	1.33	14	1
2	B	173	ARG	CA-CB	5.57	1.61	1.53	6	1
2	C	78	GLU	CA-CB	5.57	1.62	1.53	10	1
2	B	156	LEU	CA-CB	5.57	1.62	1.53	4	1
2	C	157	HIS	C-N	5.57	1.41	1.33	9	1
2	C	248	LYS	CA-CB	5.56	1.62	1.53	9	3
2	C	233	LEU	C-O	5.56	1.30	1.24	3	1
2	B	215	HIS	CG-CD2	5.56	1.42	1.35	15	1
2	C	88	LYS	CA-CB	5.56	1.61	1.53	13	1
1	A	415	ILE	C-N	5.55	1.41	1.33	5	1
1	A	325	THR	CA-CB	5.55	1.62	1.53	7	1
2	C	100	TYR	CA-CB	5.55	1.62	1.53	5	2
2	B	177	HIS	C-O	-5.55	1.17	1.24	4	1
2	B	232	ALA	CA-C	-5.55	1.45	1.52	4	1
2	C	258	TYR	N-CA	-5.55	1.39	1.46	7	1
2	C	135	GLU	C-O	-5.55	1.17	1.24	12	1
2	B	227	GLU	C-O	5.55	1.31	1.24	12	2
2	C	171	ARG	CZ-NH2	-5.55	1.26	1.33	6	2
1	A	504	ASP	C-O	5.55	1.30	1.24	7	1
2	B	236	LEU	CA-CB	5.55	1.62	1.53	10	2
2	C	246	SER	C-N	-5.55	1.26	1.33	10	1
2	C	142	GLU	CA-C	5.54	1.59	1.52	9	1
2	B	105	GLN	CA-C	5.54	1.59	1.52	8	3
1	A	438	PHE	CA-CB	5.54	1.60	1.53	12	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	C	146	ALA	N-CA	-5.54	1.39	1.46	8	1
2	C	222	LEU	C-O	-5.54	1.17	1.24	10	1
1	A	403	ILE	C-N	5.54	1.41	1.33	11	1
1	A	437	ARG	C-N	5.54	1.41	1.33	14	1
2	C	182	ARG	CZ-NH2	-5.54	1.26	1.33	6	1
2	B	174	ALA	CA-CB	-5.54	1.44	1.53	14	1
1	A	484	TRP	CA-C	-5.54	1.46	1.52	7	1
2	B	213	GLU	CA-C	-5.54	1.45	1.52	14	1
1	A	439	ASN	N-CA	-5.54	1.39	1.46	2	1
2	C	193	ARG	C-N	5.54	1.41	1.33	14	1
1	A	326	VAL	N-CA	5.53	1.53	1.46	11	2
2	B	261	LYS	CA-CB	5.53	1.62	1.53	11	1
2	C	235	ASP	CA-CB	5.53	1.62	1.53	1	2
1	A	394	SER	N-CA	5.53	1.52	1.46	4	1
2	B	87	SER	CA-C	5.53	1.59	1.52	7	2
2	C	145	ARG	N-CA	-5.53	1.39	1.46	8	1
2	B	133	GLU	CA-C	5.53	1.59	1.52	1	2
2	C	221	HIS	C-N	5.53	1.41	1.33	5	2
2	B	128	LYS	N-CA	-5.52	1.39	1.46	10	1
2	C	65	GLY	C-N	5.52	1.40	1.34	1	2
1	A	365	PRO	N-CD	-5.52	1.40	1.47	6	1
2	C	174	ALA	N-CA	-5.52	1.39	1.46	6	1
2	B	249	VAL	N-CA	-5.52	1.40	1.46	12	2
2	C	214	TYR	N-CA	-5.52	1.39	1.46	15	2
2	B	131	GLN	N-CA	5.52	1.52	1.46	4	2
2	C	195	ARG	CD-NE	5.51	1.53	1.46	14	3
1	A	378	LYS	C-N	5.51	1.41	1.33	4	1
1	A	461	GLU	N-CA	-5.51	1.39	1.46	7	1
2	B	242	PRO	N-CA	-5.51	1.40	1.47	9	1
2	C	156	LEU	CA-C	5.51	1.59	1.52	11	2
1	A	392	GLU	CA-C	5.51	1.60	1.52	9	1
2	C	159	LEU	C-N	5.51	1.41	1.33	11	1
2	C	130	TRP	CZ2-CH2	5.51	1.47	1.37	3	1
2	C	205	GLU	C-N	5.51	1.41	1.33	4	1
1	A	383	LYS	N-CA	-5.51	1.39	1.46	14	1
1	A	503	ARG	CD-NE	5.51	1.53	1.46	10	4
2	C	235	ASP	C-O	-5.51	1.17	1.24	8	1
1	A	456	TRP	CA-C	5.51	1.59	1.52	13	1
1	A	503	ARG	CA-C	5.51	1.59	1.52	14	1
2	B	251	PHE	N-CA	-5.51	1.39	1.46	11	1
2	C	131	GLN	CA-CB	5.51	1.61	1.53	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	377	GLY	CA-C	-5.51	1.43	1.51	9	2
1	A	364	LEU	C-N	5.51	1.41	1.33	13	1
1	A	487	ASN	CA-CB	5.50	1.60	1.53	7	3
2	B	154	GLN	CA-C	-5.50	1.45	1.52	11	2
2	B	171	ARG	NE-CZ	5.50	1.39	1.33	11	1
2	C	98	GLN	CA-C	5.50	1.59	1.52	10	1
2	C	168	GLU	CA-C	5.50	1.60	1.52	6	1
1	A	456	TRP	CA-CB	5.50	1.61	1.53	15	3
2	C	60	LEU	C-N	-5.50	1.26	1.33	15	1
1	A	390	PHE	CA-CB	5.50	1.63	1.53	5	2
2	C	91	GLU	N-CA	-5.50	1.39	1.46	12	1
2	C	228	LYS	C-N	5.50	1.41	1.34	4	1
2	C	167	GLY	C-N	5.50	1.41	1.33	14	2
2	B	76	GLU	CA-C	-5.50	1.45	1.52	13	2
2	B	189	SER	CA-C	5.49	1.59	1.52	4	1
2	B	144	LEU	N-CA	5.49	1.52	1.46	8	1
2	C	65	GLY	CA-C	5.49	1.55	1.51	8	1
1	A	434	LYS	N-CA	-5.49	1.39	1.45	14	1
1	A	455	VAL	CA-C	-5.49	1.46	1.52	15	1
2	B	142	GLU	CA-C	-5.49	1.47	1.52	5	1
1	A	395	LEU	N-CA	5.49	1.53	1.46	8	1
2	B	214	TYR	CA-CB	5.49	1.61	1.53	15	1
2	C	121	PRO	CA-CB	5.49	1.61	1.53	6	1
2	B	261	LYS	N-CA	-5.49	1.39	1.46	1	1
2	C	200	LEU	N-CA	5.49	1.52	1.46	7	1
1	A	430	PHE	CA-CB	5.49	1.61	1.53	4	1
1	A	328	MET	C-N	5.49	1.41	1.33	12	1
2	B	78	GLU	CA-CB	5.48	1.61	1.53	1	1
2	C	214	TYR	CZ-OH	5.48	1.49	1.38	6	1
1	A	363	GLY	CA-C	5.48	1.57	1.51	8	1
1	A	385	ASP	N-CA	-5.48	1.40	1.46	10	1
1	A	335	VAL	CA-C	-5.48	1.45	1.52	14	1
2	B	214	TYR	CA-C	-5.48	1.45	1.52	5	1
2	B	103	ASP	CA-C	5.48	1.59	1.52	15	1
2	C	112	MET	CA-C	-5.48	1.45	1.52	15	1
2	C	75	LEU	N-CA	-5.48	1.39	1.46	2	1
2	B	121	PRO	C-O	-5.48	1.17	1.24	6	2
2	C	176	ALA	CA-CB	5.48	1.62	1.53	8	1
1	A	441	GLU	N-CA	5.47	1.53	1.46	1	2
2	C	217	LYS	C-N	5.47	1.40	1.33	1	2
2	B	157	HIS	C-N	5.47	1.41	1.33	7	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	488	ASN	CA-CB	5.47	1.61	1.53	11	1
1	A	399	TYR	C-O	-5.47	1.17	1.24	2	1
2	B	199	ARG	NE-CZ	-5.47	1.27	1.33	15	1
1	A	452	ASN	C-O	-5.47	1.17	1.23	3	1
2	B	170	MET	C-N	5.47	1.40	1.33	11	1
1	A	440	GLU	CA-C	-5.47	1.45	1.52	14	1
1	A	323	PHE	C-N	5.46	1.40	1.33	15	2
2	C	237	ARG	CZ-NH2	-5.46	1.26	1.33	15	1
1	A	354	PRO	C-N	5.46	1.40	1.33	6	1
1	A	480	GLY	N-CA	5.46	1.53	1.45	14	1
1	A	373	GLU	N-CA	5.46	1.53	1.46	1	2
2	C	70	GLU	C-N	5.46	1.40	1.33	15	1
2	C	204	LYS	C-N	5.46	1.41	1.34	4	2
1	A	450	PRO	C-N	5.46	1.41	1.33	7	1
2	C	215	HIS	CB-CG	5.46	1.57	1.50	8	1
1	A	468	MET	N-CA	-5.46	1.39	1.46	2	1
2	C	202	ALA	C-O	-5.46	1.17	1.24	11	1
1	A	494	GLU	C-N	5.45	1.40	1.33	6	3
2	B	201	GLU	CA-CB	5.45	1.62	1.53	6	1
2	B	251	PHE	C-N	5.45	1.41	1.33	8	1
2	C	192	LEU	C-O	-5.45	1.17	1.24	14	1
2	C	101	LEU	C-N	5.45	1.41	1.33	6	2
2	C	145	ARG	CZ-NH2	-5.45	1.26	1.33	8	1
1	A	365	PRO	CA-C	-5.44	1.46	1.52	13	1
1	A	502	LEU	CB-CG	5.44	1.64	1.53	13	1
1	A	343	ARG	C-O	-5.44	1.17	1.23	10	1
2	B	244	LEU	CA-CB	5.44	1.62	1.53	12	1
2	C	135	GLU	C-N	5.44	1.41	1.34	13	1
2	B	196	LEU	CA-CB	5.44	1.61	1.53	6	1
2	C	258	TYR	CA-CB	5.44	1.61	1.53	9	1
1	A	375	LYS	CA-CB	5.43	1.61	1.53	7	2
1	A	489	GLN	CA-C	-5.43	1.46	1.52	5	1
2	B	171	ARG	CZ-NH2	-5.43	1.26	1.33	5	1
2	B	235	ASP	CA-C	-5.43	1.46	1.52	6	1
2	C	149	GLN	CA-C	-5.43	1.46	1.52	8	1
1	A	358	GLY	N-CA	-5.43	1.36	1.45	3	1
2	B	153	ARG	CZ-NH2	-5.43	1.26	1.33	2	1
2	B	241	LEU	N-CA	-5.43	1.40	1.46	2	2
2	C	72	TRP	NE1-CE2	-5.43	1.31	1.37	13	1
1	A	455	VAL	CA-CB	5.42	1.61	1.54	8	1
2	C	189	SER	N-CA	5.42	1.52	1.46	10	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	218	ALA	C-O	-5.42	1.17	1.24	12	1
1	A	415	ILE	CA-CB	5.42	1.60	1.53	1	2
2	B	220	GLU	C-O	-5.42	1.17	1.24	2	1
2	C	194	GLN	CA-C	5.42	1.59	1.52	5	2
2	B	122	TYR	C-O	-5.42	1.17	1.24	8	1
2	C	242	PRO	C-N	5.42	1.40	1.33	8	1
2	C	105	GLN	C-N	5.42	1.40	1.33	13	1
2	C	64	LEU	CA-CB	5.42	1.61	1.53	15	1
2	C	195	ARG	NE-CZ	5.42	1.39	1.33	11	1
2	B	237	ARG	C-N	5.41	1.41	1.33	5	1
2	C	117	GLN	CA-CB	5.41	1.62	1.53	14	1
2	B	79	THR	CA-C	-5.41	1.46	1.52	6	1
2	C	179	ASP	CA-CB	5.41	1.61	1.53	3	3
2	C	222	LEU	C-N	5.41	1.40	1.33	7	1
2	B	202	ALA	CA-C	5.41	1.59	1.52	11	1
1	A	491	LEU	CA-C	5.40	1.59	1.53	14	1
2	B	112	MET	C-N	5.40	1.41	1.33	14	1
2	C	155	LYS	CA-C	5.40	1.59	1.52	12	2
2	B	107	LYS	C-N	5.40	1.41	1.33	3	1
2	B	162	LYS	N-CA	5.40	1.52	1.46	8	1
1	A	367	SER	C-N	5.40	1.41	1.33	13	1
1	A	402	HIS	CA-C	5.40	1.60	1.52	13	1
2	C	175	ARG	N-CA	-5.39	1.39	1.46	1	1
2	C	82	LEU	CA-C	-5.39	1.45	1.52	2	2
2	C	60	LEU	CA-C	5.39	1.59	1.52	9	1
2	C	193	ARG	CZ-NH2	-5.39	1.26	1.33	14	1
2	B	55	SER	CA-CB	5.39	1.64	1.53	15	1
2	C	63	GLN	CA-C	-5.39	1.46	1.52	2	1
1	A	361	TRP	CA-C	5.39	1.59	1.52	11	1
1	A	416	ASP	N-CA	-5.39	1.39	1.46	13	1
2	B	227	GLU	CA-CB	5.39	1.62	1.53	1	1
2	B	210	ARG	CD-NE	5.39	1.53	1.46	11	2
1	A	406	LEU	C-O	-5.39	1.17	1.24	1	1
2	B	69	GLN	C-N	5.39	1.41	1.34	12	1
2	B	62	GLU	CA-C	-5.38	1.45	1.52	3	1
2	C	251	PHE	N-CA	-5.38	1.40	1.46	4	2
2	B	130	TRP	CA-CB	5.38	1.61	1.53	8	1
1	A	453	ILE	C-N	5.38	1.42	1.33	11	2
2	B	207	GLY	N-CA	-5.38	1.39	1.45	6	1
2	C	94	LYS	CA-CB	5.38	1.61	1.53	15	1
2	B	102	ASP	CA-CB	5.38	1.61	1.53	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	C	158	GLU	C-O	-5.38	1.18	1.24	15	1
2	B	95	ALA	CA-C	5.38	1.60	1.52	2	1
1	A	319	CYS	CA-C	5.38	1.60	1.52	4	1
1	A	410	LEU	CA-CB	5.38	1.60	1.53	9	1
2	B	124	ASP	C-N	5.38	1.41	1.33	14	2
2	B	116	ARG	NE-CZ	5.38	1.39	1.33	6	1
2	C	100	TYR	C-O	-5.37	1.17	1.24	10	1
1	A	408	ARG	C-N	5.37	1.40	1.33	14	1
2	C	67	VAL	C-N	5.37	1.41	1.33	15	1
2	C	161	GLU	CA-CB	5.37	1.61	1.53	1	1
1	A	430	PHE	C-N	5.37	1.40	1.33	2	2
1	A	484	TRP	C-N	5.37	1.41	1.33	3	1
1	A	416	ASP	CA-CB	5.37	1.61	1.53	4	1
2	C	202	ALA	CA-C	-5.37	1.46	1.52	5	1
1	A	340	TRP	N-CA	5.36	1.52	1.45	4	1
1	A	332	GLU	CA-C	5.36	1.59	1.52	6	1
2	C	182	ARG	N-CA	-5.36	1.40	1.46	10	1
1	A	339	ARG	N-CA	5.36	1.52	1.46	9	1
2	B	258	TYR	N-CA	-5.36	1.40	1.46	11	1
2	C	92	GLU	C-O	5.36	1.30	1.24	12	1
2	C	108	TRP	N-CA	5.36	1.52	1.46	6	1
1	A	436	TYR	CA-C	-5.36	1.46	1.52	5	1
2	B	58	SER	CA-C	-5.35	1.46	1.52	14	1
2	B	199	ARG	C-N	5.35	1.41	1.33	1	1
2	B	192	LEU	CA-CB	5.35	1.61	1.53	14	1
1	A	348	GLN	C-O	-5.35	1.17	1.23	1	1
2	C	134	MET	CA-C	5.35	1.60	1.52	8	1
2	C	192	LEU	C-N	5.35	1.40	1.33	2	1
1	A	393	ALA	C-N	5.35	1.40	1.33	6	1
2	C	127	GLN	C-N	5.35	1.40	1.33	10	1
2	B	222	LEU	C-N	5.34	1.41	1.33	9	1
2	C	137	TYR	CZ-OH	5.34	1.49	1.38	12	1
1	A	479	LYS	N-CA	-5.34	1.40	1.46	7	2
2	C	216	ALA	C-N	5.34	1.41	1.33	9	1
2	C	173	ARG	CD-NE	5.34	1.53	1.46	11	1
1	A	510	SER	C-N	5.34	1.40	1.33	6	1
2	B	79	THR	C-O	-5.34	1.18	1.24	6	1
2	B	248	LYS	C-N	5.34	1.40	1.33	1	1
2	B	59	LYS	CA-C	5.34	1.59	1.52	10	2
2	C	102	ASP	CA-CB	5.34	1.61	1.53	3	1
2	B	222	LEU	CA-CB	5.33	1.61	1.53	4	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	215	HIS	CD2-NE2	5.33	1.43	1.37	12	1
2	C	171	ARG	C-O	5.33	1.30	1.24	6	1
2	C	221	HIS	CB-CG	-5.33	1.42	1.50	8	1
2	B	246	SER	C-N	5.33	1.41	1.33	14	1
1	A	421	TRP	C-N	5.33	1.40	1.33	14	1
2	B	55	SER	N-CA	5.33	1.56	1.46	5	2
1	A	321	GLY	C-N	5.33	1.41	1.33	3	1
2	B	180	ALA	CA-C	5.32	1.59	1.52	4	2
1	A	431	ARG	CA-C	-5.32	1.46	1.52	15	2
1	A	394	SER	CA-C	-5.32	1.46	1.52	3	1
1	A	381	PHE	C-N	5.32	1.41	1.33	10	1
1	A	341	PHE	CA-CB	5.32	1.62	1.53	15	1
2	C	91	GLU	CA-CB	5.31	1.61	1.53	8	1
1	A	370	THR	C-N	5.31	1.40	1.33	14	2
2	C	115	TYR	CA-C	-5.31	1.46	1.52	13	1
2	C	181	LEU	CA-C	-5.31	1.46	1.52	5	1
1	A	472	GLU	CA-CB	5.31	1.60	1.53	11	1
2	B	203	LEU	N-CA	5.31	1.52	1.46	12	1
2	B	190	ASP	CA-C	5.31	1.59	1.52	13	1
2	C	85	GLU	N-CA	5.31	1.52	1.46	15	1
2	B	161	GLU	C-O	-5.31	1.18	1.24	2	1
2	C	143	PRO	C-O	5.31	1.30	1.24	13	1
2	C	84	GLN	C-N	5.31	1.40	1.33	11	1
1	A	495	PRO	C-N	5.30	1.40	1.33	10	1
2	C	195	ARG	CZ-NH2	-5.30	1.26	1.33	13	1
2	C	111	GLU	N-CA	-5.30	1.39	1.46	1	1
2	C	151	GLY	N-CA	-5.30	1.39	1.45	10	2
1	A	419	LEU	C-N	5.30	1.41	1.33	5	2
2	C	254	ALA	CA-CB	5.30	1.61	1.53	8	1
2	C	200	LEU	CA-CB	5.30	1.61	1.53	15	1
2	B	236	LEU	C-N	5.30	1.40	1.33	3	1
1	A	388	TRP	CA-C	5.30	1.58	1.52	7	1
2	C	258	TYR	C-O	-5.30	1.18	1.24	9	1
2	C	162	LYS	CA-C	-5.29	1.45	1.52	2	2
2	B	129	LYS	C-N	5.29	1.40	1.33	6	1
2	C	69	GLN	C-N	5.29	1.41	1.33	9	2
2	C	234	GLU	CA-CB	5.29	1.61	1.53	9	1
2	C	83	ARG	NE-CZ	5.29	1.38	1.33	10	2
1	A	505	TRP	C-N	5.29	1.41	1.33	15	1
2	B	194	GLN	CA-CB	5.29	1.61	1.53	7	3
2	C	72	TRP	C-N	5.29	1.40	1.33	11	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	343	ARG	CZ-NH2	-5.29	1.26	1.33	1	1
2	B	142	GLU	N-CA	5.29	1.51	1.46	1	2
2	B	148	LEU	C-N	-5.29	1.27	1.33	2	1
2	B	165	PRO	N-CA	-5.28	1.40	1.47	2	2
1	A	471	ASP	CA-C	5.28	1.59	1.52	3	2
2	C	206	ASN	CA-C	5.28	1.59	1.53	4	1
2	B	179	ASP	CA-C	5.28	1.59	1.52	7	1
1	A	440	GLU	C-N	5.28	1.40	1.33	14	1
2	B	227	GLU	CA-C	-5.28	1.45	1.52	14	1
2	C	193	ARG	CA-CB	5.28	1.61	1.53	15	1
2	B	56	THR	CA-CB	-5.28	1.45	1.53	2	1
1	A	382	PHE	CA-CB	5.28	1.61	1.53	11	1
2	C	229	ALA	CA-C	5.28	1.59	1.52	6	1
2	B	175	ARG	CZ-NH2	-5.28	1.26	1.33	8	1
1	A	398	GLY	CA-C	-5.28	1.44	1.51	12	1
2	C	138	ARG	CA-C	5.27	1.59	1.52	12	1
1	A	491	LEU	CA-CB	5.27	1.61	1.53	4	1
2	C	211	LEU	C-N	5.27	1.40	1.33	2	2
2	C	92	GLU	C-N	-5.26	1.27	1.33	14	2
2	B	142	GLU	CA-CB	-5.26	1.47	1.53	15	1
2	B	189	SER	C-O	-5.26	1.18	1.24	2	1
2	C	150	GLU	CA-C	-5.26	1.46	1.52	2	1
2	B	97	VAL	CA-C	5.26	1.59	1.52	7	1
2	B	206	ASN	N-CA	-5.26	1.40	1.46	10	1
2	C	113	GLU	N-CA	-5.26	1.40	1.46	12	1
2	B	70	GLU	CA-C	5.26	1.59	1.52	11	1
2	B	147	GLU	N-CA	-5.26	1.39	1.46	10	1
1	A	355	MET	SD-CE	5.26	1.92	1.79	13	1
2	B	228	LYS	CA-CB	5.26	1.61	1.53	8	1
2	C	162	LYS	N-CA	-5.25	1.39	1.46	1	1
2	C	183	THR	CA-C	5.25	1.59	1.52	11	2
2	B	84	GLN	C-O	-5.25	1.17	1.24	8	1
2	B	200	LEU	C-N	5.25	1.40	1.33	10	1
2	B	57	PHE	C-N	5.25	1.41	1.34	1	1
1	A	415	ILE	N-CA	-5.24	1.40	1.46	13	1
2	C	99	PRO	N-CD	-5.24	1.40	1.47	10	1
2	C	215	HIS	CD2-NE2	-5.24	1.32	1.37	9	1
2	B	130	TRP	C-N	5.24	1.40	1.33	10	1
1	A	415	ILE	C-O	-5.24	1.18	1.24	14	1
1	A	459	ILE	CB-CG1	5.24	1.64	1.53	14	1
1	A	404	LYS	N-CA	5.24	1.53	1.46	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	159	LEU	C-O	-5.24	1.18	1.24	9	1
2	C	62	GLU	CA-CB	5.24	1.61	1.53	11	1
2	C	264	THR	C-N	5.23	1.40	1.33	6	1
1	A	388	TRP	N-CA	-5.23	1.39	1.46	8	1
1	A	318	ILE	CA-C	5.23	1.59	1.52	13	1
2	B	119	VAL	C-N	-5.23	1.27	1.33	13	1
1	A	338	GLU	C-N	5.23	1.40	1.33	4	1
2	C	244	LEU	N-CA	-5.23	1.40	1.46	2	1
2	B	115	TYR	N-CA	5.23	1.52	1.46	5	1
1	A	486	PHE	C-O	-5.22	1.18	1.24	7	1
2	B	183	THR	CB-OG1	-5.22	1.35	1.43	6	1
2	C	87	SER	CA-CB	-5.22	1.45	1.53	11	1
2	C	150	GLU	CA-CB	5.22	1.61	1.53	3	1
2	C	128	LYS	C-N	5.22	1.40	1.33	3	1
2	C	117	GLN	N-CA	-5.22	1.39	1.46	4	1
1	A	502	LEU	N-CA	-5.22	1.40	1.46	1	1
1	A	389	VAL	N-CA	5.22	1.53	1.46	3	1
2	C	229	ALA	N-CA	-5.22	1.39	1.46	9	1
2	C	85	GLU	CA-C	-5.21	1.46	1.52	8	1
1	A	360	PHE	N-CA	-5.21	1.39	1.46	9	1
2	C	204	LYS	CA-C	5.21	1.59	1.53	9	1
1	A	376	ASP	CA-C	5.21	1.59	1.52	5	1
2	C	92	GLU	N-CA	-5.21	1.40	1.46	8	1
2	B	137	TYR	CA-CB	5.21	1.61	1.53	9	2
1	A	382	PHE	CA-C	-5.21	1.46	1.52	15	1
2	C	132	GLU	C-N	5.21	1.41	1.33	1	1
1	A	350	MET	N-CA	5.21	1.51	1.45	10	1
1	A	322	ASN	N-CA	5.21	1.54	1.46	14	1
2	B	157	HIS	CD2-NE2	-5.21	1.32	1.37	9	2
2	B	255	LEU	C-N	5.20	1.41	1.33	1	1
1	A	420	PHE	N-CA	-5.20	1.39	1.46	2	1
2	B	234	GLU	CA-C	5.20	1.59	1.52	2	1
2	B	211	LEU	C-N	5.20	1.40	1.33	2	1
2	B	244	LEU	N-CA	-5.20	1.40	1.46	4	1
2	B	68	THR	CA-C	-5.20	1.46	1.52	6	1
1	A	356	PRO	C-N	5.20	1.40	1.33	13	1
1	A	503	ARG	CA-CB	5.20	1.61	1.53	3	1
1	A	497	TYR	N-CA	-5.20	1.39	1.45	5	1
2	C	118	LYS	CA-CB	5.20	1.61	1.53	14	1
1	A	466	SER	CA-C	5.20	1.58	1.52	11	2
2	B	187	PRO	CA-C	-5.20	1.44	1.52	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	98	GLN	CA-CB	5.20	1.60	1.53	10	1
2	C	131	GLN	N-CA	5.20	1.52	1.46	11	1
2	C	84	GLN	C-O	-5.20	1.18	1.24	2	1
1	A	378	LYS	CA-CB	5.20	1.61	1.53	12	2
2	B	127	GLN	C-O	-5.19	1.17	1.24	9	1
2	C	157	HIS	CA-CB	5.19	1.61	1.53	9	1
2	B	83	ARG	CZ-NH2	-5.19	1.26	1.33	12	1
1	A	495	PRO	CA-C	5.19	1.58	1.52	13	1
2	B	195	ARG	NE-CZ	5.19	1.38	1.33	12	1
2	C	154	GLN	C-N	-5.19	1.26	1.33	14	1
1	A	372	TYR	CA-CB	5.18	1.62	1.53	2	1
2	C	99	PRO	CA-C	-5.18	1.45	1.52	2	1
2	B	263	ASN	CA-C	5.18	1.58	1.52	11	2
2	B	265	GLN	C-OXT	5.18	1.33	1.23	14	1
2	C	261	LYS	N-CA	5.18	1.52	1.46	4	1
2	B	136	LEU	CB-CG	5.18	1.63	1.53	5	1
2	B	252	LEU	CA-CB	5.18	1.61	1.53	5	1
1	A	324	ASP	C-N	-5.18	1.27	1.33	9	1
2	B	185	LEU	CA-CB	5.18	1.61	1.53	5	1
2	B	173	ARG	CD-NE	5.18	1.53	1.46	14	1
2	C	232	ALA	CA-CB	5.18	1.62	1.53	8	1
2	C	72	TRP	CA-CB	5.17	1.61	1.53	11	1
2	B	130	TRP	CG-CD2	5.17	1.53	1.43	1	1
2	C	72	TRP	CA-C	5.17	1.59	1.52	14	2
1	A	333	MET	CG-SD	5.17	1.93	1.80	5	1
1	A	357	ILE	N-CA	5.17	1.52	1.46	12	1
2	C	109	GLN	CA-CB	5.17	1.61	1.53	12	1
2	B	236	LEU	CA-C	5.17	1.59	1.52	2	1
1	A	334	PHE	N-CA	-5.17	1.39	1.45	3	1
2	C	198	ALA	N-CA	-5.17	1.39	1.46	14	2
1	A	355	MET	CA-CB	5.17	1.60	1.53	13	1
1	A	417	ALA	CA-C	5.17	1.58	1.52	14	1
1	A	393	ALA	N-CA	-5.16	1.41	1.46	9	1
1	A	474	PHE	C-O	-5.16	1.18	1.23	13	1
2	C	136	LEU	CA-CB	5.16	1.61	1.53	14	1
2	B	127	GLN	CA-C	-5.16	1.46	1.52	14	1
2	B	173	ARG	N-CA	5.15	1.52	1.46	2	2
1	A	426	LYS	N-CA	-5.15	1.39	1.45	7	1
2	C	249	VAL	N-CA	5.15	1.52	1.46	7	2
2	B	140	LYS	C-O	-5.15	1.18	1.24	8	1
2	B	137	TYR	CB-CG	-5.15	1.40	1.51	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	165	PRO	N-CD	-5.15	1.40	1.47	8	1
1	A	502	LEU	C-N	5.15	1.40	1.33	11	1
1	A	341	PHE	C-N	5.15	1.40	1.33	12	1
1	A	492	LYS	CA-CB	5.15	1.63	1.53	4	1
2	B	199	ARG	CA-CB	5.15	1.61	1.53	7	1
1	A	355	MET	CG-SD	5.14	1.93	1.80	1	1
1	A	426	LYS	C-N	5.14	1.40	1.33	4	1
1	A	477	PHE	N-CA	5.14	1.52	1.45	6	1
2	C	262	LEU	CB-CG	5.14	1.63	1.53	15	1
2	C	261	LYS	CA-C	5.14	1.59	1.52	5	1
2	B	191	GLU	CA-CB	5.14	1.61	1.53	9	2
2	C	195	ARG	CA-C	-5.14	1.46	1.52	2	1
1	A	501	ALA	C-N	5.14	1.40	1.33	3	1
2	B	91	GLU	C-N	5.14	1.41	1.33	10	1
2	C	177	HIS	CD2-NE2	5.13	1.43	1.37	6	1
2	B	162	LYS	C-N	5.13	1.41	1.33	10	1
2	C	205	GLU	N-CA	5.13	1.52	1.46	9	1
1	A	508	CYS	CA-C	5.13	1.58	1.53	3	2
2	B	160	GLN	CA-CB	5.13	1.61	1.53	7	1
2	C	89	ASP	C-N	5.13	1.40	1.33	5	1
1	A	435	TYR	CG-CD2	5.13	1.50	1.39	13	1
1	A	409	GLY	N-CA	5.12	1.52	1.45	5	1
2	B	118	LYS	C-N	5.12	1.40	1.33	3	1
2	B	262	LEU	C-N	5.12	1.39	1.33	9	1
2	C	134	MET	N-CA	-5.12	1.39	1.46	15	1
2	C	194	GLN	CA-CB	5.12	1.61	1.53	2	1
2	B	107	LYS	CA-C	-5.12	1.46	1.52	3	1
1	A	333	MET	CA-C	5.12	1.59	1.52	7	1
2	B	75	LEU	CA-CB	5.12	1.61	1.53	9	2
1	A	353	TYR	CA-CB	5.12	1.61	1.53	11	1
2	C	199	ARG	CD-NE	5.12	1.53	1.46	7	1
2	C	232	ALA	C-N	5.12	1.40	1.33	7	1
2	C	130	TRP	CD2-CE3	5.12	1.48	1.40	14	1
2	B	130	TRP	CA-C	-5.12	1.46	1.52	7	1
2	C	214	TYR	C-N	5.12	1.40	1.33	5	1
1	A	462	SER	C-N	5.12	1.40	1.33	8	1
2	B	136	LEU	N-CA	5.12	1.52	1.46	9	1
1	A	362	ARG	CA-C	5.11	1.59	1.52	5	1
2	B	189	SER	CA-CB	5.11	1.61	1.53	8	1
1	A	354	PRO	CA-CB	5.11	1.62	1.53	11	1
2	B	125	ASP	C-N	5.11	1.40	1.33	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	77	LYS	CA-C	5.11	1.59	1.52	8	1
1	A	374	ARG	C-N	5.11	1.40	1.33	3	1
2	B	181	LEU	C-N	5.11	1.40	1.33	7	1
2	C	245	GLU	CA-CB	5.11	1.61	1.53	8	2
1	A	451	LYS	N-CA	-5.11	1.39	1.45	14	1
2	B	165	PRO	C-N	5.10	1.41	1.33	4	1
2	B	131	GLN	CA-CB	5.10	1.61	1.53	8	1
2	C	60	LEU	C-O	-5.10	1.17	1.24	14	1
2	B	121	PRO	N-CA	-5.10	1.40	1.47	1	2
2	B	122	TYR	CZ-OH	5.10	1.48	1.38	1	1
1	A	412	THR	CA-C	-5.10	1.45	1.52	7	1
2	B	263	ASN	N-CA	-5.10	1.39	1.45	14	1
2	B	218	ALA	N-CA	-5.10	1.39	1.46	5	1
1	A	402	HIS	C-N	5.10	1.40	1.34	5	1
2	B	199	ARG	N-CA	5.10	1.52	1.46	7	1
2	B	172	ASP	N-CA	5.09	1.52	1.46	3	1
2	C	141	VAL	N-CA	5.09	1.52	1.46	3	1
1	A	471	ASP	C-N	5.09	1.40	1.33	8	1
2	B	123	LEU	C-N	5.09	1.40	1.33	9	1
2	C	259	THR	C-N	5.08	1.40	1.33	8	1
2	C	87	SER	CA-C	-5.08	1.46	1.52	12	1
1	A	334	PHE	CA-CB	5.08	1.61	1.53	10	1
1	A	450	PRO	N-CD	5.08	1.54	1.47	4	1
2	C	75	LEU	CA-CB	5.08	1.61	1.53	14	2
2	B	123	LEU	C-O	-5.08	1.18	1.24	4	1
2	C	249	VAL	CA-CB	5.08	1.60	1.54	5	1
1	A	469	GLY	CA-C	-5.08	1.47	1.52	10	1
1	A	347	ASN	C-N	5.08	1.40	1.33	9	1
2	B	95	ALA	N-CA	-5.08	1.40	1.46	7	1
2	C	181	LEU	N-CA	5.07	1.52	1.46	1	1
2	C	259	THR	CA-C	5.07	1.59	1.52	12	1
1	A	506	MET	C-O	5.07	1.30	1.24	4	1
2	B	157	HIS	C-O	-5.07	1.18	1.24	9	1
2	C	96	LYS	N-CA	-5.07	1.40	1.46	3	1
2	B	215	HIS	CA-CB	5.07	1.61	1.53	3	1
1	A	326	VAL	CA-CB	5.07	1.61	1.54	5	1
1	A	343	ARG	CZ-NH1	-5.07	1.25	1.32	15	1
2	B	193	ARG	N-CA	-5.07	1.40	1.46	1	1
2	B	154	GLN	CA-CB	5.07	1.61	1.53	6	1
1	A	476	TYR	CZ-OH	5.07	1.48	1.38	7	1
1	A	407	GLY	C-N	5.07	1.40	1.33	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	498	PRO	N-CD	-5.07	1.40	1.47	15	1
2	B	201	GLU	C-O	5.06	1.30	1.24	2	1
2	C	255	LEU	C-O	-5.06	1.18	1.24	2	1
1	A	412	THR	CA-CB	5.06	1.61	1.53	10	1
1	A	330	ARG	NE-CZ	-5.06	1.27	1.33	12	1
1	A	466	SER	CA-CB	5.06	1.62	1.53	5	1
1	A	429	PHE	CA-C	-5.06	1.46	1.52	2	1
2	B	183	THR	CA-CB	5.06	1.61	1.53	12	1
2	C	255	LEU	C-N	5.05	1.40	1.33	10	1
1	A	336	PHE	C-N	5.05	1.40	1.33	15	1
2	C	108	TRP	CD2-CE3	5.05	1.48	1.40	9	1
1	A	396	GLU	CA-CB	5.05	1.60	1.53	2	1
2	C	64	LEU	C-N	5.05	1.41	1.33	3	1
1	A	442	LEU	CA-C	5.05	1.59	1.52	9	1
2	B	131	GLN	CA-C	5.05	1.59	1.52	14	1
2	B	113	GLU	N-CA	5.05	1.52	1.46	1	1
1	A	465	GLY	N-CA	5.05	1.52	1.45	1	1
2	C	166	LEU	CA-CB	5.05	1.61	1.53	3	1
2	B	77	LYS	N-CA	5.04	1.52	1.46	10	1
1	A	354	PRO	N-CD	-5.04	1.40	1.47	15	1
2	B	174	ALA	CA-C	5.04	1.59	1.52	7	1
2	B	105	GLN	CA-CB	5.04	1.61	1.53	8	1
2	B	241	LEU	C-N	5.04	1.40	1.34	6	1
2	C	96	LYS	CA-C	-5.04	1.45	1.52	9	1
2	B	98	GLN	C-O	-5.04	1.19	1.24	11	1
2	C	191	GLU	N-CA	5.04	1.52	1.46	12	1
2	B	228	LYS	C-O	-5.04	1.18	1.24	8	1
1	A	424	ASN	N-CA	5.04	1.52	1.45	11	1
2	C	159	LEU	CA-CB	5.04	1.61	1.53	2	1
1	A	356	PRO	CA-C	-5.04	1.46	1.52	13	1
1	A	508	CYS	C-N	5.03	1.40	1.33	10	1
2	C	108	TRP	CA-CB	5.03	1.61	1.53	14	1
1	A	412	THR	CB-OG1	-5.03	1.35	1.43	12	1
2	B	106	LYS	C-O	-5.03	1.18	1.24	2	1
2	B	224	THR	CA-C	-5.03	1.46	1.52	8	1
1	A	394	SER	C-N	5.03	1.40	1.33	12	1
2	C	178	VAL	CA-C	5.03	1.58	1.52	13	1
1	A	362	ARG	CD-NE	5.02	1.53	1.46	10	1
1	A	329	LEU	N-CA	-5.02	1.40	1.46	8	1
2	C	162	LYS	C-O	-5.02	1.17	1.24	9	1
1	A	373	GLU	CA-CB	5.02	1.60	1.53	14	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	217	LYS	N-CA	5.02	1.52	1.46	14	1
2	C	208	GLY	CA-C	5.02	1.58	1.51	4	1
1	A	417	ALA	N-CA	-5.02	1.39	1.46	8	1
2	B	200	LEU	C-O	-5.02	1.18	1.24	2	1
2	B	63	GLN	C-N	5.02	1.40	1.33	11	1
2	C	105	GLN	N-CA	-5.02	1.39	1.46	12	1
2	B	195	ARG	CD-NE	5.02	1.53	1.46	5	1
2	C	263	ASN	N-CA	-5.02	1.39	1.46	8	1
2	C	254	ALA	N-CA	5.02	1.52	1.46	12	1
2	B	152	ALA	CA-CB	5.02	1.61	1.53	13	1
2	C	263	ASN	CA-CB	5.01	1.62	1.53	3	1
2	B	57	PHE	CG-CD1	5.01	1.49	1.38	7	1
2	C	141	VAL	C-O	-5.01	1.18	1.24	3	1
1	A	464	ARG	CZ-NH1	-5.01	1.25	1.32	6	1
1	A	342	TRP	N-CA	-5.01	1.39	1.45	10	1
2	C	190	ASP	C-N	5.01	1.40	1.33	10	1
1	A	368	ILE	N-CA	5.01	1.52	1.46	15	1
1	A	480	GLY	C-O	-5.01	1.17	1.23	4	1
2	B	259	THR	N-CA	-5.01	1.40	1.46	6	1
2	C	149	GLN	CG-CD	5.01	1.64	1.52	6	1
2	C	236	LEU	C-O	-5.01	1.18	1.24	11	1
1	A	418	ALA	C-O	-5.01	1.18	1.23	15	1
2	C	106	LYS	C-N	5.01	1.40	1.33	2	1
1	A	443	ARG	C-N	5.01	1.40	1.33	5	1
2	B	149	GLN	CA-CB	5.01	1.61	1.53	5	1
1	A	356	PRO	C-O	-5.01	1.18	1.23	13	1
2	C	220	GLU	N-CA	-5.00	1.40	1.46	6	1
1	A	428	TYR	CE1-CZ	5.00	1.50	1.38	2	1
2	B	219	THR	N-CA	-5.00	1.40	1.46	3	1
1	A	407	GLY	CA-C	-5.00	1.44	1.51	7	1
1	A	388	TRP	CD2-CE3	5.00	1.48	1.40	10	1
2	B	184	HIS	CG-CD2	5.00	1.41	1.35	13	1
1	A	405	GLU	CA-CB	5.00	1.61	1.53	14	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	459	ILE	O-C-N	-14.86	112.01	121.37	3	3
2	B	193	ARG	NE-CZ-NH2	14.81	132.53	119.20	8	5
2	C	61	ARG	NE-CZ-NH2	14.06	131.86	119.20	11	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	497	TYR	O-C-N	-13.71	112.93	121.71	8	8
2	C	71	PHE	CA-CB-CG	13.68	127.48	113.80	14	5
2	C	116	ARG	NE-CZ-NH2	13.66	131.49	119.20	10	7
2	B	199	ARG	NE-CZ-NH2	13.60	131.44	119.20	14	8
2	C	153	ARG	NE-CZ-NH2	13.50	131.35	119.20	12	9
2	B	116	ARG	NE-CZ-NH2	12.93	130.84	119.20	12	4
1	A	353	TYR	CA-C-O	-12.85	108.68	120.50	10	4
2	C	83	ARG	NE-CZ-NH2	12.81	130.72	119.20	12	8
2	B	175	ARG	NE-CZ-NH2	12.78	130.70	119.20	13	12
1	A	346	ASN	CA-CB-CG	-12.64	99.96	112.60	10	4
2	B	119	VAL	N-CA-C	12.63	122.54	110.42	3	6
2	B	195	ARG	NE-CZ-NH2	12.56	130.50	119.20	3	10
2	C	175	ARG	NE-CZ-NH2	12.26	130.23	119.20	2	9
1	A	464	ARG	NE-CZ-NH2	12.06	130.06	119.20	1	8
2	C	195	ARG	NE-CZ-NH2	12.04	130.04	119.20	4	10
1	A	462	SER	CA-C-O	-12.04	110.63	120.26	5	2
1	A	343	ARG	NE-CZ-NH2	11.94	129.94	119.20	4	9
2	C	237	ARG	NE-CZ-NH2	11.80	129.82	119.20	14	9
2	C	138	ARG	NE-CZ-NH2	11.71	129.74	119.20	9	6
1	A	317	ASN	CA-CB-CG	-11.68	100.92	112.60	15	2
1	A	336	PHE	CA-CB-CG	-11.67	102.13	113.80	3	4
1	A	323	PHE	CA-CB-CG	-11.66	102.14	113.80	3	6
2	B	124	ASP	CA-CB-CG	11.62	124.22	112.60	10	5
2	B	237	ARG	NE-CZ-NH2	11.59	129.63	119.20	8	7
2	B	248	LYS	N-CA-C	11.59	123.99	111.36	3	4
2	C	171	ARG	NE-CZ-NH2	11.57	129.61	119.20	15	11
2	B	256	GLU	N-CA-C	11.50	123.81	111.28	12	6
2	B	173	ARG	NE-CZ-NH1	-11.49	110.01	121.50	5	5
2	B	61	ARG	NE-CZ-NH2	11.45	129.50	119.20	7	2
2	C	61	ARG	NE-CZ-NH1	-11.42	110.08	121.50	11	2
2	C	259	THR	N-CA-C	11.38	123.24	111.07	11	1
2	C	145	ARG	NE-CZ-NH2	11.35	129.42	119.20	1	10
1	A	322	ASN	CA-CB-CG	-11.33	101.27	112.60	10	4
2	C	210	ARG	NE-CZ-NH2	11.30	129.37	119.20	9	10
2	B	110	GLU	N-CA-C	11.25	123.11	111.07	5	4
1	A	353	TYR	O-C-N	-11.21	114.54	121.71	7	6
2	C	202	ALA	CA-C-N	11.17	136.37	120.28	9	2
2	C	202	ALA	C-N-CA	11.17	136.37	120.28	9	2
2	B	238	GLN	CA-C-N	11.10	132.26	119.94	10	4
2	B	238	GLN	C-N-CA	11.10	132.26	119.94	10	4
1	A	422	MET	CA-C-N	11.08	131.95	119.32	2	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	422	MET	C-N-CA	11.08	131.95	119.32	2	4
1	A	399	TYR	O-C-N	-11.07	112.28	121.80	8	3
2	C	73	ASP	CA-CB-CG	-10.98	101.62	112.60	3	3
2	B	178	VAL	CA-C-N	10.94	134.66	120.44	1	1
2	B	178	VAL	C-N-CA	10.94	134.66	120.44	1	1
2	B	83	ARG	NE-CZ-NH2	10.93	129.03	119.20	13	6
1	A	468	MET	CA-C-N	10.92	130.48	120.10	10	5
1	A	468	MET	C-N-CA	10.92	130.48	120.10	10	5
2	B	219	THR	N-CA-C	10.92	122.75	111.07	7	2
1	A	357	ILE	N-CA-C	10.88	120.86	110.42	2	1
2	B	173	ARG	NE-CZ-NH2	10.86	128.98	119.20	14	5
2	B	209	ALA	N-CA-C	10.81	122.64	111.07	12	1
2	C	171	ARG	NE-CZ-NH1	-10.80	110.70	121.50	14	6
2	C	204	LYS	N-CA-C	10.79	123.12	111.36	7	2
1	A	452	ASN	CA-CB-CG	10.79	123.39	112.60	10	3
2	C	234	GLU	O-C-N	-10.73	111.01	122.07	5	2
2	C	150	GLU	N-CA-C	10.72	122.55	111.07	2	3
2	B	239	GLY	CA-C-N	10.71	134.37	120.44	13	6
2	B	239	GLY	C-N-CA	10.71	134.37	120.44	13	6
2	B	164	SER	N-CA-C	10.70	127.31	112.75	10	5
2	B	150	GLU	CA-C-N	10.70	132.07	119.99	4	5
2	B	150	GLU	C-N-CA	10.70	132.07	119.99	4	5
2	B	153	ARG	NE-CZ-NH2	10.68	128.81	119.20	14	11
2	C	72	TRP	N-CA-C	10.63	122.45	111.07	5	3
2	C	199	ARG	NE-CZ-NH2	10.62	128.76	119.20	14	6
2	C	62	GLU	N-CA-C	10.60	122.84	111.28	4	5
2	B	132	GLU	N-CA-C	10.60	122.84	111.28	7	1
2	C	76	GLU	N-CA-C	10.60	122.83	111.28	13	5
2	B	116	ARG	N-CA-C	10.56	122.37	111.07	5	1
2	B	157	HIS	CA-CB-CG	-10.54	103.26	113.80	2	3
2	B	178	VAL	N-CA-C	10.47	121.36	110.36	13	7
2	C	193	ARG	NE-CZ-NH2	10.41	128.57	119.20	4	7
2	B	177	HIS	CA-C-N	10.37	133.63	120.56	10	3
2	B	177	HIS	C-N-CA	10.37	133.63	120.56	10	3
1	A	474	PHE	CA-CB-CG	-10.34	103.46	113.80	1	4
2	C	122	TYR	N-CA-C	10.27	122.56	111.36	7	3
2	C	186	ALA	CA-C-O	-10.27	108.67	118.73	4	1
1	A	446	ASP	CA-CB-CG	10.23	122.83	112.60	9	7
1	A	408	ARG	NE-CZ-NH2	10.21	128.39	119.20	13	9
2	C	127	GLN	OE1-CD-NE2	-10.22	112.38	122.60	7	3
2	B	182	ARG	NE-CZ-NH2	10.21	128.39	119.20	12	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	238	GLN	CA-C-N	10.21	131.52	119.99	8	6
2	C	238	GLN	C-N-CA	10.21	131.52	119.99	8	6
2	B	157	HIS	CE1-NE2-CD2	-10.19	98.81	109.00	14	6
1	A	439	ASN	OD1-CG-ND2	-10.18	112.42	122.60	5	3
2	B	205	GLU	CA-C-N	10.15	133.64	120.44	15	1
2	B	205	GLU	C-N-CA	10.15	133.64	120.44	15	1
2	B	120	GLU	N-CA-C	10.15	126.45	113.25	14	7
1	A	381	PHE	CA-CB-CG	-10.12	103.68	113.80	3	4
2	B	84	GLN	N-CA-C	10.11	122.38	111.36	15	2
2	B	171	ARG	N-CA-C	10.07	121.84	111.07	7	8
1	A	462	SER	CB-CA-C	-10.04	102.27	111.00	4	3
2	C	217	LYS	N-CA-C	10.01	122.27	111.36	4	3
1	A	390	PHE	CA-CB-CG	-10.01	103.79	113.80	12	3
2	B	169	GLU	N-CA-C	10.01	121.78	111.07	4	5
2	B	66	PRO	CA-C-N	9.98	133.18	120.70	2	5
2	B	66	PRO	C-N-CA	9.98	133.18	120.70	2	5
2	C	87	SER	N-CA-C	9.97	121.74	111.07	4	4
2	B	218	ALA	N-CA-C	9.96	123.16	111.71	13	7
2	B	139	GLN	N-CA-C	9.89	122.06	111.28	6	5
2	B	216	ALA	N-CA-C	9.89	122.06	111.28	13	5
2	C	181	LEU	CA-C-O	9.88	131.19	120.82	5	1
1	A	343	ARG	NE-CZ-NH1	-9.87	111.63	121.50	4	7
2	C	262	LEU	N-CA-C	9.87	121.63	111.07	13	3
2	C	182	ARG	NE-CZ-NH2	9.87	128.08	119.20	8	6
2	C	253	SER	N-CA-C	9.81	123.20	111.33	2	4
2	C	63	GLN	N-CA-C	9.81	121.57	111.07	14	3
1	A	365	PRO	CA-C-N	9.80	134.63	120.71	13	5
1	A	365	PRO	C-N-CA	9.80	134.63	120.71	13	5
1	A	368	ILE	N-CA-C	9.80	123.52	109.51	14	3
2	C	144	LEU	N-CA-C	9.79	121.95	111.28	5	2
2	B	162	LYS	N-CA-C	9.78	124.27	111.75	15	8
2	B	157	HIS	N-CA-C	9.77	121.93	111.28	1	3
1	A	387	HIS	CA-CB-CG	9.75	123.55	113.80	5	6
1	A	345	ARG	NE-CZ-NH2	9.75	127.97	119.20	6	5
2	C	97	VAL	N-CA-C	9.75	119.78	110.42	5	6
1	A	413	ASP	CA-CB-CG	9.74	122.34	112.60	10	6
2	C	153	ARG	N-CA-C	9.70	123.07	111.82	10	5
2	B	145	ARG	NE-CZ-NH2	9.65	127.88	119.20	7	5
2	C	88	LYS	N-CA-C	9.65	121.39	111.07	5	4
1	A	493	VAL	N-CA-C	9.64	121.93	109.30	6	3
2	B	102	ASP	N-CA-C	9.62	121.77	111.28	9	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	210	ARG	NE-CZ-NH2	9.60	127.84	119.20	5	5
2	B	63	GLN	CA-C-O	9.59	130.59	120.42	2	1
2	B	151	GLY	CA-C-N	9.58	132.90	120.44	4	1
2	B	151	GLY	C-N-CA	9.58	132.90	120.44	4	1
2	C	222	LEU	N-CA-C	9.58	121.32	111.07	1	3
1	A	345	ARG	NE-CZ-NH1	-9.57	111.93	121.50	15	4
2	B	188	TYR	CA-C-N	9.56	133.09	120.28	12	5
2	B	188	TYR	C-N-CA	9.56	133.09	120.28	12	5
1	A	457	GLU	CA-C-O	9.55	130.68	120.36	4	2
2	B	102	ASP	CA-CB-CG	9.54	122.14	112.60	7	3
2	B	94	LYS	CA-C-N	9.53	133.82	120.29	7	6
2	B	94	LYS	C-N-CA	9.53	133.82	120.29	7	6
1	A	475	THR	O-C-N	-9.53	111.80	123.33	5	3
2	B	195	ARG	NE-CZ-NH1	-9.51	111.99	121.50	7	7
2	C	186	ALA	N-CA-C	9.50	125.60	113.25	13	3
2	B	63	GLN	N-CA-C	9.50	121.32	110.97	1	4
1	A	321	GLY	CA-C-N	9.48	135.83	122.46	13	1
1	A	321	GLY	C-N-CA	9.48	135.83	122.46	13	1
2	B	166	LEU	CA-C-N	9.46	130.68	119.99	2	2
2	B	166	LEU	C-N-CA	9.46	130.68	119.99	2	2
2	C	103	ASP	CA-C-N	9.46	133.34	120.38	4	1
2	C	103	ASP	C-N-CA	9.46	133.34	120.38	4	1
1	A	449	TYR	O-C-N	-9.46	115.66	121.71	13	1
1	A	431	ARG	NE-CZ-NH2	9.44	127.70	119.20	14	8
2	B	205	GLU	N-CA-C	9.44	121.34	111.14	5	2
1	A	439	ASN	CA-C-O	9.41	130.49	120.33	5	2
2	C	169	GLU	N-CA-C	9.37	121.10	111.07	14	3
1	A	464	ARG	NE-CZ-NH1	-9.36	112.14	121.50	1	5
2	C	206	ASN	CA-CB-CG	-9.36	103.24	112.60	10	3
2	C	148	LEU	N-CA-C	9.35	121.47	111.28	11	1
2	B	194	GLN	CA-C-N	9.35	132.59	120.44	4	1
2	B	194	GLN	C-N-CA	9.35	132.59	120.44	4	1
2	B	186	ALA	O-C-N	-9.34	111.68	120.55	9	5
2	C	128	LYS	O-C-N	-9.34	112.22	122.12	4	1
2	B	105	GLN	N-CA-C	9.31	121.03	111.07	11	6
2	C	142	GLU	O-C-N	-9.31	111.70	120.55	10	2
1	A	375	LYS	N-CA-C	9.29	122.57	111.33	13	5
2	B	120	GLU	O-C-N	-9.28	113.05	120.38	5	2
2	C	119	VAL	N-CA-C	9.27	122.68	111.09	3	1
2	B	175	ARG	NE-CZ-NH1	-9.27	112.23	121.50	11	7
2	B	63	GLN	OE1-CD-NE2	9.26	131.86	122.60	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	176	ALA	CA-C-O	-9.25	111.10	120.82	8	2
2	B	154	GLN	O-C-N	-9.25	112.31	122.12	10	1
1	A	408	ARG	NE-CZ-NH1	-9.23	112.27	121.50	15	3
1	A	422	MET	O-C-N	-9.23	110.71	121.32	1	3
2	B	208	GLY	N-CA-C	9.23	123.80	112.73	6	1
2	B	221	HIS	CA-CB-CG	-9.23	104.57	113.80	9	1
1	A	389	VAL	N-CA-CB	9.22	123.90	112.10	3	2
1	A	414	LYS	O-C-N	-9.22	113.56	123.42	4	2
2	C	91	GLU	N-CA-C	9.21	121.32	111.28	9	4
2	B	179	ASP	CA-CB-CG	9.21	121.81	112.60	2	3
1	A	506	MET	CA-C-O	9.21	130.43	119.28	4	2
2	B	64	LEU	N-CA-C	9.21	120.92	111.07	8	2
2	C	133	GLU	N-CA-C	9.20	121.08	111.14	11	1
2	C	188	TYR	CA-C-O	9.20	130.74	120.90	11	1
2	C	226	SER	CA-C-N	9.18	132.38	120.44	14	4
2	C	226	SER	C-N-CA	9.18	132.38	120.44	14	4
1	A	419	LEU	CA-C-N	9.18	135.03	121.72	14	1
1	A	419	LEU	C-N-CA	9.18	135.03	121.72	14	1
1	A	385	ASP	CA-CB-CG	9.16	121.76	112.60	15	6
2	C	197	ALA	N-CA-C	9.16	121.26	111.28	13	4
2	C	182	ARG	NE-CZ-NH1	-9.16	112.34	121.50	7	6
2	B	153	ARG	CA-C-N	9.15	132.89	120.54	3	5
2	B	153	ARG	C-N-CA	9.15	132.89	120.54	3	5
2	B	58	SER	CA-C-O	9.15	130.25	120.55	12	3
2	C	105	GLN	OE1-CD-NE2	-9.15	113.45	122.60	11	2
1	A	396	GLU	CA-C-N	9.14	129.71	119.93	3	8
1	A	396	GLU	C-N-CA	9.14	129.71	119.93	3	8
2	C	162	LYS	N-CA-C	9.13	121.23	111.28	6	3
2	C	184	HIS	O-C-N	-9.11	112.47	122.12	11	1
2	B	61	ARG	NH1-CZ-NH2	-9.11	107.46	119.30	7	4
2	B	157	HIS	ND1-CE1-NE2	9.11	117.51	108.40	14	5
2	C	177	HIS	CE1-NE2-CD2	-9.09	99.91	109.00	15	4
1	A	487	ASN	CA-CB-CG	9.09	121.69	112.60	3	3
2	C	94	LYS	O-C-N	-9.09	112.49	122.12	1	2
2	B	149	GLN	N-CA-C	9.08	120.79	111.07	2	2
1	A	471	ASP	CA-CB-CG	9.06	121.66	112.60	5	4
2	C	102	ASP	CA-C-O	9.05	130.02	120.70	6	3
1	A	382	PHE	CA-CB-CG	9.05	122.85	113.80	2	1
2	B	104	PHE	CA-C-N	9.04	132.75	120.54	9	4
2	B	104	PHE	C-N-CA	9.04	132.75	120.54	9	4
1	A	415	ILE	CA-C-O	9.04	130.06	120.48	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	173	ARG	NE-CZ-NH2	9.02	127.32	119.20	3	7
2	C	229	ALA	N-CA-C	9.01	122.07	111.71	4	3
2	B	134	MET	CA-C-N	9.00	132.14	120.44	14	3
2	B	134	MET	C-N-CA	9.00	132.14	120.44	14	3
2	C	251	PHE	CA-CB-CG	8.99	122.79	113.80	11	4
2	C	86	MET	CA-C-N	8.98	132.12	120.44	9	1
2	C	86	MET	C-N-CA	8.98	132.12	120.44	9	1
2	B	145	ARG	NE-CZ-NH1	-8.98	112.52	121.50	12	4
2	C	100	TYR	CA-C-N	8.96	132.29	120.28	4	9
2	C	100	TYR	C-N-CA	8.96	132.29	120.28	4	9
2	C	129	LYS	N-CA-C	8.96	121.04	111.28	4	5
2	C	202	ALA	N-CA-C	8.96	121.05	111.28	7	1
1	A	452	ASN	CB-CA-C	8.92	122.11	109.71	13	1
2	C	131	GLN	N-CA-C	8.90	121.95	111.71	3	3
2	C	153	ARG	NE-CZ-NH1	-8.90	112.60	121.50	5	5
1	A	411	PRO	CA-C-N	8.89	132.00	120.44	5	3
1	A	411	PRO	C-N-CA	8.89	132.00	120.44	5	3
2	B	226	SER	CA-C-N	8.89	132.92	120.29	7	1
2	B	226	SER	C-N-CA	8.89	132.92	120.29	7	1
1	A	422	MET	N-CA-C	8.89	125.81	113.45	11	10
2	B	199	ARG	NE-CZ-NH1	-8.89	112.61	121.50	14	5
1	A	439	ASN	O-C-N	-8.86	112.99	123.27	4	2
2	C	177	HIS	N-CA-C	8.86	120.93	111.28	6	5
2	B	160	GLN	CA-C-N	8.85	132.13	120.28	6	4
2	B	160	GLN	C-N-CA	8.85	132.13	120.28	6	4
2	B	250	SER	CA-C-N	8.84	133.07	120.79	2	3
2	B	250	SER	C-N-CA	8.84	133.07	120.79	2	3
2	C	120	GLU	CA-C-O	-8.83	110.51	118.63	15	1
2	B	173	ARG	N-CA-C	8.82	120.51	111.07	1	3
2	C	116	ARG	NH1-CZ-NH2	-8.82	107.83	119.30	10	2
2	B	204	LYS	N-CA-C	8.79	120.86	111.28	7	3
2	C	126	PHE	CA-C-O	8.79	130.74	121.07	8	3
1	A	433	ASN	N-CA-C	-8.78	102.72	112.72	2	2
2	B	255	LEU	N-CA-C	8.78	120.46	111.07	6	1
2	B	177	HIS	CE1-NE2-CD2	-8.77	100.23	109.00	5	5
2	B	115	TYR	CA-C-O	-8.75	111.17	120.63	13	1
2	B	73	ASP	CA-C-N	8.73	131.99	120.28	3	2
2	B	73	ASP	C-N-CA	8.73	131.99	120.28	3	2
2	C	250	SER	N-CA-C	8.73	120.87	111.36	3	4
2	B	73	ASP	CA-CB-CG	8.73	121.33	112.60	6	4
2	B	115	TYR	N-CA-C	8.73	120.79	111.28	8	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	141	VAL	N-CA-C	8.72	118.80	110.42	14	6
2	C	191	GLU	CA-C-O	-8.72	111.18	120.42	1	1
2	C	171	ARG	CA-C-O	8.72	129.66	120.42	6	3
2	C	66	PRO	CA-C-N	8.71	132.40	120.46	8	4
2	C	66	PRO	C-N-CA	8.71	132.40	120.46	8	4
2	B	174	ALA	N-CA-C	8.71	120.77	111.28	6	1
2	C	254	ALA	N-CA-C	8.70	121.86	111.33	11	4
2	C	77	LYS	CA-C-N	8.70	131.75	120.44	7	1
2	C	77	LYS	C-N-CA	8.70	131.75	120.44	7	1
1	A	424	ASN	CA-CB-CG	8.69	121.28	112.60	11	5
2	C	201	GLU	CA-C-N	8.68	131.92	120.28	11	4
2	C	201	GLU	C-N-CA	8.68	131.92	120.28	11	4
2	C	58	SER	N-CA-C	8.68	120.35	111.07	11	1
2	B	191	GLU	O-C-N	-8.67	112.26	122.15	10	2
2	B	131	GLN	N-CA-C	8.67	120.73	111.28	3	2
2	C	57	PHE	CA-CB-CG	-8.65	105.15	113.80	15	4
2	C	77	LYS	N-CA-C	8.65	120.48	111.14	3	2
2	B	72	TRP	CA-C-N	8.64	131.85	120.28	15	3
2	B	72	TRP	C-N-CA	8.64	131.85	120.28	15	3
1	A	510	SER	N-CA-C	8.63	121.81	111.02	11	2
2	B	92	GLU	CA-C-N	8.63	131.60	120.56	11	4
2	B	92	GLU	C-N-CA	8.63	131.60	120.56	11	4
2	C	134	MET	N-CA-C	8.62	120.30	111.07	3	5
1	A	354	PRO	N-CD-CG	8.60	114.12	103.80	5	1
1	A	503	ARG	NE-CZ-NH1	-8.59	112.91	121.50	11	1
2	C	188	TYR	O-C-N	-8.59	113.01	122.12	5	3
2	C	158	GLU	CA-C-N	8.59	131.78	120.28	7	2
2	C	158	GLU	C-N-CA	8.59	131.78	120.28	7	2
1	A	502	LEU	O-C-N	8.58	130.91	122.07	10	2
2	B	241	LEU	CA-C-N	-8.58	110.90	119.56	14	4
2	B	241	LEU	C-N-CA	-8.58	110.90	119.56	14	4
2	C	147	GLU	CA-C-N	8.57	131.97	120.65	12	3
2	C	147	GLU	C-N-CA	8.57	131.97	120.65	12	3
2	B	237	ARG	N-CA-CB	8.56	122.83	110.16	9	6
2	C	149	GLN	O-C-N	-8.55	113.20	122.09	4	2
1	A	474	PHE	N-CA-C	8.55	122.83	108.90	15	2
1	A	483	TYR	CA-C-N	8.54	134.13	122.77	12	2
1	A	483	TYR	C-N-CA	8.54	134.13	122.77	12	2
2	C	126	PHE	CA-CB-CG	-8.52	105.28	113.80	1	6
2	B	133	GLU	N-CA-C	8.51	121.69	111.82	6	4
2	B	262	LEU	N-CA-C	8.51	121.69	111.82	4	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	177	HIS	ND1-CE1-NE2	8.51	116.91	108.40	15	3
2	C	151	GLY	CA-C-N	8.50	131.68	120.28	14	3
2	C	151	GLY	C-N-CA	8.50	131.68	120.28	14	3
2	C	78	GLU	CA-C-O	8.50	129.56	120.55	5	2
1	A	470	SER	N-CA-C	8.50	120.16	111.07	1	6
2	C	210	ARG	NE-CZ-NH1	-8.49	113.01	121.50	10	3
2	C	118	LYS	N-CA-C	8.48	120.52	111.28	9	3
1	A	342	TRP	CA-C-O	8.47	129.69	120.71	9	1
1	A	385	ASP	N-CA-C	-8.46	104.00	112.97	12	2
1	A	466	SER	O-C-N	-8.46	114.38	123.26	12	2
2	B	226	SER	N-CA-CB	8.46	122.27	110.01	6	1
2	B	171	ARG	CA-C-O	8.46	129.95	120.90	15	1
2	C	148	LEU	N-CA-CB	-8.46	97.64	110.16	15	1
2	B	157	HIS	CG-CD2-NE2	8.45	115.65	107.20	13	2
1	A	443	ARG	NE-CZ-NH1	-8.45	113.05	121.50	9	3
2	B	226	SER	N-CA-C	8.45	120.11	111.07	15	2
1	A	328	MET	CA-C-O	8.45	129.71	120.92	15	2
2	C	156	LEU	CA-C-N	8.44	131.41	120.44	12	3
2	C	156	LEU	C-N-CA	8.44	131.41	120.44	12	3
2	B	183	THR	N-CA-CB	8.44	122.24	110.01	11	2
2	C	206	ASN	CA-C-N	8.43	129.30	119.94	9	8
2	C	206	ASN	C-N-CA	8.43	129.30	119.94	9	8
1	A	345	ARG	NH1-CZ-NH2	-8.43	108.34	119.30	6	2
2	B	92	GLU	N-CA-C	8.42	120.24	111.14	3	2
2	C	265	GLN	OE1-CD-NE2	-8.42	114.18	122.60	3	5
1	A	462	SER	O-C-N	8.42	125.40	121.53	5	3
1	A	461	GLU	O-C-N	-8.41	112.96	123.06	12	1
2	B	244	LEU	CA-C-N	8.41	131.38	120.44	5	1
2	B	244	LEU	C-N-CA	8.41	131.38	120.44	5	1
2	B	178	VAL	O-C-N	-8.41	113.67	121.91	14	1
2	B	69	GLN	N-CA-C	8.41	120.07	111.07	7	8
2	C	241	LEU	O-C-N	-8.41	112.38	120.70	2	4
2	C	226	SER	N-CA-C	8.41	121.20	111.11	9	1
2	B	176	ALA	CA-C-N	8.41	131.37	120.44	12	1
2	B	176	ALA	C-N-CA	8.41	131.37	120.44	12	1
2	C	106	LYS	O-C-N	-8.40	113.21	122.12	7	2
2	B	78	GLU	N-CA-C	8.39	120.43	111.28	8	4
2	C	243	VAL	N-CA-C	-8.39	102.68	111.58	8	4
2	C	236	LEU	N-CA-C	-8.39	102.21	111.36	1	2
2	C	131	GLN	OE1-CD-NE2	-8.39	114.21	122.60	10	5
2	B	68	THR	CA-C-N	8.38	131.34	120.44	3	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	68	THR	C-N-CA	8.38	131.34	120.44	3	4
2	B	60	LEU	CA-C-N	8.38	131.33	120.44	7	2
2	B	60	LEU	C-N-CA	8.38	131.33	120.44	7	2
1	A	396	GLU	O-C-N	-8.37	112.32	121.53	5	3
2	C	221	HIS	CA-C-O	-8.37	111.54	120.42	8	2
1	A	375	LYS	O-C-N	-8.37	113.25	122.12	3	1
2	C	133	GLU	CA-C-N	8.36	131.49	120.28	13	3
2	C	133	GLU	C-N-CA	8.36	131.49	120.28	13	3
1	A	489	GLN	CA-C-N	8.36	132.17	120.29	10	1
1	A	489	GLN	C-N-CA	8.36	132.17	120.29	10	1
2	C	196	LEU	CA-C-N	8.35	131.29	120.44	9	3
2	C	196	LEU	C-N-CA	8.35	131.29	120.44	9	3
2	C	123	LEU	CA-C-O	-8.35	111.57	120.42	3	2
1	A	403	ILE	O-C-N	-8.35	113.71	121.89	5	1
2	C	146	ALA	CA-C-N	8.35	131.46	120.28	7	2
2	C	146	ALA	C-N-CA	8.35	131.46	120.28	7	2
2	C	120	GLU	O-C-N	-8.34	112.75	120.51	11	3
1	A	459	ILE	CA-C-O	-8.34	111.81	119.82	13	4
2	B	139	GLN	CA-C-N	8.33	132.12	120.29	6	2
2	B	139	GLN	C-N-CA	8.33	132.12	120.29	6	2
1	A	510	SER	CB-CA-C	8.33	122.95	111.63	12	2
1	A	486	PHE	O-C-N	-8.32	113.61	123.27	15	1
2	C	167	GLY	CA-C-O	-8.32	112.18	120.75	15	2
1	A	330	ARG	NE-CZ-NH2	8.32	126.69	119.20	9	8
2	C	100	TYR	N-CA-C	8.31	120.34	111.28	6	2
2	B	123	LEU	CA-C-N	8.31	131.42	120.28	6	2
2	B	123	LEU	C-N-CA	8.31	131.42	120.28	6	2
2	B	227	GLU	CA-C-O	-8.31	111.75	120.55	5	1
1	A	374	ARG	NE-CZ-NH2	8.30	126.67	119.20	9	6
1	A	493	VAL	O-C-N	-8.30	114.74	122.79	6	3
2	B	129	LYS	N-CA-C	8.29	120.31	111.28	5	3
2	B	214	TYR	CA-C-N	8.29	131.21	120.44	2	3
2	B	214	TYR	C-N-CA	8.29	131.21	120.44	2	3
1	A	403	ILE	CB-CA-C	8.28	123.32	112.14	4	3
2	C	179	ASP	O-C-N	-8.28	113.34	122.12	10	6
2	C	89	ASP	CA-C-N	8.28	131.70	120.44	14	3
2	C	89	ASP	C-N-CA	8.28	131.70	120.44	14	3
2	B	171	ARG	NE-CZ-NH2	8.28	126.65	119.20	12	7
2	C	230	LYS	N-CA-C	8.28	124.01	113.25	12	5
2	C	201	GLU	N-CA-C	8.27	121.03	111.11	1	4
2	B	67	VAL	CB-CA-C	8.27	122.56	111.97	14	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	492	LYS	CA-C-N	8.27	131.58	120.50	1	5
1	A	492	LYS	C-N-CA	8.27	131.58	120.50	1	5
2	B	215	HIS	CE1-NE2-CD2	-8.26	100.74	109.00	3	4
2	B	193	ARG	NE-CZ-NH1	-8.26	113.25	121.50	1	4
2	B	203	LEU	O-C-N	-8.25	113.37	122.12	14	3
2	B	223	SER	N-CA-C	8.25	120.27	111.28	9	2
2	B	57	PHE	N-CA-C	8.25	120.27	111.28	8	4
2	B	140	LYS	CA-C-N	8.24	131.24	120.60	9	5
2	B	140	LYS	C-N-CA	8.24	131.24	120.60	9	5
2	C	234	GLU	CA-C-N	8.24	131.65	120.44	5	4
2	C	234	GLU	C-N-CA	8.24	131.65	120.44	5	4
2	C	184	HIS	CA-C-O	8.24	129.28	120.55	11	1
2	B	102	ASP	CA-C-N	8.24	131.32	120.28	4	1
2	B	102	ASP	C-N-CA	8.24	131.32	120.28	4	1
2	B	97	VAL	N-CA-C	8.23	119.03	110.72	10	4
2	C	261	LYS	N-CA-C	8.23	120.25	111.28	7	3
2	C	101	LEU	N-CA-C	8.23	120.25	111.28	8	1
2	B	83	ARG	N-CA-C	8.23	121.28	111.33	15	4
1	A	462	SER	CA-C-N	8.22	128.29	119.90	6	4
1	A	462	SER	C-N-CA	8.22	128.29	119.90	6	4
2	C	193	ARG	NH1-CZ-NH2	-8.21	108.62	119.30	4	1
1	A	326	VAL	O-C-N	-8.20	113.51	123.10	11	2
2	B	191	GLU	CA-C-O	8.20	129.11	120.42	8	3
2	C	93	VAL	N-CA-C	8.20	118.29	110.42	6	4
2	C	257	GLU	N-CA-C	8.20	119.84	111.07	5	3
2	C	83	ARG	NH1-CZ-NH2	-8.20	108.65	119.30	12	3
2	B	135	GLU	N-CA-C	8.19	121.24	111.33	2	2
2	C	88	LYS	CA-C-N	8.18	131.25	120.28	3	4
2	C	88	LYS	C-N-CA	8.18	131.25	120.28	3	4
2	B	238	GLN	N-CA-C	8.18	122.22	111.75	14	1
2	B	170	MET	O-C-N	-8.18	112.22	122.27	10	2
1	A	405	GLU	CA-C-O	8.17	129.43	119.38	8	2
2	C	56	THR	CA-C-O	-8.17	112.24	120.82	13	1
1	A	487	ASN	OD1-CG-ND2	-8.17	114.43	122.60	1	2
2	B	241	LEU	N-CA-C	8.17	124.80	113.45	1	4
2	B	71	PHE	CA-C-N	8.16	131.22	120.28	11	4
2	B	71	PHE	C-N-CA	8.16	131.22	120.28	11	4
1	A	477	PHE	CA-CB-CG	-8.16	105.64	113.80	15	3
1	A	350	MET	N-CA-C	8.16	120.85	110.24	4	3
2	B	89	ASP	N-CA-C	8.15	120.16	111.28	12	2
2	B	166	LEU	N-CA-C	-8.15	102.48	111.36	14	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	401	LYS	CA-C-O	8.14	129.36	120.32	3	2
2	B	198	ALA	CA-C-N	8.14	131.19	120.28	15	2
2	B	198	ALA	C-N-CA	8.14	131.19	120.28	15	2
2	B	120	GLU	CA-C-O	-8.14	111.14	118.63	8	3
1	A	402	HIS	CA-C-N	8.14	132.00	120.53	13	5
1	A	402	HIS	C-N-CA	8.14	132.00	120.53	13	5
2	B	112	MET	N-CA-C	8.14	121.07	111.71	14	4
2	C	103	ASP	CA-C-O	8.13	128.00	119.05	2	1
2	B	194	GLN	N-CA-C	8.13	119.92	111.14	2	4
2	C	79	THR	CA-C-N	8.12	131.00	120.44	12	7
2	C	79	THR	C-N-CA	8.12	131.00	120.44	12	7
2	B	189	SER	N-CA-C	8.12	120.13	111.28	14	2
2	C	147	GLU	N-CA-C	8.11	120.12	111.28	3	1
2	B	68	THR	N-CA-C	8.11	120.19	111.36	8	5
2	B	101	LEU	CA-C-N	8.11	131.49	120.38	3	5
2	B	101	LEU	C-N-CA	8.11	131.49	120.38	3	5
2	C	227	GLU	CA-C-N	8.11	131.14	120.28	12	4
2	C	227	GLU	C-N-CA	8.11	131.14	120.28	12	4
2	B	71	PHE	CB-CA-C	8.10	123.77	110.81	2	1
1	A	393	ALA	N-CA-CB	-8.10	99.03	111.66	5	1
2	C	184	HIS	CA-CB-CG	8.10	121.89	113.80	12	2
2	C	161	GLU	CA-C-O	-8.10	112.32	120.82	14	2
2	C	57	PHE	N-CA-C	8.09	120.10	111.28	10	2
2	C	64	LEU	O-C-N	-8.08	112.89	122.27	3	1
2	C	198	ALA	CA-C-N	8.08	131.76	120.29	4	5
2	C	198	ALA	C-N-CA	8.08	131.76	120.29	4	5
2	C	123	LEU	CA-C-N	8.08	131.10	120.28	9	3
2	C	123	LEU	C-N-CA	8.08	131.10	120.28	9	3
1	A	347	ASN	N-CA-CB	8.08	124.14	110.49	14	1
2	C	174	ALA	N-CA-C	8.07	119.71	111.07	15	3
2	C	203	LEU	N-CA-C	8.07	120.08	111.28	12	2
1	A	317	ASN	OD1-CG-ND2	-8.07	114.53	122.60	8	1
2	C	98	GLN	N-CA-C	8.06	123.72	112.75	3	7
2	B	187	PRO	CA-C-N	8.06	131.09	120.28	6	3
2	B	187	PRO	C-N-CA	8.06	131.09	120.28	6	3
2	C	74	ASN	CA-C-N	8.06	131.41	120.44	7	5
2	C	74	ASN	C-N-CA	8.06	131.41	120.44	7	5
2	B	221	HIS	N-CA-C	8.06	120.07	111.28	13	1
1	A	357	ILE	CA-C-N	8.06	130.21	120.14	15	2
1	A	357	ILE	C-N-CA	8.06	130.21	120.14	15	2
2	C	221	HIS	CA-CB-CG	-8.04	105.76	113.80	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	216	ALA	N-CA-C	8.04	119.67	111.07	12	4
2	B	237	ARG	NE-CZ-NH1	-8.04	113.47	121.50	6	4
2	B	261	LYS	CA-C-O	8.04	129.26	119.38	4	2
1	A	473	VAL	CA-C-N	8.03	135.15	122.62	2	1
1	A	473	VAL	C-N-CA	8.03	135.15	122.62	2	1
2	C	142	GLU	N-CA-C	8.03	124.61	113.45	1	4
2	C	220	GLU	CA-C-N	8.02	131.37	120.54	15	2
2	C	220	GLU	C-N-CA	8.02	131.37	120.54	15	2
2	B	181	LEU	N-CA-C	8.02	119.81	111.14	14	3
2	C	248	LYS	N-CA-C	8.02	119.65	111.07	1	6
2	B	261	LYS	N-CA-C	8.02	119.65	111.07	12	2
1	A	414	LYS	CA-CB-CG	8.02	130.13	114.10	11	1
1	A	437	ARG	NE-CZ-NH1	8.01	129.51	121.50	2	4
2	C	138	ARG	CA-C-O	8.01	129.04	120.55	14	2
1	A	440	GLU	N-CA-C	8.00	120.08	111.36	10	2
2	C	109	GLN	OE1-CD-NE2	-7.99	114.61	122.60	7	1
2	B	170	MET	N-CA-C	7.99	119.62	111.07	13	2
1	A	463	PRO	CA-C-N	7.99	134.67	122.37	12	1
1	A	463	PRO	C-N-CA	7.99	134.67	122.37	12	1
2	C	138	ARG	NE-CZ-NH1	-7.98	113.52	121.50	1	4
1	A	318	ILE	CA-C-N	7.98	131.77	120.28	8	2
1	A	318	ILE	C-N-CA	7.98	131.77	120.28	8	2
1	A	319	CYS	CA-C-O	7.98	129.12	120.10	10	1
2	B	199	ARG	N-CA-C	7.98	119.75	111.14	14	4
2	C	252	LEU	CA-C-N	7.98	131.62	120.29	13	1
2	C	252	LEU	C-N-CA	7.98	131.62	120.29	13	1
2	B	160	GLN	OE1-CD-NE2	-7.97	114.63	122.60	7	2
2	C	195	ARG	N-CA-C	7.97	119.96	111.28	11	5
2	B	218	ALA	CA-C-N	7.97	130.80	120.44	13	3
2	B	218	ALA	C-N-CA	7.97	130.80	120.44	13	3
2	C	183	THR	CA-C-N	7.97	130.96	120.28	15	1
2	C	183	THR	C-N-CA	7.97	130.96	120.28	15	1
2	B	134	MET	N-CA-C	7.96	119.96	111.28	14	3
2	B	140	LYS	CA-C-O	-7.96	112.32	121.07	4	2
1	A	446	ASP	O-C-N	-7.95	113.30	122.68	12	2
2	C	110	GLU	O-C-N	-7.95	113.89	122.07	14	1
2	B	153	ARG	NE-CZ-NH1	-7.94	113.56	121.50	11	7
2	C	140	LYS	N-CA-C	7.94	120.01	111.36	12	3
2	B	214	TYR	CB-CG-CD1	7.94	132.71	120.80	11	2
2	B	118	LYS	N-CA-C	7.94	119.56	111.07	3	5
1	A	341	PHE	CA-C-N	7.93	135.06	122.21	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	341	PHE	C-N-CA	7.93	135.06	122.21	6	1
1	A	488	ASN	N-CA-C	7.93	121.02	111.82	6	3
2	B	184	HIS	CA-CB-CG	7.92	121.72	113.80	7	4
1	A	394	SER	CA-C-O	7.92	129.03	120.32	10	1
2	B	206	ASN	O-C-N	7.92	130.22	122.07	15	2
2	C	153	ARG	O-C-N	-7.92	113.73	122.12	12	2
2	C	140	LYS	CA-C-N	7.91	130.53	120.56	8	2
2	C	140	LYS	C-N-CA	7.91	130.53	120.56	8	2
1	A	399	TYR	CA-C-O	-7.91	112.09	120.87	13	3
2	B	177	HIS	ND1-CE1-NE2	7.90	116.30	108.40	5	5
2	C	179	ASP	CA-C-N	7.90	131.51	120.29	10	3
2	C	179	ASP	C-N-CA	7.90	131.51	120.29	10	3
2	C	205	GLU	N-CA-C	7.90	119.53	111.07	14	6
2	C	177	HIS	CG-CD2-NE2	7.90	115.10	107.20	15	2
2	B	126	PHE	CA-CB-CG	7.90	121.70	113.80	10	1
1	A	468	MET	O-C-N	-7.90	113.80	123.04	2	1
2	C	127	GLN	N-CA-C	7.89	119.88	111.28	3	4
2	B	228	LYS	N-CA-C	7.89	119.96	111.36	4	4
1	A	459	ILE	CA-C-N	7.89	127.65	119.76	6	3
1	A	459	ILE	C-N-CA	7.89	127.65	119.76	6	3
2	C	233	LEU	N-CA-C	7.89	119.66	111.14	14	4
2	B	96	LYS	N-CA-C	7.89	120.58	111.11	5	3
2	B	87	SER	N-CA-C	7.88	120.78	111.71	8	3
2	C	186	ALA	O-C-N	-7.88	112.90	120.70	14	7
2	C	152	ALA	N-CA-C	7.88	119.87	111.28	5	4
2	C	106	LYS	CA-C-O	7.88	128.90	120.55	7	1
2	B	184	HIS	CA-C-N	7.86	130.82	120.28	6	2
2	B	184	HIS	C-N-CA	7.86	130.82	120.28	6	2
2	B	108	TRP	N-CA-C	7.86	120.54	111.11	1	3
1	A	321	GLY	N-CA-C	7.85	125.05	111.78	4	1
2	B	172	ASP	CA-CB-CG	-7.85	104.75	112.60	8	2
1	A	494	GLU	N-CA-C	7.85	118.63	109.60	9	4
2	C	59	LYS	CA-C-N	7.84	130.79	120.28	6	3
2	C	59	LYS	C-N-CA	7.84	130.79	120.28	6	3
1	A	412	THR	N-CA-C	7.84	119.46	111.07	12	6
2	B	248	LYS	O-C-N	-7.84	113.81	122.12	1	4
2	B	136	LEU	CA-C-N	7.84	130.79	120.28	2	2
2	B	136	LEU	C-N-CA	7.84	130.79	120.28	2	2
1	A	351	ASP	CA-C-O	7.83	130.10	121.56	7	2
2	B	114	LEU	CA-C-N	7.83	130.62	120.44	9	3
2	B	114	LEU	C-N-CA	7.83	130.62	120.44	9	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	180	ALA	CA-C-N	7.83	130.62	120.44	9	3
2	C	180	ALA	C-N-CA	7.83	130.62	120.44	9	3
2	C	134	MET	O-C-N	-7.83	113.22	122.15	9	1
2	C	67	VAL	N-CA-C	7.83	118.60	110.62	14	2
2	B	116	ARG	CA-C-N	7.82	131.54	120.28	9	2
2	B	116	ARG	C-N-CA	7.82	131.54	120.28	9	2
1	A	433	ASN	CB-CA-C	7.81	124.54	110.72	11	2
2	C	131	GLN	CA-C-N	7.80	130.59	120.44	1	4
2	C	131	GLN	C-N-CA	7.80	130.59	120.44	1	4
2	C	145	ARG	NE-CZ-NH1	-7.80	113.70	121.50	2	5
1	A	431	ARG	NE-CZ-NH1	-7.79	113.70	121.50	5	3
2	B	69	GLN	OE1-CD-NE2	-7.79	114.81	122.60	5	1
2	C	195	ARG	CA-C-O	-7.79	112.29	120.55	4	1
2	C	95	ALA	N-CA-C	7.79	120.85	111.82	5	3
2	B	74	ASN	CA-C-O	-7.78	112.65	120.82	6	3
2	C	107	LYS	N-CA-C	7.78	119.39	111.07	9	2
2	B	164	SER	CA-C-O	-7.78	110.80	118.34	9	5
2	C	222	LEU	CA-C-O	7.78	128.99	120.82	7	3
2	B	70	GLU	CB-CG-CD	7.77	125.81	112.60	7	2
1	A	500	SER	CA-C-N	7.77	131.32	120.29	15	3
1	A	500	SER	C-N-CA	7.77	131.32	120.29	15	3
2	B	215	HIS	CG-CD2-NE2	7.77	114.97	107.20	2	3
2	C	104	PHE	N-CA-C	7.77	120.43	111.11	11	4
1	A	442	LEU	CA-C-O	7.77	128.00	119.15	5	2
1	A	443	ARG	NE-CZ-NH2	7.76	126.19	119.20	14	7
2	B	103	ASP	N-CA-C	7.76	119.74	111.28	11	3
2	B	251	PHE	N-CA-C	7.76	119.37	111.07	9	4
2	B	182	ARG	N-CA-C	7.75	119.81	111.36	8	3
1	A	347	ASN	CA-CB-CG	-7.75	104.85	112.60	11	3
2	C	168	GLU	N-CA-C	7.75	119.81	111.36	13	3
1	A	470	SER	CA-C-O	7.75	129.00	120.63	11	1
1	A	381	PHE	CA-C-O	7.74	129.06	120.70	15	2
2	C	195	ARG	NE-CZ-NH1	-7.74	113.76	121.50	9	5
2	C	126	PHE	CA-C-N	7.74	130.50	120.44	2	6
2	C	126	PHE	C-N-CA	7.74	130.50	120.44	2	6
2	C	125	ASP	N-CA-CB	-7.74	98.71	110.16	5	2
2	B	66	PRO	N-CA-CB	7.73	111.37	103.25	9	1
2	B	197	ALA	N-CA-C	7.73	120.60	111.71	10	1
1	A	508	CYS	CA-C-N	7.73	127.74	119.78	10	2
1	A	508	CYS	C-N-CA	7.73	127.74	119.78	10	2
2	B	125	ASP	CA-C-N	7.73	130.63	120.28	2	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	125	ASP	C-N-CA	7.73	130.63	120.28	2	2
1	A	424	ASN	O-C-N	-7.73	113.89	121.85	8	3
1	A	416	ASP	CB-CA-C	-7.72	98.70	110.90	4	1
1	A	438	PHE	CA-C-O	7.72	128.84	120.43	9	2
2	C	228	LYS	CA-C-N	7.72	131.39	120.28	4	1
2	C	228	LYS	C-N-CA	7.72	131.39	120.28	4	1
2	C	61	ARG	N-CA-C	7.71	119.68	111.28	12	3
2	B	185	LEU	N-CA-CB	-7.71	98.36	110.46	12	1
2	B	245	GLU	N-CA-C	7.71	119.32	111.07	2	3
2	B	172	ASP	CA-C-O	7.71	128.88	119.79	10	4
2	C	199	ARG	NE-CZ-NH1	-7.70	113.80	121.50	1	5
2	B	230	LYS	O-C-N	-7.69	114.31	120.38	14	2
2	B	250	SER	CA-C-O	7.69	128.57	120.42	9	1
2	B	154	GLN	OE1-CD-NE2	-7.68	114.92	122.60	7	1
2	B	98	GLN	O-C-N	-7.68	113.49	120.71	15	3
2	B	69	GLN	CA-C-N	7.68	130.57	120.28	6	2
2	B	69	GLN	C-N-CA	7.68	130.57	120.28	6	2
2	C	152	ALA	O-C-N	-7.67	113.99	122.12	2	1
2	B	234	GLU	CA-C-O	7.67	128.68	120.55	8	2
2	B	143	PRO	CA-C-N	7.67	130.41	120.44	12	3
2	B	143	PRO	C-N-CA	7.67	130.41	120.44	12	3
2	B	160	GLN	N-CA-C	7.67	119.28	111.07	4	1
2	C	182	ARG	N-CA-C	7.67	119.28	111.07	5	6
2	C	245	GLU	CA-C-N	7.67	130.41	120.44	2	1
2	C	245	GLU	C-N-CA	7.67	130.41	120.44	2	1
2	B	72	TRP	N-CA-C	7.66	119.63	111.28	12	3
2	C	81	GLY	O-C-N	7.66	129.53	122.18	9	1
2	C	139	GLN	N-CA-C	7.66	120.70	111.82	13	3
2	B	108	TRP	CB-CG-CD2	7.66	137.52	126.80	14	2
2	C	75	LEU	CA-C-N	7.66	130.87	120.38	2	3
2	C	75	LEU	C-N-CA	7.66	130.87	120.38	2	3
2	C	225	LEU	N-CA-C	7.66	119.62	111.28	14	1
2	C	237	ARG	NH1-CZ-NH2	-7.65	109.35	119.30	8	4
2	C	193	ARG	N-CA-C	-7.65	103.02	111.36	14	5
1	A	401	LYS	O-C-N	-7.64	114.37	123.31	3	3
2	C	263	ASN	OD1-CG-ND2	-7.64	114.96	122.60	5	1
2	C	260	LYS	CA-C-N	7.64	130.51	120.28	1	3
2	C	260	LYS	C-N-CA	7.64	130.51	120.28	1	3
2	B	137	TYR	CA-C-N	7.64	130.37	120.44	11	2
2	B	137	TYR	C-N-CA	7.64	130.37	120.44	11	2
2	C	231	PRO	CA-C-N	7.64	130.51	120.28	14	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	231	PRO	C-N-CA	7.64	130.51	120.28	14	2
2	B	199	ARG	NH1-CZ-NH2	-7.63	109.38	119.30	10	1
2	B	241	LEU	O-C-N	-7.63	112.54	121.32	6	1
2	C	212	ALA	N-CA-C	7.63	119.59	111.28	12	3
1	A	449	TYR	CA-C-O	-7.63	113.09	120.64	6	2
2	C	196	LEU	N-CA-C	7.63	119.23	111.07	14	3
2	B	154	GLN	CA-C-O	7.63	128.63	120.55	10	1
2	B	219	THR	CA-C-O	7.61	128.81	120.82	4	1
1	A	435	TYR	CB-CA-C	7.61	122.98	110.74	8	2
1	A	427	THR	CA-C-N	7.61	132.57	122.30	12	2
1	A	427	THR	C-N-CA	7.61	132.57	122.30	12	2
2	C	223	SER	CA-C-N	7.59	131.34	120.79	7	4
2	C	223	SER	C-N-CA	7.59	131.34	120.79	7	4
2	B	210	ARG	N-CA-C	7.59	120.51	111.33	9	3
2	B	238	GLN	N-CA-CB	7.58	121.27	110.12	6	1
2	C	71	PHE	O-C-N	7.58	129.97	122.09	4	1
2	B	185	LEU	N-CA-C	7.58	119.18	111.07	14	1
1	A	323	PHE	CA-C-N	7.57	130.28	120.44	15	3
1	A	323	PHE	C-N-CA	7.57	130.28	120.44	15	3
2	B	98	GLN	CG-CD-NE2	7.57	127.75	116.40	8	1
1	A	404	LYS	CA-C-O	7.56	128.88	119.05	9	4
2	C	213	GLU	CA-C-N	7.56	130.27	120.44	7	3
2	C	213	GLU	C-N-CA	7.56	130.27	120.44	7	3
2	B	130	TRP	CB-CG-CD2	7.56	137.38	126.80	15	4
2	B	80	GLU	CA-C-O	7.56	128.66	119.97	8	2
2	B	125	ASP	CB-CA-C	-7.56	98.01	110.85	14	1
2	B	259	THR	N-CA-C	7.55	119.51	111.28	7	2
2	B	154	GLN	CA-C-N	7.54	130.38	120.28	13	2
2	B	154	GLN	C-N-CA	7.54	130.38	120.28	13	2
2	C	227	GLU	O-C-N	7.54	130.11	122.12	2	1
2	C	75	LEU	N-CA-C	7.53	120.15	111.11	10	2
2	B	74	ASN	N-CA-C	7.52	119.56	111.36	8	2
2	C	203	LEU	CA-C-N	7.52	130.58	120.65	15	4
2	C	203	LEU	C-N-CA	7.52	130.58	120.65	15	4
2	B	146	ALA	N-CA-C	7.52	119.48	111.28	7	4
2	B	183	THR	CA-C-N	7.52	130.35	120.28	11	1
2	B	183	THR	C-N-CA	7.52	130.35	120.28	11	1
1	A	334	PHE	CA-CB-CG	7.51	121.31	113.80	8	2
2	B	86	MET	N-CA-C	7.51	122.27	113.18	1	3
1	A	483	TYR	CA-C-O	7.51	130.23	121.44	13	3
2	B	249	VAL	O-C-N	-7.51	114.55	121.91	12	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	165	PRO	N-CA-CB	7.51	111.13	103.25	1	3
2	C	130	TRP	N-CA-C	7.51	120.18	111.02	10	2
2	C	60	LEU	CA-C-N	7.51	130.34	120.28	10	2
2	C	60	LEU	C-N-CA	7.51	130.34	120.28	10	2
2	B	58	SER	O-C-N	-7.50	114.17	122.12	12	2
2	C	84	GLN	OE1-CD-NE2	-7.50	115.10	122.60	4	2
2	B	171	ARG	NE-CZ-NH1	-7.50	114.00	121.50	8	2
2	C	105	GLN	N-CA-C	-7.50	104.26	113.41	15	1
1	A	325	THR	O-C-N	-7.50	114.64	123.41	10	2
2	C	88	LYS	O-C-N	-7.49	114.35	122.07	4	1
2	B	249	VAL	N-CA-C	7.49	118.26	110.62	5	3
2	C	194	GLN	O-C-N	-7.49	114.18	122.12	5	2
1	A	440	GLU	CA-C-N	7.49	130.31	120.28	9	4
1	A	440	GLU	C-N-CA	7.49	130.31	120.28	9	4
2	B	109	GLN	N-CA-C	7.49	120.39	111.33	6	2
2	C	164	SER	CA-C-O	-7.48	111.61	118.79	1	4
2	C	74	ASN	N-CA-C	7.48	119.07	111.07	12	4
2	B	63	GLN	N-CA-CB	-7.48	99.09	110.16	5	1
1	A	424	ASN	CA-C-O	7.47	128.30	119.48	13	3
2	C	71	PHE	N-CA-C	7.47	119.07	111.07	9	1
2	B	227	GLU	N-CA-C	7.47	119.42	111.28	10	4
2	C	241	LEU	CA-C-N	7.47	129.18	119.84	4	1
2	C	241	LEU	C-N-CA	7.47	129.18	119.84	4	1
2	B	128	LYS	N-CA-CB	-7.47	99.13	110.12	7	1
2	C	175	ARG	O-C-N	-7.47	114.20	122.12	14	2
1	A	413	ASP	O-C-N	-7.46	112.66	122.59	11	2
2	B	58	SER	N-CA-C	7.46	119.49	111.36	11	5
2	B	133	GLU	CA-C-O	7.45	128.54	119.97	6	1
1	A	493	VAL	CA-C-O	7.45	129.55	121.36	14	3
2	C	210	ARG	CA-C-O	-7.45	112.58	120.92	1	4
2	B	150	GLU	N-CA-C	7.44	119.39	111.28	8	2
2	B	244	LEU	O-C-N	7.44	129.73	122.07	1	2
2	B	181	LEU	CA-C-N	7.44	130.47	120.65	4	4
2	B	181	LEU	C-N-CA	7.44	130.47	120.65	4	4
2	B	85	GLU	CA-C-O	7.43	128.27	119.28	8	2
2	B	184	HIS	ND1-CE1-NE2	7.43	115.83	108.40	3	5
1	A	506	MET	N-CA-C	7.41	122.35	113.16	4	1
2	C	111	GLU	N-CA-C	7.41	120.23	111.71	4	3
1	A	450	PRO	N-CA-C	7.41	131.36	112.10	6	2
2	B	217	LYS	N-CA-C	7.41	119.35	111.28	15	3
2	C	193	ARG	CA-C-N	7.41	130.07	120.44	11	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	193	ARG	C-N-CA	7.41	130.07	120.44	11	2
2	C	264	THR	N-CA-CB	7.40	121.02	109.69	13	2
1	A	340	TRP	CA-C-O	7.40	129.80	121.51	10	1
1	A	502	LEU	N-CA-C	7.40	119.34	111.28	12	5
2	C	258	TYR	N-CA-CB	-7.40	99.25	110.12	2	1
2	B	199	ARG	CA-C-N	7.39	130.19	120.28	15	2
2	B	199	ARG	C-N-CA	7.39	130.19	120.28	15	2
2	C	94	LYS	CA-C-N	7.39	130.05	120.44	14	3
2	C	94	LYS	C-N-CA	7.39	130.05	120.44	14	3
1	A	357	ILE	CA-C-O	-7.39	113.36	121.05	11	2
2	B	264	THR	N-CA-C	7.39	120.94	110.23	8	4
2	B	94	LYS	O-C-N	-7.39	113.73	122.15	8	3
1	A	430	PHE	CA-CB-CG	-7.39	106.41	113.80	8	4
1	A	421	TRP	CB-CG-CD2	7.39	137.14	126.80	2	1
2	C	162	LYS	CA-C-N	7.39	130.18	120.28	4	7
2	C	162	LYS	C-N-CA	7.39	130.18	120.28	4	7
2	B	63	GLN	CA-C-N	7.39	130.18	120.28	10	1
2	B	63	GLN	C-N-CA	7.39	130.18	120.28	10	1
1	A	404	LYS	O-C-N	-7.38	113.79	122.20	2	3
2	B	86	MET	CA-C-N	7.37	131.03	120.79	14	2
2	B	86	MET	C-N-CA	7.37	131.03	120.79	14	2
2	B	202	ALA	N-CA-C	7.36	119.31	111.28	13	4
2	C	137	TYR	CA-C-N	7.36	130.15	120.28	15	3
2	C	137	TYR	C-N-CA	7.36	130.15	120.28	15	3
1	A	455	VAL	CA-CB-CG2	7.36	122.91	110.40	12	1
2	C	182	ARG	O-C-N	-7.36	114.44	122.09	10	1
2	B	106	LYS	N-CA-C	7.35	119.29	111.28	3	1
1	A	344	VAL	O-C-N	-7.35	115.26	123.20	8	2
2	B	76	GLU	CA-C-N	7.35	130.13	120.28	15	1
2	B	76	GLU	C-N-CA	7.35	130.13	120.28	15	1
2	B	200	LEU	N-CA-C	7.34	118.93	111.07	14	2
2	B	259	THR	O-C-N	-7.34	113.78	122.15	3	3
2	C	187	PRO	CA-C-N	7.34	129.98	120.44	15	6
2	C	187	PRO	C-N-CA	7.34	129.98	120.44	15	6
1	A	360	PHE	CA-CB-CG	-7.34	106.46	113.80	9	2
2	B	128	LYS	N-CA-C	7.34	118.92	111.07	8	3
1	A	417	ALA	O-C-N	-7.33	115.45	123.52	10	3
2	B	253	SER	N-CA-C	-7.33	103.23	111.07	15	2
2	C	110	GLU	N-CA-C	7.33	118.91	111.07	4	3
1	A	463	PRO	N-CA-CB	7.32	110.94	103.25	4	2
2	C	130	TRP	CA-C-N	7.32	130.09	120.28	1	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	130	TRP	C-N-CA	7.32	130.09	120.28	1	2
2	C	154	GLN	CA-C-O	-7.32	113.13	120.82	8	1
2	B	145	ARG	CA-C-N	7.31	130.40	120.38	3	2
2	B	145	ARG	C-N-CA	7.31	130.40	120.38	3	2
2	C	113	GLU	N-CA-C	7.31	119.25	111.28	3	3
1	A	429	PHE	CA-CB-CG	-7.31	106.49	113.80	10	2
2	C	225	LEU	CA-C-N	7.31	130.29	120.65	5	1
2	C	225	LEU	C-N-CA	7.31	130.29	120.65	5	1
2	C	59	LYS	N-CA-C	7.30	120.29	111.82	4	6
2	C	128	LYS	N-CA-CB	7.30	120.85	110.12	13	1
2	C	207	GLY	CA-C-N	7.30	128.24	119.99	6	3
2	C	207	GLY	C-N-CA	7.30	128.24	119.99	6	3
2	C	93	VAL	CA-C-N	7.29	130.05	120.28	15	2
2	C	93	VAL	C-N-CA	7.29	130.05	120.28	15	2
1	A	325	THR	CA-C-O	-7.29	112.58	120.75	2	2
2	B	223	SER	CA-C-N	7.29	129.92	120.44	5	5
2	B	223	SER	C-N-CA	7.29	129.92	120.44	5	5
2	B	90	LEU	CA-C-O	-7.29	112.83	120.55	1	1
2	B	226	SER	O-C-N	-7.28	114.57	122.07	14	3
1	A	336	PHE	N-CA-C	7.28	120.79	109.07	9	2
2	B	132	GLU	CA-C-N	7.28	130.03	120.28	12	2
2	B	132	GLU	C-N-CA	7.28	130.03	120.28	12	2
2	C	201	GLU	O-C-N	7.28	129.83	122.12	9	2
2	C	55	SER	CA-C-N	7.27	130.03	120.28	14	2
2	C	55	SER	C-N-CA	7.27	130.03	120.28	14	2
2	B	168	GLU	N-CA-C	7.27	119.21	111.28	2	3
1	A	457	GLU	O-C-N	-7.27	114.64	123.30	4	3
1	A	446	ASP	N-CA-C	7.27	119.71	110.33	12	4
1	A	442	LEU	CB-CA-C	-7.27	97.95	110.09	8	1
2	C	178	VAL	CA-C-N	7.26	129.88	120.44	13	3
2	C	178	VAL	C-N-CA	7.26	129.88	120.44	13	3
2	B	90	LEU	CA-C-N	7.26	129.88	120.44	4	3
2	B	90	LEU	C-N-CA	7.26	129.88	120.44	4	3
2	B	263	ASN	CA-CB-CG	-7.26	105.34	112.60	11	3
2	B	59	LYS	CA-C-N	7.26	129.88	120.44	13	3
2	B	59	LYS	C-N-CA	7.26	129.88	120.44	13	3
2	B	79	THR	N-CA-C	7.26	120.11	111.33	2	3
1	A	491	LEU	O-C-N	-7.26	114.47	122.67	4	1
2	C	175	ARG	NE-CZ-NH1	-7.25	114.25	121.50	5	5
1	A	389	VAL	CA-C-N	7.25	132.83	122.09	14	2
1	A	389	VAL	C-N-CA	7.25	132.83	122.09	14	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	170	MET	O-C-N	7.25	130.42	122.15	4	2
1	A	409	GLY	CA-C-O	7.25	127.06	119.01	5	1
2	B	244	LEU	N-CA-CB	7.25	120.53	110.01	8	1
2	B	113	GLU	N-CA-C	7.25	119.19	111.28	2	2
2	B	83	ARG	NE-CZ-NH1	-7.25	114.25	121.50	10	3
1	A	324	ASP	CA-CB-CG	-7.25	105.35	112.60	3	3
2	B	145	ARG	CA-C-O	7.24	127.41	119.15	12	2
2	C	215	HIS	CE1-NE2-CD2	-7.24	101.76	109.00	10	5
2	B	62	GLU	CA-C-N	7.24	129.98	120.28	15	4
2	B	62	GLU	C-N-CA	7.24	129.98	120.28	15	4
2	B	67	VAL	CA-C-N	7.24	130.30	120.38	14	1
2	B	67	VAL	C-N-CA	7.24	130.30	120.38	14	1
2	C	116	ARG	N-CA-C	7.24	119.17	111.28	2	2
2	C	250	SER	CA-C-O	-7.24	112.21	120.24	2	3
2	C	116	ARG	NE-CZ-NH1	-7.23	114.27	121.50	11	4
2	C	223	SER	N-CA-C	7.23	119.17	111.28	9	1
1	A	488	ASN	OD1-CG-ND2	-7.23	115.37	122.60	15	3
2	B	77	LYS	N-CA-C	7.23	119.16	111.28	9	1
2	B	85	GLU	N-CA-C	7.23	118.81	111.07	1	1
2	B	118	LYS	CA-C-N	7.23	130.36	120.46	9	2
2	B	118	LYS	C-N-CA	7.23	130.36	120.46	9	2
2	C	176	ALA	N-CA-C	7.23	119.16	111.28	9	2
2	C	130	TRP	CB-CG-CD2	7.23	136.92	126.80	4	2
2	B	138	ARG	N-CA-C	7.22	118.80	111.07	10	2
2	B	156	LEU	N-CA-C	7.22	119.15	111.28	3	3
1	A	426	LYS	CA-C-O	7.22	128.70	120.54	1	2
2	B	91	GLU	O-C-N	-7.22	113.92	122.15	14	2
2	B	59	LYS	N-CA-C	7.21	119.22	111.36	1	2
2	B	261	LYS	O-C-N	-7.21	113.98	122.20	6	1
2	C	85	GLU	N-CA-C	7.21	119.14	111.28	1	3
2	C	209	ALA	CA-C-N	7.21	129.94	120.28	12	3
2	C	209	ALA	C-N-CA	7.21	129.94	120.28	12	3
2	B	256	GLU	CA-C-O	7.21	128.39	120.82	5	2
2	C	97	VAL	O-C-N	-7.20	114.41	121.83	13	2
2	C	138	ARG	N-CA-CB	7.20	120.67	109.94	13	1
2	C	171	ARG	CA-C-N	7.20	129.80	120.44	9	2
2	C	171	ARG	C-N-CA	7.20	129.80	120.44	9	2
2	C	97	VAL	CA-C-N	7.19	130.08	120.58	7	2
2	C	97	VAL	C-N-CA	7.19	130.08	120.58	7	2
2	C	122	TYR	O-C-N	-7.19	113.95	122.15	1	1
2	C	239	GLY	O-C-N	-7.19	115.22	122.19	5	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	494	GLU	N-CA-CB	7.19	120.27	110.14	8	1
2	B	192	LEU	N-CA-C	7.18	119.73	111.11	3	1
2	B	164	SER	O-C-N	-7.18	113.88	120.92	12	4
2	C	173	ARG	NH1-CZ-NH2	7.18	128.64	119.30	10	2
2	C	109	GLN	CA-C-N	7.18	130.77	120.79	5	1
2	C	109	GLN	C-N-CA	7.18	130.77	120.79	5	1
2	C	221	HIS	ND1-CE1-NE2	7.18	115.58	108.40	13	3
2	C	185	LEU	CA-C-O	7.17	127.74	119.35	9	1
2	C	137	TYR	CA-C-O	-7.17	112.95	120.55	3	1
2	C	191	GLU	N-CA-C	7.17	118.74	111.07	10	5
1	A	383	LYS	CB-CA-C	-7.17	99.78	110.24	5	1
2	B	61	ARG	NE-CZ-NH1	7.17	128.67	121.50	11	2
2	C	109	GLN	O-C-N	-7.17	114.69	122.07	8	2
2	B	142	GLU	N-CA-C	7.16	122.49	112.75	1	3
2	C	89	ASP	N-CA-C	7.16	120.13	111.82	15	1
1	A	490	LYS	CA-C-N	7.15	132.28	122.19	14	3
1	A	490	LYS	C-N-CA	7.15	132.28	122.19	14	3
1	A	364	LEU	O-C-N	-7.15	113.42	121.36	12	2
1	A	484	TRP	CB-CG-CD2	7.15	136.81	126.80	10	5
2	C	195	ARG	CA-C-N	7.15	129.73	120.44	13	1
2	C	195	ARG	C-N-CA	7.15	129.73	120.44	13	1
2	B	138	ARG	NE-CZ-NH1	-7.15	114.35	121.50	8	3
1	A	362	ARG	NE-CZ-NH1	7.15	128.65	121.50	5	2
1	A	350	MET	CA-C-N	7.14	130.89	120.82	1	3
1	A	350	MET	C-N-CA	7.14	130.89	120.82	1	3
2	B	202	ALA	CA-C-N	7.13	129.84	120.28	5	1
2	B	202	ALA	C-N-CA	7.13	129.84	120.28	5	1
2	B	152	ALA	O-C-N	-7.13	114.73	122.07	7	1
1	A	481	ASN	O-C-N	-7.12	114.73	122.00	10	1
2	C	137	TYR	N-CA-C	-7.12	103.45	111.07	9	3
2	B	248	LYS	CA-C-O	-7.12	113.36	120.70	8	2
2	B	110	GLU	O-C-N	7.12	129.40	122.07	1	1
2	B	188	TYR	N-CA-C	7.12	119.12	111.36	7	4
2	B	229	ALA	N-CA-C	7.12	118.83	111.14	2	7
2	B	201	GLU	N-CA-C	7.12	119.04	111.28	1	3
2	B	240	LEU	N-CA-C	7.12	119.04	111.28	15	4
2	B	108	TRP	CA-C-O	-7.12	113.35	120.82	8	2
2	C	199	ARG	N-CA-C	-7.11	103.46	111.14	1	2
1	A	402	HIS	CG-CD2-NE2	7.11	114.31	107.20	3	2
1	A	410	LEU	O-C-N	-7.11	113.14	121.32	7	1
2	C	119	VAL	O-C-N	-7.11	113.87	122.12	10	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	117	GLN	N-CA-C	7.11	119.89	111.71	3	5
1	A	349	VAL	N-CA-C	7.11	119.25	109.80	14	5
2	C	170	MET	N-CA-C	7.11	119.11	111.36	6	2
1	A	382	PHE	N-CA-CB	7.10	122.61	110.68	1	3
2	C	215	HIS	N-CA-C	7.10	118.67	111.07	12	3
2	C	102	ASP	O-C-N	-7.10	113.91	122.22	4	2
1	A	456	TRP	N-CA-C	-7.10	98.36	109.72	4	1
2	B	79	THR	N-CA-CB	7.10	120.36	110.07	6	4
1	A	507	GLY	N-CA-C	7.09	124.81	114.10	14	2
2	C	249	VAL	CA-C-N	7.09	129.78	120.28	1	4
2	C	249	VAL	C-N-CA	7.09	129.78	120.28	1	4
2	B	177	HIS	N-CA-C	7.09	119.01	111.28	11	2
1	A	405	GLU	CA-C-N	7.09	129.78	120.28	7	2
1	A	405	GLU	C-N-CA	7.09	129.78	120.28	7	2
2	B	217	LYS	CB-CA-C	-7.09	99.02	110.79	9	1
2	C	221	HIS	CE1-NE2-CD2	-7.09	101.91	109.00	13	5
2	C	105	GLN	CA-C-O	7.08	126.93	119.14	1	2
2	C	134	MET	CA-C-N	7.08	129.77	120.28	4	5
2	C	134	MET	C-N-CA	7.08	129.77	120.28	4	5
1	A	441	GLU	N-CA-C	7.08	119.86	111.71	10	4
2	B	141	VAL	N-CA-C	7.08	117.87	110.72	10	4
1	A	503	ARG	N-CA-C	7.08	118.69	110.97	11	1
1	A	486	PHE	CB-CA-C	7.08	121.43	109.75	2	2
1	A	396	GLU	N-CA-C	7.08	118.62	109.64	2	1
2	C	69	GLN	N-CA-C	7.08	118.99	111.28	10	2
2	C	123	LEU	O-C-N	-7.08	114.62	122.12	7	1
1	A	491	LEU	CA-C-O	-7.07	112.86	121.28	14	2
2	C	154	GLN	OE1-CD-NE2	-7.07	115.53	122.60	8	1
1	A	487	ASN	O-C-N	-7.07	115.16	123.22	5	2
2	C	188	TYR	CA-C-N	7.07	129.75	120.28	10	2
2	C	188	TYR	C-N-CA	7.07	129.75	120.28	10	2
2	C	126	PHE	O-C-N	7.07	129.61	122.12	10	2
1	A	484	TRP	CB-CG-CD1	-7.06	116.30	126.90	10	5
2	B	254	ALA	CA-C-N	7.06	129.62	120.44	8	4
2	B	254	ALA	C-N-CA	7.06	129.62	120.44	8	4
1	A	380	VAL	O-C-N	-7.06	115.64	123.26	8	2
2	C	260	LYS	O-C-N	-7.06	114.64	122.12	8	1
2	C	247	PHE	N-CA-C	7.05	118.61	111.07	1	5
2	B	236	LEU	N-CA-C	7.05	119.62	111.02	13	1
1	A	347	ASN	N-CA-C	7.05	121.20	111.90	1	2
2	C	251	PHE	N-CA-C	-7.05	103.53	111.14	1	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	146	ALA	O-C-N	-7.04	114.65	122.12	5	1
2	C	235	ASP	N-CA-C	7.04	118.96	111.28	4	1
2	C	246	SER	CA-C-N	7.04	130.04	120.54	13	1
2	C	246	SER	C-N-CA	7.04	130.04	120.54	13	1
2	C	83	ARG	N-CA-C	7.04	118.60	111.07	1	3
2	C	70	GLU	O-C-N	7.04	129.58	122.12	10	1
2	B	207	GLY	N-CA-C	7.03	122.80	113.37	1	2
2	B	164	SER	CA-C-N	7.03	126.52	118.85	12	1
2	B	164	SER	C-N-CA	7.03	126.52	118.85	12	1
2	C	149	GLN	N-CA-C	7.03	118.94	111.28	5	3
2	C	219	THR	CA-C-N	7.03	129.70	120.28	5	3
2	C	219	THR	C-N-CA	7.03	129.70	120.28	5	3
2	B	135	GLU	CB-CA-C	7.03	122.46	110.79	6	1
2	B	253	SER	CA-C-N	7.03	129.58	120.44	14	3
2	B	253	SER	C-N-CA	7.03	129.58	120.44	14	3
1	A	339	ARG	NE-CZ-NH1	7.03	128.53	121.50	3	4
2	C	151	GLY	O-C-N	-7.03	115.45	122.19	9	2
2	C	93	VAL	CB-CA-C	7.02	120.59	111.81	12	1
2	C	98	GLN	O-C-N	-7.02	113.25	121.32	5	4
1	A	373	GLU	O-C-N	-7.02	115.06	123.13	4	2
2	C	170	MET	CA-C-O	-7.01	113.47	120.70	13	2
2	B	196	LEU	CA-C-N	7.01	129.68	120.28	5	1
2	B	196	LEU	C-N-CA	7.01	129.68	120.28	5	1
2	C	125	ASP	CA-CB-CG	7.01	119.61	112.60	8	3
2	C	78	GLU	CA-C-N	7.01	129.99	120.38	2	2
2	C	78	GLU	C-N-CA	7.01	129.99	120.38	2	2
1	A	383	LYS	CA-C-N	7.01	131.36	120.07	11	1
1	A	383	LYS	C-N-CA	7.01	131.36	120.07	11	1
1	A	477	PHE	CA-C-O	7.01	129.31	121.11	15	1
1	A	422	MET	CA-C-O	-7.01	112.18	118.63	5	3
2	B	99	PRO	N-CA-CB	7.01	111.29	103.44	9	1
2	B	222	LEU	CA-C-O	7.00	127.97	120.55	14	1
2	B	76	GLU	N-CA-CB	7.00	120.37	109.94	2	2
1	A	325	THR	CA-CB-OG1	7.00	120.10	109.60	3	2
2	C	242	PRO	CA-C-N	7.00	130.75	120.74	12	2
2	C	242	PRO	C-N-CA	7.00	130.75	120.74	12	2
2	B	83	ARG	CA-C-O	6.99	127.96	120.55	7	3
1	A	491	LEU	CB-CA-C	6.99	121.66	111.73	14	1
1	A	369	ASN	CA-C-O	6.99	127.31	119.41	13	1
2	B	243	VAL	O-C-N	6.99	128.65	121.87	5	3
2	B	154	GLN	N-CA-C	6.99	118.89	111.28	15	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	130	TRP	CB-CG-CD1	-6.98	116.42	126.90	15	3
2	B	136	LEU	N-CA-C	6.98	118.54	111.07	13	2
2	B	140	LYS	N-CA-C	6.98	118.97	111.36	9	2
2	B	264	THR	N-CA-CB	6.98	120.90	110.29	5	1
2	C	120	GLU	N-CA-C	6.98	122.98	113.77	5	4
2	B	211	LEU	CA-C-N	6.98	129.63	120.28	11	2
2	B	211	LEU	C-N-CA	6.98	129.63	120.28	11	2
2	C	120	GLU	CA-C-N	6.98	126.45	118.85	1	4
2	C	120	GLU	C-N-CA	6.98	126.45	118.85	1	4
2	C	124	ASP	CA-C-N	6.97	129.50	120.44	11	4
2	C	124	ASP	C-N-CA	6.97	129.50	120.44	11	4
2	C	124	ASP	N-CA-CB	-6.97	99.96	110.07	10	5
2	B	75	LEU	CA-C-N	6.97	129.62	120.28	10	4
2	B	75	LEU	C-N-CA	6.97	129.62	120.28	10	4
1	A	349	VAL	O-C-N	-6.97	115.24	122.63	5	1
2	B	247	PHE	CA-CB-CG	6.96	120.76	113.80	8	3
2	B	115	TYR	O-C-N	6.96	129.50	122.12	13	3
2	C	88	LYS	CA-C-O	-6.96	113.17	120.55	13	3
2	B	206	ASN	CA-CB-CG	-6.96	105.64	112.60	14	4
2	B	195	ARG	N-CA-C	6.96	119.46	111.11	8	3
1	A	436	TYR	O-C-N	-6.96	114.91	123.33	14	3
2	C	82	LEU	CA-C-O	6.96	127.93	120.55	12	1
2	C	193	ARG	N-CA-CB	6.96	120.46	110.16	14	1
2	B	250	SER	N-CA-CB	6.96	120.46	110.16	9	2
2	C	111	GLU	O-C-N	-6.96	114.75	122.12	7	3
2	C	72	TRP	O-C-N	-6.96	114.91	122.07	7	4
2	B	142	GLU	CA-C-N	6.95	126.56	119.19	13	2
2	B	142	GLU	C-N-CA	6.95	126.56	119.19	13	2
2	B	234	GLU	CA-C-N	6.95	129.59	120.28	11	2
2	B	234	GLU	C-N-CA	6.95	129.59	120.28	11	2
2	B	202	ALA	CA-C-O	6.95	127.92	120.55	13	1
1	A	426	LYS	N-CA-C	6.95	120.22	108.90	9	2
2	B	183	THR	N-CA-C	6.95	118.93	111.36	3	3
2	C	233	LEU	O-C-N	-6.95	114.76	122.12	7	1
1	A	500	SER	N-CA-C	6.95	120.72	110.30	8	2
1	A	324	ASP	CB-CA-C	-6.95	99.04	110.85	10	1
2	B	90	LEU	O-C-N	-6.95	114.76	122.12	13	1
2	C	58	SER	CA-C-N	6.94	129.91	120.54	15	2
2	C	58	SER	C-N-CA	6.94	129.91	120.54	15	2
2	B	72	TRP	CD2-CE2-CZ2	-6.94	115.46	122.40	12	1
2	B	202	ALA	O-C-N	-6.94	114.92	122.07	14	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	338	GLU	N-CA-C	6.94	118.86	108.31	2	2
2	B	221	HIS	O-C-N	-6.94	114.24	122.15	12	2
2	C	128	LYS	N-CA-C	-6.93	104.30	112.89	12	2
2	C	157	HIS	CA-CB-CG	-6.93	106.87	113.80	8	4
2	B	258	TYR	CA-C-N	6.93	129.90	120.54	6	2
2	B	258	TYR	C-N-CA	6.93	129.90	120.54	6	2
2	B	253	SER	N-CA-CB	6.93	120.12	110.07	9	1
1	A	502	LEU	CA-C-N	6.93	129.56	120.28	13	1
1	A	502	LEU	C-N-CA	6.93	129.56	120.28	13	1
2	C	131	GLN	CA-C-O	-6.93	113.49	120.90	4	2
2	B	148	LEU	CA-C-O	6.93	128.03	120.90	13	2
2	B	84	GLN	CB-CG-CD	6.92	124.37	112.60	7	2
1	A	364	LEU	CA-C-N	6.92	128.49	119.84	12	4
1	A	364	LEU	C-N-CA	6.92	128.49	119.84	12	4
2	B	184	HIS	CE1-NE2-CD2	-6.92	102.08	109.00	4	4
2	C	166	LEU	N-CA-C	-6.92	103.18	111.69	1	1
2	B	98	GLN	CA-C-N	6.92	126.39	118.85	9	2
2	B	98	GLN	C-N-CA	6.92	126.39	118.85	9	2
2	C	175	ARG	CB-CA-C	6.91	122.27	110.79	15	1
2	B	235	ASP	CA-C-N	6.91	129.43	120.44	1	3
2	B	235	ASP	C-N-CA	6.91	129.43	120.44	1	3
2	B	122	TYR	CA-C-N	6.91	130.40	120.79	7	2
2	B	122	TYR	C-N-CA	6.91	130.40	120.79	7	2
2	B	231	PRO	CA-C-N	6.91	129.42	120.44	2	3
2	B	231	PRO	C-N-CA	6.91	129.42	120.44	2	3
2	C	197	ALA	CA-C-N	6.90	129.53	120.28	5	4
2	C	197	ALA	C-N-CA	6.90	129.53	120.28	5	4
2	B	124	ASP	CA-C-O	6.90	128.07	120.82	13	1
2	B	142	GLU	O-C-N	-6.90	113.38	121.32	11	3
2	C	104	PHE	CA-CB-CG	6.90	120.70	113.80	5	1
2	C	190	ASP	O-C-N	-6.90	113.78	122.27	11	3
2	C	179	ASP	CA-C-O	6.90	127.86	120.55	10	2
2	C	245	GLU	N-CA-C	6.90	118.88	111.36	4	5
2	C	130	TRP	CG-CD2-CE3	-6.90	127.00	133.90	13	1
2	B	257	GLU	N-CA-C	6.89	118.79	111.28	7	5
2	C	220	GLU	N-CA-CB	6.89	120.35	110.16	14	2
2	C	157	HIS	CA-C-N	6.88	130.06	120.29	5	4
2	C	157	HIS	C-N-CA	6.88	130.06	120.29	5	4
2	C	83	ARG	CA-C-N	6.88	129.80	120.44	12	2
2	C	83	ARG	C-N-CA	6.88	129.80	120.44	12	2
2	B	95	ALA	CA-C-N	6.88	129.74	120.65	12	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	95	ALA	C-N-CA	6.88	129.74	120.65	12	2
2	B	173	ARG	NH1-CZ-NH2	-6.88	110.36	119.30	15	1
2	B	255	LEU	O-C-N	-6.87	114.99	122.07	6	1
2	B	170	MET	N-CA-CB	6.87	120.33	110.16	8	1
2	C	156	LEU	N-CA-C	6.87	118.42	111.07	12	4
1	A	387	HIS	CB-CG-CD2	-6.87	122.27	131.20	11	2
2	B	122	TYR	N-CA-C	6.87	118.77	111.28	12	2
2	C	191	GLU	O-C-N	-6.87	114.84	122.12	9	1
2	B	126	PHE	N-CA-C	6.86	118.41	111.07	8	2
2	C	161	GLU	CA-C-N	6.86	129.36	120.44	15	1
2	C	161	GLU	C-N-CA	6.86	129.36	120.44	15	1
2	C	60	LEU	N-CA-C	6.85	118.75	111.28	5	1
2	C	102	ASP	N-CA-C	6.85	119.62	111.33	15	1
2	B	182	ARG	NE-CZ-NH1	-6.85	114.65	121.50	3	3
2	C	217	LYS	CA-C-O	6.85	127.68	120.42	13	2
1	A	379	PHE	O-C-N	6.85	131.01	123.27	4	2
1	A	347	ASN	OD1-CG-ND2	-6.85	115.75	122.60	8	2
1	A	371	ALA	O-C-N	-6.85	115.30	123.31	6	2
1	A	431	ARG	O-C-N	-6.84	114.77	123.26	9	1
1	A	374	ARG	NE-CZ-NH1	-6.84	114.66	121.50	3	4
1	A	341	PHE	CA-CB-CG	6.84	120.64	113.80	14	5
1	A	326	VAL	N-CA-CB	6.84	121.51	111.52	13	1
2	B	257	GLU	CB-CG-CD	6.84	124.23	112.60	10	1
2	C	253	SER	CA-C-N	6.84	129.44	120.28	5	5
2	C	253	SER	C-N-CA	6.84	129.44	120.28	5	5
2	C	87	SER	CA-C-O	6.84	127.67	120.42	13	2
2	B	254	ALA	N-CA-C	6.84	118.73	111.28	6	3
1	A	434	LYS	O-C-N	-6.83	115.61	123.33	12	2
2	C	79	THR	N-CA-C	6.83	118.38	111.07	9	2
2	B	129	LYS	CA-C-N	6.83	129.43	120.28	2	3
2	B	129	LYS	C-N-CA	6.83	129.43	120.28	2	3
2	C	235	ASP	CA-C-N	6.83	129.31	120.44	6	4
2	C	235	ASP	C-N-CA	6.83	129.31	120.44	6	4
2	C	250	SER	N-CA-CB	6.83	119.91	110.01	6	2
2	C	174	ALA	CA-C-N	6.82	129.31	120.44	12	3
2	C	174	ALA	C-N-CA	6.82	129.31	120.44	12	3
2	C	135	GLU	N-CA-C	6.82	118.71	111.28	13	2
1	A	445	VAL	CA-C-O	6.82	129.04	121.13	1	2
1	A	493	VAL	CA-C-N	6.82	131.03	120.60	6	3
1	A	493	VAL	C-N-CA	6.82	131.03	120.60	6	3
2	B	213	GLU	N-CA-C	6.82	118.50	111.14	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	477	PHE	O-C-N	-6.82	115.33	123.31	13	2
2	C	84	GLN	CA-C-N	6.81	129.71	120.44	9	4
2	C	84	GLN	C-N-CA	6.81	129.71	120.44	9	4
2	C	80	GLU	CA-C-N	6.81	127.49	120.00	2	3
2	C	80	GLU	C-N-CA	6.81	127.49	120.00	2	3
2	C	184	HIS	N-CA-C	6.81	118.70	111.28	10	3
2	C	157	HIS	CA-C-O	6.81	127.80	119.97	2	2
1	A	404	LYS	N-CA-CB	6.81	120.27	110.06	3	1
2	B	106	LYS	CA-C-N	6.80	129.40	120.28	7	2
2	B	106	LYS	C-N-CA	6.80	129.40	120.28	7	2
1	A	369	ASN	OD1-CG-ND2	-6.80	115.80	122.60	11	2
2	C	208	GLY	CA-C-O	6.80	127.48	119.45	11	1
2	C	111	GLU	CB-CA-C	6.80	121.55	110.88	8	2
1	A	503	ARG	CA-C-N	6.80	129.39	120.28	12	2
1	A	503	ARG	C-N-CA	6.80	129.39	120.28	12	2
2	B	250	SER	CB-CA-C	6.79	121.54	110.88	1	1
1	A	431	ARG	NH1-CZ-NH2	-6.79	110.48	119.30	12	3
2	C	214	TYR	CA-C-N	6.79	129.26	120.44	2	3
2	C	214	TYR	C-N-CA	6.79	129.26	120.44	2	3
2	C	130	TRP	CE3-CZ3-CH2	-6.79	112.28	121.10	11	2
2	B	93	VAL	CA-C-O	6.78	128.04	120.85	3	1
2	C	122	TYR	CB-CG-CD2	6.78	130.96	120.80	8	1
2	B	246	SER	CA-C-N	6.77	129.24	120.44	8	3
2	B	246	SER	C-N-CA	6.77	129.24	120.44	8	3
2	B	149	GLN	O-C-N	6.77	129.04	122.07	11	1
2	B	84	GLN	CA-C-N	6.77	129.24	120.44	14	1
2	B	84	GLN	C-N-CA	6.77	129.24	120.44	14	1
2	B	156	LEU	CA-C-N	6.76	129.89	120.29	2	2
2	B	156	LEU	C-N-CA	6.76	129.89	120.29	2	2
2	B	97	VAL	O-C-N	-6.76	115.31	121.87	5	2
1	A	505	TRP	N-CA-CB	6.76	120.68	110.14	6	1
1	A	377	GLY	CA-C-O	6.76	126.64	119.07	2	2
2	C	154	GLN	O-C-N	-6.76	115.11	122.07	2	2
2	B	264	THR	O-C-N	-6.76	115.52	123.22	4	2
1	A	372	TYR	CA-CB-CG	6.75	126.06	113.90	5	2
1	A	383	LYS	O-C-N	-6.75	115.51	123.41	2	1
2	B	210	ARG	NE-CZ-NH1	-6.75	114.75	121.50	1	6
2	C	154	GLN	N-CA-C	6.74	118.71	111.36	14	1
2	B	223	SER	CB-CA-C	-6.74	99.60	110.79	1	3
2	B	56	THR	CA-C-O	6.74	127.70	120.55	2	2
2	B	175	ARG	CA-C-O	-6.74	113.27	120.42	4	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	106	LYS	N-CA-C	6.74	118.28	111.07	2	8
1	A	410	LEU	CA-C-N	6.74	128.26	119.84	2	1
1	A	410	LEU	C-N-CA	6.74	128.26	119.84	2	1
2	B	107	LYS	O-C-N	-6.74	115.13	122.07	2	2
2	B	201	GLU	N-CA-CB	6.74	119.84	110.07	15	1
2	B	109	GLN	OE1-CD-NE2	-6.73	115.87	122.60	8	4
2	C	257	GLU	CA-C-N	6.73	129.84	120.29	15	5
2	C	257	GLU	C-N-CA	6.73	129.84	120.29	15	5
1	A	332	GLU	O-C-N	-6.73	115.44	123.31	2	3
2	B	215	HIS	CA-C-N	6.72	129.18	120.44	15	2
2	B	215	HIS	C-N-CA	6.72	129.18	120.44	15	2
1	A	327	ALA	N-CA-C	6.72	119.65	109.23	11	3
2	B	110	GLU	CA-C-N	6.72	129.83	120.29	3	3
2	B	110	GLU	C-N-CA	6.72	129.83	120.29	3	3
2	C	224	THR	CA-CB-OG1	6.72	119.68	109.60	10	1
2	B	118	LYS	O-C-N	6.72	128.99	122.07	1	1
2	B	115	TYR	CA-C-N	6.71	129.17	120.44	15	3
2	B	115	TYR	C-N-CA	6.71	129.17	120.44	15	3
1	A	351	ASP	O-C-N	-6.71	114.94	122.86	4	3
2	C	65	GLY	O-C-N	-6.71	115.06	121.77	5	2
2	C	93	VAL	CA-C-O	-6.71	113.97	120.95	14	1
2	C	70	GLU	CA-C-N	6.71	129.59	120.54	6	5
2	C	70	GLU	C-N-CA	6.71	129.59	120.54	6	5
2	C	90	LEU	N-CA-C	6.71	118.59	111.28	2	1
2	C	101	LEU	CA-C-N	6.71	129.26	120.28	8	4
2	C	101	LEU	C-N-CA	6.71	129.26	120.28	8	4
2	C	214	TYR	N-CA-C	6.70	118.24	111.07	1	1
2	B	63	GLN	O-C-N	-6.70	113.41	122.19	10	2
2	C	221	HIS	CG-CD2-NE2	6.70	113.90	107.20	9	1
1	A	322	ASN	N-CA-C	6.70	119.39	111.02	2	2
2	B	193	ARG	NH1-CZ-NH2	6.70	128.01	119.30	14	3
2	B	88	LYS	N-CA-CB	6.70	119.72	110.01	7	1
2	C	164	SER	O-C-N	-6.69	114.19	120.55	2	4
2	C	166	LEU	CA-C-N	6.69	127.55	119.99	11	3
2	C	166	LEU	C-N-CA	6.69	127.55	119.99	11	3
2	C	64	LEU	CA-C-O	6.69	126.26	118.90	3	1
2	C	259	THR	CA-C-O	6.69	127.65	120.55	8	1
2	B	262	LEU	CA-C-O	6.69	127.75	119.78	9	3
2	B	258	TYR	N-CA-C	6.69	118.58	111.28	13	6
2	C	236	LEU	N-CA-CB	-6.69	100.31	110.01	10	2
2	B	206	ASN	CA-C-N	6.69	127.36	120.00	11	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	206	ASN	C-N-CA	6.69	127.36	120.00	11	5
2	B	165	PRO	CA-C-N	6.69	129.79	120.29	14	2
2	B	165	PRO	C-N-CA	6.69	129.79	120.29	14	2
1	A	408	ARG	CA-C-N	6.69	131.75	120.91	12	1
1	A	408	ARG	C-N-CA	6.69	131.75	120.91	12	1
2	B	193	ARG	N-CA-C	6.69	118.57	111.28	2	2
1	A	353	TYR	CA-CB-CG	-6.69	101.86	113.90	15	1
2	C	171	ARG	N-CA-C	6.68	118.56	111.28	15	3
2	C	157	HIS	CB-CG-CD2	-6.67	122.53	131.20	12	2
2	B	74	ASN	CA-CB-CG	-6.67	105.93	112.60	15	2
2	B	82	LEU	CA-C-O	6.67	127.83	120.63	1	2
1	A	497	TYR	CA-C-O	-6.67	113.79	120.66	9	4
2	C	105	GLN	CA-C-N	6.67	129.22	120.28	7	1
2	C	105	GLN	C-N-CA	6.67	129.22	120.28	7	1
2	B	103	ASP	CA-C-N	6.67	129.10	120.44	10	5
2	B	103	ASP	C-N-CA	6.67	129.10	120.44	10	5
2	B	221	HIS	CB-CG-CD2	-6.67	122.53	131.20	3	1
2	C	102	ASP	CA-CB-CG	6.66	119.26	112.60	14	1
2	B	201	GLU	CA-C-N	6.66	129.20	120.28	12	2
2	B	201	GLU	C-N-CA	6.66	129.20	120.28	12	2
2	C	90	LEU	CA-C-N	6.66	129.75	120.29	13	1
2	C	90	LEU	C-N-CA	6.66	129.75	120.29	13	1
2	C	108	TRP	CG-CD2-CE3	-6.66	127.24	133.90	15	1
2	B	249	VAL	CA-C-O	6.66	128.23	121.17	12	1
2	C	221	HIS	N-CA-C	6.65	118.53	111.28	2	2
2	C	190	ASP	N-CA-CB	6.65	119.85	109.94	7	2
2	C	99	PRO	CA-C-N	6.65	129.49	120.38	1	3
2	C	99	PRO	C-N-CA	6.65	129.49	120.38	1	3
1	A	335	VAL	O-C-N	-6.65	116.15	123.20	14	3
2	B	184	HIS	CB-CG-CD2	-6.65	122.56	131.20	4	1
2	B	198	ALA	N-CA-C	6.65	118.61	111.36	5	4
2	B	138	ARG	N-CA-CB	6.65	119.65	110.01	11	1
2	B	215	HIS	CA-CB-CG	6.65	120.45	113.80	8	2
2	B	111	GLU	CA-C-N	6.65	129.08	120.44	3	3
2	B	111	GLU	C-N-CA	6.65	129.08	120.44	3	3
2	C	68	THR	O-C-N	-6.65	114.57	122.15	13	3
2	B	201	GLU	CA-C-O	-6.65	113.79	120.90	14	2
2	B	206	ASN	CA-C-O	-6.65	113.84	120.82	15	1
1	A	479	LYS	CA-C-N	6.64	134.43	121.41	8	3
1	A	479	LYS	C-N-CA	6.64	134.43	121.41	8	3
2	B	175	ARG	O-C-N	-6.64	115.08	122.12	11	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	121	PRO	CA-C-N	6.64	129.07	120.44	10	2
2	B	121	PRO	C-N-CA	6.64	129.07	120.44	10	2
1	A	390	PHE	N-CA-CB	6.63	120.98	110.57	4	1
2	C	70	GLU	N-CA-C	6.63	118.59	111.36	13	4
2	B	167	GLY	CA-C-N	6.63	129.07	120.44	12	2
2	B	167	GLY	C-N-CA	6.63	129.07	120.44	12	2
2	B	233	LEU	O-C-N	-6.63	114.59	122.15	4	4
2	C	182	ARG	CA-C-N	6.63	129.17	120.28	4	5
2	C	182	ARG	C-N-CA	6.63	129.17	120.28	4	5
2	C	170	MET	CG-SD-CE	-6.63	86.31	100.90	5	4
2	C	237	ARG	CA-C-N	6.63	129.16	120.28	6	4
2	C	237	ARG	C-N-CA	6.63	129.16	120.28	6	4
1	A	471	ASP	CA-C-O	6.63	127.41	119.59	8	1
1	A	501	ALA	CA-C-N	6.63	130.39	120.31	9	2
1	A	501	ALA	C-N-CA	6.63	130.39	120.31	9	2
1	A	504	ASP	N-CA-CB	6.63	119.94	110.13	14	1
2	B	89	ASP	CA-C-N	6.62	129.16	120.28	4	3
2	B	89	ASP	C-N-CA	6.62	129.16	120.28	4	3
2	C	241	LEU	CA-C-O	-6.62	112.24	118.73	12	2
2	B	246	SER	CA-C-O	6.62	127.57	120.55	1	1
2	B	251	PHE	CB-CG-CD1	6.62	131.95	120.70	11	1
2	C	253	SER	CA-C-O	6.62	127.57	120.55	9	1
2	B	161	GLU	CA-C-N	6.62	129.15	120.28	11	1
2	B	161	GLU	C-N-CA	6.62	129.15	120.28	11	1
2	C	58	SER	N-CA-CB	6.62	119.61	110.01	15	2
2	C	109	GLN	N-CA-C	6.62	118.49	111.28	5	4
2	C	56	THR	O-C-N	6.61	128.88	122.07	13	3
1	A	376	ASP	CA-C-N	6.61	132.91	121.07	11	1
1	A	376	ASP	C-N-CA	6.61	132.91	121.07	11	1
2	C	178	VAL	N-CA-C	6.61	117.30	110.36	2	4
2	C	139	GLN	OE1-CD-NE2	-6.61	115.99	122.60	12	1
2	B	259	THR	N-CA-CB	6.61	119.78	109.94	6	2
2	B	259	THR	CA-C-N	6.60	129.13	120.28	3	2
2	B	259	THR	C-N-CA	6.60	129.13	120.28	3	2
2	B	57	PHE	CA-CB-CG	-6.60	107.20	113.80	5	4
2	C	110	GLU	CA-C-N	6.60	129.02	120.44	10	5
2	C	110	GLU	C-N-CA	6.60	129.02	120.44	10	5
1	A	324	ASP	O-C-N	-6.60	115.27	122.07	3	3
2	B	181	LEU	O-C-N	-6.60	114.96	122.09	10	1
2	C	146	ALA	CA-C-O	6.60	127.75	120.82	1	3
1	A	399	TYR	CB-CA-C	-6.60	98.99	108.88	12	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	355	MET	N-CA-C	-6.59	100.36	110.32	1	1
1	A	451	LYS	CA-C-N	6.59	130.71	120.75	3	2
1	A	451	LYS	C-N-CA	6.59	130.71	120.75	3	2
2	C	221	HIS	CA-C-N	6.59	129.65	120.29	10	2
2	C	221	HIS	C-N-CA	6.59	129.65	120.29	10	2
1	A	424	ASN	CB-CA-C	6.59	119.70	109.03	5	1
2	B	207	GLY	CA-C-N	6.59	127.25	120.00	2	3
2	B	207	GLY	C-N-CA	6.59	127.25	120.00	2	3
2	C	217	LYS	N-CA-CB	6.59	120.02	110.20	14	1
2	B	98	GLN	CA-C-O	-6.59	111.14	120.16	3	1
2	C	248	LYS	CA-C-N	6.59	128.86	120.56	6	2
2	C	248	LYS	C-N-CA	6.59	128.86	120.56	6	2
2	C	206	ASN	N-CA-CB	6.59	120.02	110.47	10	1
1	A	355	MET	CG-SD-CE	-6.58	86.42	100.90	9	3
2	B	125	ASP	O-C-N	6.58	129.65	122.15	5	3
1	A	479	LYS	O-C-N	-6.58	113.84	122.59	11	2
2	C	190	ASP	CA-CB-CG	-6.57	106.03	112.60	1	2
2	C	58	SER	CB-CA-C	-6.57	100.56	110.88	15	2
2	B	86	MET	O-C-N	-6.57	114.46	122.34	6	2
2	B	134	MET	CG-SD-CE	6.57	115.35	100.90	12	2
2	B	77	LYS	CA-C-N	6.57	129.08	120.28	6	3
2	B	77	LYS	C-N-CA	6.57	129.08	120.28	6	3
2	B	107	LYS	CA-C-O	-6.57	113.59	120.55	4	2
2	C	72	TRP	CB-CG-CD2	6.57	135.99	126.80	2	2
1	A	484	TRP	O-C-N	-6.57	115.65	123.27	9	1
1	A	394	SER	CA-C-N	6.56	130.73	121.02	6	3
1	A	394	SER	C-N-CA	6.56	130.73	121.02	6	3
1	A	460	PRO	N-CA-C	6.56	121.54	111.11	9	1
1	A	433	ASN	N-CA-CB	-6.56	102.03	111.54	5	2
2	C	232	ALA	CA-C-N	6.56	129.60	120.29	5	2
2	C	232	ALA	C-N-CA	6.56	129.60	120.29	5	2
2	B	225	LEU	O-C-N	-6.56	113.64	122.43	10	1
2	C	236	LEU	CA-C-N	6.55	129.35	120.44	15	3
2	C	236	LEU	C-N-CA	6.55	129.35	120.44	15	3
2	C	162	LYS	O-C-N	-6.55	115.32	122.07	15	2
2	C	112	MET	CB-CA-C	6.55	121.67	110.79	8	1
2	C	82	LEU	CB-CA-C	-6.55	99.54	110.68	14	1
2	C	199	ARG	CA-C-N	6.55	129.06	120.28	5	2
2	C	199	ARG	C-N-CA	6.55	129.06	120.28	5	2
2	B	83	ARG	NH1-CZ-NH2	-6.55	110.78	119.30	11	2
1	A	415	ILE	O-C-N	-6.55	116.30	123.18	8	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	98	GLN	CB-CG-CD	-6.55	101.47	112.60	14	2
1	A	444	ALA	CA-C-N	6.55	129.53	120.49	12	2
1	A	444	ALA	C-N-CA	6.55	129.53	120.49	12	2
1	A	319	CYS	N-CA-C	6.55	121.12	113.20	7	2
2	C	229	ALA	CA-C-N	6.54	129.22	120.58	8	3
2	C	229	ALA	C-N-CA	6.54	129.22	120.58	8	3
2	B	217	LYS	O-C-N	-6.54	115.33	122.07	13	2
2	C	134	MET	N-CA-CB	-6.54	99.73	110.40	10	1
2	B	193	ARG	CA-C-O	6.54	127.49	120.10	11	1
2	C	208	GLY	N-CA-C	6.54	120.09	112.50	14	1
2	C	73	ASP	N-CA-C	-6.54	104.23	111.36	8	3
2	B	206	ASN	N-CA-CB	6.54	119.73	110.12	3	1
2	C	56	THR	CA-C-N	6.54	129.57	120.29	3	2
2	C	56	THR	C-N-CA	6.54	129.57	120.29	3	2
1	A	422	MET	CG-SD-CE	-6.54	86.52	100.90	1	1
1	A	424	ASN	OD1-CG-ND2	-6.54	116.06	122.60	5	3
1	A	377	GLY	CA-C-N	6.54	131.91	120.87	11	1
1	A	377	GLY	C-N-CA	6.54	131.91	120.87	11	1
2	C	73	ASP	CA-C-N	6.53	131.75	120.58	9	2
2	C	73	ASP	C-N-CA	6.53	131.75	120.58	9	2
2	C	215	HIS	N-CA-CB	6.53	119.48	110.01	2	1
2	B	212	ALA	N-CA-C	6.53	119.23	111.33	4	2
2	C	158	GLU	N-CA-C	6.53	118.40	111.28	6	1
1	A	402	HIS	N-CA-C	6.53	119.70	110.23	14	2
2	C	237	ARG	CA-C-O	6.53	127.67	120.82	7	2
1	A	342	TRP	N-CA-C	-6.53	99.19	109.50	11	2
2	B	127	GLN	OE1-CD-NE2	-6.53	116.07	122.60	12	1
1	A	342	TRP	CZ3-CH2-CZ2	-6.53	113.01	121.50	13	1
1	A	359	GLN	N-CA-CB	6.53	119.71	110.12	13	1
2	B	69	GLN	CA-C-O	-6.52	113.97	120.82	3	1
1	A	348	GLN	O-C-N	-6.52	115.28	123.17	12	2
2	B	200	LEU	CA-C-N	6.52	129.02	120.28	5	3
2	B	200	LEU	C-N-CA	6.52	129.02	120.28	5	3
2	C	75	LEU	CA-C-O	-6.52	113.64	120.55	6	2
1	A	376	ASP	N-CA-CB	6.52	120.83	110.73	10	1
1	A	317	ASN	CA-C-N	6.51	129.67	120.42	1	1
1	A	317	ASN	C-N-CA	6.51	129.67	120.42	1	1
2	C	63	GLN	OE1-CD-NE2	-6.51	116.09	122.60	8	1
2	B	149	GLN	CA-C-O	-6.51	113.98	120.82	11	1
1	A	370	THR	CA-CB-CG2	6.51	121.57	110.50	8	3
1	A	494	GLU	CA-C-N	6.51	127.53	119.98	14	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	494	GLU	C-N-CA	6.51	127.53	119.98	14	4
2	C	147	GLU	CA-C-O	-6.51	113.65	120.55	5	3
1	A	508	CYS	O-C-N	-6.51	114.52	121.42	1	3
2	B	125	ASP	N-CA-C	6.50	118.45	111.36	14	3
1	A	416	ASP	CA-CB-CG	6.50	119.10	112.60	2	2
1	A	505	TRP	CB-CG-CD2	-6.50	117.70	126.80	2	1
2	C	184	HIS	ND1-CE1-NE2	6.50	114.90	108.40	11	2
2	B	92	GLU	CA-C-O	6.50	127.64	120.82	5	2
2	C	106	LYS	CA-C-N	6.50	129.28	120.38	14	2
2	C	106	LYS	C-N-CA	6.50	129.28	120.38	14	2
1	A	461	GLU	N-CA-C	6.50	119.79	110.24	12	2
2	C	200	LEU	O-C-N	-6.49	114.75	122.15	12	2
2	C	212	ALA	CA-C-N	6.49	128.98	120.28	13	2
2	C	212	ALA	C-N-CA	6.49	128.98	120.28	13	2
2	C	59	LYS	O-C-N	-6.49	115.25	122.12	9	1
2	C	121	PRO	CA-C-N	6.48	130.17	120.31	9	4
2	C	121	PRO	C-N-CA	6.48	130.17	120.31	9	4
2	C	114	LEU	CA-C-N	6.48	129.50	120.29	5	2
2	C	114	LEU	C-N-CA	6.48	129.50	120.29	5	2
2	C	186	ALA	CA-C-N	6.48	125.92	118.85	10	3
2	C	186	ALA	C-N-CA	6.48	125.92	118.85	10	3
2	B	78	GLU	CA-C-N	6.48	128.96	120.28	5	2
2	B	78	GLU	C-N-CA	6.48	128.96	120.28	5	2
2	B	197	ALA	O-C-N	6.48	129.80	122.22	10	2
2	B	224	THR	O-C-N	-6.48	115.40	122.07	10	4
2	C	113	GLU	CA-C-N	6.48	129.25	120.38	13	4
2	C	113	GLU	C-N-CA	6.48	129.25	120.38	13	4
2	C	56	THR	OG1-CB-CG2	-6.48	96.34	109.30	14	1
2	C	184	HIS	CB-CG-CD2	-6.48	122.78	131.20	15	1
1	A	344	VAL	CA-C-O	6.47	127.22	120.36	14	1
2	B	251	PHE	N-CA-CB	-6.47	100.63	110.01	10	1
2	C	114	LEU	N-CA-C	6.47	118.33	111.28	3	2
1	A	322	ASN	OD1-CG-ND2	-6.47	116.13	122.60	7	3
2	C	147	GLU	O-C-N	-6.47	115.26	122.12	7	1
2	C	65	GLY	CA-C-O	-6.47	112.27	121.52	15	1
2	C	206	ASN	N-CA-C	6.47	120.09	112.72	6	3
2	B	196	LEU	CA-C-O	-6.46	113.58	120.42	10	1
2	C	196	LEU	N-CA-CB	-6.46	100.64	110.01	14	1
2	B	59	LYS	N-CA-CB	-6.46	100.61	110.16	7	1
2	C	124	ASP	CA-CB-CG	-6.45	106.15	112.60	9	1
2	C	197	ALA	CA-C-O	6.45	127.39	120.55	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	105	GLN	N-CA-CB	-6.45	102.42	111.00	14	2
2	B	153	ARG	O-C-N	-6.45	114.33	122.27	13	3
1	A	402	HIS	CE1-NE2-CD2	-6.45	102.55	109.00	11	7
2	C	181	LEU	O-C-N	-6.45	115.43	122.07	5	3
1	A	323	PHE	CA-C-O	6.45	128.24	121.15	5	2
1	A	478	TYR	N-CA-C	6.45	120.10	108.69	8	1
2	B	204	LYS	CA-C-N	6.45	129.40	120.63	15	5
2	B	204	LYS	C-N-CA	6.45	129.40	120.63	15	5
2	C	73	ASP	N-CA-CB	6.45	119.70	110.16	8	3
2	C	219	THR	N-CA-C	6.45	118.39	111.36	9	2
2	C	233	LEU	CA-C-O	6.44	127.58	120.63	7	1
2	C	219	THR	O-C-N	-6.44	114.81	122.15	9	1
2	B	73	ASP	CA-C-O	6.44	127.25	120.42	7	3
2	C	246	SER	CA-C-O	-6.44	114.06	120.82	13	1
2	B	160	GLN	O-C-N	-6.43	115.30	122.12	13	2
1	A	439	ASN	CA-C-N	6.43	128.90	120.28	5	3
1	A	439	ASN	C-N-CA	6.43	128.90	120.28	5	3
1	A	457	GLU	N-CA-C	6.43	119.61	109.96	6	1
2	C	181	LEU	CA-C-N	6.43	128.81	120.44	7	1
2	C	181	LEU	C-N-CA	6.43	128.81	120.44	7	1
2	C	95	ALA	O-C-N	-6.43	114.36	122.27	3	1
1	A	411	PRO	N-CA-C	6.43	121.75	111.26	9	3
1	A	442	LEU	CA-C-N	6.43	131.53	122.46	12	2
1	A	442	LEU	C-N-CA	6.43	131.53	122.46	12	2
2	B	213	GLU	CA-C-N	6.43	130.08	120.31	6	2
2	B	213	GLU	C-N-CA	6.43	130.08	120.31	6	2
2	C	262	LEU	CA-C-N	6.43	128.90	120.28	6	1
2	C	262	LEU	C-N-CA	6.43	128.90	120.28	6	1
2	B	172	ASP	N-CA-C	-6.43	104.13	112.23	12	4
1	A	408	ARG	N-CA-C	6.43	120.36	110.20	10	1
2	C	224	THR	CA-C-N	6.43	129.22	120.54	15	1
2	C	224	THR	C-N-CA	6.43	129.22	120.54	15	1
1	A	471	ASP	N-CA-C	-6.43	105.07	113.17	5	3
2	B	215	HIS	N-CA-CB	6.42	119.56	110.12	9	1
2	C	67	VAL	CB-CA-C	-6.42	103.47	112.14	8	2
2	C	108	TRP	CA-C-O	6.42	127.22	120.42	1	2
1	A	412	THR	CA-CB-CG2	6.42	121.41	110.50	15	2
2	C	215	HIS	CG-CD2-NE2	6.42	113.61	107.20	4	1
2	C	235	ASP	CA-CB-CG	-6.42	106.19	112.60	5	2
1	A	433	ASN	OD1-CG-ND2	6.41	129.01	122.60	11	1
2	C	57	PHE	N-CA-CB	6.41	119.27	109.91	14	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	355	MET	CA-C-N	6.41	126.75	119.83	12	3
1	A	355	MET	C-N-CA	6.41	126.75	119.83	12	3
2	C	152	ALA	CA-C-N	6.41	128.77	120.44	5	3
2	C	152	ALA	C-N-CA	6.41	128.77	120.44	5	3
2	C	61	ARG	O-C-N	-6.41	115.47	122.07	3	1
2	B	108	TRP	CA-C-N	6.41	129.16	120.38	11	1
2	B	108	TRP	C-N-CA	6.41	129.16	120.38	11	1
2	C	221	HIS	N-CA-CB	6.41	119.30	110.01	11	1
2	B	230	LYS	CA-C-N	6.41	125.98	119.19	15	1
2	B	230	LYS	C-N-CA	6.41	125.98	119.19	15	1
2	B	88	LYS	CA-C-N	6.40	128.86	120.28	15	2
2	B	88	LYS	C-N-CA	6.40	128.86	120.28	15	2
2	B	222	LEU	CA-C-N	6.40	129.38	120.29	7	2
2	B	222	LEU	C-N-CA	6.40	129.38	120.29	7	2
1	A	430	PHE	O-C-N	-6.40	115.73	123.29	10	1
2	B	221	HIS	CA-C-N	6.40	128.76	120.44	11	3
2	B	221	HIS	C-N-CA	6.40	128.76	120.44	11	3
2	B	130	TRP	N-CA-C	6.40	117.92	111.07	4	1
2	C	68	THR	CA-CB-CG2	6.40	121.38	110.50	4	2
2	C	84	GLN	N-CA-C	6.40	117.92	111.07	4	3
2	B	101	LEU	N-CA-C	6.40	118.25	111.28	1	3
2	C	238	GLN	CA-C-O	6.40	127.33	120.55	4	2
2	C	164	SER	CA-C-N	6.40	126.15	119.05	10	1
2	C	164	SER	C-N-CA	6.40	126.15	119.05	10	1
1	A	352	GLY	O-C-N	-6.39	116.49	122.50	11	1
2	C	148	LEU	CA-C-N	6.39	129.17	120.54	4	4
2	C	148	LEU	C-N-CA	6.39	129.17	120.54	4	4
2	B	177	HIS	N-CA-CB	6.39	120.19	110.28	3	2
1	A	333	MET	N-CA-C	6.39	118.35	109.15	10	4
2	C	207	GLY	CA-C-O	-6.39	113.89	120.66	7	2
1	A	364	LEU	CA-C-O	-6.39	112.46	119.61	4	1
2	C	175	ARG	CB-CG-CD	6.38	125.99	111.30	6	2
2	C	78	GLU	N-CA-C	6.38	119.05	111.33	9	3
1	A	495	PRO	CA-C-O	-6.38	114.06	121.34	7	1
2	C	119	VAL	CA-C-N	6.38	129.01	120.58	9	1
2	C	119	VAL	C-N-CA	6.38	129.01	120.58	9	1
2	B	128	LYS	O-C-N	-6.38	115.45	122.09	12	2
1	A	472	GLU	O-C-N	-6.38	115.49	122.00	15	1
2	C	173	ARG	NE-CZ-NH1	-6.38	115.12	121.50	5	2
1	A	435	TYR	CA-C-N	6.38	132.38	123.07	13	1
1	A	435	TYR	C-N-CA	6.38	132.38	123.07	13	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	82	LEU	CA-C-N	6.38	129.15	120.54	3	1
2	B	82	LEU	C-N-CA	6.38	129.15	120.54	3	1
2	B	224	THR	N-CA-CB	6.38	119.60	110.16	8	2
2	B	176	ALA	N-CA-CB	-6.38	100.72	110.16	10	1
1	A	351	ASP	CA-CB-CG	-6.38	106.22	112.60	8	3
2	B	76	GLU	N-CA-C	6.37	118.23	111.28	6	1
1	A	473	VAL	CB-CA-C	-6.37	103.53	112.14	15	2
2	B	243	VAL	N-CA-CB	6.37	118.73	110.57	13	2
2	B	149	GLN	CA-C-N	6.37	129.14	120.54	14	3
2	B	149	GLN	C-N-CA	6.37	129.14	120.54	14	3
2	B	201	GLU	O-C-N	-6.37	113.89	122.43	8	1
2	C	200	LEU	CB-CA-C	6.37	120.88	110.88	9	1
2	B	68	THR	CA-C-O	-6.37	114.08	120.90	13	1
2	C	210	ARG	CA-CB-CG	6.37	126.83	114.10	2	1
2	C	112	MET	N-CA-C	6.37	118.22	111.28	13	4
2	B	61	ARG	O-C-N	-6.36	115.38	122.12	8	1
2	C	258	TYR	CA-C-O	-6.36	114.10	120.90	9	3
2	B	160	GLN	CA-C-O	6.36	127.29	120.55	13	3
2	B	56	THR	O-C-N	6.35	128.70	122.09	6	1
2	C	211	LEU	CA-C-O	-6.35	114.15	120.82	9	1
2	C	89	ASP	CA-CB-CG	6.35	118.95	112.60	13	2
2	B	188	TYR	CA-C-O	-6.35	114.15	120.82	2	1
1	A	421	TRP	CB-CA-C	6.35	120.48	110.19	4	1
2	B	111	GLU	O-C-N	-6.35	115.53	122.07	10	2
2	C	117	GLN	CB-CG-CD	-6.35	101.81	112.60	15	2
1	A	384	GLY	O-C-N	-6.35	115.44	122.61	12	2
1	A	503	ARG	NE-CZ-NH2	6.35	124.91	119.20	5	6
2	C	200	LEU	CA-C-N	6.35	128.78	120.28	9	5
2	C	200	LEU	C-N-CA	6.35	128.78	120.28	9	5
2	C	161	GLU	O-C-N	6.34	128.60	122.07	14	3
2	C	209	ALA	N-CA-C	6.34	118.19	111.28	15	1
2	B	193	ARG	O-C-N	-6.34	115.40	122.12	13	3
1	A	505	TRP	N-CA-C	-6.34	105.44	113.43	11	2
2	B	117	GLN	CA-C-N	6.34	129.06	120.44	4	2
2	B	117	GLN	C-N-CA	6.34	129.06	120.44	4	2
1	A	361	TRP	CB-CG-CD1	6.34	136.41	126.90	10	1
1	A	401	LYS	CA-C-N	6.33	129.70	120.71	14	1
1	A	401	LYS	C-N-CA	6.33	129.70	120.71	14	1
2	B	218	ALA	N-CA-CB	-6.33	100.81	110.12	10	3
2	B	162	LYS	CA-C-O	-6.33	113.84	120.55	11	4
1	A	365	PRO	N-CA-C	6.33	120.38	111.33	3	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	404	LYS	N-CA-C	6.33	118.71	111.11	6	4
2	C	127	GLN	O-C-N	6.33	128.83	122.12	3	3
1	A	387	HIS	CE1-NE2-CD2	-6.33	102.67	109.00	12	2
2	C	147	GLU	CB-CA-C	6.33	121.29	110.79	7	1
2	C	115	TYR	O-C-N	-6.32	115.56	122.07	11	4
2	B	212	ALA	CA-C-N	6.32	128.75	120.28	3	3
2	B	212	ALA	C-N-CA	6.32	128.75	120.28	3	3
2	C	220	GLU	N-CA-C	6.32	118.17	111.28	4	1
2	B	137	TYR	N-CA-C	6.32	117.84	111.07	11	2
1	A	374	ARG	CD-NE-CZ	-6.32	115.55	124.40	8	2
1	A	359	GLN	N-CA-C	6.32	118.98	111.71	2	1
2	B	243	VAL	CA-C-O	6.32	127.55	120.85	2	1
1	A	453	ILE	CA-CB-CG1	6.32	121.14	110.40	3	1
2	C	117	GLN	CA-C-N	6.32	128.66	120.44	3	3
2	C	117	GLN	C-N-CA	6.32	128.66	120.44	3	3
2	C	99	PRO	CB-CA-C	-6.32	101.92	110.52	9	1
1	A	460	PRO	CA-C-O	-6.32	114.23	121.56	14	2
1	A	388	TRP	CB-CG-CD2	-6.32	117.96	126.80	12	1
2	B	238	GLN	O-C-N	-6.31	113.97	122.43	3	1
2	C	129	LYS	CA-C-N	6.31	128.65	120.44	14	2
2	C	129	LYS	C-N-CA	6.31	128.65	120.44	14	2
2	C	170	MET	CA-C-N	6.31	128.74	120.28	9	4
2	C	170	MET	C-N-CA	6.31	128.74	120.28	9	4
1	A	464	ARG	N-CA-C	-6.31	104.89	112.59	9	2
2	C	172	ASP	N-CA-C	6.31	118.24	111.36	6	4
1	A	355	MET	O-C-N	-6.30	114.16	121.60	9	2
2	C	161	GLU	N-CA-C	6.30	118.23	111.36	9	2
2	C	237	ARG	NE-CZ-NH1	-6.30	115.20	121.50	14	2
1	A	368	ILE	CB-CA-C	-6.30	101.11	111.51	14	2
2	C	160	GLN	CA-C-O	6.30	127.10	120.42	9	2
2	B	111	GLU	CA-C-O	6.30	127.21	119.97	4	1
1	A	348	GLN	CA-C-N	6.30	129.66	120.91	8	1
1	A	348	GLN	C-N-CA	6.30	129.66	120.91	8	1
2	B	192	LEU	CA-C-N	6.29	128.71	120.28	2	2
2	B	192	LEU	C-N-CA	6.29	128.71	120.28	2	2
2	C	122	TYR	CA-C-N	6.29	128.62	120.44	10	3
2	C	122	TYR	C-N-CA	6.29	128.62	120.44	10	3
2	B	120	GLU	CA-C-N	6.29	125.71	118.85	10	1
2	B	120	GLU	C-N-CA	6.29	125.71	118.85	10	1
2	C	213	GLU	CB-CA-C	6.29	120.76	110.88	11	1
2	B	190	ASP	N-CA-C	6.29	117.93	111.14	3	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	395	LEU	CA-C-O	6.29	127.78	120.49	5	2
1	A	332	GLU	CA-C-O	6.29	127.37	120.71	4	1
1	A	456	TRP	CB-CG-CD2	-6.29	118.00	126.80	11	1
2	B	61	ARG	CA-C-N	6.29	128.61	120.44	14	1
2	B	61	ARG	C-N-CA	6.29	128.61	120.44	14	1
1	A	464	ARG	O-C-N	-6.28	114.53	122.26	9	2
1	A	381	PHE	CA-C-N	6.28	131.85	122.99	13	1
1	A	381	PHE	C-N-CA	6.28	131.85	122.99	13	1
2	B	171	ARG	O-C-N	-6.28	115.56	122.09	15	1
1	A	421	TRP	O-C-N	-6.28	115.57	123.05	9	2
2	B	173	ARG	O-C-N	-6.28	115.60	122.07	12	1
1	A	477	PHE	CA-C-N	6.28	132.36	122.94	2	1
1	A	477	PHE	C-N-CA	6.28	132.36	122.94	2	1
2	C	59	LYS	CA-C-O	6.28	127.21	120.55	9	1
2	B	109	GLN	CA-C-N	6.28	128.69	120.28	15	3
2	B	109	GLN	C-N-CA	6.28	128.69	120.28	15	3
2	C	250	SER	CA-C-N	6.28	128.60	120.44	8	2
2	C	250	SER	C-N-CA	6.28	128.60	120.44	8	2
2	B	70	GLU	O-C-N	-6.27	115.47	122.12	14	2
2	B	66	PRO	CB-CA-C	-6.27	102.53	111.68	2	1
2	C	256	GLU	N-CA-C	-6.27	104.33	112.23	3	3
2	C	73	ASP	CA-C-O	6.27	127.61	120.90	12	1
2	C	152	ALA	CA-C-O	-6.27	113.91	120.55	14	1
2	B	175	ARG	CA-C-N	6.26	128.96	120.38	4	4
2	B	175	ARG	C-N-CA	6.26	128.96	120.38	4	4
1	A	416	ASP	N-CA-CB	6.26	119.15	110.07	13	3
1	A	433	ASN	CA-CB-CG	6.26	118.86	112.60	7	2
1	A	503	ARG	CB-CA-C	-6.26	101.01	110.90	1	2
2	B	238	GLN	OE1-CD-NE2	-6.26	116.34	122.60	4	3
1	A	452	ASN	CA-C-O	6.26	128.07	121.19	14	2
1	A	421	TRP	CB-CG-CD1	-6.26	117.52	126.90	2	1
2	C	158	GLU	CA-C-O	6.26	127.14	120.70	2	2
2	C	68	THR	CA-C-N	6.26	128.57	120.44	6	2
2	C	68	THR	C-N-CA	6.26	128.57	120.44	6	2
2	C	61	ARG	NH1-CZ-NH2	-6.26	111.17	119.30	9	2
2	C	234	GLU	N-CA-C	6.25	117.76	111.07	9	2
2	B	110	GLU	CA-C-O	6.25	127.59	120.90	7	3
2	B	70	GLU	CA-C-N	6.25	129.16	120.29	15	3
2	B	70	GLU	C-N-CA	6.25	129.16	120.29	15	3
2	B	94	LYS	N-CA-C	6.25	118.09	111.28	6	6
2	C	100	TYR	CA-C-O	6.25	127.34	119.78	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	180	ALA	O-C-N	-6.25	115.50	122.12	3	1
1	A	459	ILE	CB-CA-C	-6.25	103.59	110.52	10	3
1	A	402	HIS	ND1-CE1-NE2	6.24	114.64	108.40	3	2
2	B	100	TYR	CA-C-O	6.24	127.17	120.55	4	1
1	A	475	THR	N-CA-C	-6.24	99.02	109.07	10	2
1	A	501	ALA	O-C-N	-6.24	113.91	122.46	10	1
1	A	421	TRP	CA-C-O	6.24	127.18	120.32	2	3
2	B	158	GLU	O-C-N	-6.24	115.64	122.07	8	2
2	C	98	GLN	OE1-CD-NE2	-6.24	116.36	122.60	13	1
2	B	142	GLU	CA-C-O	-6.24	111.62	120.16	2	2
1	A	460	PRO	CA-C-N	6.24	129.56	120.71	4	2
1	A	460	PRO	C-N-CA	6.24	129.56	120.71	4	2
2	B	200	LEU	CA-C-O	6.24	127.03	120.42	3	1
2	B	100	TYR	N-CA-CB	6.24	119.29	110.12	9	2
2	C	66	PRO	CB-CA-C	-6.24	103.01	112.11	8	2
2	C	144	LEU	CA-C-N	6.23	128.54	120.44	2	1
2	C	144	LEU	C-N-CA	6.23	128.54	120.44	2	1
2	C	121	PRO	N-CA-CB	6.23	110.42	103.44	1	1
2	C	175	ARG	NH1-CZ-NH2	-6.23	111.20	119.30	6	1
1	A	425	GLY	CA-C-N	6.23	132.59	122.81	14	1
1	A	425	GLY	C-N-CA	6.23	132.59	122.81	14	1
2	C	157	HIS	N-CA-CB	6.23	119.27	110.12	8	2
2	C	85	GLU	CA-C-N	6.22	128.62	120.28	12	1
2	C	85	GLU	C-N-CA	6.22	128.62	120.28	12	1
2	C	103	ASP	N-CA-C	6.22	120.61	112.89	8	2
1	A	445	VAL	N-CA-CB	6.22	120.58	110.13	4	1
2	B	241	LEU	CA-C-O	-6.22	112.31	118.34	12	2
2	C	91	GLU	O-C-N	-6.22	115.06	122.15	11	2
2	B	117	GLN	CA-CB-CG	6.21	126.53	114.10	14	1
2	B	81	GLY	CA-C-N	6.21	129.22	120.28	12	5
2	B	81	GLY	C-N-CA	6.21	129.22	120.28	12	5
2	C	212	ALA	O-C-N	-6.21	115.67	122.07	9	1
2	C	251	PHE	O-C-N	-6.21	115.67	122.07	11	2
2	B	75	LEU	N-CA-C	6.21	118.05	111.28	2	2
2	B	251	PHE	CB-CA-C	6.21	120.79	110.92	2	1
2	B	258	TYR	CB-CG-CD2	-6.21	111.49	120.80	11	1
1	A	444	ALA	O-C-N	-6.21	117.32	123.46	13	2
2	B	104	PHE	CA-CB-CG	6.21	120.00	113.80	11	4
2	C	157	HIS	CE1-NE2-CD2	-6.20	102.80	109.00	13	5
2	B	60	LEU	CA-C-O	-6.20	113.09	120.10	7	1
2	B	159	LEU	CB-CA-C	-6.20	101.10	110.90	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	115	TYR	CB-CA-C	6.20	120.62	110.88	11	1
1	A	437	ARG	NH1-CZ-NH2	-6.20	111.24	119.30	9	3
1	A	346	ASN	OD1-CG-ND2	-6.20	116.40	122.60	11	2
1	A	388	TRP	CA-C-N	6.20	130.74	122.93	12	2
1	A	388	TRP	C-N-CA	6.20	130.74	122.93	12	2
2	C	238	GLN	OE1-CD-NE2	-6.20	116.40	122.60	4	1
1	A	343	ARG	CA-C-N	6.20	131.61	123.06	9	1
1	A	343	ARG	C-N-CA	6.20	131.61	123.06	9	1
2	C	203	LEU	N-CA-CB	-6.19	101.02	110.12	2	1
2	C	112	MET	CA-C-N	6.19	128.49	120.44	12	4
2	C	112	MET	C-N-CA	6.19	128.49	120.44	12	4
1	A	453	ILE	N-CA-CB	6.19	118.96	110.54	11	1
2	B	157	HIS	CB-CG-CD2	-6.19	123.15	131.20	12	1
2	B	221	HIS	CA-C-O	6.19	126.98	120.42	12	2
1	A	322	ASN	CA-C-N	6.19	129.62	120.90	5	3
1	A	322	ASN	C-N-CA	6.19	129.62	120.90	5	3
1	A	446	ASP	CA-C-O	6.19	129.05	121.87	8	1
2	B	80	GLU	CA-C-N	6.19	127.87	120.14	11	3
2	B	80	GLU	C-N-CA	6.19	127.87	120.14	11	3
2	C	184	HIS	CB-CG-ND1	6.19	131.98	122.70	15	1
2	B	147	GLU	CA-C-N	6.18	128.57	120.28	3	2
2	B	147	GLU	C-N-CA	6.18	128.57	120.28	3	2
2	B	232	ALA	CB-CA-C	-6.18	101.17	110.88	6	1
2	C	159	LEU	CA-C-N	6.18	128.56	120.28	11	3
2	C	159	LEU	C-N-CA	6.18	128.56	120.28	11	3
2	B	163	LEU	N-CA-C	6.18	118.99	111.82	12	2
2	C	95	ALA	CA-C-N	6.18	129.07	120.29	8	1
2	C	95	ALA	C-N-CA	6.18	129.07	120.29	8	1
2	C	70	GLU	CB-CA-C	-6.18	101.18	110.88	1	1
2	B	176	ALA	O-C-N	-6.18	115.67	122.09	3	2
2	B	243	VAL	CA-C-N	6.18	128.47	120.44	3	2
2	B	243	VAL	C-N-CA	6.18	128.47	120.44	3	2
1	A	378	LYS	N-CA-CB	6.18	119.06	110.17	4	1
2	B	108	TRP	O-C-N	-6.18	115.67	122.09	11	1
2	B	237	ARG	N-CA-C	6.17	118.01	111.28	1	3
2	B	180	ALA	N-CA-C	6.17	118.01	111.28	3	2
2	B	130	TRP	CE2-CD2-CE3	6.17	124.97	118.80	13	1
2	C	176	ALA	CA-C-O	6.17	126.96	120.42	7	1
2	B	138	ARG	NE-CZ-NH2	6.17	124.75	119.20	12	6
2	C	178	VAL	O-C-N	-6.17	115.64	121.87	6	2
1	A	491	LEU	N-CA-CB	6.17	122.12	112.25	10	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	256	GLU	O-C-N	6.17	128.66	122.12	7	2
2	B	137	TYR	O-C-N	-6.16	115.59	122.12	3	1
2	B	152	ALA	CA-C-N	6.16	129.04	120.29	5	2
2	B	152	ALA	C-N-CA	6.16	129.04	120.29	5	2
2	B	214	TYR	CB-CA-C	-6.16	100.57	110.79	8	1
2	C	215	HIS	ND1-CE1-NE2	6.15	114.55	108.40	15	3
2	B	216	ALA	CA-C-N	6.15	128.44	120.44	14	2
2	B	216	ALA	C-N-CA	6.15	128.44	120.44	14	2
2	C	196	LEU	CB-CA-C	6.15	120.54	110.88	13	1
1	A	330	ARG	NE-CZ-NH1	6.15	127.65	121.50	5	4
2	C	238	GLN	N-CA-C	6.15	117.98	111.28	14	2
2	C	244	LEU	N-CA-C	6.14	118.77	111.33	10	2
2	C	185	LEU	O-C-N	-6.14	114.66	122.34	14	1
2	C	222	LEU	O-C-N	-6.14	115.75	122.07	4	2
2	C	139	GLN	CB-CG-CD	6.14	123.04	112.60	15	1
2	B	89	ASP	O-C-N	-6.14	115.61	122.12	11	2
2	C	245	GLU	N-CA-CB	-6.14	101.08	110.16	4	1
2	C	100	TYR	O-C-N	-6.14	113.24	122.20	9	2
2	C	62	GLU	CA-C-N	6.13	128.41	120.44	2	2
2	C	62	GLU	C-N-CA	6.13	128.41	120.44	2	2
2	C	127	GLN	CG-CD-OE1	6.13	133.07	120.80	3	1
2	B	250	SER	O-C-N	-6.13	115.16	122.15	4	2
2	B	182	ARG	CD-NE-CZ	6.13	132.99	124.40	4	1
2	C	72	TRP	CA-C-O	-6.13	114.38	120.82	5	1
2	B	264	THR	CA-C-N	6.13	132.74	121.70	15	2
2	B	264	THR	C-N-CA	6.13	132.74	121.70	15	2
2	B	60	LEU	O-C-N	-6.13	115.62	122.12	8	1
2	B	177	HIS	CA-C-O	6.13	127.05	120.55	11	1
2	C	97	VAL	N-CA-CB	6.12	118.87	110.54	15	1
2	B	117	GLN	N-CA-C	6.12	117.62	111.07	1	2
2	B	148	LEU	CA-C-N	6.12	128.99	120.29	4	2
2	B	148	LEU	C-N-CA	6.12	128.99	120.29	4	2
2	C	227	GLU	N-CA-C	6.12	117.62	111.07	15	4
1	A	479	LYS	CA-C-O	6.12	128.47	120.21	5	1
2	B	263	ASN	CA-C-N	6.12	131.54	121.39	5	1
2	B	263	ASN	C-N-CA	6.12	131.54	121.39	5	1
2	B	124	ASP	N-CA-C	6.12	117.64	110.97	7	1
2	B	124	ASP	CB-CA-C	6.12	120.48	110.88	3	1
2	C	111	GLU	CA-C-O	6.12	127.03	120.55	14	2
2	B	171	ARG	CA-C-N	6.11	128.47	120.28	3	2
2	B	171	ARG	C-N-CA	6.11	128.47	120.28	3	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	252	LEU	N-CA-C	6.11	117.61	111.07	14	3
2	B	172	ASP	CB-CA-C	6.11	120.93	110.79	7	3
1	A	358	GLY	N-CA-C	6.11	121.25	113.24	12	1
1	A	472	GLU	CA-C-O	6.11	128.20	118.92	15	2
2	B	213	GLU	CA-C-O	-6.10	114.08	120.55	3	1
1	A	414	LYS	N-CA-C	6.10	118.05	108.96	6	1
2	C	222	LEU	CA-C-N	6.10	128.95	120.29	1	4
2	C	222	LEU	C-N-CA	6.10	128.95	120.29	1	4
2	C	69	GLN	OE1-CD-NE2	-6.10	116.50	122.60	12	2
2	B	158	GLU	N-CA-C	6.10	117.93	111.28	4	2
2	B	182	ARG	O-C-N	6.10	128.35	122.07	11	2
1	A	370	THR	N-CA-CB	6.09	121.01	111.56	13	1
2	B	264	THR	CA-CB-OG1	6.09	118.74	109.60	14	1
1	A	386	LYS	N-CA-C	6.09	118.44	109.24	10	2
1	A	432	GLY	CA-C-N	6.09	132.39	122.65	4	2
1	A	432	GLY	C-N-CA	6.09	132.39	122.65	4	2
2	C	160	GLN	OE1-CD-NE2	-6.09	116.51	122.60	13	2
2	B	102	ASP	CA-C-O	6.09	127.00	120.55	7	1
2	B	219	THR	O-C-N	-6.08	115.80	122.07	4	1
2	C	193	ARG	NE-CZ-NH1	-6.08	115.42	121.50	1	4
2	B	109	GLN	CB-CA-C	6.08	120.43	110.88	8	1
2	B	263	ASN	OD1-CG-ND2	-6.08	116.52	122.60	15	3
2	B	203	LEU	CA-C-N	6.08	128.43	120.28	14	3
2	B	203	LEU	C-N-CA	6.08	128.43	120.28	14	3
2	B	260	LYS	N-CA-C	-6.08	105.86	113.28	12	1
1	A	386	LYS	CA-C-N	6.08	132.84	122.37	14	1
1	A	386	LYS	C-N-CA	6.08	132.84	122.37	14	1
2	C	80	GLU	N-CA-C	6.08	117.91	111.28	1	1
2	B	169	GLU	CA-C-O	6.08	127.21	120.82	4	1
1	A	367	SER	N-CA-C	6.08	119.63	111.24	1	5
2	C	180	ALA	CA-C-O	6.08	127.40	120.90	7	1
1	A	456	TRP	O-C-N	-6.08	116.22	123.27	8	2
2	B	227	GLU	CA-C-N	6.08	128.42	120.28	9	2
2	B	227	GLU	C-N-CA	6.08	128.42	120.28	9	2
2	C	162	LYS	CB-CA-C	6.08	120.42	110.88	15	1
2	C	116	ARG	N-CA-CB	6.07	119.69	110.28	14	1
2	B	64	LEU	CA-C-O	6.07	126.84	119.31	6	2
2	C	208	GLY	O-C-N	-6.07	116.30	122.19	8	1
2	B	228	LYS	CA-C-O	6.07	126.98	120.55	3	3
1	A	416	ASP	CA-C-O	-6.07	112.72	120.31	12	3
2	B	94	LYS	CB-CG-CD	6.07	125.26	111.30	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	361	TRP	CB-CG-CD2	-6.07	118.31	126.80	10	2
2	B	249	VAL	CA-C-N	6.06	128.41	120.28	8	2
2	B	249	VAL	C-N-CA	6.06	128.41	120.28	8	2
1	A	415	ILE	CB-CA-C	6.06	117.78	111.23	4	1
1	A	374	ARG	NH1-CZ-NH2	-6.06	111.42	119.30	9	1
1	A	440	GLU	CA-C-O	6.06	126.95	119.79	11	1
1	A	387	HIS	ND1-CE1-NE2	6.06	114.46	108.40	12	3
1	A	500	SER	CB-CA-C	-6.06	102.34	109.80	11	1
1	A	439	ASN	CA-CB-CG	6.06	118.66	112.60	8	2
1	A	374	ARG	CA-C-N	6.06	133.11	121.54	1	3
1	A	374	ARG	C-N-CA	6.06	133.11	121.54	1	3
2	B	193	ARG	CB-CA-C	6.06	120.39	110.88	9	1
2	B	138	ARG	CA-C-N	6.05	128.39	120.28	10	3
2	B	138	ARG	C-N-CA	6.05	128.39	120.28	10	3
2	B	158	GLU	CA-C-O	-6.05	114.14	120.55	7	3
1	A	334	PHE	CA-C-O	6.05	126.90	120.36	14	1
2	B	179	ASP	O-C-N	-6.05	115.25	122.15	9	2
2	B	263	ASN	CB-CA-C	-6.05	99.68	109.72	8	1
1	A	438	PHE	CA-CB-CG	6.05	119.85	113.80	7	1
2	C	95	ALA	CA-C-O	-6.04	113.02	119.97	5	2
1	A	452	ASN	O-C-N	-6.04	115.45	122.95	7	3
2	B	101	LEU	O-C-N	-6.04	115.72	122.12	11	3
2	C	255	LEU	N-CA-C	6.04	117.54	111.07	2	1
1	A	399	TYR	CA-CB-CG	-6.04	103.02	113.90	15	2
2	B	237	ARG	CA-C-O	6.04	126.83	120.42	9	2
2	C	71	PHE	CA-C-O	6.04	126.95	120.55	2	1
2	B	256	GLU	CA-C-N	6.04	128.65	120.38	10	4
2	B	256	GLU	C-N-CA	6.04	128.65	120.38	10	4
2	C	237	ARG	CD-NE-CZ	6.04	132.85	124.40	9	2
1	A	389	VAL	CG1-CB-CG2	-6.04	97.52	110.80	6	1
2	B	153	ARG	CA-C-O	6.03	126.91	119.97	13	2
1	A	408	ARG	NH1-CZ-NH2	-6.03	111.46	119.30	9	3
1	A	406	LEU	CA-C-N	6.03	129.13	120.56	9	2
1	A	406	LEU	C-N-CA	6.03	129.13	120.56	9	2
2	C	247	PHE	O-C-N	-6.03	115.73	122.12	9	2
2	B	104	PHE	N-CA-CB	6.03	118.75	110.01	2	1
1	A	420	PHE	O-C-N	-6.03	115.98	123.04	3	1
2	C	202	ALA	N-CA-CB	-6.03	101.26	110.12	7	2
2	C	173	ARG	CA-C-N	6.03	128.36	120.28	9	2
2	C	173	ARG	C-N-CA	6.03	128.36	120.28	9	2
2	B	114	LEU	CA-C-O	6.03	127.00	120.55	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	90	LEU	N-CA-CB	6.03	118.81	110.07	14	1
2	B	67	VAL	CA-C-O	-6.03	113.25	120.78	7	1
2	B	183	THR	CA-C-O	6.03	126.94	120.55	7	1
2	B	227	GLU	N-CA-CB	6.03	119.08	110.16	7	1
1	A	467	PHE	O-C-N	-6.03	117.17	123.56	6	3
2	C	167	GLY	N-CA-C	6.02	120.18	112.83	2	1
2	B	248	LYS	CA-C-N	6.02	128.71	120.46	5	1
2	B	248	LYS	C-N-CA	6.02	128.71	120.46	5	1
1	A	446	ASP	CA-C-N	6.02	129.38	120.95	12	1
1	A	446	ASP	C-N-CA	6.02	129.38	120.95	12	1
2	B	250	SER	N-CA-C	6.02	117.84	111.28	5	1
2	B	199	ARG	N-CA-CB	-6.02	101.27	110.12	13	2
1	A	486	PHE	CA-C-O	6.02	126.74	120.30	15	1
2	C	136	LEU	CA-C-N	6.02	128.26	120.44	9	1
2	C	136	LEU	C-N-CA	6.02	128.26	120.44	9	1
2	B	80	GLU	N-CA-C	6.01	117.84	111.28	7	1
2	C	147	GLU	N-CA-CB	6.01	118.73	110.01	14	1
1	A	426	LYS	O-C-N	-6.01	116.37	123.22	1	2
2	B	108	TRP	CB-CG-CD1	-6.01	117.89	126.90	2	2
2	C	83	ARG	NE-CZ-NH1	-6.00	115.50	121.50	1	1
2	B	161	GLU	CA-C-O	6.00	126.88	120.70	15	2
2	B	245	GLU	CA-C-N	6.00	128.64	120.54	2	2
2	B	245	GLU	C-N-CA	6.00	128.64	120.54	2	2
1	A	331	GLY	O-C-N	6.00	129.76	122.32	13	1
2	B	62	GLU	O-C-N	-6.00	115.76	122.12	2	1
1	A	462	SER	N-CA-CB	5.99	118.31	111.66	15	2
2	B	56	THR	CA-C-N	5.99	128.23	120.44	14	3
2	B	56	THR	C-N-CA	5.99	128.23	120.44	14	3
2	B	177	HIS	CA-CB-CG	-5.99	107.81	113.80	15	2
2	C	162	LYS	CA-C-O	5.99	126.86	119.79	5	2
1	A	387	HIS	CG-CD2-NE2	5.99	113.19	107.20	3	1
1	A	456	TRP	CB-CG-CD1	5.99	135.88	126.90	11	1
2	B	206	ASN	OD1-CG-ND2	-5.99	116.61	122.60	14	1
1	A	449	TYR	CB-CA-C	5.99	118.07	108.91	15	1
1	A	361	TRP	O-C-N	-5.98	114.50	122.28	4	1
2	B	185	LEU	CA-C-O	5.98	127.10	120.82	14	1
1	A	317	ASN	CA-C-O	-5.98	114.16	120.80	12	2
1	A	493	VAL	CA-CB-CG2	5.98	120.56	110.40	5	1
2	B	104	PHE	CA-C-O	5.98	126.75	120.42	14	3
2	B	126	PHE	CA-C-N	5.97	130.69	120.71	1	2
2	B	126	PHE	C-N-CA	5.97	130.69	120.71	1	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	355	MET	CA-C-O	-5.97	112.87	120.04	15	2
2	B	136	LEU	CA-C-O	5.97	127.08	120.63	1	1
2	C	72	TRP	CA-C-N	5.97	128.20	120.44	3	2
2	C	72	TRP	C-N-CA	5.97	128.20	120.44	3	2
2	C	136	LEU	N-CA-C	5.97	119.40	111.75	10	3
2	C	159	LEU	N-CA-C	-5.97	104.35	111.69	13	1
2	B	195	ARG	CA-C-N	5.97	128.76	120.29	1	2
2	B	195	ARG	C-N-CA	5.97	128.76	120.29	1	2
2	B	147	GLU	N-CA-C	5.97	117.78	111.28	9	2
2	B	242	PRO	CA-C-N	5.97	128.63	120.46	10	3
2	B	242	PRO	C-N-CA	5.97	128.63	120.46	10	3
2	C	157	HIS	CG-CD2-NE2	5.97	113.17	107.20	7	3
2	C	108	TRP	CA-C-N	5.96	128.55	120.44	1	2
2	C	108	TRP	C-N-CA	5.96	128.55	120.44	1	2
2	C	145	ARG	NH1-CZ-NH2	-5.96	111.55	119.30	10	1
2	B	158	GLU	CB-CG-CD	-5.96	102.47	112.60	6	1
2	C	171	ARG	O-C-N	-5.96	115.93	122.07	2	2
2	C	231	PRO	N-CA-C	-5.96	107.05	114.68	6	1
2	B	254	ALA	O-C-N	-5.96	115.36	122.15	11	1
2	B	149	GLN	CA-CB-CG	5.96	126.02	114.10	13	1
1	A	378	LYS	N-CA-C	5.96	119.23	109.76	3	2
2	C	94	LYS	N-CA-C	5.96	117.77	111.28	13	1
2	C	213	GLU	N-CA-C	-5.96	104.70	111.07	10	2
2	B	153	ARG	CB-CA-C	5.96	120.23	110.88	11	1
2	C	101	LEU	O-C-N	-5.95	115.81	122.12	7	1
1	A	426	LYS	CB-CA-C	5.95	120.10	109.38	11	1
1	A	393	ALA	O-C-N	-5.95	114.67	122.59	1	3
2	B	175	ARG	NH1-CZ-NH2	5.95	127.04	119.30	2	2
2	C	105	GLN	O-C-N	-5.95	115.37	122.27	9	1
2	C	86	MET	CA-C-O	-5.95	114.24	120.55	15	1
2	C	130	TRP	CB-CG-CD1	-5.95	117.98	126.90	2	1
1	A	494	GLU	CB-CA-C	5.95	118.84	109.27	3	1
2	C	204	LYS	O-C-N	5.94	128.93	122.15	2	2
2	C	150	GLU	CA-C-N	5.94	127.83	120.34	10	2
2	C	150	GLU	C-N-CA	5.94	127.83	120.34	10	2
1	A	361	TRP	CD2-CE2-CZ2	-5.94	116.46	122.40	9	2
1	A	325	THR	N-CA-C	-5.94	100.11	108.96	12	1
1	A	405	GLU	O-C-N	-5.94	114.47	122.43	8	1
1	A	362	ARG	N-CA-C	5.94	118.13	108.63	15	1
2	B	105	GLN	CA-C-N	5.93	128.15	120.44	15	3
2	B	105	GLN	C-N-CA	5.93	128.15	120.44	15	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	169	GLU	CA-C-N	5.93	128.23	120.28	7	2
2	C	169	GLU	C-N-CA	5.93	128.23	120.28	7	2
1	A	385	ASP	CA-C-N	5.93	132.78	122.81	4	1
1	A	385	ASP	C-N-CA	5.93	132.78	122.81	4	1
1	A	429	PHE	O-C-N	-5.93	116.27	123.27	4	2
2	B	233	LEU	N-CA-C	5.93	117.75	111.28	8	1
1	A	394	SER	O-C-N	-5.93	116.27	123.27	10	1
2	C	156	LEU	O-C-N	-5.93	115.83	122.12	1	2
2	C	194	GLN	OE1-CD-NE2	5.93	128.53	122.60	5	2
1	A	465	GLY	O-C-N	-5.93	114.99	122.70	11	1
2	C	108	TRP	CD2-CE2-CZ2	-5.93	116.47	122.40	15	1
1	A	451	LYS	CA-C-O	-5.93	114.51	121.44	13	2
1	A	403	ILE	N-CA-C	5.93	117.38	110.62	6	1
2	C	238	GLN	CG-CD-NE2	5.93	125.29	116.40	7	1
2	C	232	ALA	N-CA-C	5.92	120.24	112.89	8	1
2	B	170	MET	CA-C-N	5.92	128.22	120.28	1	1
2	B	170	MET	C-N-CA	5.92	128.22	120.28	1	1
2	B	98	GLN	N-CA-C	5.92	120.95	113.25	13	1
1	A	504	ASP	N-CA-C	5.92	117.73	111.28	11	3
1	A	370	THR	CA-C-N	5.92	132.19	121.89	14	2
1	A	370	THR	C-N-CA	5.92	132.19	121.89	14	2
1	A	395	LEU	O-C-N	-5.92	114.78	122.77	7	2
2	C	132	GLU	O-C-N	-5.92	115.41	122.15	9	1
2	C	151	GLY	CA-C-O	5.92	126.84	120.75	9	2
2	C	224	THR	O-C-N	-5.92	115.41	122.15	6	1
2	C	150	GLU	CA-C-O	-5.91	114.56	121.07	10	1
2	C	155	LYS	N-CA-C	5.91	117.72	111.28	1	2
2	B	198	ALA	O-C-N	-5.91	115.85	122.12	4	1
2	B	172	ASP	CA-C-N	5.91	128.12	120.44	1	2
2	B	172	ASP	C-N-CA	5.91	128.12	120.44	1	2
2	B	167	GLY	N-CA-C	5.91	119.35	112.50	15	1
2	C	215	HIS	CA-C-N	5.91	128.47	120.38	7	3
2	C	215	HIS	C-N-CA	5.91	128.47	120.38	7	3
2	B	247	PHE	N-CA-C	5.91	118.23	111.02	11	2
2	C	91	GLU	N-CA-CB	5.91	119.43	110.28	1	2
2	B	155	LYS	N-CA-C	5.91	117.72	111.28	12	3
2	C	201	GLU	CA-C-O	-5.90	114.29	120.55	9	3
1	A	435	TYR	CA-C-O	5.90	127.80	120.54	4	1
2	C	237	ARG	O-C-N	-5.90	115.87	122.12	14	2
2	B	204	LYS	O-C-N	-5.90	115.86	122.12	9	1
2	C	264	THR	N-CA-C	5.90	118.28	109.25	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	56	THR	N-CA-CB	5.90	118.79	110.12	3	2
2	C	166	LEU	O-C-N	-5.90	115.01	122.27	12	1
2	B	202	ALA	N-CA-CB	-5.90	101.21	110.06	7	2
2	B	177	HIS	O-C-N	-5.90	115.02	122.27	10	1
1	A	345	ARG	O-C-N	-5.90	116.67	123.33	3	1
1	A	374	ARG	O-C-N	-5.89	115.78	122.68	5	2
2	C	63	GLN	O-C-N	-5.89	115.67	122.03	12	2
2	B	190	ASP	CA-CB-CG	5.89	118.50	112.60	7	1
1	A	421	TRP	CA-C-N	5.89	129.69	120.97	5	2
1	A	421	TRP	C-N-CA	5.89	129.69	120.97	5	2
2	B	190	ASP	CB-CA-C	5.89	120.13	110.88	8	1
2	B	85	GLU	O-C-N	5.89	128.14	122.07	6	3
2	C	243	VAL	N-CA-CB	5.89	117.44	110.55	11	2
2	C	84	GLN	O-C-N	-5.89	116.00	122.07	11	2
2	C	234	GLU	CB-CA-C	5.89	120.86	110.85	1	1
1	A	455	VAL	CA-C-O	5.89	127.41	121.17	3	1
2	C	108	TRP	CD2-CE3-CZ3	5.89	126.25	118.60	6	1
1	A	490	LYS	CA-C-O	5.89	125.52	119.05	11	1
2	C	175	ARG	N-CA-C	5.88	118.17	111.11	6	1
2	B	252	LEU	N-CA-C	5.88	117.37	111.07	10	1
1	A	368	ILE	CA-CB-CG2	-5.88	100.50	110.50	13	2
2	C	169	GLU	N-CA-CB	-5.88	101.48	110.12	6	3
2	B	210	ARG	CA-C-N	5.88	128.16	120.28	3	1
2	B	210	ARG	C-N-CA	5.88	128.16	120.28	3	1
2	C	234	GLU	CA-C-O	5.88	126.75	120.70	8	2
1	A	434	LYS	CB-CA-C	5.87	120.46	109.71	6	1
2	C	70	GLU	CA-C-O	-5.87	114.32	120.55	10	2
2	B	128	LYS	CA-C-N	5.87	128.43	120.44	10	1
2	B	128	LYS	C-N-CA	5.87	128.43	120.44	10	1
2	B	158	GLU	CA-C-N	5.87	128.15	120.28	14	1
2	B	158	GLU	C-N-CA	5.87	128.15	120.28	14	1
2	B	177	HIS	CB-CG-CD2	-5.87	123.57	131.20	11	1
2	C	154	GLN	N-CA-CB	5.87	118.75	110.12	6	3
1	A	387	HIS	N-CA-C	-5.87	99.78	108.99	15	2
2	C	259	THR	O-C-N	-5.87	115.90	122.12	8	1
2	B	174	ALA	CA-C-O	-5.87	114.33	120.55	13	1
2	B	221	HIS	ND1-CE1-NE2	5.87	114.27	108.40	15	1
2	C	92	GLU	CA-C-N	5.86	128.49	120.46	15	2
2	C	92	GLU	C-N-CA	5.86	128.49	120.46	15	2
1	A	445	VAL	CA-CB-CG1	5.86	120.36	110.40	14	1
2	B	141	VAL	CB-CA-C	5.86	119.72	112.04	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	221	HIS	CG-CD2-NE2	5.86	113.06	107.20	9	1
1	A	460	PRO	N-CA-CB	5.86	108.45	103.35	11	1
1	A	448	GLU	CA-C-O	5.85	126.94	119.16	3	1
2	B	60	LEU	N-CA-C	5.85	117.66	111.28	9	1
2	C	138	ARG	N-CA-C	5.85	118.44	111.71	4	2
2	B	178	VAL	CA-CB-CG1	5.85	120.35	110.40	6	1
2	C	225	LEU	CD1-CG-CD2	5.85	123.67	110.80	13	1
2	B	215	HIS	O-C-N	5.85	128.32	122.12	9	1
1	A	509	PRO	O-C-N	5.84	130.26	123.01	1	1
2	C	196	LEU	O-C-N	-5.84	115.49	122.15	2	3
2	B	68	THR	CA-CB-OG1	5.84	118.37	109.60	8	1
2	C	247	PHE	CA-C-O	5.84	127.15	120.90	13	1
2	B	168	GLU	CA-C-N	5.84	128.43	120.54	14	1
2	B	168	GLU	C-N-CA	5.84	128.43	120.54	14	1
1	A	342	TRP	CB-CG-CD1	-5.84	118.14	126.90	2	1
2	B	81	GLY	O-C-N	5.84	127.79	122.18	7	2
2	C	145	ARG	N-CA-CB	5.84	118.48	110.01	11	1
2	B	164	SER	N-CA-CB	5.84	119.00	110.30	6	2
2	C	80	GLU	N-CA-CB	-5.84	101.54	110.12	15	1
2	C	205	GLU	O-C-N	-5.84	116.06	122.07	1	1
1	A	449	TYR	CA-CB-CG	-5.84	103.40	113.90	5	3
2	B	134	MET	O-C-N	-5.83	115.94	122.12	14	2
2	C	130	TRP	CZ3-CH2-CZ2	-5.83	113.92	121.50	4	1
2	B	62	GLU	CB-CA-C	-5.83	101.72	110.88	12	1
1	A	462	SER	N-CA-C	5.83	122.70	109.81	13	1
2	B	96	LYS	CA-C-O	-5.83	114.37	120.55	7	1
1	A	492	LYS	CA-C-O	-5.83	113.72	120.31	8	2
1	A	407	GLY	CA-C-N	5.83	131.38	122.93	8	2
1	A	407	GLY	C-N-CA	5.83	131.38	122.93	8	2
1	A	402	HIS	O-C-N	-5.83	115.78	122.89	7	1
2	C	260	LYS	N-CA-C	5.83	118.58	111.82	10	1
1	A	392	GLU	O-C-N	5.83	130.34	122.59	15	1
2	B	83	ARG	CA-C-N	5.83	128.01	120.44	4	1
2	B	83	ARG	C-N-CA	5.83	128.01	120.44	4	1
2	C	184	HIS	CE1-NE2-CD2	-5.83	103.17	109.00	11	4
2	C	195	ARG	CD-NE-CZ	5.83	132.56	124.40	5	1
2	B	145	ARG	O-C-N	-5.82	115.32	122.25	6	2
2	B	256	GLU	N-CA-CB	5.82	118.78	110.16	9	1
2	B	105	GLN	OE1-CD-NE2	-5.82	116.78	122.60	10	1
2	C	93	VAL	O-C-N	-5.82	115.84	121.83	13	1
2	C	208	GLY	CA-C-N	5.82	128.55	120.29	5	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	208	GLY	C-N-CA	5.82	128.55	120.29	5	2
1	A	431	ARG	N-CA-C	5.82	117.92	108.26	6	2
2	C	198	ALA	CA-C-O	-5.81	114.39	120.55	9	1
1	A	339	ARG	NH1-CZ-NH2	-5.81	111.75	119.30	3	1
2	B	219	THR	N-CA-CB	5.81	118.76	110.16	3	2
2	C	170	MET	N-CA-CB	-5.81	101.56	110.16	6	1
1	A	469	GLY	CA-C-N	5.81	128.33	120.38	4	2
1	A	469	GLY	C-N-CA	5.81	128.33	120.38	4	2
2	B	180	ALA	CA-C-N	5.80	128.33	120.44	10	3
2	B	180	ALA	C-N-CA	5.80	128.33	120.44	10	3
2	C	102	ASP	CA-C-N	5.80	131.30	121.14	8	1
2	C	102	ASP	C-N-CA	5.80	131.30	121.14	8	1
2	B	78	GLU	CB-CA-C	-5.80	101.16	110.79	9	1
1	A	458	GLY	CA-C-N	5.80	129.47	122.85	3	3
1	A	458	GLY	C-N-CA	5.80	129.47	122.85	3	3
2	B	232	ALA	CA-C-N	5.80	129.13	120.31	13	3
2	B	232	ALA	C-N-CA	5.80	129.13	120.31	13	3
2	C	198	ALA	N-CA-CB	-5.80	100.94	110.40	10	1
2	C	177	HIS	CA-C-N	5.80	127.87	120.56	13	1
2	C	177	HIS	C-N-CA	5.80	127.87	120.56	13	1
2	C	111	GLU	CA-C-N	5.80	127.98	120.44	15	2
2	C	111	GLU	C-N-CA	5.80	127.98	120.44	15	2
2	B	128	LYS	CG-CD-CE	5.80	124.63	111.30	15	1
2	B	195	ARG	O-C-N	5.80	128.04	122.07	5	2
2	C	137	TYR	CB-CA-C	-5.80	101.78	110.88	12	1
1	A	503	ARG	NH1-CZ-NH2	-5.79	111.77	119.30	15	3
2	C	257	GLU	O-C-N	-5.79	116.10	122.07	3	2
1	A	410	LEU	CA-C-O	-5.79	112.93	121.27	6	1
2	C	189	SER	N-CA-C	5.79	117.59	111.28	9	2
2	B	191	GLU	CA-C-N	5.79	128.04	120.28	10	2
2	B	191	GLU	C-N-CA	5.79	128.04	120.28	10	2
1	A	326	VAL	N-CA-C	-5.79	99.72	108.17	12	1
2	C	192	LEU	N-CA-C	5.79	117.67	111.36	4	1
2	B	197	ALA	N-CA-CB	-5.79	101.62	110.01	7	1
1	A	416	ASP	N-CA-C	5.79	119.52	112.23	2	1
2	C	215	HIS	O-C-N	-5.79	116.11	122.07	7	2
1	A	420	PHE	CA-CB-CG	-5.79	108.02	113.80	12	2
1	A	447	SER	CB-CA-C	-5.78	101.17	109.84	4	1
2	C	149	GLN	CB-CA-C	-5.78	101.19	110.79	5	2
1	A	495	PRO	O-C-N	-5.78	115.84	123.01	13	1
2	B	159	LEU	CA-C-N	5.78	128.03	120.28	13	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	159	LEU	C-N-CA	5.78	128.03	120.28	13	1
2	B	155	LYS	CB-CG-CD	5.78	124.59	111.30	13	1
1	A	368	ILE	CA-C-N	5.78	129.09	120.31	4	2
1	A	368	ILE	C-N-CA	5.78	129.09	120.31	4	2
1	A	372	TYR	CA-C-O	5.78	127.41	121.23	4	1
1	A	505	TRP	CB-CG-CD1	5.78	135.56	126.90	2	1
2	C	177	HIS	CA-CB-CG	-5.78	108.02	113.80	12	1
1	A	427	THR	CA-C-O	-5.77	114.28	120.92	3	1
2	B	86	MET	CG-SD-CE	-5.77	88.20	100.90	9	1
2	B	91	GLU	N-CA-C	5.77	118.35	111.71	1	1
2	B	197	ALA	CA-C-O	5.77	127.08	120.90	4	1
2	B	223	SER	CA-C-O	5.77	126.67	120.55	9	1
2	B	116	ARG	NE-CZ-NH1	-5.77	115.73	121.50	3	2
2	B	234	GLU	N-CA-CB	5.77	118.38	110.01	5	2
1	A	386	LYS	CA-C-O	5.77	127.21	120.80	6	2
2	B	263	ASN	O-C-N	-5.77	116.67	123.25	9	1
2	C	119	VAL	N-CA-CB	5.77	119.24	110.58	14	1
1	A	399	TYR	CB-CG-CD2	-5.77	112.15	120.80	5	1
2	C	179	ASP	N-CA-CB	-5.77	101.64	110.12	11	1
2	C	240	LEU	N-CA-C	5.77	120.47	113.38	2	2
2	C	239	GLY	N-CA-C	5.77	121.14	114.16	3	1
1	A	407	GLY	O-C-N	-5.77	117.08	123.66	12	2
2	B	206	ASN	N-CA-C	5.77	117.57	111.28	9	2
2	C	177	HIS	O-C-N	-5.76	116.01	122.12	5	2
2	C	78	GLU	O-C-N	-5.76	116.01	122.12	6	2
1	A	477	PHE	N-CA-CB	5.76	120.77	110.80	4	1
2	B	172	ASP	O-C-N	-5.76	116.01	122.12	1	4
2	B	155	LYS	CB-CA-C	5.76	120.35	110.79	2	1
1	A	372	TYR	CB-CG-CD1	5.76	129.44	120.80	3	1
1	A	372	TYR	O-C-N	-5.76	117.25	123.42	4	2
2	C	87	SER	O-C-N	-5.76	115.58	122.15	13	2
2	B	252	LEU	CA-C-O	5.76	126.87	120.82	10	1
1	A	318	ILE	O-C-N	-5.76	116.05	121.87	11	1
1	A	442	LEU	O-C-N	-5.76	115.41	122.20	7	1
2	B	100	TYR	CG-CD1-CE1	-5.76	112.56	121.20	10	1
2	C	251	PHE	CA-C-O	5.76	126.86	120.82	3	1
1	A	489	GLN	OE1-CD-NE2	-5.75	116.84	122.60	1	1
2	C	65	GLY	CA-C-N	5.75	127.03	119.84	6	1
2	C	65	GLY	C-N-CA	5.75	127.03	119.84	6	1
1	A	340	TRP	O-C-N	-5.75	114.71	122.94	6	1
1	A	454	LYS	CA-C-O	5.75	126.24	119.28	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	187	PRO	O-C-N	5.75	129.64	122.22	6	1
1	A	331	GLY	CA-C-N	5.75	130.94	123.00	8	1
1	A	331	GLY	C-N-CA	5.75	130.94	123.00	8	1
2	C	214	TYR	CB-CG-CD1	-5.75	112.17	120.80	13	1
1	A	473	VAL	N-CA-C	-5.75	107.21	112.96	14	1
2	C	210	ARG	N-CA-C	5.75	117.55	111.28	7	2
1	A	328	MET	O-C-N	-5.75	115.38	122.68	15	2
1	A	367	SER	CA-C-N	5.75	129.22	120.13	2	1
1	A	367	SER	C-N-CA	5.75	129.22	120.13	2	1
2	B	116	ARG	NH1-CZ-NH2	-5.75	111.83	119.30	12	2
1	A	421	TRP	CE2-CD2-CE3	5.75	124.55	118.80	11	1
1	A	475	THR	CA-C-O	5.75	126.65	120.38	13	1
2	B	230	LYS	N-CA-C	5.75	121.44	113.45	10	4
2	C	247	PHE	CB-CA-C	5.75	120.33	110.79	4	1
2	C	167	GLY	CA-C-N	5.75	128.26	120.44	9	1
2	C	167	GLY	C-N-CA	5.75	128.26	120.44	9	1
2	B	148	LEU	N-CA-CB	-5.75	101.67	110.12	10	2
1	A	458	GLY	CA-C-O	5.75	124.17	118.77	12	1
2	B	167	GLY	CA-C-O	-5.75	113.98	120.30	13	1
1	A	388	TRP	CA-C-O	-5.75	114.62	120.71	4	1
2	C	265	GLN	CG-CD-NE2	5.75	125.02	116.40	7	1
2	B	101	LEU	CA-C-O	5.75	126.85	120.82	2	1
1	A	348	GLN	OE1-CD-NE2	-5.75	116.86	122.60	6	1
1	A	467	PHE	CA-CB-CG	5.74	119.54	113.80	5	2
1	A	494	GLU	CB-CG-CD	5.74	122.36	112.60	12	1
2	B	77	LYS	CA-C-O	-5.74	114.79	120.82	3	2
2	B	166	LEU	CA-C-O	5.74	126.51	120.42	11	2
2	B	191	GLU	N-CA-C	5.74	117.54	111.28	11	1
2	C	240	LEU	CA-C-N	5.74	127.95	120.26	14	2
2	C	240	LEU	C-N-CA	5.74	127.95	120.26	14	2
2	B	130	TRP	CA-C-N	5.74	128.24	120.44	2	4
2	B	130	TRP	C-N-CA	5.74	128.24	120.44	2	4
1	A	487	ASN	CA-C-N	5.74	129.03	120.31	6	3
1	A	487	ASN	C-N-CA	5.74	129.03	120.31	6	3
2	C	131	GLN	O-C-N	-5.74	114.77	122.23	13	2
2	C	72	TRP	CD2-CE2-CZ2	5.74	128.14	122.40	10	1
2	B	179	ASP	N-CA-C	5.73	117.53	111.28	7	2
2	B	100	TYR	N-CA-C	5.73	117.53	111.28	7	2
1	A	400	PRO	N-CA-CB	5.73	108.91	102.60	15	1
2	B	208	GLY	CA-C-O	-5.73	113.96	120.09	8	1
2	C	261	LYS	CA-C-O	5.73	126.50	120.42	12	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	189	SER	CA-C-N	5.73	128.28	120.54	7	1
2	C	189	SER	C-N-CA	5.73	128.28	120.54	7	1
1	A	499	LYS	O-C-N	-5.73	116.19	123.24	8	4
2	B	222	LEU	N-CA-C	5.73	117.60	111.36	5	1
2	B	129	LYS	O-C-N	-5.73	114.66	122.33	12	1
2	C	264	THR	O-C-N	-5.73	115.79	123.23	1	2
2	B	215	HIS	CB-CG-CD2	5.73	138.64	131.20	2	2
1	A	507	GLY	CA-C-N	5.73	129.38	120.68	13	1
1	A	507	GLY	C-N-CA	5.73	129.38	120.68	13	1
2	C	89	ASP	CA-C-O	5.72	126.61	120.55	9	2
2	C	253	SER	O-C-N	-5.72	116.06	122.12	9	1
2	C	251	PHE	CA-C-N	5.72	128.41	120.29	6	2
2	C	251	PHE	C-N-CA	5.72	128.41	120.29	6	2
2	B	141	VAL	N-CA-CB	-5.72	102.76	110.54	1	1
2	C	233	LEU	CA-C-N	5.72	127.87	120.44	5	2
2	C	233	LEU	C-N-CA	5.72	127.87	120.44	5	2
1	A	474	PHE	O-C-N	-5.72	116.62	123.31	7	1
2	C	148	LEU	O-C-N	-5.72	116.06	122.12	3	1
1	A	454	LYS	CA-C-N	5.72	127.76	120.56	15	2
1	A	454	LYS	C-N-CA	5.72	127.76	120.56	15	2
2	B	87	SER	CA-C-N	5.72	127.87	120.44	11	2
2	B	87	SER	C-N-CA	5.72	127.87	120.44	11	2
2	B	129	LYS	CA-C-O	-5.72	114.81	120.70	10	1
2	B	240	LEU	O-C-N	-5.72	116.18	122.07	10	1
2	C	168	GLU	CA-C-N	5.71	127.87	120.44	3	1
2	C	168	GLU	C-N-CA	5.71	127.87	120.44	3	1
2	C	154	GLN	CA-C-N	5.71	127.94	120.28	4	1
2	C	154	GLN	C-N-CA	5.71	127.94	120.28	4	1
1	A	456	TRP	CA-C-O	5.71	126.61	120.38	10	1
2	B	122	TYR	CA-CB-CG	-5.71	103.62	113.90	14	1
1	A	488	ASN	CA-C-N	5.71	130.13	120.88	5	1
1	A	488	ASN	C-N-CA	5.71	130.13	120.88	5	1
2	B	237	ARG	CB-CA-C	5.71	120.27	110.79	8	2
2	C	106	LYS	N-CA-CB	5.71	118.51	110.12	6	2
2	B	68	THR	OG1-CB-CG2	-5.71	97.89	109.30	6	2
1	A	349	VAL	CA-C-N	5.71	128.97	120.87	9	2
1	A	349	VAL	C-N-CA	5.71	128.97	120.87	9	2
2	C	238	GLN	CB-CG-CD	5.71	122.30	112.60	11	1
1	A	368	ILE	CA-CB-CG1	5.70	120.09	110.40	4	1
2	C	124	ASP	N-CA-C	5.70	117.50	111.28	6	1
2	B	263	ASN	N-CA-C	5.70	118.54	110.50	13	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	90	LEU	O-C-N	-5.70	116.08	122.12	8	1
2	C	139	GLN	CA-C-O	5.70	126.59	120.55	3	1
1	A	368	ILE	CA-C-O	5.70	127.46	121.59	1	2
2	B	146	ALA	O-C-N	-5.70	115.65	122.15	6	2
2	C	244	LEU	CA-C-N	5.70	127.92	120.28	9	1
2	C	244	LEU	C-N-CA	5.70	127.92	120.28	9	1
2	B	116	ARG	CA-C-O	5.70	126.57	120.70	1	1
2	C	129	LYS	CA-C-O	-5.70	114.51	120.55	5	1
2	B	184	HIS	N-CA-C	5.70	117.57	111.36	7	1
2	B	56	THR	N-CA-C	5.70	117.94	111.11	6	1
2	B	159	LEU	O-C-N	-5.70	116.08	122.12	14	1
2	B	157	HIS	CA-C-N	5.69	127.90	120.28	1	2
2	B	157	HIS	C-N-CA	5.69	127.90	120.28	1	2
2	C	181	LEU	N-CA-C	5.69	117.48	111.28	1	1
1	A	470	SER	CA-C-N	5.69	131.93	122.54	6	1
1	A	470	SER	C-N-CA	5.69	131.93	122.54	6	1
2	B	215	HIS	N-CA-C	5.69	117.48	111.28	6	1
1	A	485	LYS	CA-C-N	5.69	130.57	122.72	2	1
1	A	485	LYS	C-N-CA	5.69	130.57	122.72	2	1
1	A	380	VAL	CA-C-O	5.69	126.62	120.53	14	2
2	C	74	ASN	O-C-N	-5.69	115.57	122.22	7	1
2	C	92	GLU	N-CA-C	5.69	117.48	111.28	10	3
2	C	130	TRP	CE2-CD2-CE3	5.68	124.48	118.80	13	1
2	C	155	LYS	CA-C-N	5.68	127.90	120.28	13	1
2	C	155	LYS	C-N-CA	5.68	127.90	120.28	13	1
1	A	456	TRP	CE2-CD2-CE3	5.68	124.48	118.80	6	1
2	C	78	GLU	CB-CA-C	5.68	119.80	110.88	7	1
2	C	141	VAL	O-C-N	-5.68	115.98	121.83	7	2
1	A	359	GLN	CA-C-O	5.68	126.58	119.59	6	1
2	C	100	TYR	N-CA-CB	-5.68	101.77	110.12	2	1
2	C	160	GLN	CA-C-N	5.68	127.89	120.28	13	1
2	C	160	GLN	C-N-CA	5.68	127.89	120.28	13	1
1	A	452	ASN	CA-C-N	5.67	129.93	120.62	7	2
1	A	452	ASN	C-N-CA	5.67	129.93	120.62	7	2
2	C	193	ARG	O-C-N	-5.67	116.22	122.07	5	1
2	B	94	LYS	CA-C-O	5.67	126.77	120.82	14	2
2	B	252	LEU	CD1-CG-CD2	-5.67	98.32	110.80	10	1
2	C	212	ALA	CA-C-O	5.67	126.56	120.55	2	2
1	A	452	ASN	N-CA-C	5.67	118.57	110.24	15	1
1	A	377	GLY	O-C-N	-5.67	115.29	122.32	11	2
1	A	418	ALA	O-C-N	-5.67	116.58	123.27	14	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	126	PHE	N-CA-CB	-5.67	101.78	110.16	4	1
1	A	461	GLU	N-CA-CB	5.67	118.73	109.95	13	1
1	A	437	ARG	N-CA-C	-5.66	100.47	109.76	10	2
2	B	128	LYS	CA-C-O	-5.66	114.87	120.82	3	1
2	C	123	LEU	CB-CA-C	5.66	120.48	110.85	3	1
2	B	235	ASP	N-CA-C	5.66	117.45	111.28	12	1
2	B	186	ALA	N-CA-C	5.66	121.20	113.16	5	2
2	B	73	ASP	O-C-N	-5.66	115.70	122.15	5	1
1	A	350	MET	CA-C-O	-5.66	115.39	121.56	5	1
2	B	240	LEU	N-CA-CB	-5.66	101.77	110.20	5	1
2	C	127	GLN	CA-C-O	5.66	126.49	120.10	5	1
1	A	495	PRO	CA-C-N	5.66	130.11	121.51	10	1
1	A	495	PRO	C-N-CA	5.66	130.11	121.51	10	1
1	A	443	ARG	N-CA-C	5.66	119.38	111.74	11	1
1	A	363	GLY	O-C-N	-5.66	115.44	122.34	12	1
2	C	210	ARG	O-C-N	-5.66	115.31	122.27	14	1
1	A	320	ASP	CA-CB-CG	5.65	118.25	112.60	4	2
2	C	204	LYS	CA-C-N	5.65	128.17	120.54	12	2
2	C	204	LYS	C-N-CA	5.65	128.17	120.54	12	2
2	B	125	ASP	CA-CB-CG	-5.65	106.95	112.60	3	1
2	B	259	THR	CB-CA-C	-5.65	101.97	110.90	8	1
1	A	363	GLY	CA-C-O	-5.65	112.42	118.86	5	1
2	B	231	PRO	N-CA-CB	5.65	109.18	103.25	10	1
2	B	190	ASP	O-C-N	-5.65	115.99	122.09	1	1
2	B	215	HIS	ND1-CE1-NE2	5.65	114.05	108.40	3	2
2	C	188	TYR	N-CA-CB	-5.65	101.60	110.30	4	2
2	C	79	THR	CA-CB-CG2	5.64	120.10	110.50	4	2
1	A	501	ALA	N-CA-CB	5.64	118.19	110.01	5	1
1	A	487	ASN	CA-C-O	5.64	126.92	120.54	5	1
2	C	172	ASP	CA-CB-CG	5.64	118.24	112.60	5	2
2	B	225	LEU	CA-C-N	5.64	127.78	120.44	6	2
2	B	225	LEU	C-N-CA	5.64	127.78	120.44	6	2
2	B	162	LYS	O-C-N	-5.64	115.77	122.20	15	1
2	C	146	ALA	N-CA-CB	-5.64	101.83	110.12	4	1
1	A	453	ILE	CA-C-N	5.64	132.58	121.58	13	1
1	A	453	ILE	C-N-CA	5.64	132.58	121.58	13	1
1	A	464	ARG	CD-NE-CZ	5.64	132.29	124.40	5	1
2	C	224	THR	N-CA-CB	5.63	118.40	110.12	9	1
1	A	506	MET	CG-SD-CE	-5.63	88.51	100.90	2	4
2	C	168	GLU	O-C-N	-5.63	116.15	122.12	10	1
2	C	213	GLU	O-C-N	-5.63	116.15	122.12	13	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	369	ASN	N-CA-CB	5.63	118.59	110.20	1	1
2	B	127	GLN	CA-C-N	5.63	127.76	120.44	6	2
2	B	127	GLN	C-N-CA	5.63	127.76	120.44	6	2
1	A	444	ALA	N-CA-CB	-5.63	102.50	111.62	11	1
2	B	251	PHE	CA-C-N	5.63	127.82	120.28	5	3
2	B	251	PHE	C-N-CA	5.63	127.82	120.28	5	3
2	B	74	ASN	CA-C-N	5.63	127.75	120.44	3	1
2	B	74	ASN	C-N-CA	5.63	127.75	120.44	3	1
2	B	97	VAL	CA-CB-CG2	-5.62	100.84	110.40	7	1
2	B	256	GLU	CB-CA-C	5.62	119.81	110.81	6	1
2	C	215	HIS	CB-CG-CD2	-5.62	123.89	131.20	6	1
2	C	178	VAL	CA-C-O	-5.62	115.42	121.27	2	1
2	C	210	ARG	CA-C-N	5.62	127.75	120.44	12	2
2	C	210	ARG	C-N-CA	5.62	127.75	120.44	12	2
2	B	157	HIS	N-CA-CB	5.62	118.16	110.01	3	1
1	A	508	CYS	N-CA-C	5.62	116.73	109.65	4	4
2	C	174	ALA	CA-C-O	5.62	126.72	120.82	12	1
2	C	111	GLU	CB-CG-CD	-5.62	103.05	112.60	13	1
2	B	136	LEU	O-C-N	-5.62	116.17	122.12	1	2
1	A	345	ARG	CA-C-N	5.61	130.33	122.36	2	1
1	A	345	ARG	C-N-CA	5.61	130.33	122.36	2	1
2	C	157	HIS	ND1-CG-CD2	5.61	111.71	106.10	11	1
2	B	142	GLU	CB-CG-CD	-5.61	103.06	112.60	3	2
2	B	57	PHE	CA-C-O	-5.61	114.93	120.82	11	1
2	B	261	LYS	N-CA-CB	5.61	118.65	110.47	5	1
2	C	122	TYR	CB-CG-CD1	-5.60	112.39	120.80	8	1
2	C	74	ASN	CB-CG-ND2	-5.60	108.00	116.40	4	1
2	B	176	ALA	N-CA-C	5.60	117.06	111.07	7	1
2	B	225	LEU	N-CA-CB	5.60	118.84	110.22	3	1
1	A	423	PRO	N-CA-C	5.59	122.09	113.75	13	5
2	C	136	LEU	N-CA-CB	5.59	118.32	109.82	7	1
1	A	322	ASN	CB-CG-ND2	5.59	124.79	116.40	7	1
2	B	106	LYS	CA-C-O	-5.59	114.95	120.82	8	1
2	C	84	GLN	CA-C-O	5.59	126.35	120.42	8	1
2	B	196	LEU	N-CA-C	5.59	117.38	111.28	6	1
2	B	192	LEU	N-CA-CB	5.59	118.18	110.07	13	1
2	C	61	ARG	CA-C-O	5.59	126.34	120.42	15	2
2	B	194	GLN	CB-CA-C	5.59	120.07	110.79	5	1
1	A	394	SER	N-CA-C	5.59	117.63	108.52	10	1
2	C	185	LEU	CA-C-N	5.59	127.08	120.09	12	1
2	C	185	LEU	C-N-CA	5.59	127.08	120.09	12	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	91	GLU	CA-C-N	5.59	127.71	120.44	13	1
2	C	91	GLU	C-N-CA	5.59	127.71	120.44	13	1
2	C	240	LEU	O-C-N	-5.59	115.60	122.25	14	1
1	A	444	ALA	N-CA-C	5.59	116.45	108.74	9	1
1	A	396	GLU	CA-C-O	-5.58	114.36	120.17	9	1
1	A	386	LYS	O-C-N	-5.58	116.41	123.17	10	1
2	B	189	SER	CA-C-O	5.58	126.47	120.55	14	1
2	C	71	PHE	N-CA-CB	-5.58	101.62	109.94	3	1
2	C	174	ALA	N-CA-CB	5.58	118.26	109.94	6	1
1	A	323	PHE	CB-CA-C	-5.58	100.45	109.72	10	1
2	C	88	LYS	CB-CA-C	-5.58	102.08	110.90	8	1
2	B	131	GLN	O-C-N	-5.58	116.32	122.07	10	1
2	B	153	ARG	NH1-CZ-NH2	-5.58	112.05	119.30	14	1
2	C	107	LYS	CA-C-N	5.58	128.31	120.28	5	1
2	C	107	LYS	C-N-CA	5.58	128.31	120.28	5	1
2	B	177	HIS	CB-CG-ND1	5.58	131.07	122.70	11	1
1	A	371	ALA	CA-C-O	-5.58	114.74	120.99	15	1
1	A	356	PRO	CA-C-N	5.58	128.08	120.77	15	1
1	A	356	PRO	C-N-CA	5.58	128.08	120.77	15	1
2	B	188	TYR	CG-CD2-CE2	-5.58	112.83	121.20	3	1
1	A	471	ASP	CA-C-N	5.58	130.77	122.74	1	1
1	A	471	ASP	C-N-CA	5.58	130.77	122.74	1	1
2	C	204	LYS	CA-C-O	5.58	126.43	120.24	4	1
2	B	131	GLN	OE1-CD-NE2	5.58	128.18	122.60	15	1
2	B	214	TYR	CA-C-O	5.57	126.46	120.55	11	2
2	C	127	GLN	CA-C-N	5.57	128.02	120.44	7	2
2	C	127	GLN	C-N-CA	5.57	128.02	120.44	7	2
2	C	232	ALA	N-CA-CB	-5.57	101.32	110.40	3	1
2	C	183	THR	O-C-N	5.57	128.02	122.12	12	2
1	A	475	THR	CA-CB-CG2	5.57	119.97	110.50	7	1
2	B	233	LEU	CA-C-O	-5.57	113.56	119.97	10	1
2	B	107	LYS	CA-C-N	5.57	127.74	120.28	12	3
2	B	107	LYS	C-N-CA	5.57	127.74	120.28	12	3
2	B	91	GLU	CA-C-O	5.57	126.39	120.10	9	1
1	A	349	VAL	N-CA-CB	5.57	121.30	110.95	12	1
2	C	134	MET	CA-C-O	5.57	126.23	119.38	8	1
2	C	86	MET	N-CA-C	5.57	118.11	111.71	11	1
1	A	476	TYR	O-C-N	-5.57	116.68	123.30	12	2
2	B	232	ALA	CA-C-O	5.56	126.01	119.28	10	2
2	C	179	ASP	CA-CB-CG	-5.56	107.04	112.60	1	1
1	A	448	GLU	O-C-N	-5.56	116.03	121.87	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	492	LYS	CB-CA-C	-5.56	99.36	110.42	9	1
2	B	257	GLU	N-CA-CB	5.56	118.07	110.01	2	1
2	C	230	LYS	O-C-N	-5.56	115.49	120.71	9	2
1	A	510	SER	CA-C-N	5.56	131.70	121.70	13	1
1	A	510	SER	C-N-CA	5.56	131.70	121.70	13	1
2	B	219	THR	OG1-CB-CG2	-5.56	98.19	109.30	2	1
2	C	206	ASN	OD1-CG-ND2	-5.56	117.04	122.60	2	1
2	C	72	TRP	CE2-CD2-CE3	-5.56	113.24	118.80	10	1
1	A	477	PHE	CB-CG-CD1	5.55	130.14	120.70	8	1
2	C	171	ARG	N-CA-CB	-5.55	101.96	110.12	14	1
2	B	179	ASP	CB-CA-C	5.55	120.01	110.79	2	1
2	B	119	VAL	CA-CB-CG1	5.55	119.84	110.40	12	2
2	B	210	ARG	CB-CG-CD	5.55	124.07	111.30	4	2
1	A	507	GLY	CA-C-O	5.55	126.15	119.82	9	1
2	C	199	ARG	N-CA-CB	-5.55	101.96	110.01	10	1
1	A	376	ASP	CA-C-O	5.55	126.06	119.56	14	1
2	C	96	LYS	CA-C-N	5.55	127.55	120.56	5	2
2	C	96	LYS	C-N-CA	5.55	127.55	120.56	5	2
2	B	75	LEU	CA-C-O	5.55	126.43	120.55	8	1
1	A	437	ARG	NE-CZ-NH2	-5.55	114.21	119.20	12	1
2	B	216	ALA	CA-C-O	-5.55	115.00	120.82	15	1
2	C	215	HIS	CA-CB-CG	5.54	119.34	113.80	6	2
2	B	95	ALA	N-CA-CB	-5.54	101.68	110.22	9	1
2	B	79	THR	CA-C-N	5.54	127.64	120.44	2	1
2	B	79	THR	C-N-CA	5.54	127.64	120.44	2	1
2	C	133	GLU	CA-C-O	5.54	126.42	120.55	2	1
1	A	342	TRP	CB-CA-C	-5.54	99.67	109.70	1	1
2	B	212	ALA	N-CA-CB	-5.54	101.98	110.12	1	1
2	C	71	PHE	CA-C-N	5.54	127.64	120.44	3	1
2	C	71	PHE	C-N-CA	5.54	127.64	120.44	3	1
2	B	235	ASP	N-CA-CB	5.54	118.26	110.12	4	1
2	B	196	LEU	O-C-N	-5.54	116.37	122.07	7	3
2	C	165	PRO	CA-C-N	5.54	127.70	120.28	5	1
2	C	165	PRO	C-N-CA	5.54	127.70	120.28	5	1
2	B	232	ALA	O-C-N	-5.54	116.37	122.07	12	1
2	B	114	LEU	N-CA-C	5.54	117.31	111.28	4	1
1	A	491	LEU	CA-C-N	5.54	132.11	121.54	9	1
1	A	491	LEU	C-N-CA	5.54	132.11	121.54	9	1
1	A	488	ASN	CA-CB-CG	-5.53	107.07	112.60	2	2
2	B	239	GLY	O-C-N	-5.53	116.88	122.19	4	2
2	C	149	GLN	OE1-CD-NE2	-5.53	117.07	122.60	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	219	THR	N-CA-CB	5.53	118.50	110.26	4	1
2	C	229	ALA	CA-C-O	-5.53	112.80	119.49	7	1
1	A	351	ASP	N-CA-CB	-5.53	101.84	109.97	6	1
1	A	351	ASP	CB-CA-C	-5.53	100.73	109.80	8	1
2	C	92	GLU	O-C-N	-5.53	116.38	122.07	3	1
2	C	108	TRP	O-C-N	-5.53	116.26	122.12	12	2
2	B	88	LYS	O-C-N	-5.53	114.51	122.36	15	1
2	C	72	TRP	CB-CG-CD1	-5.53	118.61	126.90	2	2
2	C	125	ASP	CA-C-O	5.53	126.28	120.42	6	2
2	C	185	LEU	N-CA-CB	5.53	118.67	110.49	12	1
2	B	247	PHE	O-C-N	-5.52	116.27	122.12	6	3
2	B	244	LEU	CA-C-O	-5.52	114.70	120.55	14	1
1	A	328	MET	CG-SD-CE	-5.52	88.76	100.90	2	1
2	B	192	LEU	CA-C-O	-5.52	114.57	120.42	7	1
1	A	417	ALA	N-CA-C	5.52	117.18	108.96	1	2
2	C	247	PHE	CA-C-N	5.52	128.46	120.79	15	2
2	C	247	PHE	C-N-CA	5.52	128.46	120.79	15	2
2	C	116	ARG	CD-NE-CZ	5.52	132.12	124.40	13	1
2	B	206	ASN	CB-CG-ND2	5.51	124.67	116.40	1	1
1	A	467	PHE	CB-CG-CD2	-5.51	111.33	120.70	7	1
2	B	247	PHE	N-CA-CB	-5.51	102.07	110.07	15	1
1	A	335	VAL	CA-C-N	5.51	130.33	122.72	4	1
1	A	335	VAL	C-N-CA	5.51	130.33	122.72	4	1
2	C	95	ALA	N-CA-CB	-5.51	101.15	110.41	15	1
1	A	432	GLY	CA-C-O	5.51	130.16	120.57	3	1
2	B	117	GLN	N-CA-CB	-5.51	102.02	110.12	15	1
2	C	115	TYR	N-CA-CB	-5.51	102.03	110.01	1	1
2	B	174	ALA	CA-C-N	5.50	127.92	120.38	15	2
2	B	174	ALA	C-N-CA	5.50	127.92	120.38	15	2
1	A	405	GLU	N-CA-C	5.50	119.26	112.54	15	1
2	B	230	LYS	CA-C-O	-5.50	113.57	118.63	2	3
2	C	230	LYS	CA-C-O	-5.50	113.27	118.33	6	3
1	A	497	TYR	CA-CB-CG	-5.50	104.00	113.90	12	1
2	C	125	ASP	O-C-N	5.50	127.73	122.07	7	1
1	A	509	PRO	CA-C-N	5.50	130.37	122.40	6	4
1	A	509	PRO	C-N-CA	5.50	130.37	122.40	6	4
2	C	64	LEU	CA-C-N	5.50	130.50	121.87	15	2
2	C	64	LEU	C-N-CA	5.50	130.50	121.87	15	2
2	B	91	GLU	CA-C-N	5.50	127.65	120.28	6	2
2	B	91	GLU	C-N-CA	5.50	127.65	120.28	6	2
2	B	96	LYS	CA-C-N	5.50	127.49	120.56	12	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	96	LYS	C-N-CA	5.50	127.49	120.56	12	2
2	B	93	VAL	CA-CB-CG1	-5.50	101.05	110.40	10	1
2	B	166	LEU	N-CA-CB	5.50	118.20	110.12	10	1
2	B	171	ARG	CB-CA-C	-5.50	102.25	110.88	11	1
1	A	468	MET	CA-C-O	5.50	126.96	120.69	2	1
1	A	335	VAL	CA-C-O	-5.50	114.67	120.39	9	1
2	C	187	PRO	N-CA-CB	5.50	109.35	103.52	13	1
2	C	57	PHE	CA-C-N	5.49	127.91	120.38	4	1
2	C	57	PHE	C-N-CA	5.49	127.91	120.38	4	1
1	A	346	ASN	CB-CG-ND2	-5.49	108.16	116.40	9	1
2	C	153	ARG	NH1-CZ-NH2	-5.49	112.17	119.30	3	1
2	B	124	ASP	N-CA-CB	-5.49	102.05	110.12	4	1
2	C	247	PHE	CA-CB-CG	5.49	119.29	113.80	8	1
2	B	66	PRO	N-CA-C	5.49	120.76	113.57	14	1
1	A	398	GLY	N-CA-C	5.48	121.22	114.69	7	1
1	A	424	ASN	N-CA-CB	-5.48	103.30	110.59	5	1
1	A	415	ILE	CA-C-N	5.48	127.56	120.44	6	1
1	A	415	ILE	C-N-CA	5.48	127.56	120.44	6	1
1	A	509	PRO	CA-C-O	5.48	127.33	120.92	12	1
2	B	93	VAL	CA-CB-CG2	-5.48	101.09	110.40	11	1
2	C	140	LYS	O-C-N	-5.48	114.90	122.46	13	1
2	B	257	GLU	CA-C-O	-5.48	115.07	120.82	15	1
2	C	157	HIS	ND1-CE1-NE2	5.48	113.88	108.40	4	3
2	B	64	LEU	N-CA-CB	-5.48	102.07	110.01	8	1
2	B	57	PHE	CA-C-N	5.48	127.62	120.28	12	1
2	B	57	PHE	C-N-CA	5.48	127.62	120.28	12	1
2	C	86	MET	CG-SD-CE	-5.48	88.85	100.90	12	1
2	C	138	ARG	O-C-N	-5.47	116.32	122.12	15	2
2	C	118	LYS	CA-C-N	-5.47	114.53	122.69	13	1
2	C	118	LYS	C-N-CA	-5.47	114.53	122.69	13	1
1	A	470	SER	O-C-N	-5.47	116.32	122.12	11	1
1	A	392	GLU	CA-C-O	-5.47	112.68	120.51	15	1
1	A	477	PHE	CB-CA-C	-5.47	97.95	109.38	15	1
2	C	142	GLU	CA-C-N	5.47	124.99	119.19	5	2
2	C	142	GLU	C-N-CA	5.47	124.99	119.19	5	2
1	A	324	ASP	N-CA-C	5.47	117.32	111.36	7	1
2	B	131	GLN	N-CA-CB	5.46	117.99	110.07	2	1
2	B	225	LEU	N-CA-C	5.46	117.24	111.28	9	3
2	C	240	LEU	N-CA-CB	5.46	118.15	110.12	5	1
1	A	382	PHE	CA-C-O	5.46	126.26	120.36	15	1
2	C	71	PHE	CB-CA-C	5.46	119.54	110.81	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	190	ASP	N-CA-C	5.46	117.98	111.71	13	1
2	B	236	LEU	O-C-N	-5.45	116.45	122.07	1	1
2	B	152	ALA	N-CA-C	5.45	117.67	111.02	5	2
2	C	180	ALA	N-CA-C	5.45	117.30	111.36	13	2
2	C	69	GLN	CA-C-N	5.45	127.59	120.28	10	1
2	C	69	GLN	C-N-CA	5.45	127.59	120.28	10	1
1	A	419	LEU	CA-C-O	5.45	126.13	120.30	3	3
2	C	237	ARG	N-CA-CB	-5.45	102.11	110.12	8	1
1	A	380	VAL	CA-CB-CG2	-5.45	101.14	110.40	1	1
2	C	117	GLN	O-C-N	5.45	128.60	122.22	14	1
2	B	167	GLY	O-C-N	-5.45	116.91	122.19	3	1
1	A	332	GLU	CB-CG-CD	5.45	121.86	112.60	5	1
2	B	210	ARG	N-CA-CB	5.45	118.12	110.12	7	1
1	A	336	PHE	CA-C-O	5.45	126.24	120.36	14	2
2	C	205	GLU	CA-C-N	5.44	130.75	122.37	2	1
2	C	205	GLU	C-N-CA	5.44	130.75	122.37	2	1
2	C	184	HIS	CG-CD2-NE2	5.44	112.64	107.20	1	1
2	C	80	GLU	CB-CA-C	-5.44	101.76	110.79	11	2
2	B	93	VAL	CA-C-N	-5.44	112.99	120.28	10	2
2	B	93	VAL	C-N-CA	-5.44	112.99	120.28	10	2
2	B	184	HIS	CG-CD2-NE2	5.44	112.64	107.20	2	2
2	B	72	TRP	CB-CG-CD1	-5.44	118.75	126.90	15	1
2	B	221	HIS	CE1-NE2-CD2	-5.43	103.56	109.00	15	3
1	A	435	TYR	N-CA-CB	-5.43	102.06	110.65	8	2
1	A	455	VAL	CA-CB-CG1	5.43	119.64	110.40	10	1
2	C	94	LYS	CB-CA-C	5.43	119.81	110.79	14	1
2	C	137	TYR	O-C-N	-5.43	116.44	122.09	15	2
2	B	215	HIS	ND1-CG-CD2	-5.43	100.67	106.10	2	1
2	C	211	LEU	CB-CA-C	5.43	119.50	110.81	8	1
1	A	367	SER	O-C-N	-5.43	115.37	122.59	2	1
1	A	446	ASP	N-CA-CB	-5.43	102.68	110.44	4	1
2	C	263	ASN	CB-CG-ND2	5.43	124.54	116.40	15	1
2	C	199	ARG	CA-C-O	-5.43	114.67	120.42	12	1
1	A	359	GLN	OE1-CD-NE2	5.43	128.03	122.60	2	1
2	B	252	LEU	CA-C-N	5.43	127.49	120.44	2	2
2	B	252	LEU	C-N-CA	5.43	127.49	120.44	2	2
1	A	501	ALA	N-CA-C	5.43	117.19	111.28	6	1
2	C	178	VAL	CA-CB-CG2	-5.43	101.18	110.40	9	1
1	A	414	LYS	N-CA-CB	5.43	120.13	111.56	10	1
2	C	94	LYS	N-CA-CB	-5.43	102.14	110.12	13	1
2	B	175	ARG	N-CA-C	5.42	117.27	111.36	4	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	92	GLU	O-C-N	-5.42	115.60	122.27	11	2
2	C	220	GLU	O-C-N	-5.42	116.37	122.12	5	1
2	B	116	ARG	CA-CB-CG	-5.42	103.25	114.10	8	1
2	C	187	PRO	CB-CA-C	-5.42	103.76	111.68	1	1
1	A	428	TYR	CB-CA-C	-5.42	100.58	109.53	4	1
2	C	56	THR	CA-CB-OG1	5.42	117.73	109.60	5	1
2	C	195	ARG	NH1-CZ-NH2	-5.42	112.25	119.30	4	1
1	A	348	GLN	N-CA-C	-5.42	99.85	109.06	1	1
2	B	83	ARG	O-C-N	-5.42	116.38	122.12	13	3
2	B	214	TYR	CB-CG-CD2	-5.42	112.67	120.80	11	1
2	B	193	ARG	CA-C-N	5.42	127.81	120.44	2	3
2	B	193	ARG	C-N-CA	5.42	127.81	120.44	2	3
2	B	263	ASN	CA-C-O	5.42	128.11	121.56	4	1
2	C	132	GLU	N-CA-C	5.42	117.18	111.28	8	3
2	C	160	GLN	N-CA-C	5.41	117.88	111.33	5	1
1	A	327	ALA	O-C-N	-5.41	116.88	123.10	6	1
2	C	76	GLU	CA-C-N	5.41	127.79	120.65	6	1
2	C	76	GLU	C-N-CA	5.41	127.79	120.65	6	1
1	A	457	GLU	N-CA-CB	5.41	118.04	109.71	12	1
1	A	443	ARG	NH1-CZ-NH2	-5.41	112.27	119.30	10	1
1	A	451	LYS	N-CA-CB	5.41	119.76	110.68	6	1
2	B	213	GLU	N-CA-CB	5.41	118.04	109.82	7	1
2	B	127	GLN	N-CA-CB	-5.41	101.59	110.40	15	1
1	A	508	CYS	CB-CA-C	-5.41	100.94	109.42	3	1
2	B	75	LEU	N-CA-CB	5.41	117.85	110.01	3	1
1	A	484	TRP	CA-C-O	5.40	126.27	120.32	3	2
2	B	69	GLN	O-C-N	5.40	127.65	122.03	14	1
2	B	139	GLN	OE1-CD-NE2	-5.40	117.20	122.60	9	1
2	B	64	LEU	O-C-N	-5.40	116.39	122.12	10	1
2	B	130	TRP	O-C-N	-5.40	115.99	122.15	14	2
2	B	234	GLU	N-CA-C	5.40	117.17	111.28	4	2
2	B	223	SER	O-C-N	-5.40	116.51	122.07	10	2
1	A	413	ASP	CA-C-O	5.40	128.23	120.51	11	1
2	C	139	GLN	N-CA-CB	5.40	119.20	110.40	11	2
1	A	481	ASN	CA-C-O	5.40	126.34	119.16	8	2
2	C	55	SER	O-C-N	-5.40	114.36	123.00	1	1
1	A	431	ARG	CA-C-O	5.40	126.56	119.98	9	2
2	B	123	LEU	N-CA-CB	5.40	117.84	110.01	12	1
2	C	135	GLU	CA-C-N	5.39	127.51	120.28	14	1
2	C	135	GLU	C-N-CA	5.39	127.51	120.28	14	1
1	A	343	ARG	CD-NE-CZ	5.39	131.95	124.40	2	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	475	THR	CA-C-N	5.39	130.44	123.00	13	1
1	A	475	THR	C-N-CA	5.39	130.44	123.00	13	1
2	B	247	PHE	CA-C-N	5.39	127.45	120.44	12	1
2	B	247	PHE	C-N-CA	5.39	127.45	120.44	12	1
2	C	213	GLU	N-CA-CB	-5.39	102.18	110.16	15	1
1	A	341	PHE	CB-CA-C	5.39	122.04	110.45	5	1
2	C	200	LEU	N-CA-C	5.39	117.16	111.28	5	1
1	A	345	ARG	CA-C-O	-5.39	114.13	120.60	7	1
2	B	122	TYR	CA-C-O	5.39	126.48	120.82	11	1
1	A	330	ARG	CA-C-N	5.39	130.71	121.07	13	1
1	A	330	ARG	C-N-CA	5.39	130.71	121.07	13	1
2	B	136	LEU	CB-CA-C	-5.39	102.42	110.88	9	1
2	B	89	ASP	N-CA-CB	-5.38	102.19	110.16	5	1
2	C	203	LEU	CB-CA-C	-5.38	102.20	110.81	13	1
1	A	448	GLU	CA-C-N	5.38	134.22	123.56	12	1
1	A	448	GLU	C-N-CA	5.38	134.22	123.56	12	1
2	C	210	ARG	NH1-CZ-NH2	-5.38	112.31	119.30	4	3
2	C	261	LYS	O-C-N	-5.38	116.42	122.12	4	1
2	B	65	GLY	CA-C-N	5.38	124.71	118.85	7	1
2	B	65	GLY	C-N-CA	5.38	124.71	118.85	7	1
1	A	341	PHE	O-C-N	-5.38	116.19	122.96	3	2
1	A	369	ASN	N-CA-C	5.38	117.83	111.33	3	1
2	B	126	PHE	N-CA-CB	5.38	117.81	110.01	7	1
2	C	168	GLU	N-CA-CB	5.38	118.03	110.12	10	1
2	C	129	LYS	CA-CB-CG	5.38	124.85	114.10	9	1
2	C	203	LEU	CA-C-O	-5.37	114.03	120.10	9	1
1	A	417	ALA	CA-C-O	-5.37	114.98	120.89	11	1
1	A	334	PHE	O-C-N	-5.37	116.90	123.30	14	1
2	C	213	GLU	CA-C-O	5.37	126.23	120.70	6	1
2	B	194	GLN	N-CA-CB	-5.37	102.20	110.20	8	1
1	A	342	TRP	O-C-N	-5.37	116.25	123.23	8	1
1	A	411	PRO	CB-CA-C	5.37	118.38	111.56	7	2
1	A	319	CYS	O-C-N	-5.37	115.94	122.22	13	2
1	A	400	PRO	N-CD-CG	5.37	110.24	103.80	2	1
2	C	178	VAL	N-CA-CB	5.37	116.47	110.51	3	1
2	C	82	LEU	CA-C-N	5.37	128.47	120.31	13	2
2	C	82	LEU	C-N-CA	5.37	128.47	120.31	13	2
1	A	455	VAL	O-C-N	5.36	127.86	121.80	7	1
2	C	238	GLN	CA-CB-CG	5.36	124.83	114.10	9	1
1	A	376	ASP	CA-CB-CG	5.36	117.96	112.60	12	1
2	B	73	ASP	N-CA-CB	-5.36	102.22	110.16	1	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	167	GLY	O-C-N	-5.36	115.73	122.70	6	1
1	A	448	GLU	N-CA-CB	5.36	119.55	110.49	7	1
1	A	390	PHE	N-CA-C	-5.36	100.17	108.90	12	1
1	A	342	TRP	N-CA-CB	5.36	118.91	110.56	15	2
2	B	172	ASP	N-CA-CB	5.36	118.08	110.16	14	1
2	C	249	VAL	O-C-N	-5.36	116.66	121.91	14	1
2	C	125	ASP	CB-CA-C	-5.36	100.90	110.70	15	1
1	A	436	TYR	CB-CA-C	-5.35	102.80	110.62	7	2
1	A	329	LEU	O-C-N	-5.35	116.05	123.12	7	2
1	A	445	VAL	O-C-N	-5.35	116.96	122.63	4	3
2	B	150	GLU	CB-CA-C	5.35	119.28	110.88	13	1
2	C	264	THR	CA-C-O	5.35	126.14	120.36	14	1
1	A	343	ARG	NH1-CZ-NH2	-5.35	112.34	119.30	11	1
2	B	101	LEU	N-CA-CB	5.35	117.76	110.01	2	1
1	A	493	VAL	CB-CA-C	5.35	120.04	111.32	4	1
1	A	381	PHE	O-C-N	5.35	129.60	123.29	6	1
2	B	225	LEU	CD1-CG-CD2	-5.35	99.03	110.80	8	1
2	C	103	ASP	CA-CB-CG	-5.35	107.25	112.60	10	1
2	B	119	VAL	CA-C-N	5.35	128.88	120.97	7	2
2	B	119	VAL	C-N-CA	5.35	128.88	120.97	7	2
2	C	65	GLY	N-CA-C	5.34	123.24	112.34	5	3
1	A	413	ASP	CB-CA-C	5.34	121.05	110.42	6	2
2	C	93	VAL	CA-CB-CG2	-5.34	101.32	110.40	3	1
2	B	170	MET	CB-CA-C	5.34	119.76	110.68	12	1
1	A	475	THR	OG1-CB-CG2	-5.34	98.62	109.30	2	2
1	A	416	ASP	O-C-N	-5.34	116.32	122.09	4	2
2	C	109	GLN	CG-CD-NE2	5.34	124.41	116.40	7	1
2	C	201	GLU	CB-CG-CD	5.34	121.68	112.60	15	1
2	C	238	GLN	O-C-N	-5.34	116.46	122.12	3	2
2	C	147	GLU	CG-CD-OE2	5.34	130.67	118.40	11	1
2	B	194	GLN	O-C-N	-5.33	116.48	122.03	11	1
2	B	229	ALA	CB-CA-C	-5.33	102.47	110.90	2	1
2	B	112	MET	O-C-N	-5.33	116.58	122.07	3	1
2	B	131	GLN	CA-C-N	5.33	127.43	120.28	6	1
2	B	131	GLN	C-N-CA	5.33	127.43	120.28	6	1
1	A	322	ASN	O-C-N	-5.33	115.94	122.55	8	1
2	C	240	LEU	CA-C-O	5.33	125.73	119.28	10	1
2	C	211	LEU	CA-C-N	5.33	127.43	120.28	12	1
2	C	211	LEU	C-N-CA	5.33	127.43	120.28	12	1
1	A	360	PHE	N-CA-C	-5.33	105.84	112.93	2	1
2	B	164	SER	CB-CA-C	-5.33	102.84	112.76	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	394	SER	N-CA-CB	5.33	118.96	110.65	15	1
1	A	324	ASP	CA-C-O	5.33	126.41	120.82	3	1
1	A	325	THR	N-CA-CB	5.33	120.42	110.99	5	2
2	B	118	LYS	CB-CG-CD	5.33	123.55	111.30	4	1
2	B	58	SER	N-CA-CB	5.33	118.04	110.16	9	1
2	B	65	GLY	O-C-N	-5.33	116.44	121.77	9	1
2	B	126	PHE	CA-C-O	5.33	126.60	120.90	9	1
2	C	169	GLU	O-C-N	-5.32	116.59	122.07	1	1
2	C	228	LYS	N-CA-C	5.32	117.77	111.33	9	1
2	B	88	LYS	CB-CA-C	-5.32	101.96	110.79	1	1
2	B	195	ARG	N-CA-CB	5.32	117.94	110.12	10	1
2	C	229	ALA	CB-CA-C	-5.32	101.81	110.85	1	1
1	A	504	ASP	CA-CB-CG	-5.32	107.28	112.60	8	1
2	B	58	SER	CA-C-N	5.32	127.40	120.28	10	1
2	B	58	SER	C-N-CA	5.32	127.40	120.28	10	1
1	A	421	TRP	N-CA-CB	-5.31	102.43	110.77	3	2
2	C	139	GLN	O-C-N	-5.31	116.49	122.12	3	2
1	A	326	VAL	CA-C-O	-5.31	114.64	120.43	12	1
2	B	123	LEU	N-CA-C	5.31	116.75	111.07	15	1
2	C	264	THR	CA-C-N	5.31	131.26	121.70	4	1
2	C	264	THR	C-N-CA	5.31	131.26	121.70	4	1
2	C	135	GLU	CB-CA-C	5.31	119.61	110.79	13	1
2	C	193	ARG	CD-NE-CZ	-5.31	116.97	124.40	3	1
2	B	89	ASP	CB-CG-OD2	-5.31	106.19	118.40	13	1
2	B	109	GLN	O-C-N	-5.30	116.50	122.12	10	2
1	A	492	LYS	O-C-N	-5.30	116.89	123.36	14	1
2	B	62	GLU	N-CA-C	5.30	117.06	111.28	2	1
2	B	225	LEU	CB-CA-C	-5.30	100.83	110.63	3	1
2	B	183	THR	CA-CB-CG2	-5.30	101.49	110.50	4	1
2	C	155	LYS	O-C-N	-5.29	116.62	122.07	9	1
1	A	350	MET	N-CA-CB	5.29	117.79	110.17	2	1
1	A	438	PHE	CB-CA-C	5.29	118.56	109.51	5	1
2	B	134	MET	CA-C-O	5.29	126.38	120.82	5	1
2	B	73	ASP	CB-CA-C	5.29	119.58	110.79	12	1
1	A	323	PHE	O-C-N	-5.29	116.52	122.97	5	1
2	C	256	GLU	CA-C-N	5.29	127.63	120.44	6	1
2	C	256	GLU	C-N-CA	5.29	127.63	120.44	6	1
2	B	215	HIS	CB-CG-ND1	-5.29	114.77	122.70	14	1
1	A	439	ASN	CB-CA-C	5.29	118.60	110.62	5	1
1	A	380	VAL	N-CA-CB	5.29	118.51	111.64	11	1
2	C	209	ALA	CA-C-O	5.29	126.03	119.79	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	161	GLU	O-C-N	-5.28	116.52	122.12	6	1
2	C	78	GLU	CA-CB-CG	-5.28	103.53	114.10	6	1
1	A	391	ASP	CB-CA-C	5.28	119.40	110.79	9	1
2	B	55	SER	N-CA-CB	5.28	119.48	110.50	2	1
2	B	88	LYS	N-CA-C	5.28	117.03	111.28	1	1
1	A	387	HIS	CB-CG-ND1	5.28	130.62	122.70	6	1
1	A	366	ALA	CA-C-O	5.28	127.31	121.56	12	1
2	C	191	GLU	CA-CB-CG	5.28	124.66	114.10	12	1
1	A	380	VAL	CA-C-N	5.28	131.28	122.73	4	1
1	A	380	VAL	C-N-CA	5.28	131.28	122.73	4	1
2	C	190	ASP	CA-C-N	5.28	127.35	120.28	4	1
2	C	190	ASP	C-N-CA	5.28	127.35	120.28	4	1
2	C	143	PRO	CB-CA-C	-5.28	104.41	112.11	7	1
2	B	100	TYR	O-C-N	-5.27	116.53	122.12	4	2
1	A	464	ARG	NH1-CZ-NH2	-5.27	112.44	119.30	8	1
2	C	206	ASN	O-C-N	-5.27	115.62	122.37	12	1
2	B	234	GLU	O-C-N	-5.27	116.64	122.07	3	1
2	B	238	GLN	CA-C-O	5.27	125.85	119.31	4	1
2	B	153	ARG	N-CA-C	5.27	116.71	111.07	8	1
2	B	133	GLU	CA-C-N	5.27	127.29	120.44	13	1
2	B	133	GLU	C-N-CA	5.27	127.29	120.44	13	1
2	C	74	ASN	CA-C-O	5.27	126.13	120.55	6	1
2	B	139	GLN	N-CA-CB	5.27	117.96	110.16	13	1
2	B	218	ALA	CA-C-O	5.26	126.53	120.90	3	1
1	A	473	VAL	CA-C-O	5.26	127.36	120.78	4	1
1	A	497	TYR	CG-CD2-CE2	-5.26	113.31	121.20	6	1
1	A	437	ARG	CA-C-N	5.26	129.98	122.72	9	1
1	A	437	ARG	C-N-CA	5.26	129.98	122.72	9	1
2	C	108	TRP	CE2-CD2-CE3	5.26	124.06	118.80	15	1
2	B	171	ARG	CD-NE-CZ	-5.26	117.04	124.40	3	1
1	A	456	TRP	CG-CD2-CE3	-5.26	128.64	133.90	6	1
1	A	365	PRO	N-CA-CB	5.25	108.77	103.25	12	1
2	C	263	ASN	O-C-N	-5.25	116.04	122.34	1	1
1	A	502	LEU	CA-C-O	-5.25	113.93	119.97	5	1
2	C	250	SER	O-C-N	5.25	127.48	122.07	6	1
1	A	451	LYS	O-C-N	-5.25	116.54	123.16	10	1
2	B	137	TYR	CA-C-O	5.25	126.12	120.55	12	1
2	B	261	LYS	CA-C-N	5.25	127.74	120.29	2	1
2	B	261	LYS	C-N-CA	5.25	127.74	120.29	2	1
2	C	160	GLN	CB-CG-CD	5.25	121.52	112.60	1	2
1	A	320	ASP	N-CA-C	-5.25	106.38	112.89	5	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	177	HIS	CG-CD2-NE2	5.25	112.45	107.20	10	1
2	C	211	LEU	N-CA-C	5.25	117.00	111.28	11	1
2	C	184	HIS	N-CA-CB	-5.24	102.40	110.16	14	1
2	C	239	GLY	CA-C-O	5.24	125.70	120.09	6	1
2	B	240	LEU	CA-C-N	5.24	126.64	120.09	8	1
2	B	240	LEU	C-N-CA	5.24	126.64	120.09	8	1
2	B	79	THR	OG1-CB-CG2	-5.24	98.82	109.30	3	1
2	C	120	GLU	CB-CA-C	5.24	120.49	110.17	3	1
2	B	71	PHE	CA-C-O	5.24	126.10	120.55	6	1
1	A	477	PHE	CB-CG-CD2	-5.24	111.80	120.70	8	1
2	B	180	ALA	N-CA-CB	-5.24	102.42	110.01	4	1
2	C	73	ASP	O-C-N	-5.24	116.57	122.12	5	1
2	B	208	GLY	O-C-N	-5.24	116.11	122.71	13	1
1	A	328	MET	N-CA-C	5.24	117.15	108.20	2	1
2	C	81	GLY	CA-C-N	5.24	127.55	120.38	14	1
2	C	81	GLY	C-N-CA	5.24	127.55	120.38	14	1
2	B	200	LEU	O-C-N	-5.24	116.57	122.12	15	1
2	C	226	SER	N-CA-CB	-5.23	102.16	110.22	7	1
2	C	157	HIS	CB-CG-ND1	5.23	130.55	122.70	1	1
2	B	247	PHE	CB-CG-CD1	-5.23	111.81	120.70	9	1
2	C	118	LYS	CA-CB-CG	5.23	124.56	114.10	10	1
1	A	474	PHE	CB-CG-CD1	-5.23	111.81	120.70	14	1
2	B	183	THR	CB-CA-C	-5.23	102.64	110.90	2	1
1	A	366	ALA	O-C-N	-5.23	116.38	122.81	4	1
1	A	453	ILE	CA-CB-CG2	-5.23	101.61	110.50	8	1
2	B	162	LYS	CA-C-N	5.23	127.24	120.44	9	1
2	B	162	LYS	C-N-CA	5.23	127.24	120.44	9	1
2	B	196	LEU	N-CA-CB	5.23	117.80	110.12	5	2
1	A	402	HIS	CA-CB-CG	-5.23	108.57	113.80	10	1
2	B	100	TYR	CB-CA-C	5.23	119.09	110.88	11	1
1	A	339	ARG	CA-C-N	5.23	130.73	122.36	15	1
1	A	339	ARG	C-N-CA	5.23	130.73	122.36	15	1
2	C	226	SER	CA-CB-OG	5.23	121.55	111.10	1	1
1	A	406	LEU	O-C-N	-5.23	115.33	122.33	9	1
2	B	264	THR	CA-C-O	-5.23	116.12	121.87	11	1
2	B	219	THR	CA-CB-CG2	5.22	119.38	110.50	1	1
2	C	199	ARG	NH1-CZ-NH2	-5.22	112.51	119.30	10	2
2	B	214	TYR	N-CA-CB	5.22	117.80	110.12	8	1
1	A	478	TYR	CB-CG-CD2	-5.22	112.97	120.80	9	1
2	B	70	GLU	N-CA-C	5.22	116.97	111.28	9	1
1	A	380	VAL	N-CA-C	-5.22	100.96	108.53	12	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	456	TRP	CA-C-N	5.22	128.51	121.05	1	1
1	A	456	TRP	C-N-CA	5.22	128.51	121.05	1	1
2	C	122	TYR	CA-C-O	5.22	125.95	120.42	1	2
1	A	347	ASN	CB-CG-ND2	5.22	124.23	116.40	2	1
2	B	257	GLU	O-C-N	-5.22	116.69	122.07	2	1
2	B	107	LYS	N-CA-C	5.22	116.97	111.28	3	2
1	A	474	PHE	CA-C-O	5.22	127.57	121.46	12	2
2	C	69	GLN	N-CA-CB	5.22	117.89	110.16	13	1
2	C	171	ARG	CG-CD-NE	-5.22	100.52	112.00	14	1
2	C	211	LEU	O-C-N	-5.22	116.69	122.07	15	1
2	B	104	PHE	O-C-N	-5.22	116.20	122.15	11	2
1	A	342	TRP	CA-CB-CG	5.22	123.51	113.60	10	1
2	B	101	LEU	CB-CA-C	-5.22	102.69	110.88	7	1
2	C	97	VAL	CA-CB-CG1	5.21	119.26	110.40	15	2
2	B	144	LEU	N-CA-CB	-5.21	102.17	109.94	8	1
1	A	469	GLY	O-C-N	-5.21	116.50	122.91	10	1
2	C	222	LEU	CB-CA-C	5.21	119.15	110.81	11	1
1	A	481	ASN	OD1-CG-ND2	-5.21	117.39	122.60	12	1
2	B	144	LEU	N-CA-C	5.21	118.80	112.23	6	1
2	C	169	GLU	CA-C-O	5.21	126.29	120.82	1	1
2	C	249	VAL	CA-C-O	5.21	126.69	121.17	12	1
1	A	327	ALA	CA-C-O	5.21	126.62	120.89	13	1
2	B	146	ALA	CA-C-N	5.21	128.94	120.60	13	1
2	B	146	ALA	C-N-CA	5.21	128.94	120.60	13	1
2	B	152	ALA	CA-C-O	5.21	125.94	120.42	14	1
2	C	188	TYR	N-CA-C	5.21	117.64	111.33	7	1
1	A	318	ILE	CB-CA-C	5.21	119.41	112.22	8	1
2	C	92	GLU	N-CA-CB	-5.21	102.45	110.16	2	1
2	C	180	ALA	O-C-N	-5.21	116.70	122.07	2	1
2	C	221	HIS	O-C-N	5.21	128.09	122.15	8	2
2	C	76	GLU	CA-C-O	5.21	126.29	120.82	10	1
1	A	362	ARG	NH1-CZ-NH2	-5.21	112.53	119.30	11	1
2	C	153	ARG	N-CA-CB	5.21	117.56	110.01	11	1
2	B	56	THR	N-CA-CB	5.21	117.87	110.16	12	1
2	C	146	ALA	N-CA-C	5.21	117.63	111.33	12	1
2	C	248	LYS	CA-C-O	5.21	125.94	120.42	12	1
2	B	228	LYS	N-CA-CB	-5.20	102.47	110.12	9	1
1	A	434	LYS	CA-C-O	5.20	126.82	120.99	12	1
2	C	255	LEU	CB-CA-C	5.20	119.05	110.88	1	1
2	C	183	THR	CA-C-O	5.20	125.93	119.79	3	1
2	B	184	HIS	CB-CG-ND1	5.20	130.50	122.70	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	61	ARG	CA-CB-CG	5.20	124.50	114.10	12	1
1	A	379	PHE	CA-CB-CG	-5.20	108.60	113.80	13	1
2	B	118	LYS	CA-CB-CG	-5.20	103.70	114.10	5	1
1	A	361	TRP	NE1-CE2-CD2	5.20	114.16	107.40	11	1
2	C	80	GLU	O-C-N	-5.20	116.48	122.09	2	1
2	C	83	ARG	N-CA-CB	5.20	117.54	110.01	2	1
1	A	362	ARG	NE-CZ-NH2	-5.20	114.53	119.20	10	1
1	A	460	PRO	N-CD-CG	5.19	110.99	103.20	4	1
2	B	259	THR	CA-CB-CG2	5.19	119.33	110.50	3	1
2	C	194	GLN	CB-CG-CD	5.19	121.43	112.60	15	1
1	A	412	THR	CA-CB-OG1	5.19	117.39	109.60	2	1
2	B	73	ASP	N-CA-C	5.19	116.62	111.07	10	2
1	A	384	GLY	CA-C-N	5.19	131.10	122.54	14	2
1	A	384	GLY	C-N-CA	5.19	131.10	122.54	14	2
1	A	343	ARG	CG-CD-NE	-5.19	100.59	112.00	3	2
1	A	510	SER	N-CA-CB	5.19	119.25	110.49	13	1
1	A	459	ILE	CA-CB-CG1	5.18	119.21	110.40	15	1
1	A	398	GLY	O-C-N	-5.18	115.77	122.25	6	2
2	B	224	THR	CA-C-O	-5.18	115.36	120.70	4	1
2	B	59	LYS	CA-C-O	5.18	125.91	120.42	7	1
2	B	150	GLU	CA-C-O	5.18	126.04	120.55	8	1
1	A	432	GLY	O-C-N	-5.18	115.97	122.70	3	1
2	B	216	ALA	O-C-N	-5.18	116.74	122.07	10	1
2	B	116	ARG	O-C-N	-5.18	116.74	122.07	15	1
2	B	183	THR	CA-CB-OG1	5.17	117.36	109.60	5	1
1	A	408	ARG	N-CA-CB	5.17	117.62	110.17	11	1
2	B	240	LEU	CA-C-O	5.17	126.03	120.70	11	1
2	B	228	LYS	O-C-N	-5.17	116.25	122.15	8	1
2	B	265	GLN	OE1-CD-NE2	-5.17	117.43	122.60	10	1
2	B	169	GLU	CA-C-N	5.17	127.21	120.28	6	1
2	B	169	GLU	C-N-CA	5.17	127.21	120.28	6	1
2	C	156	LEU	N-CA-CB	5.17	117.50	110.01	10	1
1	A	441	GLU	CB-CA-C	-5.17	99.19	109.99	1	1
2	C	82	LEU	N-CA-C	5.17	117.65	111.71	5	2
1	A	388	TRP	CD2-CE2-CZ2	-5.17	117.23	122.40	9	2
1	A	339	ARG	N-CA-C	-5.17	106.22	112.88	12	1
2	B	68	THR	O-C-N	-5.17	116.72	122.09	12	1
2	C	87	SER	CA-C-N	5.17	127.16	120.44	14	1
2	C	87	SER	C-N-CA	5.17	127.16	120.44	14	1
2	C	191	GLU	CA-C-N	5.17	128.16	120.31	14	1
2	C	191	GLU	C-N-CA	5.17	128.16	120.31	14	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	483	TYR	O-C-N	-5.17	116.89	123.24	15	1
1	A	333	MET	CA-CB-CG	5.16	124.43	114.10	3	1
2	B	209	ALA	CA-C-N	5.16	127.15	120.44	6	1
2	B	209	ALA	C-N-CA	5.16	127.15	120.44	6	1
2	C	188	TYR	CB-CA-C	5.16	120.58	110.67	10	1
2	C	80	GLU	CA-C-O	-5.16	115.08	120.55	11	1
1	A	418	ALA	CB-CA-C	-5.16	100.62	109.65	8	1
2	C	63	GLN	CA-CB-CG	5.16	124.42	114.10	12	1
1	A	430	PHE	CA-C-O	-5.16	115.07	120.80	14	1
2	B	256	GLU	O-C-N	-5.16	116.65	122.12	15	1
2	C	172	ASP	CB-CA-C	5.16	119.62	110.85	7	1
2	B	89	ASP	CA-C-O	5.16	125.89	120.42	9	1
2	C	172	ASP	CA-C-O	5.16	126.24	120.82	15	1
1	A	362	ARG	CB-CA-C	5.16	117.58	110.16	3	1
1	A	398	GLY	CA-C-O	5.16	124.53	118.96	9	1
2	B	97	VAL	CA-C-N	5.15	126.17	119.78	5	1
2	B	97	VAL	C-N-CA	5.15	126.17	119.78	5	1
1	A	349	VAL	CA-CB-CG1	-5.15	101.64	110.40	6	1
2	B	107	LYS	CB-CA-C	5.15	119.05	110.81	8	1
1	A	360	PHE	CA-C-N	5.15	130.16	122.23	10	1
1	A	360	PHE	C-N-CA	5.15	130.16	122.23	10	1
2	B	242	PRO	N-CD-CG	5.15	110.93	103.20	15	1
1	A	481	ASN	CA-CB-CG	-5.15	107.45	112.60	5	1
2	B	56	THR	CB-CA-C	5.15	119.34	110.79	2	1
2	B	243	VAL	CB-CA-C	5.15	119.14	112.24	8	1
1	A	366	ALA	N-CA-C	5.15	116.57	110.19	10	1
2	C	59	LYS	CB-CG-CD	5.15	123.14	111.30	9	1
2	C	251	PHE	CB-CA-C	5.14	118.95	110.88	4	1
2	C	110	GLU	CB-CA-C	-5.14	102.80	110.88	7	1
1	A	329	LEU	CA-C-N	5.14	129.86	122.40	11	1
1	A	329	LEU	C-N-CA	5.14	129.86	122.40	11	1
2	B	190	ASP	CA-C-N	5.14	128.12	120.31	7	2
2	B	190	ASP	C-N-CA	5.14	128.12	120.31	7	2
2	B	127	GLN	N-CA-C	5.14	116.88	111.28	14	1
2	B	156	LEU	CB-CA-C	-5.14	102.82	110.88	6	1
1	A	410	LEU	N-CA-C	-5.14	102.57	110.58	8	2
2	B	112	MET	CA-CB-CG	-5.13	103.83	114.10	6	1
2	B	55	SER	O-C-N	-5.13	114.78	123.00	9	1
2	B	132	GLU	CA-C-O	-5.13	115.43	120.82	1	1
1	A	442	LEU	N-CA-CB	5.13	119.45	110.98	6	1
2	B	75	LEU	CB-CA-C	5.13	118.94	110.88	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	99	PRO	N-CA-C	-5.13	107.05	114.18	10	1
1	A	486	PHE	N-CA-C	5.13	116.78	108.41	15	1
2	C	128	LYS	CA-C-O	5.13	125.99	120.55	4	1
2	C	119	VAL	CA-CB-CG1	5.13	119.12	110.40	9	1
1	A	398	GLY	CA-C-N	5.13	132.29	123.11	4	1
1	A	398	GLY	C-N-CA	5.13	132.29	123.11	4	1
1	A	466	SER	N-CA-C	5.13	116.32	108.42	13	1
2	B	156	LEU	O-C-N	-5.13	116.68	122.12	13	1
1	A	390	PHE	CB-CA-C	5.13	118.34	110.14	2	1
2	C	145	ARG	O-C-N	-5.13	116.31	122.15	8	1
1	A	383	LYS	CA-C-O	5.13	126.45	120.20	9	1
2	C	249	VAL	N-CA-C	5.13	115.34	110.42	13	1
2	C	248	LYS	O-C-N	-5.12	116.79	122.07	1	1
2	C	135	GLU	O-C-N	-5.12	116.69	122.12	14	1
2	C	81	GLY	CA-C-O	-5.12	115.47	121.00	9	1
1	A	362	ARG	CA-CB-CG	5.12	124.34	114.10	10	1
2	B	117	GLN	O-C-N	-5.12	115.39	122.46	11	1
2	B	205	GLU	N-CA-CB	5.12	117.40	109.98	15	1
1	A	454	LYS	N-CA-CB	5.12	117.89	110.47	5	1
1	A	487	ASN	N-CA-CB	5.12	118.97	110.47	11	1
2	C	244	LEU	O-C-N	-5.12	116.69	122.12	7	1
2	B	93	VAL	N-CA-C	5.12	115.84	110.62	2	1
2	B	71	PHE	O-C-N	5.12	127.54	122.12	4	1
1	A	509	PRO	N-CA-CB	-5.12	98.19	103.15	7	1
2	B	189	SER	CB-CA-C	-5.12	102.30	110.79	8	1
1	A	489	GLN	N-CA-C	5.12	116.55	110.97	14	1
1	A	447	SER	N-CA-C	5.11	117.58	109.96	9	1
2	B	153	ARG	N-CA-CB	-5.11	102.35	110.28	15	1
2	C	194	GLN	CA-C-N	5.11	127.13	120.28	5	1
2	C	194	GLN	C-N-CA	5.11	127.13	120.28	5	1
2	C	109	GLN	CG-CD-OE1	5.11	131.02	120.80	13	1
2	C	250	SER	CB-CA-C	-5.11	101.99	110.68	13	1
2	B	123	LEU	O-C-N	5.11	127.97	122.15	3	1
2	C	153	ARG	CB-CG-CD	5.11	123.05	111.30	4	1
2	C	160	GLN	N-CA-CB	5.11	117.42	110.01	8	1
2	B	255	LEU	CA-C-O	-5.11	115.46	120.82	2	1
2	B	260	LYS	N-CA-CB	5.11	117.81	110.20	4	1
1	A	420	PHE	CA-C-O	-5.11	114.71	120.43	5	1
1	A	333	MET	CA-C-O	5.11	125.95	120.38	9	1
2	B	55	SER	CA-CB-OG	5.11	121.31	111.10	10	1
2	B	86	MET	CA-C-O	5.11	125.21	119.18	10	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	63	GLN	CB-CG-CD	5.11	121.28	112.60	13	1
2	C	122	TYR	N-CA-CB	-5.11	102.60	110.16	13	1
2	B	168	GLU	CB-CA-C	5.11	118.90	110.88	3	1
1	A	463	PRO	N-CA-C	5.11	122.99	112.47	12	1
1	A	357	ILE	CA-CB-CG2	5.10	119.18	110.50	1	1
1	A	363	GLY	N-CA-C	-5.10	107.75	114.95	9	1
2	C	62	GLU	CB-CA-C	5.10	118.97	110.81	14	1
2	B	246	SER	CB-CA-C	-5.10	102.84	110.90	3	1
1	A	329	LEU	CB-CA-C	-5.10	102.47	110.79	15	1
2	C	107	LYS	N-CA-CB	5.10	117.62	110.12	2	1
2	C	74	ASN	CA-CB-CG	5.10	117.70	112.60	12	2
2	C	117	GLN	CG-CD-NE2	5.10	124.05	116.40	3	1
1	A	484	TRP	CZ3-CH2-CZ2	-5.10	114.87	121.50	7	1
2	B	111	GLU	N-CA-C	5.10	116.83	111.28	7	2
1	A	369	ASN	CA-CB-CG	5.10	117.70	112.60	13	2
1	A	497	TYR	CB-CA-C	5.09	116.48	108.63	10	1
1	A	503	ARG	O-C-N	-5.09	116.72	122.12	13	1
2	B	212	ALA	O-C-N	-5.09	116.79	122.09	14	2
1	A	435	TYR	O-C-N	-5.09	116.74	123.21	13	1
1	A	481	ASN	N-CA-CB	5.09	119.19	114.10	1	1
1	A	429	PHE	N-CA-CB	5.09	118.88	110.69	6	2
1	A	476	TYR	CA-C-O	5.09	125.86	120.36	12	1
2	B	251	PHE	O-C-N	5.09	127.51	122.12	13	1
1	A	445	VAL	N-CA-C	5.09	116.57	109.80	8	2
2	B	152	ALA	N-CA-CB	-5.09	102.64	110.01	6	1
2	B	211	LEU	CA-C-O	5.09	126.16	120.82	7	1
2	C	116	ARG	CA-CB-CG	5.09	124.27	114.10	14	1
2	C	142	GLU	CB-CA-C	-5.08	102.34	112.05	15	1
2	C	123	LEU	N-CA-C	5.08	116.90	111.36	2	1
1	A	391	ASP	O-C-N	-5.08	117.00	123.05	5	1
2	C	79	THR	O-C-N	-5.08	116.73	122.12	2	1
2	B	262	LEU	O-C-N	-5.08	115.20	122.41	11	1
1	A	387	HIS	CA-C-N	5.08	130.54	122.62	13	1
1	A	387	HIS	C-N-CA	5.08	130.54	122.62	13	1
2	C	216	ALA	CA-C-N	5.08	127.50	120.29	13	1
2	C	216	ALA	C-N-CA	5.08	127.50	120.29	13	1
2	B	130	TRP	CB-CA-C	-5.08	102.91	110.88	1	1
2	B	231	PRO	CB-CA-C	5.08	119.52	112.11	5	1
1	A	469	GLY	N-CA-C	5.08	119.04	112.54	3	1
1	A	338	GLU	CB-CA-C	-5.08	110.74	116.63	5	2
2	B	203	LEU	N-CA-C	5.08	116.81	111.28	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	473	VAL	CA-CB-CG1	5.08	119.03	110.40	13	1
2	B	56	THR	CA-CB-CG2	5.07	119.12	110.50	6	1
2	B	232	ALA	N-CA-C	5.07	116.50	111.07	6	1
2	C	190	ASP	CA-C-O	5.07	125.93	120.55	14	1
2	B	205	GLU	O-C-N	-5.07	116.56	122.03	15	1
2	C	224	THR	N-CA-C	5.07	116.49	111.07	3	1
1	A	387	HIS	N-CA-CB	5.07	120.94	111.52	15	1
2	B	84	GLN	OE1-CD-NE2	5.07	127.67	122.60	6	1
2	C	68	THR	N-CA-CB	5.07	117.57	110.12	12	1
2	C	126	PHE	CB-CG-CD1	-5.06	112.09	120.70	4	1
1	A	388	TRP	CE2-CD2-CG	-5.06	101.12	107.20	12	1
1	A	485	LYS	CB-CA-C	5.06	118.59	110.29	3	1
2	C	258	TYR	O-C-N	-5.06	116.86	122.07	10	1
2	B	215	HIS	CB-CA-C	-5.06	102.93	110.88	2	1
2	C	107	LYS	CA-C-O	5.06	125.78	120.42	3	1
2	B	157	HIS	CA-C-O	5.06	125.91	120.55	14	1
2	B	70	GLU	N-CA-CB	5.06	117.65	110.16	15	1
2	B	245	GLU	CB-CG-CD	5.06	121.20	112.60	1	1
2	C	85	GLU	CA-CB-CG	5.06	124.22	114.10	3	1
1	A	391	ASP	CA-CB-CG	-5.06	107.54	112.60	11	2
2	B	220	GLU	CA-C-O	-5.06	115.69	121.00	6	1
1	A	478	TYR	CA-C-O	5.05	125.89	120.38	4	1
2	B	69	GLN	N-CA-CB	-5.05	102.69	110.12	6	2
2	C	258	TYR	CD1-CG-CD2	5.05	125.68	118.10	4	1
1	A	471	ASP	CB-CA-C	5.05	118.53	110.09	7	1
1	A	489	GLN	CA-C-O	5.05	125.51	119.60	12	1
2	B	98	GLN	N-CA-CB	-5.05	104.46	110.42	5	1
2	B	237	ARG	CA-C-N	5.05	129.97	121.14	12	1
2	B	237	ARG	C-N-CA	5.05	129.97	121.14	12	1
2	C	174	ALA	O-C-N	-5.04	116.64	122.09	10	1
2	B	244	LEU	N-CA-C	5.04	116.46	111.07	5	1
2	C	168	GLU	CA-C-O	-5.04	115.08	120.42	11	1
2	C	117	GLN	OE1-CD-NE2	-5.04	117.56	122.60	3	1
2	B	210	ARG	O-C-N	-5.04	116.41	122.15	3	2
1	A	337	LYS	CB-CA-C	-5.04	103.79	110.79	7	1
2	B	251	PHE	CA-C-O	5.04	125.73	119.79	15	1
1	A	490	LYS	O-C-N	5.03	129.15	122.26	2	1
2	B	237	ARG	NH1-CZ-NH2	-5.03	112.76	119.30	8	1
2	C	153	ARG	CD-NE-CZ	5.03	131.44	124.40	8	1
1	A	443	ARG	CA-C-O	-5.03	116.14	122.03	12	1
2	B	214	TYR	O-C-N	-5.03	116.79	122.12	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	244	LEU	CB-CA-C	5.03	118.77	110.88	2	1
2	C	164	SER	CA-CB-OG	5.03	121.16	111.10	5	1
2	B	207	GLY	O-C-N	-5.03	117.31	122.19	11	1
2	C	253	SER	CA-CB-OG	-5.03	101.05	111.10	11	1
2	B	62	GLU	N-CA-CB	5.03	117.30	110.01	12	1
2	C	104	PHE	CB-CA-C	5.03	120.42	110.42	12	1
2	B	75	LEU	O-C-N	-5.03	116.79	122.12	15	1
2	B	163	LEU	CA-C-O	-5.02	114.19	119.97	13	1
2	B	67	VAL	N-CA-CB	5.02	116.09	110.51	9	1
2	C	248	LYS	CB-CA-C	-5.02	102.46	110.79	14	1
2	B	103	ASP	CB-CA-C	-5.02	102.46	110.79	4	1
2	C	140	LYS	N-CA-CB	5.02	118.58	110.40	5	1
2	B	91	GLU	N-CA-CB	5.02	117.29	110.01	11	1
2	C	141	VAL	CA-CB-CG2	-5.01	101.88	110.40	4	1
1	A	430	PHE	CB-CA-C	-5.01	100.19	109.37	5	1
2	C	126	PHE	N-CA-C	5.01	117.14	111.02	5	1
2	B	173	ARG	N-CA-CB	5.01	117.49	110.12	6	1
1	A	389	VAL	O-C-N	-5.01	117.46	123.03	11	1
1	A	450	PRO	N-CD-CG	5.01	109.82	103.80	1	1
2	B	169	GLU	O-C-N	5.01	127.43	122.12	1	1
2	C	148	LEU	CA-C-O	5.01	125.86	120.55	3	1
2	B	209	ALA	N-CA-CB	-5.01	102.75	110.12	4	1
2	C	206	ASN	CA-C-O	-5.01	113.37	119.43	14	1
2	B	141	VAL	CA-C-O	-5.01	115.74	120.95	1	1
2	C	175	ARG	CA-C-N	5.01	127.49	120.28	12	1
2	C	175	ARG	C-N-CA	5.01	127.49	120.28	12	1
2	B	179	ASP	N-CA-CB	5.01	117.27	110.01	11	1
2	C	61	ARG	CB-CG-CD	5.01	122.82	111.30	14	1
2	C	147	GLU	CA-CB-CG	-5.01	104.09	114.10	5	1
1	A	421	TRP	N-CA-C	5.00	116.84	108.23	6	1
2	B	85	GLU	CB-CG-CD	5.00	121.11	112.60	7	1
2	B	170	MET	CG-SD-CE	-5.00	89.89	100.90	7	1
1	A	385	ASP	CA-C-O	5.00	125.85	119.95	9	1
1	A	478	TYR	CD1-CG-CD2	5.00	125.60	118.10	9	1
2	B	65	GLY	CA-C-O	-5.00	114.37	121.52	14	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	478	TYR	Sidechain	11
1	A	503	ARG	Sidechain	10
2	B	100	TYR	Sidechain	8
1	A	374	ARG	Sidechain	7
1	A	476	TYR	Sidechain	7
2	B	145	ARG	Sidechain	7
2	C	115	TYR	Sidechain	7
1	A	428	TYR	Sidechain	6
1	A	483	TYR	Sidechain	6
2	B	137	TYR	Sidechain	6
2	B	214	TYR	Sidechain	6
2	B	237	ARG	Sidechain	6
2	C	100	TYR	Sidechain	6
2	C	116	ARG	Sidechain	6
2	B	115	TYR	Sidechain	6
1	A	399	TYR	Sidechain,Peptide	5
2	B	193	ARG	Sidechain	5
2	C	199	ARG	Sidechain	5
1	A	362	ARG	Sidechain	5
2	C	122	TYR	Sidechain	5
1	A	353	TYR	Sidechain	4
1	A	464	ARG	Sidechain	4
1	A	497	TYR	Sidechain	4
2	C	237	ARG	Sidechain	4
2	B	122	TYR	Sidechain	4
1	A	339	ARG	Sidechain	4
1	A	390	PHE	Sidechain	4
2	B	83	ARG	Sidechain	4
2	B	199	ARG	Sidechain	4
2	B	258	TYR	Sidechain	4
2	C	210	ARG	Sidechain	4
1	A	408	ARG	Sidechain	4
1	A	436	TYR	Sidechain	4
2	C	138	ARG	Sidechain	4
2	B	138	ARG	Sidechain	3
1	A	372	TYR	Sidechain	3
1	A	431	ARG	Sidechain	3
2	C	83	ARG	Sidechain	3
2	C	145	ARG	Sidechain	3
2	C	214	TYR	Sidechain	3
1	A	343	ARG	Sidechain	3
2	C	195	ARG	Sidechain	3
1	A	429	PHE	Sidechain	3

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	330	ARG	Sidechain	3
2	B	210	ARG	Sidechain	3
2	C	61	ARG	Sidechain	3
1	A	435	TYR	Sidechain	3
2	C	175	ARG	Sidechain	3
2	B	116	ARG	Sidechain	3
2	C	251	PHE	Sidechain	3
1	A	420	PHE	Sidechain	2
1	A	486	PHE	Sidechain	2
2	B	153	ARG	Sidechain	2
2	B	157	HIS	Sidechain	2
2	C	177	HIS	Sidechain	2
2	B	104	PHE	Sidechain	2
2	B	171	ARG	Sidechain	2
2	C	182	ARG	Sidechain	2
1	A	508	CYS	Peptide	2
1	A	443	ARG	Sidechain	2
2	C	104	PHE	Sidechain	2
2	C	153	ARG	Sidechain	2
2	B	173	ARG	Sidechain	2
2	B	175	ARG	Sidechain	2
2	C	126	PHE	Sidechain	2
2	C	188	TYR	Sidechain	2
1	A	402	HIS	Sidechain	2
2	B	182	ARG	Sidechain	2
1	A	437	ARG	Sidechain	2
2	B	188	TYR	Sidechain	2
2	B	195	ARG	Sidechain	2
1	A	387	HIS	Sidechain	2
2	C	215	HIS	Sidechain	2
1	A	449	TYR	Sidechain	1
1	A	490	LYS	Peptide	1
2	B	155	LYS	Mainchain	1
1	A	345	ARG	Sidechain	1
2	B	61	ARG	Sidechain	1
2	B	263	ASN	Peptide	1
2	C	193	ARG	Sidechain	1
2	C	71	PHE	Sidechain	1
2	C	157	HIS	Sidechain	1
1	A	381	PHE	Sidechain	1
2	B	57	PHE	Sidechain	1
2	C	235	ASP	Sidechain	1

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Mol	Chain	Res	Type	Group	Models (Total)
2	B	126	PHE	Sidechain	1
2	B	251	PHE	Sidechain	1
2	C	57	PHE	Sidechain	1
2	C	73	ASP	Mainchain	1
1	A	382	PHE	Sidechain	1
1	A	474	PHE	Sidechain	1
2	C	137	TYR	Sidechain	1
1	A	379	PHE	Sidechain	1
1	A	469	GLY	Peptide	1
2	B	177	HIS	Sidechain	1
2	C	258	TYR	Sidechain	1
2	B	184	HIS	Sidechain	1
2	C	171	ARG	Sidechain	1
1	A	341	PHE	Sidechain	1
1	A	334	PHE	Sidechain	1
2	B	215	HIS	Sidechain	1
1	A	430	PHE	Sidechain	1
2	B	71	PHE	Sidechain	1

6.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1637	1565	1563	3±1
2	B	1753	1745	1742	2±1
2	C	1753	1745	1742	2±2
3	A	2208	3456	3456	32±5
3	B	4600	7200	7200	53±7
3	C	3220	5040	5040	35±5
All	All	227595	311265	311145	1694

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:618:PX4:H12	3:A:644:PX4:H13	0.80	1.50	9	1
3:A:627:PX4:H3	3:A:627:PX4:O4	0.78	1.77	3	3
3:C:363:PX4:O4	3:C:363:PX4:H3	0.74	1.82	11	1
2:C:55:SER:N	2:C:58:SER:HG	0.72	1.82	5	3
3:B:356:PX4:H9	3:C:303:PX4:O2	0.72	1.84	11	2
3:A:610:PX4:H12	3:A:629:PX4:O6	0.72	1.83	14	1
3:C:333:PX4:O3	3:C:360:PX4:H4	0.72	1.84	14	6
3:B:398:PX4:H4	3:B:399:PX4:O8	0.72	1.85	6	4
3:A:620:PX4:O4	3:A:620:PX4:H3	0.71	1.86	15	4
3:C:326:PX4:O4	3:C:345:PX4:H3	0.71	1.85	8	1
3:B:379:PX4:H4	3:B:391:PX4:O4	0.70	1.86	8	5
3:A:601:PX4:H6	3:B:381:PX4:O4	0.70	1.85	11	1
3:B:332:PX4:O3	3:B:332:PX4:H9	0.69	1.88	6	1
3:C:326:PX4:H14	3:C:345:PX4:H3	0.69	1.63	11	1
3:A:619:PX4:O4	3:A:619:PX4:H3	0.68	1.88	2	3
3:A:608:PX4:O1	3:A:608:PX4:H4	0.68	1.86	15	1
3:B:309:PX4:H3	3:B:335:PX4:O2	0.68	1.88	4	3
3:C:309:PX4:O2	3:C:344:PX4:H5	0.68	1.88	5	1
3:B:399:PX4:H8	3:C:356:PX4:C6	0.68	2.18	11	1
3:B:312:PX4:H52	3:B:317:PX4:H8	0.68	1.63	3	1
1:A:511:GLY:OXT	3:A:648:PX4:H11	0.67	1.90	1	3
3:B:398:PX4:O4	3:B:398:PX4:H3	0.67	1.90	8	4
3:B:329:PX4:H4	3:B:341:PX4:O2	0.66	1.90	3	1
3:B:356:PX4:O4	3:B:370:PX4:H3	0.66	1.90	7	2
1:A:494:GLU:OE1	3:A:646:PX4:H4	0.66	1.90	7	2
3:A:609:PX4:O4	3:A:609:PX4:H7	0.66	1.91	15	1
3:B:399:PX4:H4	3:C:336:PX4:O6	0.66	1.91	10	1
1:A:494:GLU:OE2	3:A:643:PX4:H6	0.65	1.91	3	3
3:A:620:PX4:O6	3:A:620:PX4:H6	0.65	1.92	3	3
3:C:309:PX4:O2	3:C:344:PX4:H4	0.65	1.92	7	1
3:B:379:PX4:O4	3:B:385:PX4:H13	0.65	1.92	11	2
3:C:364:PX4:O2	3:C:369:PX4:H4	0.65	1.91	5	1
3:A:634:PX4:O1	3:A:634:PX4:H3	0.65	1.91	7	1
3:B:391:PX4:H3	3:B:391:PX4:O4	0.65	1.91	4	1
3:A:608:PX4:H4	3:B:394:PX4:O3	0.65	1.92	9	2
3:A:618:PX4:C5	3:A:644:PX4:H13	0.65	2.22	9	1
3:B:330:PX4:O1	3:B:330:PX4:H3	0.65	1.92	11	3
3:B:303:PX4:H13	3:B:303:PX4:H17	0.64	1.69	13	1
3:B:382:PX4:H13	3:B:382:PX4:O2	0.64	1.92	10	2
1:A:490:LYS:O	3:A:635:PX4:H4	0.64	1.92	8	5
1:A:457:GLU:OE2	3:A:636:PX4:H10	0.64	1.93	2	1
3:B:391:PX4:O1	3:B:395:PX4:H13	0.64	1.93	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:636:PX4:O4	3:A:640:PX4:H4	0.64	1.92	1	2
3:A:644:PX4:O4	3:A:648:PX4:H3	0.64	1.91	14	5
3:A:631:PX4:O1	3:A:631:PX4:H3	0.64	1.93	9	2
3:C:306:PX4:H4	3:C:348:PX4:O2	0.64	1.92	11	2
3:C:317:PX4:O4	3:C:355:PX4:H3	0.63	1.93	7	8
3:A:610:PX4:H7	3:C:368:PX4:O6	0.63	1.92	7	1
3:B:338:PX4:H4	3:B:357:PX4:O8	0.63	1.93	8	1
3:A:619:PX4:H4	3:A:631:PX4:O3	0.63	1.92	14	1
3:C:321:PX4:H8	3:C:356:PX4:O2	0.63	1.93	14	1
3:B:368:PX4:O2	3:B:368:PX4:H7	0.63	1.92	9	1
3:A:612:PX4:C6	3:A:612:PX4:H3	0.63	2.23	10	1
3:B:335:PX4:O4	3:B:360:PX4:H8	0.63	1.93	10	1
3:B:327:PX4:H3	3:B:352:PX4:O2	0.63	1.94	3	3
3:C:333:PX4:H3	3:C:360:PX4:O3	0.63	1.93	12	3
3:B:338:PX4:O2	3:B:363:PX4:H3	0.63	1.93	4	2
3:B:324:PX4:O2	3:B:352:PX4:H4	0.63	1.93	12	4
3:A:611:PX4:H4	3:C:337:PX4:O1	0.63	1.93	8	2
3:C:364:PX4:O1	3:C:364:PX4:H3	0.63	1.93	7	1
3:A:610:PX4:H3	3:A:615:PX4:O8	0.63	1.94	15	2
3:C:369:PX4:H9	3:C:369:PX4:O1	0.63	1.93	6	1
3:B:390:PX4:O3	3:B:395:PX4:H9	0.63	1.94	1	1
3:B:390:PX4:O4	3:B:395:PX4:H4	0.63	1.93	14	7
3:C:319:PX4:O4	3:C:323:PX4:H8	0.63	1.94	6	1
3:A:620:PX4:H4	3:A:632:PX4:O4	0.63	1.94	7	1
3:A:619:PX4:H5	3:A:635:PX4:O3	0.63	1.93	14	1
3:B:337:PX4:O4	3:B:337:PX4:H3	0.62	1.93	15	1
3:B:356:PX4:H16	3:B:370:PX4:H3	0.62	1.69	1	1
3:B:309:PX4:O2	3:B:335:PX4:H9	0.62	1.94	12	1
3:B:315:PX4:H3	3:B:328:PX4:O2	0.62	1.95	2	3
3:B:356:PX4:H7	3:C:303:PX4:O3	0.62	1.94	2	1
3:B:391:PX4:O1	3:B:391:PX4:H3	0.62	1.94	5	2
3:C:316:PX4:H3	3:C:333:PX4:O1	0.61	1.95	2	1
3:B:351:PX4:H3	3:B:379:PX4:O1	0.61	1.95	7	1
3:C:342:PX4:O2	3:C:368:PX4:H5	0.61	1.95	7	1
3:B:396:PX4:O8	3:B:396:PX4:H4	0.61	1.95	2	1
3:B:341:PX4:C1	3:B:364:PX4:H13	0.61	2.24	13	1
2:B:72:TRP:CZ2	3:B:305:PX4:H9	0.61	2.30	14	1
3:A:615:PX4:O1	3:A:629:PX4:H3	0.61	1.95	15	1
3:B:305:PX4:O3	3:B:305:PX4:H7	0.61	1.95	5	3
3:C:319:PX4:H7	3:C:334:PX4:O1	0.61	1.94	14	3
3:C:327:PX4:H9	3:C:327:PX4:O3	0.61	1.96	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:322:PX4:H3	3:B:332:PX4:O6	0.61	1.95	7	1
3:C:307:PX4:O3	3:C:307:PX4:H9	0.61	1.95	10	2
3:B:339:PX4:O2	3:B:339:PX4:H4	0.60	1.96	9	2
3:A:605:PX4:O1	3:A:607:PX4:H4	0.60	1.97	13	1
3:B:340:PX4:O2	3:B:340:PX4:H4	0.60	1.96	2	2
3:A:612:PX4:H4	3:C:358:PX4:O2	0.60	1.95	14	1
3:B:364:PX4:H45	3:B:382:PX4:H57	0.60	1.71	1	1
3:B:329:PX4:O1	3:B:329:PX4:H9	0.60	1.95	3	1
3:B:373:PX4:H4	3:B:373:PX4:O4	0.60	1.97	5	4
3:A:604:PX4:H11	3:B:384:PX4:O2	0.60	1.97	10	1
3:B:308:PX4:O2	3:C:302:PX4:H4	0.60	1.96	8	2
3:B:379:PX4:H9	3:B:391:PX4:O2	0.60	1.96	9	6
3:B:313:PX4:O1	3:B:313:PX4:H4	0.60	1.97	11	1
3:A:623:PX4:O2	3:A:630:PX4:H4	0.60	1.97	1	1
3:B:392:PX4:O2	3:B:393:PX4:H10	0.60	1.97	7	2
3:B:304:PX4:H4	3:C:301:PX4:O2	0.59	1.96	9	2
3:B:327:PX4:O3	3:B:327:PX4:H9	0.59	1.97	6	1
3:B:341:PX4:H4	3:B:364:PX4:O1	0.59	1.97	10	1
3:A:626:PX4:O4	3:C:365:PX4:H11	0.59	1.97	2	1
3:B:390:PX4:O2	3:B:395:PX4:H7	0.59	1.97	14	1
3:B:384:PX4:H3	3:B:384:PX4:O1	0.59	1.97	15	3
3:B:342:PX4:O1	3:B:360:PX4:H11	0.59	1.98	5	1
3:A:625:PX4:O2	3:A:636:PX4:H6	0.59	1.97	7	1
3:B:386:PX4:H4	3:B:392:PX4:O1	0.59	1.98	6	1
3:B:379:PX4:O2	3:B:379:PX4:H10	0.59	1.96	9	1
3:A:612:PX4:H9	3:C:351:PX4:O1	0.59	1.97	1	1
3:B:378:PX4:O4	3:C:305:PX4:H11	0.59	1.97	3	1
3:C:345:PX4:O2	3:C:364:PX4:H4	0.59	1.97	10	1
3:B:352:PX4:H11	3:B:369:PX4:O8	0.59	1.97	11	2
3:A:618:PX4:H3	3:A:618:PX4:O1	0.59	1.97	14	1
3:A:609:PX4:H3	3:A:609:PX4:O1	0.59	1.98	1	1
3:A:638:PX4:O6	3:A:648:PX4:H4	0.59	1.96	14	9
3:B:379:PX4:H3	3:B:391:PX4:O2	0.59	1.98	3	1
3:A:614:PX4:O2	3:C:340:PX4:H3	0.59	1.96	8	2
3:A:645:PX4:O1	3:A:645:PX4:H7	0.59	1.98	9	2
3:A:627:PX4:O1	3:A:632:PX4:H9	0.59	1.97	14	1
3:A:605:PX4:O8	3:A:607:PX4:H4	0.59	1.98	9	6
3:B:323:PX4:H3	3:B:323:PX4:O4	0.59	1.98	4	1
3:B:352:PX4:H4	3:B:369:PX4:O8	0.59	1.96	15	1
3:B:390:PX4:H9	3:B:390:PX4:O1	0.59	1.96	2	2
3:A:627:PX4:O3	3:A:632:PX4:H7	0.59	1.98	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:633:PX4:H5	3:C:370:PX4:O6	0.59	1.97	9	2
3:B:337:PX4:O1	3:B:362:PX4:H7	0.59	1.97	12	1
3:B:314:PX4:O2	3:B:334:PX4:H6	0.59	1.97	15	1
3:B:345:PX4:O2	3:B:345:PX4:H4	0.59	1.97	12	2
3:C:326:PX4:C6	3:C:345:PX4:H3	0.59	2.28	11	2
3:A:623:PX4:O2	3:A:639:PX4:H7	0.58	1.98	3	1
3:B:392:PX4:O3	3:B:393:PX4:H4	0.58	1.98	7	1
3:C:330:PX4:H10	3:C:330:PX4:O2	0.58	1.97	14	1
3:C:341:PX4:O1	3:C:362:PX4:H4	0.58	1.98	13	2
3:A:641:PX4:H3	3:A:646:PX4:O2	0.58	1.98	7	1
3:B:342:PX4:O6	3:B:342:PX4:H6	0.58	1.97	9	1
3:B:337:PX4:H4	3:B:342:PX4:O3	0.58	1.97	11	1
3:A:626:PX4:H3	3:A:626:PX4:O4	0.58	1.98	5	1
3:A:603:PX4:O3	3:A:603:PX4:H13	0.58	1.98	8	1
3:B:325:PX4:H13	3:B:331:PX4:O1	0.58	1.99	10	2
3:C:318:PX4:O2	3:C:342:PX4:H4	0.58	1.97	12	3
3:B:369:PX4:O4	3:B:373:PX4:H5	0.58	1.97	10	1
3:B:348:PX4:O1	3:B:364:PX4:H11	0.58	1.98	14	1
3:C:306:PX4:H4	3:C:348:PX4:O3	0.58	1.99	1	1
3:C:321:PX4:O4	3:C:356:PX4:H3	0.58	1.98	4	1
3:C:359:PX4:H3	3:C:366:PX4:O2	0.58	1.99	12	2
3:B:390:PX4:H7	3:B:395:PX4:O8	0.58	1.97	7	1
1:A:491:LEU:HB2	3:A:635:PX4:H10	0.58	1.73	8	1
3:A:643:PX4:H10	3:A:643:PX4:O2	0.58	1.99	10	2
3:B:390:PX4:H11	3:B:393:PX4:O1	0.58	1.99	10	1
3:B:345:PX4:O2	3:B:352:PX4:H9	0.58	1.99	11	1
3:A:610:PX4:H6	3:C:368:PX4:O6	0.58	1.98	3	1
3:B:356:PX4:O2	3:B:356:PX4:H13	0.58	1.98	13	3
2:B:86:MET:HE1	3:B:308:PX4:H10	0.58	1.74	7	1
3:A:628:PX4:O1	3:A:644:PX4:H5	0.58	1.99	1	1
3:B:356:PX4:O3	3:B:356:PX4:H6	0.58	1.99	5	2
3:A:615:PX4:O1	3:A:629:PX4:H13	0.58	1.99	10	1
3:B:324:PX4:O8	3:B:352:PX4:H7	0.58	1.99	3	1
3:C:321:PX4:H5	3:C:356:PX4:O4	0.58	1.98	12	1
3:C:310:PX4:H5	3:C:358:PX4:O3	0.57	1.98	9	2
3:A:626:PX4:O2	3:A:626:PX4:H3	0.57	1.99	1	1
3:A:608:PX4:H7	3:B:394:PX4:H2	0.57	1.76	5	2
3:B:324:PX4:H3	3:B:325:PX4:O2	0.57	1.99	6	2
3:C:302:PX4:O2	3:C:302:PX4:H3	0.57	1.99	9	1
3:B:341:PX4:H10	3:B:371:PX4:O1	0.57	1.99	1	2
3:A:621:PX4:O8	3:A:637:PX4:H7	0.57	2.00	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:604:PX4:H6	3:A:604:PX4:O3	0.57	1.99	7	1
3:A:633:PX4:H3	3:B:400:PX4:O2	0.57	1.97	13	2
2:B:179:ASP:OD2	3:B:318:PX4:H8	0.57	1.99	14	1
3:A:630:PX4:O2	3:A:630:PX4:H6	0.57	1.99	1	1
3:B:385:PX4:O4	3:B:385:PX4:H3	0.57	1.99	13	5
3:B:342:PX4:O6	3:B:342:PX4:H13	0.57	2.00	4	3
3:A:604:PX4:O8	3:B:394:PX4:H11	0.57	1.98	6	2
3:C:355:PX4:O1	3:C:367:PX4:H3	0.57	1.99	12	1
3:A:638:PX4:O4	3:A:648:PX4:H9	0.57	1.99	1	1
3:A:629:PX4:O2	3:A:629:PX4:H4	0.57	1.97	8	2
3:A:617:PX4:O2	3:C:365:PX4:H3	0.57	2.00	15	1
3:A:615:PX4:H4	3:C:360:PX4:O6	0.57	1.99	1	2
3:B:331:PX4:H3	3:B:331:PX4:O2	0.57	2.00	3	1
3:B:399:PX4:H10	3:C:321:PX4:O2	0.57	2.00	5	1
3:A:627:PX4:O3	3:A:627:PX4:H12	0.57	1.99	5	5
2:B:55:SER:N	2:B:58:SER:HG	0.57	1.97	13	3
3:B:325:PX4:H4	3:B:331:PX4:O4	0.57	1.99	13	2
2:C:265:GLN:HA	3:C:336:PX4:H12	0.57	1.75	11	1
3:C:366:PX4:O1	3:C:366:PX4:H4	0.57	1.99	4	1
3:B:353:PX4:O2	3:B:353:PX4:H4	0.57	1.99	5	1
3:B:364:PX4:O6	3:B:382:PX4:H4	0.57	2.00	8	1
3:B:378:PX4:H4	3:B:390:PX4:O2	0.57	2.00	10	1
3:C:366:PX4:H13	3:C:369:PX4:O4	0.57	2.00	1	1
3:A:619:PX4:H4	3:A:635:PX4:O6	0.57	2.00	5	3
3:B:343:PX4:H9	3:B:343:PX4:O3	0.57	2.00	13	2
3:B:334:PX4:C6	3:B:334:PX4:H12	0.57	2.29	6	2
3:C:314:PX4:O8	3:C:349:PX4:H7	0.57	1.98	12	1
3:B:311:PX4:O2	3:B:311:PX4:H4	0.57	1.99	13	1
3:B:355:PX4:O1	3:B:367:PX4:H4	0.57	1.99	3	1
3:A:605:PX4:H10	3:A:605:PX4:O3	0.57	2.00	6	2
3:C:310:PX4:O4	3:C:310:PX4:H3	0.57	2.00	8	1
3:C:349:PX4:O8	3:C:349:PX4:H3	0.57	2.00	10	1
3:A:610:PX4:H11	3:A:631:PX4:O8	0.56	1.99	8	2
3:A:621:PX4:O1	3:A:621:PX4:H3	0.56	2.00	11	1
3:A:615:PX4:O3	3:A:615:PX4:H6	0.56	2.00	15	2
3:C:352:PX4:O8	3:C:364:PX4:H4	0.56	1.99	2	1
3:B:326:PX4:O2	3:B:326:PX4:H4	0.56	2.00	6	3
3:B:345:PX4:O2	3:B:352:PX4:H8	0.56	1.99	15	3
3:A:646:PX4:O3	3:A:646:PX4:H7	0.56	2.00	1	5
2:C:261:LYS:O	3:C:336:PX4:H4	0.56	2.00	6	1
3:B:354:PX4:H13	3:B:354:PX4:O3	0.56	2.00	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:316:PX4:O3	3:B:316:PX4:H13	0.56	1.99	13	1
2:B:73:ASP:OD2	3:B:312:PX4:H3	0.56	1.99	14	1
3:C:359:PX4:O3	3:C:366:PX4:H4	0.56	1.99	6	2
3:C:338:PX4:H3	3:C:338:PX4:O1	0.56	2.01	7	1
3:A:608:PX4:H11	3:B:394:PX4:O1	0.56	2.00	13	1
3:B:329:PX4:H13	3:B:341:PX4:O2	0.56	2.00	1	1
3:A:611:PX4:O4	3:A:611:PX4:H4	0.56	1.99	2	1
3:B:309:PX4:O4	3:B:333:PX4:H4	0.56	2.00	6	2
3:A:630:PX4:O3	3:A:630:PX4:H13	0.56	2.01	5	1
3:B:303:PX4:H10	3:B:303:PX4:O3	0.56	2.00	10	1
3:B:328:PX4:O1	3:B:328:PX4:H3	0.56	1.99	10	1
3:B:392:PX4:O3	3:B:393:PX4:H3	0.56	2.01	10	1
3:A:601:PX4:H11	3:B:389:PX4:O6	0.56	1.99	12	1
3:B:341:PX4:H4	3:B:364:PX4:O3	0.56	2.01	12	1
3:B:351:PX4:H4	3:B:351:PX4:O2	0.56	2.00	1	2
3:B:324:PX4:O3	3:B:324:PX4:H6	0.56	2.00	3	1
3:C:303:PX4:O1	3:C:303:PX4:H12	0.56	2.00	11	1
3:B:398:PX4:H6	3:B:399:PX4:O1	0.56	2.00	13	1
3:C:342:PX4:H10	3:C:342:PX4:O2	0.56	2.01	15	1
3:A:639:PX4:H7	3:A:640:PX4:O2	0.56	2.01	1	3
3:B:317:PX4:H10	3:B:317:PX4:O3	0.56	2.01	10	1
3:B:380:PX4:O4	3:B:380:PX4:H7	0.56	2.01	10	1
3:A:617:PX4:O3	3:A:617:PX4:H12	0.56	2.01	15	1
3:B:308:PX4:H10	3:B:308:PX4:O3	0.56	2.01	15	1
3:A:604:PX4:H4	3:A:605:PX4:O2	0.56	2.00	9	2
3:A:644:PX4:O1	3:A:648:PX4:H13	0.56	2.00	6	5
3:A:601:PX4:H8	3:B:381:PX4:O4	0.56	2.01	13	1
3:B:304:PX4:O2	3:B:311:PX4:H3	0.56	2.01	5	4
3:B:376:PX4:H3	3:B:389:PX4:O1	0.56	2.01	1	2
3:B:361:PX4:H4	3:B:361:PX4:O2	0.56	2.01	6	3
3:B:364:PX4:O3	3:B:364:PX4:H12	0.56	2.01	12	3
3:B:325:PX4:H60	3:B:331:PX4:H45	0.56	1.78	9	1
3:B:357:PX4:O3	3:B:372:PX4:H8	0.56	1.99	9	1
3:C:347:PX4:H3	3:C:354:PX4:O1	0.56	1.99	11	1
3:B:383:PX4:O8	3:B:386:PX4:H8	0.55	2.02	2	1
3:B:336:PX4:O2	3:B:336:PX4:H4	0.55	1.99	11	1
3:A:632:PX4:H11	3:C:369:PX4:O1	0.55	2.01	15	1
3:C:333:PX4:H3	3:C:360:PX4:O1	0.55	2.02	2	2
3:C:312:PX4:H6	3:C:325:PX4:O2	0.55	2.00	3	2
3:B:341:PX4:O3	3:B:364:PX4:H4	0.55	2.01	7	2
3:A:602:PX4:H11	3:B:382:PX4:O4	0.55	2.02	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:366:PX4:O1	3:B:385:PX4:H8	0.55	2.01	7	2
3:B:378:PX4:H4	3:B:390:PX4:O8	0.55	2.01	8	1
3:B:309:PX4:O2	3:B:335:PX4:H4	0.55	2.02	10	1
3:B:306:PX4:H6	3:B:346:PX4:O1	0.55	2.01	12	1
3:C:339:PX4:H13	3:C:346:PX4:O2	0.55	2.02	1	2
3:C:359:PX4:O2	3:C:359:PX4:H4	0.55	2.02	15	1
3:B:386:PX4:O1	3:B:386:PX4:H3	0.55	2.01	11	2
3:C:342:PX4:O1	3:C:342:PX4:H3	0.55	2.01	2	1
3:A:627:PX4:O1	3:A:632:PX4:H8	0.55	2.02	4	2
3:B:390:PX4:C6	3:B:395:PX4:H4	0.55	2.31	12	2
1:A:343:ARG:HB3	1:A:350:MET:SD	0.55	2.41	13	1
3:B:304:PX4:O1	3:B:311:PX4:H9	0.55	2.02	13	1
3:C:306:PX4:O2	3:C:348:PX4:H4	0.55	2.02	14	1
3:C:334:PX4:O4	3:C:334:PX4:H4	0.55	2.01	14	1
3:B:399:PX4:H9	3:C:336:PX4:O6	0.55	2.02	4	1
3:B:334:PX4:O2	3:B:334:PX4:H4	0.55	2.02	11	2
3:A:624:PX4:H6	3:A:624:PX4:O4	0.55	2.02	9	1
3:A:633:PX4:H7	3:B:400:PX4:O1	0.55	2.00	12	1
3:C:309:PX4:C23	3:C:344:PX4:H10	0.55	2.31	5	1
3:B:309:PX4:H10	3:B:342:PX4:H14	0.55	1.79	10	2
3:A:620:PX4:O1	3:A:628:PX4:H3	0.55	2.02	1	2
1:A:490:LYS:O	3:A:635:PX4:H9	0.55	2.01	5	1
3:B:375:PX4:O3	3:B:375:PX4:H13	0.55	2.02	9	2
3:A:641:PX4:H4	3:A:646:PX4:O2	0.55	2.01	15	1
3:B:329:PX4:O3	3:B:329:PX4:H7	0.55	2.01	9	2
3:A:643:PX4:O3	3:A:643:PX4:H12	0.55	2.01	8	3
3:C:355:PX4:H4	3:C:355:PX4:O2	0.55	2.01	6	3
3:B:310:PX4:H4	3:B:328:PX4:O6	0.55	2.02	7	1
3:A:614:PX4:H9	3:A:619:PX4:O2	0.55	2.02	10	1
3:C:353:PX4:H9	3:C:353:PX4:O3	0.55	2.01	12	1
3:C:348:PX4:O4	3:C:348:PX4:H3	0.55	2.01	13	1
3:B:314:PX4:H9	3:B:314:PX4:O3	0.54	2.03	5	1
3:B:349:PX4:H9	3:B:353:PX4:O2	0.54	2.01	7	1
3:B:338:PX4:H4	3:B:377:PX4:O2	0.54	2.02	14	1
3:A:604:PX4:O2	3:B:394:PX4:H13	0.54	2.02	15	1
3:C:367:PX4:H3	3:C:367:PX4:O4	0.54	2.02	9	5
3:B:329:PX4:O2	3:B:353:PX4:H3	0.54	2.02	7	1
3:C:362:PX4:O4	3:C:362:PX4:H3	0.54	2.02	8	1
3:B:345:PX4:O1	3:B:373:PX4:H3	0.54	2.01	15	1
3:B:305:PX4:O2	3:B:305:PX4:H4	0.54	2.02	8	2
3:C:333:PX4:O3	3:C:360:PX4:H12	0.54	2.03	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:359:PX4:H9	3:B:359:PX4:H14	0.54	1.79	12	1
3:A:602:PX4:O2	3:B:372:PX4:H5	0.54	2.01	4	1
3:C:347:PX4:H11	3:C:354:PX4:O3	0.54	2.02	4	1
3:B:336:PX4:O2	3:B:365:PX4:H10	0.54	2.03	1	1
3:C:305:PX4:O4	3:C:305:PX4:H3	0.54	2.02	2	2
3:B:349:PX4:O3	3:B:349:PX4:H13	0.54	2.02	11	4
3:A:616:PX4:O3	3:A:616:PX4:H9	0.54	2.02	15	3
3:A:624:PX4:H3	3:A:639:PX4:O1	0.54	2.02	8	1
3:B:328:PX4:H10	3:B:328:PX4:O3	0.54	2.03	12	1
3:B:338:PX4:H9	3:B:357:PX4:O1	0.54	2.03	14	2
3:A:639:PX4:H5	3:A:640:PX4:O2	0.54	2.03	3	1
3:B:377:PX4:H4	3:B:377:PX4:O2	0.54	2.03	4	2
3:B:305:PX4:H3	3:B:340:PX4:O1	0.54	2.03	3	1
3:C:307:PX4:O1	3:C:307:PX4:H3	0.54	2.03	1	1
3:B:349:PX4:O2	3:B:371:PX4:H4	0.54	2.01	8	2
3:B:340:PX4:O4	3:B:356:PX4:H11	0.54	2.03	6	3
3:A:627:PX4:O8	3:A:632:PX4:H4	0.54	2.03	8	2
3:B:383:PX4:H14	3:B:383:PX4:H3	0.54	1.79	8	1
3:B:372:PX4:O1	3:B:372:PX4:H4	0.54	2.03	14	3
3:B:329:PX4:O2	3:B:353:PX4:H7	0.54	2.02	12	1
3:A:602:PX4:O1	3:A:602:PX4:H9	0.54	2.03	1	1
3:A:637:PX4:O8	3:A:646:PX4:H10	0.54	2.03	1	3
3:C:363:PX4:H3	3:C:363:PX4:O2	0.54	2.03	8	1
3:B:304:PX4:H9	3:B:304:PX4:O3	0.54	2.02	9	1
3:B:399:PX4:H11	3:C:321:PX4:O6	0.54	2.02	12	1
3:C:325:PX4:O2	3:C:325:PX4:H4	0.54	2.03	12	1
3:A:632:PX4:O4	3:A:632:PX4:H3	0.54	2.03	14	1
3:C:367:PX4:O8	3:C:367:PX4:H3	0.54	2.03	1	1
3:A:618:PX4:O2	3:A:618:PX4:H3	0.54	2.04	2	1
2:B:73:ASP:CG	3:B:312:PX4:H3	0.54	2.27	2	1
3:A:624:PX4:H8	3:A:630:PX4:O4	0.54	2.03	4	3
3:B:304:PX4:O1	3:B:311:PX4:H10	0.54	2.03	3	1
3:B:369:PX4:O3	3:B:369:PX4:H7	0.54	2.03	12	4
3:B:349:PX4:O2	3:B:349:PX4:H4	0.54	2.02	15	1
3:A:617:PX4:O1	3:A:617:PX4:H3	0.53	2.03	4	2
3:B:353:PX4:O3	3:B:353:PX4:H7	0.53	2.03	6	1
3:A:624:PX4:O8	3:A:624:PX4:H5	0.53	2.02	9	1
3:A:604:PX4:H11	3:B:384:PX4:O4	0.53	2.03	2	1
2:C:262:LEU:O	3:C:336:PX4:H6	0.53	2.02	7	2
3:B:337:PX4:H7	3:B:337:PX4:O3	0.53	2.03	9	1
3:B:352:PX4:O8	3:B:352:PX4:H6	0.53	2.03	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:360:PX4:H9	3:B:362:PX4:O8	0.53	2.03	11	1
3:A:644:PX4:H7	3:A:644:PX4:O2	0.53	2.03	12	1
1:A:492:LYS:HG3	3:A:643:PX4:H11	0.53	1.79	3	1
3:B:320:PX4:O3	3:B:320:PX4:H13	0.53	2.03	7	3
3:B:399:PX4:H11	3:C:321:PX4:O3	0.53	2.03	8	1
3:C:366:PX4:H12	3:C:366:PX4:O3	0.53	2.03	9	1
3:A:624:PX4:O4	3:A:624:PX4:H4	0.53	2.03	1	1
3:B:367:PX4:O1	3:B:367:PX4:H3	0.53	2.03	9	1
3:B:358:PX4:O2	3:B:365:PX4:H11	0.53	2.04	1	1
3:A:615:PX4:O3	3:A:621:PX4:H9	0.53	2.03	9	1
3:C:337:PX4:H9	3:C:346:PX4:O1	0.53	2.04	11	1
3:B:356:PX4:O4	3:B:370:PX4:H4	0.53	2.03	1	1
3:C:360:PX4:O3	3:C:360:PX4:H13	0.53	2.04	5	3
3:A:633:PX4:H11	3:C:370:PX4:O4	0.53	2.03	12	2
3:A:615:PX4:H11	3:C:360:PX4:O4	0.53	2.03	10	1
3:C:334:PX4:O2	3:C:334:PX4:H4	0.53	2.04	10	1
3:B:338:PX4:H12	3:B:377:PX4:O4	0.53	2.03	15	2
3:A:634:PX4:O6	3:A:634:PX4:H13	0.53	2.03	1	1
3:C:315:PX4:H13	3:C:331:PX4:O2	0.53	2.04	5	1
3:B:391:PX4:H12	3:B:394:PX4:O4	0.53	2.04	10	1
3:A:644:PX4:O2	3:A:648:PX4:H6	0.53	2.03	13	4
3:C:358:PX4:O4	3:C:358:PX4:H3	0.53	2.04	14	2
3:B:329:PX4:O3	3:B:353:PX4:H3	0.53	2.04	13	1
3:C:334:PX4:H3	3:C:347:PX4:O1	0.53	2.03	13	1
3:A:630:PX4:H9	3:A:639:PX4:O3	0.53	2.04	2	1
3:B:334:PX4:H10	3:B:334:PX4:O3	0.53	2.04	14	2
3:B:339:PX4:O1	3:B:355:PX4:H12	0.53	2.04	14	2
3:B:358:PX4:O8	3:B:365:PX4:H4	0.53	2.04	12	1
3:C:319:PX4:O1	3:C:319:PX4:H13	0.53	2.04	12	1
3:C:333:PX4:H7	3:C:360:PX4:O1	0.53	2.03	14	2
3:A:615:PX4:H11	3:C:360:PX4:O2	0.53	2.04	8	3
3:C:310:PX4:O3	3:C:310:PX4:H9	0.53	2.03	13	3
3:B:399:PX4:H13	3:C:356:PX4:O3	0.53	2.04	8	1
2:C:164:SER:OG	3:C:325:PX4:H4	0.53	2.03	8	1
3:A:616:PX4:H13	3:C:362:PX4:O1	0.53	2.03	13	1
3:A:616:PX4:O1	3:A:616:PX4:H3	0.53	2.04	13	1
3:B:311:PX4:H9	3:B:311:PX4:O1	0.52	2.05	4	1
3:B:366:PX4:O1	3:B:366:PX4:H3	0.52	2.04	6	4
3:C:310:PX4:H12	3:C:358:PX4:O1	0.52	2.04	12	1
3:B:316:PX4:O1	3:B:316:PX4:H13	0.52	2.03	1	1
3:A:624:PX4:H7	3:C:361:PX4:O6	0.52	2.04	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:344:PX4:H53	3:C:335:PX4:H43	0.52	1.81	12	1
3:B:380:PX4:O4	3:B:380:PX4:H9	0.52	2.04	13	1
3:A:643:PX4:C6	3:A:643:PX4:H4	0.52	2.34	3	1
3:B:344:PX4:H9	3:B:344:PX4:H14	0.52	1.81	5	1
3:B:369:PX4:O1	3:B:383:PX4:H5	0.52	2.04	5	1
3:A:641:PX4:H7	3:A:641:PX4:O1	0.52	2.05	8	1
3:B:338:PX4:O2	3:B:338:PX4:H13	0.52	2.03	9	1
3:B:357:PX4:O1	3:B:357:PX4:H3	0.52	2.04	9	1
3:C:321:PX4:H11	3:C:356:PX4:O3	0.52	2.04	14	1
3:A:640:PX4:H3	3:A:640:PX4:O4	0.52	2.04	2	2
3:C:339:PX4:H4	3:C:339:PX4:O4	0.52	2.03	1	1
3:B:309:PX4:O2	3:B:309:PX4:H4	0.52	2.04	2	2
2:B:201:GLU:OE1	3:B:313:PX4:H4	0.52	2.05	5	1
3:B:376:PX4:H10	3:B:376:PX4:O1	0.52	2.05	5	1
3:C:322:PX4:O2	3:C:322:PX4:H4	0.52	2.05	6	1
3:C:347:PX4:H4	3:C:354:PX4:O6	0.52	2.04	8	1
3:A:604:PX4:O1	3:A:607:PX4:H6	0.52	2.05	1	1
3:B:318:PX4:H10	3:B:318:PX4:O1	0.52	2.04	8	1
3:B:364:PX4:O2	3:B:364:PX4:H12	0.52	2.04	10	1
3:A:604:PX4:H4	3:A:605:PX4:O4	0.52	2.05	13	1
3:B:395:PX4:O3	3:B:395:PX4:H10	0.52	2.05	1	3
3:C:318:PX4:O1	3:C:318:PX4:H3	0.52	2.05	4	2
3:C:338:PX4:O3	3:C:338:PX4:H12	0.52	2.04	5	3
3:A:639:PX4:O6	3:A:640:PX4:H13	0.52	2.04	15	1
3:B:378:PX4:H6	3:B:378:PX4:O1	0.52	2.05	5	1
3:C:343:PX4:H3	3:C:343:PX4:O1	0.52	2.05	9	2
3:B:379:PX4:H9	3:B:391:PX4:O1	0.52	2.05	11	1
3:A:622:PX4:H3	3:A:622:PX4:O1	0.52	2.05	12	1
3:C:347:PX4:H10	3:C:347:PX4:O3	0.52	2.05	13	1
3:B:394:PX4:H3	3:B:394:PX4:O2	0.52	2.04	10	2
3:B:341:PX4:O3	3:B:364:PX4:H7	0.52	2.05	6	1
3:B:387:PX4:O1	3:B:387:PX4:H3	0.52	2.05	6	1
3:C:364:PX4:H10	3:C:364:PX4:O2	0.52	2.05	1	1
3:A:619:PX4:H5	3:A:631:PX4:O7	0.52	2.05	2	1
3:B:398:PX4:H13	3:B:399:PX4:O6	0.52	2.03	3	1
3:C:312:PX4:H10	3:C:312:PX4:O3	0.52	2.05	7	1
3:C:360:PX4:H5	3:C:365:PX4:O8	0.52	2.05	7	1
3:B:324:PX4:O2	3:B:352:PX4:H9	0.52	2.04	8	1
3:B:388:PX4:O1	3:B:388:PX4:H3	0.52	2.05	10	1
3:B:378:PX4:H12	3:B:393:PX4:H14	0.52	1.81	3	1
3:A:637:PX4:O4	3:A:646:PX4:H12	0.52	2.05	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:342:PX4:O1	3:B:360:PX4:H5	0.52	2.05	4	1
3:B:304:PX4:H7	3:B:304:PX4:O4	0.52	2.05	6	1
3:A:636:PX4:H7	3:A:636:PX4:O4	0.52	2.05	8	1
3:B:311:PX4:H4	3:B:344:PX4:O4	0.52	2.05	8	1
3:A:620:PX4:H7	3:A:632:PX4:O8	0.52	2.05	11	3
3:B:388:PX4:O1	3:B:393:PX4:H11	0.52	2.05	12	2
3:A:606:PX4:H4	3:B:386:PX4:O4	0.51	2.05	1	2
3:A:636:PX4:H9	3:A:636:PX4:O3	0.51	2.05	7	2
3:B:311:PX4:H7	3:B:311:PX4:O3	0.51	2.05	1	5
3:B:336:PX4:H11	3:B:358:PX4:C1	0.51	2.34	4	1
3:A:607:PX4:H5	3:A:608:PX4:O1	0.51	2.04	7	1
2:B:60:LEU:HD11	2:C:243:VAL:HG22	0.51	1.82	10	1
3:B:379:PX4:O8	3:B:385:PX4:H4	0.51	2.05	11	2
3:A:635:PX4:H6	3:A:635:PX4:O1	0.51	2.05	11	1
3:C:320:PX4:H13	3:C:322:PX4:O1	0.51	2.06	4	2
3:C:301:PX4:O1	3:C:301:PX4:H3	0.51	2.06	3	1
3:B:309:PX4:O6	3:B:333:PX4:H9	0.51	2.05	6	1
3:B:399:PX4:H8	3:C:356:PX4:H14	0.51	1.82	11	1
3:B:350:PX4:O1	3:B:350:PX4:H3	0.51	2.05	1	2
3:B:378:PX4:H5	3:B:390:PX4:O1	0.51	2.06	1	1
3:A:632:PX4:H3	3:A:632:PX4:O1	0.51	2.05	4	1
3:C:317:PX4:O1	3:C:317:PX4:H3	0.51	2.05	4	2
3:B:308:PX4:O2	3:C:302:PX4:H9	0.51	2.05	7	1
3:A:644:PX4:O2	3:A:644:PX4:H9	0.51	2.06	11	1
3:B:318:PX4:H10	3:B:318:PX4:O2	0.51	2.06	12	1
3:B:327:PX4:H12	3:B:352:PX4:O1	0.51	2.04	12	2
2:C:84:GLN:OE1	3:C:314:PX4:H3	0.51	2.05	14	1
3:A:619:PX4:H9	3:A:635:PX4:H18	0.51	1.81	5	1
3:B:390:PX4:H3	3:B:395:PX4:H9	0.51	1.82	7	1
3:B:366:PX4:O3	3:B:366:PX4:H6	0.51	2.06	12	2
1:A:494:GLU:OE1	3:A:646:PX4:H6	0.51	2.05	14	2
3:C:328:PX4:H15	3:C:328:PX4:H9	0.51	1.82	2	1
3:B:364:PX4:O8	3:B:382:PX4:H12	0.51	2.06	4	1
3:A:607:PX4:O3	3:A:607:PX4:H12	0.51	2.06	6	2
3:C:319:PX4:O1	3:C:323:PX4:H11	0.51	2.05	5	1
3:B:342:PX4:H7	3:B:342:PX4:O3	0.51	2.06	10	2
3:B:380:PX4:H4	3:B:380:PX4:O2	0.51	2.04	8	2
3:B:364:PX4:O8	3:B:382:PX4:H4	0.51	2.06	1	1
3:B:366:PX4:H4	3:B:367:PX4:O1	0.51	2.06	5	1
3:C:357:PX4:O3	3:C:357:PX4:H6	0.51	2.06	13	2
3:B:304:PX4:O4	3:B:304:PX4:H9	0.51	2.06	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:614:PX4:O1	3:C:368:PX4:H5	0.51	2.06	5	1
3:B:349:PX4:C1	3:B:371:PX4:H12	0.51	2.35	7	1
2:B:73:ASP:OD2	3:B:312:PX4:H6	0.51	2.05	10	1
3:A:607:PX4:H9	3:A:607:PX4:O2	0.51	2.05	13	2
3:A:614:PX4:O1	3:C:340:PX4:H3	0.51	2.06	12	1
3:C:367:PX4:O2	3:C:367:PX4:H7	0.51	2.06	12	1
3:A:636:PX4:H11	3:A:645:PX4:O5	0.51	2.06	3	1
3:A:629:PX4:O2	3:A:637:PX4:H5	0.51	2.04	9	2
3:C:339:PX4:O3	3:C:339:PX4:H7	0.51	2.06	12	2
3:B:330:PX4:H6	3:B:330:PX4:O3	0.51	2.05	12	1
3:B:386:PX4:H10	3:B:392:PX4:O1	0.51	2.05	13	1
3:B:308:PX4:H72	3:C:345:PX4:H71	0.51	1.82	7	1
3:B:399:PX4:H12	3:C:321:PX4:O6	0.51	2.05	10	1
3:B:352:PX4:H12	3:B:352:PX4:O3	0.51	2.06	14	1
3:C:316:PX4:H4	3:C:316:PX4:O2	0.51	2.06	15	1
3:B:343:PX4:O1	3:B:343:PX4:H3	0.51	2.06	2	1
3:C:347:PX4:O1	3:C:347:PX4:H3	0.51	2.06	7	1
3:A:625:PX4:H7	3:A:625:PX4:O3	0.51	2.06	9	2
3:C:332:PX4:O1	3:C:332:PX4:H10	0.50	2.06	6	1
3:B:304:PX4:O1	3:B:304:PX4:H3	0.50	2.06	7	1
3:B:356:PX4:O4	3:B:370:PX4:H5	0.50	2.06	13	1
3:C:338:PX4:H9	3:C:347:PX4:O2	0.50	2.06	1	1
3:B:321:PX4:O1	3:B:321:PX4:H3	0.50	2.07	2	3
3:A:633:PX4:H8	3:C:370:PX4:O2	0.50	2.04	4	1
3:B:304:PX4:O1	3:B:304:PX4:H9	0.50	2.05	5	1
3:B:389:PX4:O3	3:B:389:PX4:H7	0.50	2.06	6	1
3:C:365:PX4:O3	3:C:365:PX4:H9	0.50	2.06	8	1
3:B:365:PX4:H6	3:B:365:PX4:O3	0.50	2.06	9	2
3:B:392:PX4:C6	3:B:393:PX4:H9	0.50	2.36	14	1
3:A:616:PX4:O1	3:C:367:PX4:H11	0.50	2.06	15	1
3:B:341:PX4:O1	3:B:364:PX4:H4	0.50	2.07	2	5
3:C:347:PX4:H4	3:C:366:PX4:O1	0.50	2.06	2	1
3:A:620:PX4:H4	3:A:632:PX4:C6	0.50	2.36	8	2
3:C:350:PX4:H9	3:C:367:PX4:O2	0.50	2.06	10	1
3:B:390:PX4:H14	3:B:395:PX4:H4	0.50	1.82	12	1
3:B:326:PX4:H7	3:B:326:PX4:O3	0.50	2.06	15	2
3:C:321:PX4:O1	3:C:321:PX4:H3	0.50	2.07	2	1
3:C:364:PX4:O1	3:C:364:PX4:H12	0.50	2.05	2	1
3:C:360:PX4:H8	3:C:365:PX4:O8	0.50	2.07	4	1
3:A:614:PX4:H6	3:C:368:PX4:O2	0.50	2.07	11	1
3:A:633:PX4:H10	3:B:400:PX4:O2	0.50	2.06	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:350:PX4:O3	3:B:350:PX4:H12	0.50	2.06	4	1
3:C:368:PX4:O3	3:C:368:PX4:H12	0.50	2.07	4	1
3:B:347:PX4:H9	3:B:374:PX4:O2	0.50	2.07	5	1
3:B:306:PX4:H3	3:B:346:PX4:O4	0.50	2.06	6	1
3:A:602:PX4:H11	3:B:382:PX4:O1	0.50	2.06	7	1
3:B:324:PX4:H9	3:B:325:PX4:O1	0.50	2.06	7	1
3:C:329:PX4:O4	3:C:329:PX4:H3	0.50	2.07	14	2
3:B:337:PX4:H8	3:B:342:PX4:O3	0.50	2.07	8	1
3:A:620:PX4:H5	3:C:359:PX4:O8	0.50	2.07	9	1
3:C:338:PX4:O4	3:C:363:PX4:H4	0.50	2.06	9	1
3:A:615:PX4:O4	3:A:629:PX4:H3	0.50	2.06	12	1
3:A:615:PX4:O2	3:A:621:PX4:H9	0.50	2.07	2	1
3:C:359:PX4:C1	3:C:366:PX4:H4	0.50	2.36	5	1
3:A:617:PX4:H10	3:A:617:PX4:O4	0.50	2.07	7	1
3:C:338:PX4:O4	3:C:363:PX4:H7	0.50	2.07	7	1
3:C:333:PX4:O1	3:C:360:PX4:H10	0.50	2.06	8	2
3:B:351:PX4:H7	3:B:351:PX4:O3	0.50	2.07	10	3
3:B:329:PX4:H12	3:B:332:PX4:O1	0.50	2.07	5	1
3:B:387:PX4:H9	3:B:393:PX4:O1	0.50	2.07	14	1
3:B:308:PX4:O6	3:C:302:PX4:H6	0.50	2.07	15	1
3:A:620:PX4:H9	3:A:632:PX4:O1	0.50	2.07	8	2
3:A:630:PX4:H8	3:A:639:PX4:O3	0.50	2.07	4	1
3:B:349:PX4:O3	3:B:371:PX4:H12	0.50	2.07	8	2
3:B:338:PX4:O3	3:B:338:PX4:H6	0.50	2.06	5	1
3:B:351:PX4:C3	3:B:361:PX4:H6	0.50	2.36	5	1
3:A:608:PX4:H9	3:B:394:PX4:O1	0.50	2.07	6	1
3:B:377:PX4:O1	3:B:377:PX4:H4	0.50	2.06	9	1
3:C:332:PX4:H12	3:C:332:PX4:O4	0.50	2.06	9	1
3:B:342:PX4:O7	3:B:342:PX4:H6	0.50	2.07	12	1
3:B:368:PX4:H10	3:B:368:PX4:O2	0.50	2.07	15	1
3:B:354:PX4:O2	3:B:354:PX4:H13	0.49	2.07	1	1
3:B:352:PX4:H3	3:B:352:PX4:O4	0.49	2.07	9	4
3:B:366:PX4:H4	3:B:367:PX4:O4	0.49	2.06	14	2
3:C:327:PX4:O1	3:C:327:PX4:H3	0.49	2.07	12	1
3:B:383:PX4:C1	3:B:386:PX4:H11	0.49	2.37	3	1
3:A:604:PX4:O2	3:B:394:PX4:H5	0.49	2.07	5	1
3:B:314:PX4:O2	3:B:314:PX4:H7	0.49	2.07	6	2
3:B:383:PX4:H3	3:B:383:PX4:C6	0.49	2.36	8	1
2:B:263:ASN:OD1	3:B:325:PX4:H5	0.49	2.07	11	1
3:C:323:PX4:O3	3:C:323:PX4:H12	0.49	2.08	11	1
3:A:611:PX4:H3	3:C:337:PX4:O1	0.49	2.08	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:336:PX4:O3	3:B:365:PX4:H10	0.49	2.06	5	1
3:B:338:PX4:O4	3:B:338:PX4:H13	0.49	2.06	7	2
3:B:371:PX4:O3	3:B:371:PX4:H6	0.49	2.07	10	2
3:C:326:PX4:O1	3:C:326:PX4:H4	0.49	2.08	11	1
3:A:637:PX4:O6	3:A:646:PX4:H8	0.49	2.07	13	1
3:A:604:PX4:H4	3:A:605:PX4:H14	0.49	1.82	15	1
3:A:619:PX4:H9	3:A:631:PX4:O4	0.49	2.08	15	1
3:A:647:PX4:H10	3:A:647:PX4:H14	0.49	1.84	1	1
3:C:370:PX4:H10	3:C:370:PX4:O3	0.49	2.07	7	3
3:A:614:PX4:O1	3:A:614:PX4:H3	0.49	2.07	9	1
2:C:84:GLN:OE1	3:C:314:PX4:H7	0.49	2.07	11	1
3:A:627:PX4:O2	3:A:642:PX4:H13	0.49	2.07	14	1
3:A:612:PX4:H3	3:C:351:PX4:O4	0.49	2.07	1	1
3:A:620:PX4:O4	3:A:620:PX4:C2	0.49	2.58	5	2
3:C:333:PX4:O3	3:C:333:PX4:H7	0.49	2.08	4	1
1:A:495:PRO:HD3	3:A:643:PX4:H7	0.49	1.83	6	1
3:A:610:PX4:H4	3:A:615:PX4:O8	0.49	2.07	7	1
3:A:611:PX4:O2	3:C:351:PX4:H10	0.49	2.07	12	1
3:B:341:PX4:O3	3:B:364:PX4:H6	0.49	2.07	14	1
3:C:362:PX4:O3	3:C:362:PX4:H12	0.49	2.07	6	3
3:A:611:PX4:H10	3:A:611:PX4:O3	0.49	2.08	5	1
3:C:347:PX4:O3	3:C:347:PX4:H12	0.49	2.07	10	2
3:C:309:PX4:O3	3:C:309:PX4:H7	0.49	2.08	9	2
3:B:368:PX4:O2	3:B:368:PX4:H4	0.49	2.07	1	1
3:B:374:PX4:O2	3:B:374:PX4:H4	0.49	2.07	1	1
3:A:607:PX4:O2	3:A:607:PX4:H12	0.49	2.07	4	1
3:A:621:PX4:H3	3:A:621:PX4:O4	0.49	2.08	4	1
3:A:609:PX4:H66	3:A:646:PX4:H42	0.49	1.84	7	1
3:C:328:PX4:O2	3:C:328:PX4:H3	0.49	2.07	8	1
3:C:307:PX4:H13	3:C:339:PX4:O3	0.49	2.08	9	1
3:C:317:PX4:O4	3:C:355:PX4:H13	0.49	2.08	12	3
3:C:364:PX4:O2	3:C:369:PX4:H3	0.49	2.07	10	1
2:C:153:ARG:HH11	2:C:157:HIS:CE1	0.49	2.25	11	1
2:C:262:LEU:O	3:C:336:PX4:H4	0.49	2.07	11	1
3:C:364:PX4:O1	3:C:369:PX4:H3	0.49	2.08	11	2
3:A:634:PX4:P1	3:A:644:PX4:H6	0.49	2.47	13	1
3:A:619:PX4:H4	3:A:631:PX4:H2	0.49	1.84	15	1
3:A:614:PX4:H4	3:A:619:PX4:O1	0.49	2.08	1	1
3:B:309:PX4:O1	3:B:333:PX4:H12	0.49	2.08	2	1
3:A:639:PX4:H11	3:A:640:PX4:O3	0.49	2.08	3	1
2:C:84:GLN:OE1	3:C:314:PX4:H13	0.49	2.07	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:316:PX4:H10	3:C:316:PX4:P1	0.49	2.47	5	1
3:C:328:PX4:H8	3:C:350:PX4:O2	0.49	2.08	11	1
3:C:333:PX4:H10	3:C:360:PX4:O4	0.49	2.08	11	1
3:B:338:PX4:O4	3:B:338:PX4:H6	0.49	2.08	13	1
3:C:311:PX4:O3	3:C:311:PX4:H6	0.49	2.08	4	4
3:C:323:PX4:H10	3:C:323:PX4:H14	0.49	1.84	6	1
3:A:644:PX4:O2	3:A:644:PX4:H3	0.49	2.08	7	1
3:B:338:PX4:H9	3:B:357:PX4:O2	0.49	2.08	8	1
3:B:330:PX4:H3	3:B:330:PX4:O2	0.49	2.07	13	1
3:C:362:PX4:H3	3:C:362:PX4:O1	0.49	2.07	15	1
3:C:340:PX4:H4	3:C:340:PX4:O2	0.49	2.08	9	1
3:B:310:PX4:O8	3:B:342:PX4:H11	0.49	2.08	10	2
3:A:604:PX4:H8	3:B:384:PX4:O2	0.49	2.07	12	1
3:B:354:PX4:O4	3:B:354:PX4:H6	0.49	2.08	13	1
3:A:615:PX4:O1	3:A:629:PX4:H9	0.49	2.07	14	1
3:C:360:PX4:H11	3:C:365:PX4:O8	0.48	2.07	1	1
3:B:396:PX4:H8	3:C:342:PX4:O4	0.48	2.08	2	1
3:B:342:PX4:H17	3:B:342:PX4:H4	0.48	1.85	3	1
3:A:624:PX4:H3	3:C:361:PX4:O6	0.48	2.07	5	1
3:B:329:PX4:H10	3:B:332:PX4:O3	0.48	2.08	5	1
3:B:335:PX4:O2	3:B:360:PX4:H8	0.48	2.08	6	1
3:A:642:PX4:O2	3:A:647:PX4:H4	0.48	2.08	8	1
3:B:327:PX4:H4	3:B:327:PX4:O1	0.48	2.08	11	1
3:B:339:PX4:O3	3:B:355:PX4:H12	0.48	2.08	13	1
3:C:360:PX4:H9	3:C:365:PX4:O1	0.48	2.07	8	2
3:A:647:PX4:H13	3:A:648:PX4:O8	0.48	2.08	11	1
3:A:601:PX4:H20	3:A:604:PX4:H7	0.48	1.83	12	1
3:A:606:PX4:O3	3:A:606:PX4:H9	0.48	2.07	13	1
3:A:617:PX4:H9	3:C:353:PX4:O3	0.48	2.07	13	1
3:B:349:PX4:O2	3:B:371:PX4:H12	0.48	2.08	15	1
3:A:611:PX4:O4	3:A:611:PX4:H9	0.48	2.06	1	1
3:B:339:PX4:H10	3:B:339:PX4:O3	0.48	2.08	3	3
3:A:614:PX4:O3	3:C:368:PX4:H8	0.48	2.07	5	1
3:B:369:PX4:O2	3:B:383:PX4:H10	0.48	2.08	7	1
3:C:310:PX4:H10	3:C:310:PX4:H14	0.48	1.85	7	1
3:C:348:PX4:O3	3:C:348:PX4:H12	0.48	2.08	9	3
3:B:346:PX4:O1	3:B:363:PX4:H12	0.48	2.07	14	1
3:C:306:PX4:O3	3:C:306:PX4:H6	0.48	2.08	2	2
3:B:308:PX4:H10	3:B:323:PX4:O2	0.48	2.09	6	1
3:C:353:PX4:O3	3:C:353:PX4:C4	0.48	2.60	12	1
3:B:370:PX4:H47	3:B:370:PX4:H6	0.48	1.84	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:604:PX4:O1	3:B:394:PX4:H8	0.48	2.08	4	1
3:B:357:PX4:H12	3:B:357:PX4:O3	0.48	2.09	5	2
2:C:86:MET:CG	3:C:314:PX4:H19	0.48	2.39	5	1
3:C:322:PX4:H10	3:C:322:PX4:O3	0.48	2.08	11	3
3:A:620:PX4:O2	3:A:638:PX4:H9	0.48	2.09	7	1
3:B:308:PX4:O2	3:B:308:PX4:H3	0.48	2.09	9	1
3:B:341:PX4:O4	3:B:364:PX4:H3	0.48	2.09	10	2
3:A:621:PX4:O2	3:A:637:PX4:H3	0.48	2.09	11	1
3:C:348:PX4:H6	3:C:370:PX4:O8	0.48	2.09	11	1
2:C:145:ARG:HG3	3:C:320:PX4:H10	0.48	1.84	12	1
3:A:640:PX4:H10	3:A:647:PX4:O2	0.48	2.09	13	1
3:B:332:PX4:O1	3:B:332:PX4:H3	0.48	2.08	13	2
3:C:349:PX4:O2	3:C:353:PX4:H4	0.48	2.08	2	1
3:B:318:PX4:O2	3:B:334:PX4:H3	0.48	2.08	3	2
3:C:369:PX4:O3	3:C:369:PX4:H7	0.48	2.08	5	1
3:C:346:PX4:H10	3:C:346:PX4:O3	0.48	2.09	6	2
3:C:310:PX4:H11	3:C:340:PX4:O2	0.48	2.09	12	1
3:A:605:PX4:O8	3:A:607:PX4:H13	0.48	2.09	15	1
3:B:398:PX4:O3	3:B:400:PX4:H4	0.48	2.08	15	1
3:B:324:PX4:H37	3:C:356:PX4:H70	0.48	1.85	2	1
3:B:305:PX4:H10	3:B:340:PX4:O4	0.48	2.09	3	1
3:B:306:PX4:H3	3:B:346:PX4:O1	0.48	2.09	4	1
3:B:336:PX4:H11	3:B:358:PX4:H2	0.48	1.85	4	1
3:A:604:PX4:H3	3:A:605:PX4:O2	0.48	2.09	5	1
3:A:621:PX4:H2	3:C:365:PX4:H9	0.48	1.84	10	1
3:B:388:PX4:H9	3:B:388:PX4:O3	0.48	2.09	13	2
3:B:303:PX4:O5	3:B:303:PX4:C23	0.48	2.61	14	1
3:C:326:PX4:H7	3:C:326:PX4:O3	0.48	2.09	15	1
3:C:357:PX4:H13	3:C:357:PX4:O2	0.48	2.08	15	1
3:A:636:PX4:H8	3:A:645:PX4:H22	0.48	1.85	1	1
3:C:314:PX4:O4	3:C:314:PX4:H3	0.48	2.08	2	1
3:B:360:PX4:H11	3:B:362:PX4:H3	0.48	1.86	3	1
3:C:310:PX4:H11	3:C:358:PX4:O2	0.48	2.09	9	2
3:A:627:PX4:O1	3:A:632:PX4:H4	0.48	2.08	6	1
3:B:309:PX4:O1	3:B:333:PX4:H10	0.48	2.08	6	1
3:B:372:PX4:O3	3:B:382:PX4:H11	0.48	2.09	9	1
3:B:335:PX4:O1	3:B:360:PX4:H11	0.48	2.09	10	1
3:A:604:PX4:H5	3:B:384:PX4:O2	0.48	2.09	13	2
3:B:319:PX4:O8	3:B:319:PX4:H7	0.48	2.08	2	1
3:A:614:PX4:H10	3:A:619:PX4:O2	0.48	2.09	9	1
3:B:336:PX4:O4	3:B:336:PX4:H4	0.48	2.08	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:632:PX4:O3	3:A:632:PX4:H12	0.48	2.08	3	1
3:B:318:PX4:O3	3:B:318:PX4:H9	0.48	2.09	4	1
3:B:323:PX4:H12	3:B:323:PX4:O3	0.48	2.08	11	2
3:B:351:PX4:H12	3:B:379:PX4:O1	0.48	2.07	14	1
3:B:400:PX4:O3	3:C:370:PX4:H6	0.47	2.09	1	1
3:B:363:PX4:O2	3:B:363:PX4:H4	0.47	2.09	4	1
3:A:611:PX4:O2	3:C:351:PX4:H4	0.47	2.08	9	2
3:A:625:PX4:H6	3:A:625:PX4:C6	0.47	2.39	8	1
3:C:342:PX4:O3	3:C:342:PX4:H12	0.47	2.08	9	2
3:B:390:PX4:O3	3:B:395:PX4:H7	0.47	2.09	10	1
3:A:630:PX4:O3	3:A:630:PX4:H6	0.47	2.09	11	1
3:B:392:PX4:O2	3:B:393:PX4:H9	0.47	2.09	11	1
3:C:326:PX4:O2	3:C:345:PX4:H6	0.47	2.08	11	1
3:C:340:PX4:H10	3:C:340:PX4:O3	0.47	2.09	13	1
2:B:73:ASP:OD1	3:B:312:PX4:H12	0.47	2.10	1	1
3:A:623:PX4:O4	3:A:623:PX4:H4	0.47	2.09	10	3
3:A:608:PX4:H3	3:A:608:PX4:O1	0.47	2.09	5	2
2:B:73:ASP:OD1	3:B:312:PX4:H3	0.47	2.08	5	1
3:B:302:PX4:O1	3:B:307:PX4:H10	0.47	2.09	5	1
3:A:601:PX4:O3	3:A:601:PX4:H9	0.47	2.09	9	4
3:B:336:PX4:H7	3:B:336:PX4:H14	0.47	1.87	8	1
3:C:357:PX4:O3	3:C:357:PX4:H13	0.47	2.10	8	1
3:C:355:PX4:H17	3:C:367:PX4:H4	0.47	1.86	14	1
3:C:329:PX4:H7	3:C:329:PX4:O1	0.47	2.09	2	1
3:C:340:PX4:H10	3:C:340:PX4:O1	0.47	2.09	5	1
3:B:349:PX4:H3	3:B:353:PX4:O1	0.47	2.09	9	1
3:B:318:PX4:O3	3:B:334:PX4:H13	0.47	2.10	10	1
3:C:351:PX4:H6	3:C:351:PX4:O1	0.47	2.09	12	1
3:B:374:PX4:H3	3:B:374:PX4:O1	0.47	2.08	13	1
3:B:376:PX4:H12	3:B:376:PX4:O2	0.47	2.10	13	1
3:B:330:PX4:H4	3:B:330:PX4:O1	0.47	2.09	14	1
3:B:378:PX4:H8	3:B:390:PX4:O2	0.47	2.09	1	1
3:A:624:PX4:H11	3:A:630:PX4:O2	0.47	2.10	3	1
3:B:312:PX4:H7	3:B:312:PX4:O3	0.47	2.09	5	1
3:B:356:PX4:O2	3:B:370:PX4:H9	0.47	2.10	6	1
3:B:388:PX4:O2	3:B:393:PX4:H11	0.47	2.09	9	1
3:B:388:PX4:O4	3:B:393:PX4:H5	0.47	2.09	12	2
3:C:330:PX4:O1	3:C:357:PX4:H10	0.47	2.08	15	1
2:C:153:ARG:O	2:C:157:HIS:CD2	0.47	2.67	5	2
3:B:347:PX4:O2	3:B:354:PX4:H5	0.47	2.09	5	1
3:C:369:PX4:O2	3:C:369:PX4:H4	0.47	2.09	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:493:VAL:O	3:A:643:PX4:H7	0.47	2.09	10	1
3:C:316:PX4:O1	3:C:316:PX4:H12	0.47	2.09	12	1
3:B:341:PX4:O3	3:B:341:PX4:H12	0.47	2.10	14	1
3:C:355:PX4:O5	3:C:367:PX4:H4	0.47	2.09	15	1
3:A:618:PX4:O1	3:B:400:PX4:H4	0.47	2.09	3	1
3:B:344:PX4:H9	3:B:344:PX4:C6	0.47	2.40	5	1
3:C:303:PX4:H10	3:C:303:PX4:O3	0.47	2.10	6	1
3:A:619:PX4:H3	3:A:631:PX4:H14	0.47	1.86	13	1
3:A:619:PX4:H10	3:A:635:PX4:O4	0.47	2.08	1	1
3:B:387:PX4:O3	3:B:387:PX4:H9	0.47	2.10	1	1
3:C:347:PX4:H6	3:C:354:PX4:O8	0.47	2.10	1	2
3:A:627:PX4:H3	3:A:627:PX4:C6	0.47	2.38	3	1
3:B:378:PX4:C6	3:C:305:PX4:H11	0.47	2.39	3	1
3:C:309:PX4:O2	3:C:309:PX4:H4	0.47	2.10	3	2
3:A:619:PX4:H9	3:A:635:PX4:O4	0.47	2.09	6	1
3:A:640:PX4:O3	3:A:640:PX4:H6	0.47	2.09	6	3
3:C:354:PX4:O1	3:C:354:PX4:H3	0.47	2.09	7	1
3:C:309:PX4:H13	3:C:312:PX4:O1	0.47	2.09	8	1
3:B:351:PX4:H11	3:B:361:PX4:H7	0.47	1.86	10	1
3:A:618:PX4:O1	3:B:400:PX4:H11	0.47	2.10	13	1
1:A:492:LYS:HB2	3:A:643:PX4:H8	0.47	1.87	14	1
3:C:314:PX4:H3	3:C:314:PX4:O1	0.47	2.10	3	2
3:C:306:PX4:O2	3:C:306:PX4:H13	0.47	2.10	5	1
3:C:337:PX4:H4	3:C:346:PX4:O3	0.47	2.10	6	1
3:A:606:PX4:H3	3:B:386:PX4:O1	0.47	2.09	8	1
3:C:336:PX4:O3	3:C:336:PX4:H9	0.47	2.09	14	1
3:B:336:PX4:O3	3:B:336:PX4:H13	0.47	2.10	15	1
3:C:315:PX4:H7	3:C:315:PX4:O3	0.47	2.10	3	2
3:C:309:PX4:O4	3:C:344:PX4:H8	0.47	2.09	5	1
3:B:308:PX4:O2	3:B:308:PX4:H12	0.47	2.09	6	1
3:B:308:PX4:H12	3:B:323:PX4:O2	0.47	2.10	10	1
3:B:334:PX4:H4	3:B:334:PX4:O4	0.47	2.10	15	1
3:B:388:PX4:O6	3:B:393:PX4:H5	0.47	2.10	1	1
3:C:325:PX4:O4	3:C:325:PX4:H4	0.47	2.10	5	1
3:B:316:PX4:O3	3:B:316:PX4:C5	0.47	2.63	13	1
3:B:397:PX4:H5	2:C:120:GLU:OE1	0.47	2.09	14	1
3:B:392:PX4:O1	3:B:392:PX4:H3	0.46	2.10	7	2
3:B:397:PX4:O1	3:B:397:PX4:H3	0.46	2.09	9	1
3:B:352:PX4:H14	3:B:352:PX4:H3	0.46	1.86	13	1
3:B:368:PX4:H71	3:C:345:PX4:H72	0.46	1.87	13	1
3:A:612:PX4:H3	3:C:351:PX4:O1	0.46	2.10	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:624:PX4:O4	3:A:624:PX4:H3	0.46	2.10	15	1
3:B:386:PX4:H4	3:B:392:PX4:O2	0.46	2.10	2	1
3:B:352:PX4:O4	3:B:352:PX4:H13	0.46	2.10	11	1
3:B:325:PX4:H8	3:B:331:PX4:O4	0.46	2.10	2	1
3:C:325:PX4:O3	3:C:325:PX4:H10	0.46	2.11	5	3
3:A:647:PX4:H11	3:A:648:PX4:O8	0.46	2.10	3	1
3:B:318:PX4:H12	3:B:318:PX4:O3	0.46	2.11	8	3
1:A:495:PRO:O	3:A:646:PX4:H5	0.46	2.10	7	1
3:C:341:PX4:H4	3:C:341:PX4:O2	0.46	2.10	7	2
3:A:629:PX4:O2	3:A:637:PX4:H11	0.46	2.11	8	1
3:B:370:PX4:O3	3:B:370:PX4:H13	0.46	2.10	8	3
3:B:306:PX4:H10	3:B:346:PX4:O1	0.46	2.09	9	1
3:B:379:PX4:O3	3:B:379:PX4:H12	0.46	2.09	9	1
3:B:396:PX4:H4	3:B:396:PX4:O2	0.46	2.11	9	1
3:C:318:PX4:H5	3:C:324:PX4:O1	0.46	2.11	11	1
3:C:330:PX4:H12	3:C:330:PX4:O3	0.46	2.10	11	1
3:C:338:PX4:H9	3:C:338:PX4:O3	0.46	2.10	15	1
3:B:340:PX4:O4	3:B:340:PX4:H4	0.46	2.09	1	1
3:A:642:PX4:H3	3:A:647:PX4:O2	0.46	2.10	3	1
3:A:625:PX4:H9	3:A:625:PX4:O1	0.46	2.10	4	1
3:B:322:PX4:O1	3:B:322:PX4:H7	0.46	2.10	8	1
3:A:608:PX4:H9	3:B:395:PX4:O2	0.46	2.10	12	1
3:C:310:PX4:H3	3:C:310:PX4:C6	0.46	2.40	14	1
3:B:379:PX4:O4	3:B:385:PX4:H4	0.46	2.11	15	1
3:B:314:PX4:O1	3:B:314:PX4:H3	0.46	2.10	1	1
3:B:362:PX4:H12	3:B:362:PX4:O3	0.46	2.11	3	2
2:C:86:MET:HG3	3:C:314:PX4:H19	0.46	1.88	5	1
3:B:332:PX4:O2	3:B:332:PX4:H7	0.46	2.10	6	1
3:B:337:PX4:H15	3:B:339:PX4:H3	0.46	1.86	6	1
3:B:318:PX4:O4	3:B:334:PX4:H3	0.46	2.11	2	1
3:C:355:PX4:O1	3:C:367:PX4:H11	0.46	2.10	9	1
3:B:341:PX4:C2	3:B:364:PX4:O3	0.46	2.64	12	1
2:B:119:VAL:HG13	2:B:120:GLU:N	0.46	2.25	13	1
3:B:315:PX4:O3	3:B:315:PX4:H13	0.46	2.10	2	3
3:C:356:PX4:H10	3:C:356:PX4:O3	0.46	2.10	2	1
3:A:639:PX4:H8	3:A:640:PX4:O4	0.46	2.11	3	1
3:C:315:PX4:H4	3:C:331:PX4:O1	0.46	2.10	5	2
3:A:645:PX4:H13	3:A:647:PX4:O1	0.46	2.11	5	1
1:A:386:LYS:HD2	1:A:402:HIS:CE1	0.46	2.45	9	1
3:B:345:PX4:O8	3:B:373:PX4:H3	0.46	2.10	9	1
3:C:360:PX4:C6	3:C:360:PX4:H13	0.46	2.41	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:633:PX4:H3	3:B:400:PX4:O1	0.46	2.11	11	1
3:C:316:PX4:H10	3:C:316:PX4:O3	0.46	2.10	12	1
3:C:345:PX4:H10	3:C:345:PX4:O3	0.46	2.11	13	1
3:B:324:PX4:O3	3:B:324:PX4:C3	0.46	2.64	3	1
3:A:648:PX4:H10	3:A:648:PX4:O2	0.46	2.10	4	1
3:A:631:PX4:O3	3:A:631:PX4:H6	0.46	2.09	7	1
3:B:360:PX4:H4	3:B:360:PX4:O1	0.46	2.11	9	1
3:C:366:PX4:H3	3:C:366:PX4:O4	0.46	2.11	11	2
3:C:367:PX4:H9	3:C:367:PX4:O3	0.46	2.11	13	1
3:B:310:PX4:H9	3:B:310:PX4:O3	0.46	2.11	4	2
3:B:400:PX4:O1	3:C:370:PX4:H3	0.46	2.10	2	1
3:A:604:PX4:H16	3:B:394:PX4:H8	0.46	1.86	7	1
3:C:362:PX4:H3	3:C:362:PX4:C6	0.46	2.41	8	1
3:B:302:PX4:H7	3:B:302:PX4:O3	0.46	2.10	9	1
3:A:610:PX4:H5	3:C:368:PX4:O6	0.46	2.11	11	1
3:C:335:PX4:H4	3:C:335:PX4:O2	0.46	2.10	12	1
3:B:332:PX4:O3	3:B:332:PX4:H6	0.46	2.11	15	1
3:B:319:PX4:H8	3:B:320:PX4:O1	0.46	2.11	2	1
3:C:343:PX4:O3	3:C:343:PX4:H12	0.46	2.10	2	2
3:A:610:PX4:H9	3:A:610:PX4:O2	0.46	2.10	4	1
3:B:341:PX4:H12	3:B:364:PX4:H15	0.46	1.87	11	1
3:B:371:PX4:O2	3:B:375:PX4:H7	0.46	2.11	12	1
3:C:305:PX4:O3	3:C:305:PX4:H9	0.46	2.11	13	3
3:B:338:PX4:H3	3:B:357:PX4:H1	0.46	1.86	13	1
3:B:341:PX4:H1	3:B:364:PX4:H13	0.46	1.87	13	1
3:A:641:PX4:H9	3:A:641:PX4:O3	0.46	2.11	15	1
3:C:363:PX4:H10	3:C:363:PX4:O2	0.46	2.10	15	1
2:B:69:GLN:OE1	3:B:317:PX4:H5	0.45	2.11	1	1
3:B:351:PX4:H43	3:C:361:PX4:H41	0.45	1.88	1	1
3:A:602:PX4:H6	3:B:382:PX4:O2	0.45	2.11	2	1
3:C:326:PX4:O1	3:C:326:PX4:H3	0.45	2.11	2	1
3:B:350:PX4:H40	3:C:340:PX4:H43	0.45	1.88	6	1
3:B:400:PX4:O3	3:B:400:PX4:H6	0.45	2.11	6	2
3:A:621:PX4:O4	3:A:621:PX4:C23	0.45	2.64	8	1
3:C:306:PX4:H9	3:C:348:PX4:O2	0.45	2.12	9	1
3:C:309:PX4:H9	3:C:309:PX4:O3	0.45	2.11	15	1
3:C:368:PX4:O4	3:C:368:PX4:H3	0.45	2.11	15	1
3:C:306:PX4:O4	3:C:306:PX4:H3	0.45	2.11	1	1
3:B:360:PX4:H12	3:B:362:PX4:O3	0.45	2.11	3	1
3:A:619:PX4:O3	3:A:619:PX4:H12	0.45	2.11	4	1
3:B:391:PX4:H8	3:B:394:PX4:O1	0.45	2.12	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:349:PX4:O3	3:B:371:PX4:H4	0.45	2.11	5	1
3:B:332:PX4:O8	3:B:332:PX4:H3	0.45	2.12	9	1
3:A:638:PX4:O3	3:A:638:PX4:H13	0.45	2.10	15	2
3:C:302:PX4:O1	3:C:302:PX4:H3	0.45	2.11	15	1
3:A:637:PX4:O3	3:A:637:PX4:H13	0.45	2.11	1	1
3:A:614:PX4:O8	3:A:614:PX4:H4	0.45	2.11	3	1
3:C:323:PX4:H10	3:C:323:PX4:O3	0.45	2.12	6	1
3:B:320:PX4:O3	3:B:320:PX4:C5	0.45	2.64	7	1
3:B:321:PX4:H12	3:B:330:PX4:C6	0.45	2.40	10	1
3:A:602:PX4:H4	3:B:382:PX4:O2	0.45	2.10	12	1
3:B:400:PX4:O4	3:B:400:PX4:H3	0.45	2.11	1	1
3:B:377:PX4:O3	3:B:377:PX4:H7	0.45	2.11	3	3
3:C:329:PX4:H8	3:C:347:PX4:O8	0.45	2.12	8	1
3:C:359:PX4:H3	3:C:366:PX4:O4	0.45	2.11	8	1
3:A:604:PX4:O1	3:B:394:PX4:H7	0.45	2.11	9	1
3:B:399:PX4:H5	3:C:321:PX4:O6	0.45	2.11	13	2
3:B:385:PX4:H9	3:B:385:PX4:O1	0.45	2.12	14	1
3:A:643:PX4:H10	3:A:643:PX4:O4	0.45	2.11	6	1
3:B:376:PX4:H4	3:B:381:PX4:P1	0.45	2.52	7	1
3:A:626:PX4:O3	3:A:626:PX4:H6	0.45	2.12	8	1
3:B:356:PX4:O4	3:B:370:PX4:H7	0.45	2.11	8	1
3:C:326:PX4:O1	3:C:345:PX4:H6	0.45	2.12	12	1
3:A:617:PX4:O2	3:C:365:PX4:H12	0.45	2.12	13	1
3:B:308:PX4:H12	3:B:308:PX4:O3	0.45	2.11	3	1
3:B:394:PX4:O3	3:B:394:PX4:H12	0.45	2.11	3	1
1:A:487:ASN:CB	3:A:643:PX4:H6	0.45	2.42	4	1
3:B:398:PX4:H17	3:B:398:PX4:H12	0.45	1.89	5	1
3:C:353:PX4:H3	3:C:353:PX4:O1	0.45	2.12	8	1
3:A:644:PX4:H10	3:A:644:PX4:O6	0.45	2.11	14	1
3:A:608:PX4:H4	3:B:394:PX4:O6	0.45	2.12	7	1
3:A:633:PX4:H7	3:B:400:PX4:H16	0.45	1.88	8	1
3:B:378:PX4:O2	3:C:305:PX4:H11	0.45	2.11	8	1
3:C:317:PX4:H12	3:C:317:PX4:O3	0.45	2.12	10	2
3:B:340:PX4:O8	3:B:356:PX4:H12	0.45	2.11	11	1
3:B:392:PX4:H15	3:B:393:PX4:H9	0.45	1.89	14	1
3:A:608:PX4:H10	3:B:394:PX4:O1	0.45	2.11	2	1
3:B:378:PX4:H9	3:B:378:PX4:O3	0.45	2.12	3	1
3:B:378:PX4:H12	3:B:390:PX4:O2	0.45	2.12	5	1
3:A:616:PX4:H13	3:A:616:PX4:O8	0.45	2.12	7	1
3:B:377:PX4:H7	3:B:377:PX4:H14	0.45	1.88	12	1
3:C:321:PX4:O1	3:C:321:PX4:H4	0.45	2.12	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:365:PX4:O1	3:C:365:PX4:H6	0.45	2.11	14	1
3:A:604:PX4:H4	3:A:605:PX4:C6	0.45	2.41	15	1
3:C:347:PX4:O1	3:C:347:PX4:H12	0.45	2.11	15	1
3:B:392:PX4:O8	3:B:393:PX4:H3	0.45	2.10	4	2
1:A:468:MET:HE1	1:A:488:ASN:ND2	0.45	2.27	4	1
3:B:325:PX4:H5	3:B:331:PX4:O3	0.45	2.12	4	1
3:B:336:PX4:H8	3:B:358:PX4:O3	0.45	2.12	4	1
3:C:333:PX4:H12	3:C:360:PX4:O1	0.45	2.12	6	1
3:C:327:PX4:H8	3:C:332:PX4:O3	0.45	2.12	8	1
2:B:115:TYR:O	2:B:119:VAL:HG12	0.45	2.12	12	1
2:C:104:PHE:CE1	3:C:324:PX4:H28	0.45	2.47	15	1
3:A:602:PX4:O5	3:A:603:PX4:H7	0.45	2.11	2	1
3:C:355:PX4:O3	3:C:367:PX4:H8	0.45	2.12	2	1
2:C:101:LEU:HD11	3:C:324:PX4:C8	0.45	2.42	9	1
3:C:366:PX4:O6	3:C:366:PX4:H6	0.45	2.12	9	1
3:A:638:PX4:H4	3:A:638:PX4:O4	0.45	2.11	11	1
1:A:474:PHE:CE2	1:A:485:LYS:HE2	0.45	2.47	12	1
2:B:171:ARG:NH1	3:B:307:PX4:H3	0.45	2.27	12	1
1:A:503:ARG:NH2	3:A:644:PX4:O1	0.45	2.51	13	1
3:C:368:PX4:O8	3:C:368:PX4:H3	0.45	2.12	13	1
3:B:333:PX4:C1	3:B:333:PX4:C6	0.45	2.95	14	1
3:B:369:PX4:O2	3:B:369:PX4:H7	0.45	2.11	14	1
3:A:620:PX4:H8	3:C:359:PX4:O1	0.44	2.12	1	1
3:A:613:PX4:H42	3:A:622:PX4:H44	0.44	1.87	2	1
3:B:312:PX4:H4	3:B:312:PX4:O2	0.44	2.12	7	2
3:B:349:PX4:O2	3:B:371:PX4:H3	0.44	2.12	6	1
3:C:333:PX4:O4	3:C:360:PX4:H10	0.44	2.12	6	1
3:B:322:PX4:O4	3:B:322:PX4:H3	0.44	2.12	9	1
3:B:397:PX4:H5	2:C:120:GLU:OE2	0.44	2.12	11	1
3:C:344:PX4:H3	3:C:344:PX4:O1	0.44	2.12	11	1
3:B:388:PX4:O2	3:B:393:PX4:H8	0.44	2.12	12	1
3:B:366:PX4:H12	3:B:367:PX4:O1	0.44	2.12	13	1
3:C:334:PX4:H7	3:C:347:PX4:O6	0.44	2.11	14	1
3:C:301:PX4:O4	3:C:301:PX4:H3	0.44	2.12	1	1
3:A:615:PX4:O4	3:A:615:PX4:H3	0.44	2.12	2	1
3:C:330:PX4:O1	3:C:330:PX4:H3	0.44	2.13	2	1
3:B:378:PX4:H3	3:B:378:PX4:O4	0.44	2.13	4	1
3:C:309:PX4:O1	3:C:344:PX4:H7	0.44	2.13	4	1
3:A:620:PX4:H12	3:A:620:PX4:O3	0.44	2.12	6	1
3:A:639:PX4:H14	3:A:640:PX4:H6	0.44	1.90	6	1
3:B:347:PX4:P1	3:B:354:PX4:H11	0.44	2.51	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:321:PX4:O3	3:B:321:PX4:H9	0.44	2.12	8	3
3:C:309:PX4:O1	3:C:309:PX4:H9	0.44	2.12	9	1
3:C:333:PX4:O1	3:C:360:PX4:H4	0.44	2.13	5	1
3:A:642:PX4:O4	3:A:647:PX4:H10	0.44	2.13	14	2
3:A:602:PX4:O6	3:A:603:PX4:H3	0.44	2.11	7	1
3:C:320:PX4:O1	3:C:320:PX4:H4	0.44	2.11	7	1
3:B:366:PX4:H45	3:C:367:PX4:C22	0.44	2.43	8	1
3:B:336:PX4:O3	3:B:350:PX4:H7	0.44	2.12	7	1
3:B:338:PX4:H10	3:B:377:PX4:O2	0.44	2.11	13	1
3:B:393:PX4:H13	3:B:393:PX4:O3	0.44	2.12	14	2
3:C:359:PX4:O3	3:C:359:PX4:H10	0.44	2.12	1	1
3:A:617:PX4:H10	3:A:617:PX4:O8	0.44	2.13	6	1
3:B:340:PX4:H13	3:B:370:PX4:H2	0.44	1.89	10	1
3:B:396:PX4:H6	3:B:396:PX4:O1	0.44	2.12	12	1
3:B:359:PX4:H9	3:B:359:PX4:O3	0.44	2.12	13	1
3:B:384:PX4:O3	3:B:384:PX4:H12	0.44	2.13	13	1
3:B:302:PX4:H4	3:B:302:PX4:C6	0.44	2.42	1	1
3:A:648:PX4:O3	3:A:648:PX4:H12	0.44	2.13	3	1
1:A:457:GLU:OE2	3:A:636:PX4:H13	0.44	2.12	4	1
3:B:314:PX4:O2	3:B:334:PX4:H8	0.44	2.12	6	1
3:A:625:PX4:H6	3:A:625:PX4:H15	0.44	1.89	8	1
3:A:618:PX4:H12	3:A:644:PX4:C5	0.44	2.34	9	1
3:B:301:PX4:H4	3:B:301:PX4:O1	0.44	2.13	10	1
3:B:347:PX4:O3	3:B:347:PX4:H9	0.44	2.13	13	1
3:C:345:PX4:O2	3:C:364:PX4:H3	0.44	2.13	4	2
1:A:493:VAL:O	3:A:643:PX4:H5	0.44	2.12	7	1
3:C:341:PX4:O3	3:C:341:PX4:H7	0.44	2.13	1	1
3:A:639:PX4:H12	3:A:639:PX4:O2	0.44	2.12	4	1
3:B:336:PX4:O1	3:B:350:PX4:H8	0.44	2.12	8	1
3:B:341:PX4:O1	3:B:341:PX4:H3	0.44	2.13	9	2
3:A:633:PX4:O2	3:A:633:PX4:H4	0.44	2.13	12	1
3:B:354:PX4:H18	3:B:354:PX4:O8	0.44	2.13	15	1
3:A:611:PX4:O3	3:C:351:PX4:H12	0.44	2.13	2	1
3:C:302:PX4:O3	3:C:302:PX4:H6	0.44	2.13	3	1
3:C:305:PX4:H3	3:C:305:PX4:O2	0.44	2.13	4	1
3:C:344:PX4:O2	3:C:344:PX4:H4	0.44	2.13	4	1
3:B:396:PX4:O1	3:B:397:PX4:H10	0.44	2.12	7	1
3:B:307:PX4:O1	3:B:307:PX4:H3	0.44	2.13	8	2
3:A:647:PX4:H7	3:A:647:PX4:H15	0.44	1.88	14	1
3:B:345:PX4:H2	3:B:373:PX4:H13	0.44	1.90	15	1
3:A:625:PX4:O2	3:A:636:PX4:H4	0.43	2.13	6	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:644:PX4:O3	3:A:644:PX4:H6	0.43	2.13	6	1
3:B:368:PX4:H9	3:B:368:PX4:O3	0.43	2.13	9	2
2:B:217:LYS:O	2:B:221:HIS:CD2	0.43	2.71	12	1
3:B:321:PX4:H4	3:B:330:PX4:O2	0.43	2.13	14	1
3:A:627:PX4:O4	3:A:627:PX4:C2	0.43	2.57	3	1
3:A:601:PX4:H5	3:B:381:PX4:O1	0.43	2.12	4	2
3:C:344:PX4:H7	3:C:344:PX4:O2	0.43	2.13	7	1
3:C:337:PX4:H12	3:C:346:PX4:O7	0.43	2.13	8	1
3:C:301:PX4:H10	3:C:301:PX4:O2	0.43	2.13	10	1
3:C:366:PX4:H7	3:C:369:PX4:O1	0.43	2.12	10	1
3:B:372:PX4:O2	3:B:382:PX4:H4	0.43	2.14	11	1
3:B:376:PX4:O1	3:B:376:PX4:H12	0.43	2.13	12	1
1:A:494:GLU:OE1	3:A:646:PX4:H13	0.43	2.13	13	1
3:C:349:PX4:O3	3:C:349:PX4:H13	0.43	2.13	13	1
3:A:639:PX4:H7	3:A:639:PX4:O3	0.43	2.12	15	1
3:A:621:PX4:H33	3:C:360:PX4:H45	0.43	1.89	2	1
3:A:605:PX4:O8	3:A:607:PX4:H3	0.43	2.12	3	1
3:A:614:PX4:H7	3:A:619:PX4:H14	0.43	1.90	3	1
3:A:601:PX4:H13	3:B:389:PX4:O2	0.43	2.13	7	1
3:A:633:PX4:H7	3:B:400:PX4:C6	0.43	2.43	7	1
1:A:493:VAL:HG13	3:A:645:PX4:H9	0.43	1.90	8	1
3:C:334:PX4:O3	3:C:334:PX4:H10	0.43	2.13	9	2
3:C:312:PX4:H8	3:C:325:PX4:O4	0.43	2.13	10	1
3:B:399:PX4:H13	3:C:336:PX4:O6	0.43	2.13	13	1
3:C:352:PX4:H8	3:C:361:PX4:O4	0.43	2.14	14	1
3:A:602:PX4:C8	3:A:603:PX4:H7	0.43	2.44	2	1
3:A:613:PX4:O2	3:C:346:PX4:H6	0.43	2.12	2	1
3:A:619:PX4:O3	3:A:635:PX4:H7	0.43	2.14	2	1
3:B:342:PX4:H4	3:B:342:PX4:O4	0.43	2.13	3	1
3:C:347:PX4:H5	3:C:354:PX4:O4	0.43	2.13	3	1
3:B:336:PX4:H7	3:B:336:PX4:O3	0.43	2.13	4	1
3:C:324:PX4:O4	3:C:324:PX4:H3	0.43	2.13	6	1
3:C:321:PX4:H4	3:C:356:PX4:O2	0.43	2.13	10	2
3:A:644:PX4:O1	3:A:648:PX4:H6	0.43	2.14	9	1
3:B:319:PX4:O1	3:B:319:PX4:H4	0.43	2.14	9	1
3:C:359:PX4:O3	3:C:359:PX4:H13	0.43	2.13	12	1
3:B:341:PX4:O3	3:B:364:PX4:H13	0.43	2.13	13	1
3:B:340:PX4:O3	3:B:340:PX4:H9	0.43	2.13	14	1
1:A:456:TRP:CE3	1:A:459:ILE:HD11	0.43	2.48	15	1
3:A:646:PX4:O3	3:A:646:PX4:C3	0.43	2.66	1	1
3:B:399:PX4:O2	3:C:356:PX4:H12	0.43	2.13	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:606:PX4:O1	3:A:606:PX4:H3	0.43	2.13	4	2
3:B:360:PX4:H13	3:B:362:PX4:O8	0.43	2.13	4	1
3:B:390:PX4:H7	3:B:390:PX4:O3	0.43	2.13	4	1
3:B:379:PX4:H3	3:B:391:PX4:O4	0.43	2.12	5	1
3:B:332:PX4:O3	3:B:332:PX4:C4	0.43	2.64	6	1
3:A:636:PX4:H9	3:A:636:PX4:O2	0.43	2.14	8	1
3:C:333:PX4:H10	3:C:360:PX4:P1	0.43	2.53	11	1
3:A:617:PX4:H6	3:C:349:PX4:O2	0.43	2.13	13	1
3:C:344:PX4:O4	3:C:344:PX4:H3	0.43	2.14	14	1
3:A:622:PX4:O3	3:A:622:PX4:H6	0.43	2.14	2	1
3:B:302:PX4:O1	3:B:307:PX4:H4	0.43	2.14	3	2
3:B:309:PX4:H8	3:B:342:PX4:O1	0.43	2.14	7	1
3:C:365:PX4:O1	3:C:365:PX4:H3	0.43	2.13	13	1
3:B:365:PX4:H7	3:B:365:PX4:O6	0.43	2.14	14	1
3:B:303:PX4:H3	3:B:303:PX4:O4	0.43	2.14	15	1
3:C:359:PX4:O3	3:C:366:PX4:H9	0.43	2.14	2	1
3:C:329:PX4:H10	3:C:347:PX4:O2	0.43	2.14	3	1
3:C:333:PX4:O1	3:C:333:PX4:H9	0.43	2.14	4	1
3:B:341:PX4:O4	3:B:364:PX4:H9	0.43	2.14	6	1
3:C:318:PX4:O3	3:C:318:PX4:H6	0.43	2.14	6	2
1:A:321:GLY:HA2	1:A:323:PHE:CZ	0.43	2.49	7	1
3:A:603:PX4:O3	3:A:603:PX4:C5	0.43	2.67	8	1
3:C:352:PX4:H9	3:C:361:PX4:O1	0.43	2.14	12	1
3:B:331:PX4:O2	3:B:331:PX4:H6	0.43	2.14	2	1
3:B:336:PX4:O1	3:B:350:PX4:H9	0.43	2.14	4	1
3:B:302:PX4:O4	3:B:302:PX4:H4	0.43	2.14	5	1
3:A:618:PX4:H6	3:A:618:PX4:O3	0.43	2.14	7	2
3:B:319:PX4:H5	3:B:320:PX4:O4	0.43	2.13	7	1
3:B:387:PX4:O3	3:B:387:PX4:H6	0.43	2.14	11	1
3:C:369:PX4:H7	3:C:369:PX4:O2	0.43	2.13	1	1
2:C:211:LEU:HD12	2:C:215:HIS:CD2	0.43	2.49	3	1
3:C:361:PX4:O3	3:C:361:PX4:H12	0.43	2.13	9	2
3:A:610:PX4:H13	3:A:629:PX4:O6	0.43	2.14	8	2
3:A:611:PX4:H15	3:A:613:PX4:H11	0.43	1.90	7	1
3:B:357:PX4:O3	3:B:357:PX4:C5	0.43	2.67	7	1
3:C:313:PX4:O8	3:C:337:PX4:H3	0.43	2.14	11	1
3:B:356:PX4:H16	3:B:370:PX4:C2	0.43	2.43	1	1
3:C:305:PX4:H18	3:C:305:PX4:O8	0.43	2.13	1	1
3:C:352:PX4:O8	3:C:364:PX4:H7	0.43	2.14	1	1
3:C:344:PX4:O3	3:C:344:PX4:H9	0.43	2.13	6	1
1:A:486:PHE:CZ	1:A:491:LEU:HA	0.43	2.49	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:359:PX4:O1	3:B:359:PX4:H3	0.43	2.14	7	1
3:B:332:PX4:H9	3:B:332:PX4:O2	0.43	2.14	8	1
3:C:321:PX4:H12	3:C:321:PX4:O3	0.42	2.14	1	1
3:B:365:PX4:O1	3:B:365:PX4:H3	0.42	2.14	4	1
3:C:309:PX4:H2	3:C:344:PX4:H11	0.42	1.90	5	1
1:A:430:PHE:CD1	1:A:435:TYR:HB3	0.42	2.49	7	1
3:A:633:PX4:H9	3:B:400:PX4:O4	0.42	2.13	8	1
3:A:627:PX4:H5	3:C:361:PX4:H7	0.42	1.91	9	1
3:C:335:PX4:C28	3:C:335:PX4:H47	0.42	2.44	10	1
3:B:338:PX4:H3	3:B:357:PX4:O1	0.42	2.14	15	2
3:A:639:PX4:O2	3:A:640:PX4:H11	0.42	2.14	13	1
3:B:394:PX4:O2	3:B:394:PX4:H9	0.42	2.13	13	1
3:A:642:PX4:O1	3:A:647:PX4:H3	0.42	2.13	15	1
3:B:373:PX4:O1	3:B:388:PX4:H8	0.42	2.14	15	1
3:A:619:PX4:H9	3:A:635:PX4:O6	0.42	2.13	3	1
3:A:601:PX4:O3	3:A:601:PX4:H7	0.42	2.14	5	1
3:B:378:PX4:O2	3:C:305:PX4:H10	0.42	2.14	9	1
3:A:634:PX4:O4	3:A:644:PX4:H6	0.42	2.14	10	1
3:C:319:PX4:H13	3:C:319:PX4:O3	0.42	2.14	11	1
3:C:326:PX4:C9	3:C:328:PX4:H24	0.42	2.45	13	1
1:A:457:GLU:OE1	3:A:636:PX4:H12	0.42	2.14	1	1
3:C:337:PX4:O3	3:C:337:PX4:H6	0.42	2.14	3	1
3:B:356:PX4:O8	3:B:370:PX4:H10	0.42	2.14	4	1
3:A:615:PX4:H8	3:C:360:PX4:O2	0.42	2.14	7	1
3:B:358:PX4:O2	3:B:365:PX4:H13	0.42	2.13	7	1
3:C:329:PX4:H6	3:C:329:PX4:O3	0.42	2.14	10	2
3:B:352:PX4:O3	3:B:369:PX4:H10	0.42	2.14	9	1
2:B:184:HIS:CE1	2:C:123:LEU:HA	0.42	2.49	12	1
3:B:379:PX4:O2	3:B:385:PX4:H6	0.42	2.14	12	1
3:B:383:PX4:H3	3:B:383:PX4:O1	0.42	2.15	12	1
3:B:325:PX4:O3	3:B:325:PX4:H9	0.42	2.14	15	1
3:B:386:PX4:O2	3:B:386:PX4:H3	0.42	2.14	15	1
3:A:605:PX4:O4	3:A:607:PX4:H3	0.42	2.15	9	2
3:C:305:PX4:O8	3:C:305:PX4:C8	0.42	2.67	1	1
3:B:307:PX4:H6	3:B:307:PX4:O3	0.42	2.15	2	1
3:C:352:PX4:H10	3:C:352:PX4:O3	0.42	2.14	2	2
3:B:376:PX4:H10	3:B:376:PX4:O3	0.42	2.14	9	3
3:B:325:PX4:H9	3:B:325:PX4:O3	0.42	2.14	13	3
3:B:342:PX4:O4	3:B:342:PX4:H4	0.42	2.14	8	1
3:B:399:PX4:H3	3:B:399:PX4:O1	0.42	2.14	9	1
3:C:323:PX4:C6	3:C:323:PX4:H10	0.42	2.44	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:612:PX4:H3	3:A:612:PX4:O4	0.42	2.12	10	1
3:B:382:PX4:O3	3:B:382:PX4:H6	0.42	2.14	14	2
3:B:334:PX4:O1	3:B:346:PX4:H7	0.42	2.14	15	1
3:B:304:PX4:O3	3:B:304:PX4:H7	0.42	2.15	3	1
3:B:313:PX4:O3	3:B:313:PX4:H9	0.42	2.14	5	1
3:A:634:PX4:H4	3:A:641:PX4:O1	0.42	2.13	8	1
3:B:399:PX4:O3	3:C:356:PX4:H3	0.42	2.13	9	1
3:A:628:PX4:O1	3:A:644:PX4:H11	0.42	2.14	11	1
3:A:633:PX4:H6	3:C:370:PX4:H47	0.42	1.91	11	1
3:C:351:PX4:O3	3:C:351:PX4:H13	0.42	2.14	15	1
3:A:624:PX4:O3	3:A:624:PX4:H13	0.42	2.15	13	3
3:B:385:PX4:H22	3:B:389:PX4:H48	0.42	1.92	2	1
3:B:312:PX4:C27	3:B:317:PX4:H8	0.42	2.38	3	1
2:C:193:ARG:NH2	3:C:311:PX4:O1	0.42	2.53	5	1
3:B:328:PX4:H12	3:B:328:PX4:O3	0.42	2.14	9	1
3:B:320:PX4:P1	3:B:320:PX4:H13	0.42	2.54	11	1
3:C:306:PX4:O1	3:C:306:PX4:H3	0.42	2.14	11	1
3:C:364:PX4:O3	3:C:364:PX4:H12	0.42	2.14	12	1
3:A:633:PX4:H9	3:C:370:PX4:O6	0.42	2.15	1	1
1:A:490:LYS:HB2	3:A:643:PX4:H12	0.42	1.91	2	1
3:A:623:PX4:H10	3:A:623:PX4:O6	0.42	2.13	5	1
3:C:329:PX4:H14	3:C:329:PX4:H7	0.42	1.91	7	1
3:B:303:PX4:H4	3:B:303:PX4:O2	0.42	2.15	8	1
3:C:348:PX4:O3	3:C:370:PX4:H12	0.42	2.15	8	1
3:B:386:PX4:H12	3:B:386:PX4:O3	0.42	2.14	9	1
3:B:309:PX4:O6	3:B:315:PX4:H4	0.42	2.15	10	1
3:B:331:PX4:O1	3:B:331:PX4:H3	0.42	2.15	10	1
3:B:378:PX4:H1	3:B:378:PX4:C6	0.42	2.44	10	1
3:B:367:PX4:O3	3:B:367:PX4:H6	0.42	2.13	11	2
3:B:378:PX4:O2	3:B:387:PX4:H4	0.42	2.13	13	1
3:A:635:PX4:O3	3:A:635:PX4:H6	0.42	2.13	10	2
3:B:392:PX4:O8	3:B:393:PX4:H7	0.42	2.14	14	2
3:A:642:PX4:O3	3:A:642:PX4:H10	0.42	2.14	3	1
3:C:365:PX4:H4	3:C:365:PX4:C6	0.42	2.45	4	1
3:A:615:PX4:H7	3:A:615:PX4:O6	0.42	2.15	6	1
3:B:349:PX4:O3	3:B:371:PX4:H9	0.42	2.15	6	1
3:C:337:PX4:H4	3:C:346:PX4:P1	0.42	2.54	6	1
3:C:348:PX4:H9	3:C:348:PX4:O3	0.42	2.15	6	1
3:B:326:PX4:H70	3:C:327:PX4:H71	0.42	1.92	8	1
3:C:333:PX4:H4	3:C:360:PX4:O3	0.42	2.14	9	1
3:C:312:PX4:H5	3:C:325:PX4:O2	0.42	2.15	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:359:PX4:H6	3:C:363:PX4:O2	0.42	2.15	12	1
3:A:642:PX4:O6	3:A:647:PX4:H9	0.42	2.15	15	1
2:B:112:MET:HE1	3:B:304:PX4:H50	0.42	1.90	2	1
1:A:457:GLU:OE2	3:A:636:PX4:H3	0.42	2.14	3	1
3:A:621:PX4:O8	3:A:637:PX4:H6	0.42	2.15	4	1
3:B:323:PX4:H9	3:B:323:PX4:O3	0.42	2.14	5	1
3:B:360:PX4:O2	3:B:381:PX4:H6	0.42	2.13	7	1
3:C:331:PX4:O1	3:C:331:PX4:H3	0.42	2.15	7	1
3:A:647:PX4:H9	3:A:647:PX4:O4	0.42	2.14	11	1
3:C:341:PX4:P1	3:C:362:PX4:H9	0.42	2.54	11	1
3:B:321:PX4:H5	3:B:330:PX4:O2	0.42	2.15	12	1
3:B:381:PX4:H71	3:B:394:PX4:H35	0.42	1.91	14	1
3:C:312:PX4:O2	3:C:312:PX4:H4	0.42	2.14	1	1
3:A:642:PX4:O3	3:A:642:PX4:C4	0.42	2.67	3	1
3:B:345:PX4:O3	3:B:345:PX4:H10	0.42	2.15	3	1
3:A:639:PX4:O3	3:A:639:PX4:H10	0.42	2.15	4	1
3:B:331:PX4:H14	3:B:331:PX4:H6	0.42	1.91	6	1
3:B:349:PX4:H7	3:B:353:PX4:O2	0.42	2.15	9	1
3:C:321:PX4:H3	3:C:321:PX4:O4	0.42	2.15	10	1
3:C:324:PX4:H3	3:C:324:PX4:O2	0.42	2.15	11	1
3:B:312:PX4:H54	3:B:317:PX4:H10	0.42	1.90	13	1
3:A:613:PX4:O4	3:A:613:PX4:H13	0.42	2.15	14	1
3:A:610:PX4:H4	3:C:368:PX4:O6	0.42	2.13	15	1
3:B:308:PX4:H17	3:C:302:PX4:H13	0.42	1.91	15	1
2:B:98:GLN:CD	3:B:303:PX4:H13	0.41	2.40	2	1
3:C:315:PX4:O4	3:C:315:PX4:H4	0.41	2.14	6	1
3:C:366:PX4:H6	3:C:369:PX4:O4	0.41	2.14	7	1
1:A:504:ASP:OD2	3:A:641:PX4:H11	0.41	2.15	10	1
3:B:330:PX4:O3	3:B:330:PX4:C3	0.41	2.68	12	1
3:A:614:PX4:O3	3:A:614:PX4:H12	0.41	2.14	14	1
3:A:623:PX4:O3	3:A:623:PX4:H13	0.41	2.15	2	1
3:B:339:PX4:O4	3:B:339:PX4:H4	0.41	2.15	2	1
3:B:388:PX4:O3	3:B:388:PX4:H7	0.41	2.15	6	1
3:C:368:PX4:H12	3:C:368:PX4:O3	0.41	2.16	6	1
3:B:359:PX4:H8	3:B:363:PX4:O2	0.41	2.16	8	1
3:B:362:PX4:O2	3:B:362:PX4:H12	0.41	2.15	9	1
2:B:100:TYR:CD2	2:C:209:ALA:HB2	0.41	2.50	11	1
2:B:126:PHE:HB2	2:C:184:HIS:CE1	0.41	2.50	11	1
3:A:626:PX4:O8	3:C:365:PX4:H5	0.41	2.16	3	1
3:C:350:PX4:H12	3:C:352:PX4:O1	0.41	2.15	3	1
3:B:358:PX4:O1	3:B:365:PX4:H11	0.41	2.15	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:635:PX4:O2	3:A:635:PX4:H3	0.41	2.15	6	1
3:C:309:PX4:H4	3:C:309:PX4:C6	0.41	2.45	6	1
3:B:397:PX4:O3	3:B:397:PX4:H9	0.41	2.15	11	1
3:A:639:PX4:H4	3:A:639:PX4:O1	0.41	2.15	12	1
3:B:334:PX4:O2	3:B:346:PX4:H9	0.41	2.15	12	1
3:A:615:PX4:H12	3:C:360:PX4:O1	0.41	2.15	13	1
3:B:361:PX4:H7	3:B:361:PX4:O3	0.41	2.16	14	1
1:A:483:TYR:CD2	1:A:505:TRP:CZ2	0.41	3.08	2	1
3:C:319:PX4:O1	3:C:323:PX4:H5	0.41	2.15	6	1
3:A:613:PX4:O3	3:A:613:PX4:H6	0.41	2.16	9	1
3:A:638:PX4:C6	3:A:638:PX4:H4	0.41	2.45	10	1
3:C:355:PX4:H10	3:C:367:PX4:O3	0.41	2.15	13	1
3:B:358:PX4:H10	3:B:360:PX4:O1	0.41	2.14	1	1
3:A:626:PX4:H6	3:A:626:PX4:O3	0.41	2.16	6	1
3:A:635:PX4:H34	3:C:358:PX4:H68	0.41	1.93	7	1
3:B:337:PX4:O1	3:B:362:PX4:H4	0.41	2.15	8	1
3:B:346:PX4:H6	3:B:346:PX4:O3	0.41	2.15	9	1
3:B:312:PX4:O8	3:C:304:PX4:H10	0.41	2.16	12	1
3:B:309:PX4:O4	3:B:335:PX4:H7	0.41	2.16	14	1
3:B:347:PX4:O1	3:B:374:PX4:H10	0.41	2.15	14	1
3:A:633:PX4:H11	3:B:400:PX4:O2	0.41	2.16	2	1
3:C:350:PX4:H7	3:C:350:PX4:O3	0.41	2.16	4	1
3:C:342:PX4:H9	3:C:342:PX4:O3	0.41	2.16	5	1
3:C:349:PX4:O1	3:C:349:PX4:H13	0.41	2.15	7	1
1:A:476:TYR:CE1	1:A:485:LYS:HG3	0.41	2.51	9	1
3:A:601:PX4:O5	3:A:604:PX4:H9	0.41	2.16	12	1
3:A:633:PX4:H5	3:C:370:PX4:O4	0.41	2.16	14	1
3:B:392:PX4:H12	3:B:393:PX4:O6	0.41	2.15	15	1
3:A:642:PX4:O2	3:A:642:PX4:H4	0.41	2.15	10	2
3:C:348:PX4:O3	3:C:348:PX4:H9	0.41	2.16	5	1
3:A:613:PX4:O1	3:C:346:PX4:H6	0.41	2.15	7	1
3:A:601:PX4:H3	3:A:601:PX4:O8	0.41	2.15	8	1
3:A:630:PX4:O2	3:A:630:PX4:H13	0.41	2.16	11	1
3:B:373:PX4:H10	3:B:373:PX4:O3	0.41	2.15	11	1
3:C:304:PX4:O2	3:C:304:PX4:H3	0.41	2.16	11	1
3:B:355:PX4:H6	3:B:355:PX4:O3	0.41	2.16	2	2
3:C:359:PX4:H9	3:C:359:PX4:H15	0.41	1.92	2	1
3:B:380:PX4:H10	3:B:380:PX4:O3	0.41	2.15	4	1
3:C:360:PX4:O3	3:C:360:PX4:C5	0.41	2.68	5	1
3:B:349:PX4:H30	3:B:353:PX4:H48	0.41	1.91	6	1
3:B:370:PX4:O3	3:C:305:PX4:H13	0.41	2.15	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:604:PX4:H8	3:B:384:PX4:C6	0.41	2.46	7	1
3:B:345:PX4:O1	3:B:373:PX4:H13	0.41	2.15	8	1
3:B:400:PX4:O3	3:B:400:PX4:C3	0.41	2.69	10	1
3:C:335:PX4:H47	3:C:335:PX4:H54	0.41	1.92	10	1
3:A:620:PX4:H54	3:A:628:PX4:H27	0.41	1.92	11	1
3:B:320:PX4:O1	3:B:320:PX4:H6	0.41	2.15	11	1
3:B:356:PX4:H14	3:B:356:PX4:H1	0.41	1.93	15	1
3:C:350:PX4:H3	3:C:352:PX4:O1	0.41	2.16	15	1
3:C:365:PX4:O3	3:C:365:PX4:H13	0.41	2.16	15	1
3:A:621:PX4:O2	3:C:365:PX4:H10	0.41	2.16	1	1
3:C:328:PX4:O3	3:C:328:PX4:H9	0.41	2.16	1	1
3:C:332:PX4:H10	3:C:332:PX4:O3	0.41	2.16	1	1
3:C:363:PX4:O3	3:C:363:PX4:H12	0.41	2.15	1	1
3:B:326:PX4:H42	3:C:327:PX4:H45	0.41	1.93	3	1
3:B:304:PX4:H3	3:C:301:PX4:O1	0.41	2.16	4	1
3:B:396:PX4:O4	3:B:396:PX4:H4	0.41	2.16	5	1
3:C:347:PX4:H7	3:C:366:PX4:O1	0.41	2.16	5	1
3:C:323:PX4:H10	3:C:323:PX4:C6	0.41	2.46	6	1
2:C:130:TRP:CE3	2:C:130:TRP:HA	0.41	2.50	7	1
3:B:356:PX4:H6	3:B:356:PX4:O3	0.41	2.16	8	1
3:A:602:PX4:H9	3:A:602:PX4:H14	0.41	1.93	9	1
3:C:305:PX4:O3	3:C:305:PX4:H6	0.41	2.16	9	1
3:B:347:PX4:H45	3:C:363:PX4:H42	0.41	1.93	10	1
3:B:358:PX4:O3	3:B:358:PX4:H7	0.41	2.15	10	1
3:B:379:PX4:H12	3:B:379:PX4:O3	0.41	2.15	10	1
3:B:318:PX4:O1	3:B:318:PX4:H10	0.41	2.16	15	1
3:B:390:PX4:H4	3:B:390:PX4:O1	0.41	2.16	15	1
3:C:335:PX4:O2	3:C:335:PX4:H12	0.41	2.15	15	1
3:A:608:PX4:O1	3:A:608:PX4:H3	0.41	2.16	4	1
3:B:340:PX4:O3	3:B:340:PX4:H7	0.41	2.15	4	1
3:B:337:PX4:C6	3:B:339:PX4:H3	0.41	2.46	6	1
3:B:398:PX4:H3	3:B:398:PX4:O4	0.41	2.16	6	1
3:C:309:PX4:H4	3:C:309:PX4:O4	0.41	2.16	6	1
3:B:302:PX4:O2	3:B:307:PX4:H7	0.41	2.17	8	1
3:B:336:PX4:H7	3:B:336:PX4:C6	0.41	2.46	8	1
3:C:333:PX4:H4	3:C:360:PX4:C1	0.41	2.46	10	1
3:B:359:PX4:O3	3:B:359:PX4:C4	0.41	2.67	12	1
3:A:607:PX4:H10	3:A:608:PX4:O1	0.41	2.16	13	1
3:A:608:PX4:O8	3:B:390:PX4:H11	0.41	2.16	13	1
3:C:354:PX4:H3	3:C:354:PX4:O1	0.41	2.15	13	1
3:B:349:PX4:C1	3:B:349:PX4:H15	0.41	2.45	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:397:PX4:H67	3:C:318:PX4:H69	0.41	1.92	14	1
3:A:628:PX4:O3	3:A:628:PX4:H10	0.41	2.16	15	1
3:B:305:PX4:H7	3:B:305:PX4:O3	0.41	2.16	15	1
3:B:338:PX4:H10	3:B:357:PX4:O1	0.40	2.15	1	1
3:B:366:PX4:O1	3:B:385:PX4:H5	0.40	2.16	1	1
3:B:355:PX4:H7	3:B:376:PX4:O2	0.40	2.16	2	1
3:A:613:PX4:H6	3:A:613:PX4:O3	0.40	2.16	5	1
3:A:633:PX4:O1	3:A:633:PX4:H13	0.40	2.15	5	1
3:C:357:PX4:C25	3:C:363:PX4:H11	0.40	2.45	6	1
3:B:327:PX4:H3	3:B:327:PX4:O1	0.40	2.16	7	1
3:B:388:PX4:O6	3:B:393:PX4:H9	0.40	2.16	7	1
3:A:612:PX4:H3	3:C:351:PX4:H18	0.40	1.92	8	1
2:B:128:LYS:HA	3:B:320:PX4:H8	0.40	1.92	9	1
3:B:311:PX4:H3	3:B:344:PX4:O2	0.40	2.16	11	1
3:B:324:PX4:H4	3:B:327:PX4:O2	0.40	2.16	11	1
3:C:351:PX4:H13	3:C:351:PX4:O3	0.40	2.16	11	1
3:C:352:PX4:H7	3:C:361:PX4:O3	0.40	2.16	12	1
3:B:385:PX4:H3	3:B:385:PX4:O4	0.40	2.16	5	1
3:C:323:PX4:O3	3:C:323:PX4:H10	0.40	2.15	5	1
3:A:602:PX4:H14	3:A:602:PX4:H7	0.40	1.92	6	1
3:C:324:PX4:O2	3:C:324:PX4:H3	0.40	2.16	8	1
3:B:369:PX4:O1	3:B:373:PX4:H11	0.40	2.16	10	1
3:A:641:PX4:H22	3:A:646:PX4:H20	0.40	1.93	12	1
2:C:244:LEU:HD22	3:C:331:PX4:H31	0.40	1.92	14	1
1:A:449:TYR:HA	1:A:450:PRO:C	0.40	2.42	15	1
3:C:313:PX4:H72	3:C:346:PX4:H68	0.40	1.92	2	1
3:B:353:PX4:O4	3:B:371:PX4:H4	0.40	2.16	6	1
3:B:391:PX4:O3	3:B:391:PX4:H6	0.40	2.16	6	1
3:B:370:PX4:O2	3:B:370:PX4:H4	0.40	2.16	7	1
3:B:366:PX4:O3	3:B:366:PX4:C3	0.40	2.69	8	1
3:A:608:PX4:H4	3:B:394:PX4:C1	0.40	2.46	9	1
3:B:324:PX4:O1	3:B:352:PX4:H9	0.40	2.17	9	1
3:C:307:PX4:H20	3:C:313:PX4:H14	0.40	1.92	10	1
2:C:84:GLN:HE21	2:C:88:LYS:HG3	0.40	1.77	15	1
3:B:301:PX4:O2	3:B:301:PX4:H4	0.40	2.16	2	1
3:C:337:PX4:O3	3:C:346:PX4:H12	0.40	2.16	2	1
3:B:358:PX4:O3	3:B:358:PX4:H9	0.40	2.16	5	1
3:C:359:PX4:O3	3:C:366:PX4:C2	0.40	2.70	6	1
1:A:437:ARG:HH21	1:A:446:ASP:CG	0.40	2.24	8	1
3:A:638:PX4:H18	3:A:648:PX4:H9	0.40	1.93	8	1
3:B:310:PX4:O1	3:B:342:PX4:H10	0.40	2.16	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:347:PX4:O3	3:C:347:PX4:C5	0.40	2.68	10	1
3:C:361:PX4:H3	3:C:361:PX4:O2	0.40	2.16	14	1
3:C:315:PX4:O2	3:C:315:PX4:H9	0.40	2.16	4	1
3:C:354:PX4:O2	3:C:354:PX4:H3	0.40	2.16	4	1
3:C:350:PX4:O3	3:C:350:PX4:H7	0.40	2.17	5	1
3:A:620:PX4:O2	3:A:638:PX4:H3	0.40	2.17	8	1
3:B:387:PX4:O3	3:B:387:PX4:H13	0.40	2.16	9	1
3:A:604:PX4:H13	3:A:605:PX4:O4	0.40	2.16	11	1
3:A:630:PX4:H6	3:A:630:PX4:O3	0.40	2.17	14	1
3:C:311:PX4:O8	3:C:317:PX4:H7	0.40	2.17	15	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	194/196 (99%)	176±3 (91±2%)	15±3 (8±2%)	3±2 (1±1%)	11	57
2	B	209/211 (99%)	204±1 (98±1%)	4±1 (2±1%)	0±0 (0±0%)	44	80
2	C	209/211 (99%)	205±1 (98±0%)	4±1 (2±1%)	0±0 (0±0%)	44	80
All	All	9180/9270 (99%)	8779 (96%)	344 (4%)	57 (1%)	23	72

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

Mol	Chain	Res	Type	Models (Total)
1	A	392	GLU	9
2	C	231	PRO	6
1	A	393	ALA	4
1	A	448	GLU	4
1	A	375	LYS	3
1	A	354	PRO	3
2	B	143	PRO	3
2	B	142	GLU	2
1	A	472	GLU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	510	SER	2
1	A	397	PRO	2
1	A	411	PRO	2
1	A	479	LYS	1
1	A	362	ARG	1
1	A	432	GLY	1
1	A	491	LEU	1
1	A	498	PRO	1
2	B	187	PRO	1
2	C	104	PHE	1
1	A	400	PRO	1
1	A	414	LYS	1
1	A	323	PHE	1
1	A	338	GLU	1
1	A	367	SER	1
2	B	119	VAL	1
1	A	322	ASN	1
1	A	503	ARG	1

6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	169/169 (100%)	165±1 (98±1%)	4±1 (2±1%)	43	89
2	B	187/187 (100%)	182±3 (98±1%)	5±3 (2±1%)	43	89
2	C	187/187 (100%)	182±3 (97±1%)	5±3 (3±1%)	41	88
All	All	8145/8145 (100%)	7942 (98%)	203 (2%)	42	88

All 117 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	210	ARG	14
1	A	372	TYR	7
1	A	411	PRO	6
2	B	127	GLN	4
2	C	210	ARG	4

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Mol	Chain	Res	Type	Models (Total)
1	A	365	PRO	4
2	C	236	LEU	4
2	C	219	THR	4
2	C	56	THR	4
2	C	139	GLN	4
2	B	123	LEU	4
2	C	63	GLN	4
1	A	435	TYR	3
1	A	368	ILE	3
2	C	58	SER	3
2	C	119	VAL	3
2	C	97	VAL	3
2	C	242	PRO	3
1	A	375	LYS	3
1	A	470	SER	2
2	B	119	VAL	2
2	B	237	ARG	2
2	B	224	THR	2
2	B	242	PRO	2
1	A	348	GLN	2
2	B	145	ARG	2
2	C	204	LYS	2
1	A	433	ASN	2
2	B	99	PRO	2
2	B	165	PRO	2
1	A	436	TYR	2
2	B	66	PRO	2
2	C	224	THR	2
2	C	183	THR	2
2	B	86	MET	2
2	B	141	VAL	2
2	C	238	GLN	2
2	B	181	LEU	2
1	A	342	TRP	2
1	A	397	PRO	2
1	A	340	TRP	1
2	C	104	PHE	1
1	A	388	TRP	1
1	A	478	TYR	1
1	A	509	PRO	1
2	C	132	GLU	1
1	A	370	THR	1

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Mol	Chain	Res	Type	Models (Total)
2	C	206	ASN	1
2	C	252	LEU	1
1	A	382	PHE	1
1	A	491	LEU	1
2	B	93	VAL	1
2	B	121	PRO	1
2	B	150	GLU	1
2	B	159	LEU	1
2	B	194	GLN	1
2	B	243	VAL	1
2	B	245	GLU	1
2	B	255	LEU	1
2	C	147	GLU	1
2	C	154	GLN	1
1	A	357	ILE	1
1	A	422	MET	1
2	C	247	PHE	1
1	A	412	THR	1
1	A	445	VAL	1
2	C	75	LEU	1
2	C	100	TYR	1
2	B	187	PRO	1
2	B	241	LEU	1
2	C	192	LEU	1
2	C	196	LEU	1
1	A	359	GLN	1
1	A	453	ILE	1
1	A	492	LYS	1
2	C	93	VAL	1
2	C	112	MET	1
2	C	255	LEU	1
1	A	374	ARG	1
2	B	90	LEU	1
2	B	166	LEU	1
2	C	71	PHE	1
2	C	143	PRO	1
2	C	170	MET	1
1	A	404	LYS	1
1	A	475	THR	1
1	A	484	TRP	1
2	B	67	VAL	1
2	B	201	GLU	1

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Mol	Chain	Res	Type	Models (Total)
2	C	177	HIS	1
1	A	316	PRO	1
1	A	455	VAL	1
1	A	468	MET	1
2	B	92	GLU	1
2	B	139	GLN	1
2	B	222	LEU	1
2	B	231	PRO	1
2	C	69	GLN	1
2	C	102	ASP	1
2	B	84	GLN	1
2	B	264	THR	1
1	A	419	LEU	1
2	B	219	THR	1
2	C	57	PHE	1
2	C	109	GLN	1
2	C	128	LYS	1
2	C	246	SER	1
1	A	341	PHE	1
2	B	56	THR	1
2	B	170	MET	1
2	B	259	THR	1
2	C	116	ARG	1
2	C	165	PRO	1
2	C	166	LEU	1
2	C	175	ARG	1
2	C	199	ARG	1
1	A	430	PHE	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 oligosaccharides in this entry.

6.6 Ligand geometry (i)

Of 220 ligands modelled in this entry, 2 are monoatomic - leaving 218 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	PX4	C	308	-	45,45,45	1.08±0.11	3±1 (6±2%)
3	PX4	C	306	-	45,45,45	1.04±0.16	3±2 (6±4%)
3	PX4	B	360	-	45,45,45	1.03±0.09	3±1 (5±2%)
3	PX4	B	367	-	45,45,45	1.10±0.11	4±2 (8±3%)
3	PX4	B	338	-	45,45,45	1.08±0.16	3±2 (6±4%)
3	PX4	C	350	-	45,45,45	1.13±0.15	3±2 (7±4%)
3	PX4	C	309	-	45,45,45	1.02±0.13	2±2 (5±3%)
3	PX4	C	339	-	45,45,45	1.08±0.11	3±1 (6±2%)
3	PX4	B	363	-	45,45,45	1.12±0.13	3±2 (7±4%)
3	PX4	A	639	-	45,45,45	1.05±0.10	2±1 (5±3%)
3	PX4	A	616	-	45,45,45	1.09±0.11	3±1 (6±2%)
3	PX4	B	339	-	45,45,45	1.07±0.13	3±2 (7±3%)
3	PX4	C	361	-	45,45,45	1.05±0.11	3±2 (6±3%)
3	PX4	C	344	-	45,45,45	1.10±0.11	3±2 (7±3%)
3	PX4	B	372	-	45,45,45	1.06±0.17	3±2 (6±3%)
3	PX4	C	324	-	45,45,45	1.04±0.12	2±1 (5±3%)
3	PX4	B	337	-	45,45,45	1.08±0.10	3±1 (7±2%)
3	PX4	C	320	-	45,45,45	1.04±0.10	3±1 (5±2%)
3	PX4	A	629	-	45,45,45	1.09±0.15	3±1 (6±2%)
3	PX4	C	316	-	45,45,45	1.08±0.15	3±2 (6±4%)
3	PX4	B	319	-	45,45,45	1.09±0.11	4±2 (8±3%)
3	PX4	C	327	-	45,45,45	1.09±0.09	3±1 (6±2%)
3	PX4	B	364	-	45,45,45	1.02±0.09	2±2 (4±3%)
3	PX4	A	606	-	45,45,45	1.09±0.11	3±2 (6±3%)
3	PX4	C	337	-	45,45,45	1.06±0.08	3±1 (5±2%)
3	PX4	B	342	-	45,45,45	1.04±0.09	3±1 (5±3%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	PX4	B	321	-	45,45,45	1.09±0.10	3±1 (7±3%)
3	PX4	C	369	-	45,45,45	1.08±0.09	4±1 (8±3%)
3	PX4	B	324	-	45,45,45	1.11±0.13	3±1 (6±3%)
3	PX4	B	332	-	45,45,45	1.04±0.12	3±2 (6±3%)
3	PX4	C	323	-	45,45,45	1.10±0.17	4±2 (8±4%)
3	PX4	B	340	-	45,45,45	1.11±0.12	4±2 (9±4%)
3	PX4	C	304	-	45,45,45	1.08±0.13	3±2 (6±3%)
3	PX4	B	387	-	45,45,45	1.09±0.11	3±1 (7±3%)
3	PX4	B	373	-	45,45,45	1.12±0.10	4±1 (8±3%)
3	PX4	C	334	-	45,45,45	1.07±0.10	3±2 (6±3%)
3	PX4	A	614	-	45,45,45	1.10±0.10	3±1 (7±2%)
3	PX4	C	364	-	45,45,45	1.07±0.09	2±1 (5±3%)
3	PX4	C	326	-	45,45,45	1.01±0.08	2±1 (4±2%)
3	PX4	B	395	-	45,45,45	1.10±0.12	3±2 (6±4%)
3	PX4	B	325	-	45,45,45	1.05±0.11	3±1 (6±2%)
3	PX4	A	620	-	45,45,45	1.07±0.12	3±2 (6±3%)
3	PX4	B	390	-	45,45,45	1.08±0.15	4±2 (7±3%)
3	PX4	B	391	-	45,45,45	1.10±0.08	3±1 (7±2%)
3	PX4	B	350	-	45,45,45	1.09±0.19	3±2 (6±4%)
3	PX4	C	348	-	45,45,45	1.11±0.12	3±1 (7±3%)
3	PX4	C	356	-	45,45,45	1.03±0.09	3±1 (5±3%)
3	PX4	A	642	-	45,45,45	1.06±0.12	3±2 (6±3%)
3	PX4	B	381	-	45,45,45	1.06±0.10	2±1 (5±2%)
3	PX4	B	345	-	45,45,45	1.07±0.08	3±1 (5±2%)
3	PX4	C	322	-	45,45,45	1.03±0.11	3±2 (6±3%)
3	PX4	B	320	-	45,45,45	1.09±0.11	3±1 (7±2%)
3	PX4	B	307	-	45,45,45	1.17±0.08	4±1 (8±3%)
3	PX4	C	307	-	45,45,45	1.07±0.11	3±2 (5±3%)
3	PX4	C	340	-	45,45,45	1.06±0.10	2±1 (5±2%)
3	PX4	C	347	-	45,45,45	1.07±0.13	3±2 (6±3%)
3	PX4	B	366	-	45,45,45	1.11±0.09	4±1 (7±2%)
3	PX4	C	314	-	45,45,45	1.12±0.08	3±1 (7±2%)
3	PX4	B	311	-	45,45,45	1.09±0.14	3±2 (6±4%)
3	PX4	B	308	-	45,45,45	1.02±0.11	3±2 (5±3%)
3	PX4	A	638	-	45,45,45	1.02±0.11	3±2 (5±3%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	PX4	B	349	-	45,45,45	1.03±0.13	3±2 (5±3%)
3	PX4	B	388	-	45,45,45	1.07±0.10	2±1 (5±2%)
3	PX4	B	361	-	45,45,45	1.04±0.09	3±1 (6±3%)
3	PX4	B	304	-	45,45,45	1.13±0.17	4±2 (8±3%)
3	PX4	B	333	-	45,45,45	1.11±0.14	3±1 (7±3%)
3	PX4	C	336	-	45,45,45	1.09±0.13	3±2 (7±4%)
3	PX4	B	326	-	45,45,45	1.03±0.09	3±1 (5±3%)
3	PX4	C	366	-	45,45,45	1.09±0.11	3±1 (6±2%)
3	PX4	B	334	-	45,45,45	1.04±0.09	3±1 (5±3%)
3	PX4	A	637	-	45,45,45	1.07±0.13	3±2 (7±3%)
3	PX4	B	368	-	45,45,45	1.06±0.07	3±1 (6±2%)
3	PX4	A	646	-	45,45,45	1.08±0.10	3±1 (6±3%)
3	PX4	B	392	-	45,45,45	1.06±0.14	3±2 (7±4%)
3	PX4	C	354	-	45,45,45	1.10±0.12	3±1 (7±2%)
3	PX4	B	306	-	45,45,45	1.07±0.13	3±2 (6±3%)
3	PX4	B	336	-	45,45,45	1.12±0.13	3±2 (7±4%)
3	PX4	B	313	-	45,45,45	1.05±0.12	3±2 (6±4%)
3	PX4	B	383	-	45,45,45	1.03±0.12	3±1 (6±2%)
3	PX4	A	631	-	45,45,45	1.04±0.11	3±1 (6±3%)
3	PX4	B	317	-	45,45,45	1.11±0.11	3±2 (7±3%)
3	PX4	B	385	-	45,45,45	1.05±0.13	3±1 (5±3%)
3	PX4	B	389	-	45,45,45	1.07±0.13	3±1 (6±3%)
3	PX4	B	359	-	45,45,45	1.05±0.15	3±2 (6±3%)
3	PX4	C	338	-	45,45,45	1.07±0.11	3±2 (6±3%)
3	PX4	C	321	-	45,45,45	1.12±0.16	4±1 (7±2%)
3	PX4	A	608	-	45,45,45	1.11±0.14	3±2 (7±4%)
3	PX4	A	628	-	45,45,45	1.07±0.10	3±2 (5±3%)
3	PX4	C	345	-	45,45,45	1.11±0.12	4±2 (8±3%)
3	PX4	B	374	-	45,45,45	1.04±0.09	2±1 (5±3%)
3	PX4	B	382	-	45,45,45	1.04±0.10	2±1 (5±3%)
3	PX4	A	618	-	45,45,45	1.02±0.11	2±2 (5±4%)
3	PX4	C	357	-	45,45,45	1.09±0.12	3±2 (6±3%)
3	PX4	B	397	-	45,45,45	1.12±0.12	3±1 (7±3%)
3	PX4	B	301	-	45,45,45	1.12±0.12	4±2 (8±4%)
3	PX4	B	362	-	45,45,45	1.05±0.09	3±1 (6±3%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	PX4	A	610	-	45,45,45	1.08±0.12	3±2 (6±3%)
3	PX4	A	619	-	45,45,45	1.11±0.13	3±1 (7±2%)
3	PX4	B	315	-	45,45,45	1.07±0.14	3±1 (6±3%)
3	PX4	A	602	-	45,45,45	1.08±0.10	3±1 (6±2%)
3	PX4	B	309	-	45,45,45	1.07±0.07	3±1 (6±2%)
3	PX4	C	318	-	45,45,45	1.03±0.13	2±2 (5±3%)
3	PX4	A	647	-	45,45,45	1.07±0.13	4±2 (8±4%)
3	PX4	B	348	-	45,45,45	1.06±0.08	3±2 (7±3%)
3	PX4	A	611	-	45,45,45	1.03±0.13	2±1 (5±3%)
3	PX4	A	635	-	45,45,45	1.09±0.13	3±1 (6±2%)
3	PX4	C	331	-	45,45,45	1.04±0.15	3±1 (5±3%)
3	PX4	B	399	-	45,45,45	1.10±0.07	4±1 (8±2%)
3	PX4	A	622	-	45,45,45	1.04±0.09	2±1 (5±2%)
3	PX4	C	352	-	45,45,45	1.06±0.10	2±1 (5±2%)
3	PX4	B	379	-	45,45,45	1.10±0.10	3±1 (7±2%)
3	PX4	A	603	-	45,45,45	1.05±0.11	3±2 (6±3%)
3	PX4	B	327	-	45,45,45	1.09±0.09	3±1 (7±2%)
3	PX4	C	341	-	45,45,45	1.10±0.12	4±1 (8±3%)
3	PX4	B	353	-	45,45,45	1.03±0.13	2±2 (5±3%)
3	PX4	B	354	-	45,45,45	1.09±0.09	3±1 (6±2%)
3	PX4	B	371	-	45,45,45	1.04±0.12	3±1 (6±2%)
3	PX4	B	314	-	45,45,45	1.13±0.13	4±2 (8±4%)
3	PX4	B	310	-	45,45,45	1.12±0.09	4±1 (8±2%)
3	PX4	C	330	-	45,45,45	1.10±0.12	3±1 (7±3%)
3	PX4	C	325	-	45,45,45	1.11±0.11	3±1 (7±2%)
3	PX4	B	323	-	45,45,45	1.03±0.15	2±1 (5±2%)
3	PX4	B	386	-	45,45,45	1.06±0.07	3±1 (6±3%)
3	PX4	B	370	-	45,45,45	1.05±0.09	3±1 (5±2%)
3	PX4	A	644	-	45,45,45	1.03±0.12	3±2 (6±4%)
3	PX4	A	607	-	45,45,45	1.11±0.07	4±1 (7±2%)
3	PX4	C	365	-	45,45,45	1.07±0.09	3±1 (6±3%)
3	PX4	C	303	-	45,45,45	1.12±0.15	4±2 (7±4%)
3	PX4	A	601	-	45,45,45	1.08±0.12	3±2 (6±4%)
3	PX4	B	352	-	45,45,45	1.08±0.14	3±2 (6±3%)
3	PX4	B	322	-	45,45,45	1.05±0.05	3±1 (6±2%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	PX4	B	365	-	45,45,45	1.09±0.16	3±2 (6±4%)
3	PX4	C	353	-	45,45,45	1.04±0.10	3±2 (6±4%)
3	PX4	B	356	-	45,45,45	1.09±0.11	3±1 (6±2%)
3	PX4	B	357	-	45,45,45	1.03±0.10	2±1 (5±2%)
3	PX4	B	396	-	45,45,45	1.08±0.10	3±1 (6±2%)
3	PX4	C	319	-	45,45,45	1.03±0.07	2±1 (5±2%)
3	PX4	A	623	-	45,45,45	1.04±0.11	3±2 (6±3%)
3	PX4	A	643	-	45,45,45	1.06±0.13	3±1 (5±3%)
3	PX4	C	302	-	45,45,45	1.09±0.10	3±1 (6±3%)
3	PX4	B	331	-	45,45,45	1.11±0.12	3±1 (7±3%)
3	PX4	B	329	-	45,45,45	1.10±0.08	3±1 (7±3%)
3	PX4	C	317	-	45,45,45	1.08±0.14	3±1 (7±2%)
3	PX4	C	329	-	45,45,45	1.05±0.10	3±1 (5±1%)
3	PX4	C	370	-	45,45,45	1.11±0.13	3±1 (6±3%)
3	PX4	B	375	-	45,45,45	1.09±0.14	3±2 (6±4%)
3	PX4	A	633	-	45,45,45	1.08±0.12	3±2 (6±4%)
3	PX4	C	311	-	45,45,45	1.06±0.07	3±1 (7±2%)
3	PX4	A	609	-	45,45,45	1.10±0.16	3±2 (7±3%)
3	PX4	B	303	-	45,45,45	1.07±0.13	3±1 (6±3%)
3	PX4	C	335	-	45,45,45	1.08±0.10	3±1 (6±2%)
3	PX4	B	347	-	45,45,45	1.05±0.07	3±1 (6±2%)
3	PX4	C	351	-	45,45,45	1.10±0.08	3±1 (7±3%)
3	PX4	C	360	-	45,45,45	1.08±0.08	3±1 (6±2%)
3	PX4	B	376	-	45,45,45	1.07±0.12	3±2 (6±3%)
3	PX4	A	612	-	45,45,45	1.05±0.08	2±1 (5±2%)
3	PX4	C	312	-	45,45,45	1.06±0.12	3±1 (6±2%)
3	PX4	B	380	-	45,45,45	1.07±0.13	3±2 (7±3%)
3	PX4	B	377	-	45,45,45	1.10±0.08	4±1 (7±2%)
3	PX4	C	313	-	45,45,45	1.09±0.12	4±2 (8±4%)
3	PX4	C	305	-	45,45,45	1.03±0.09	3±1 (6±2%)
3	PX4	B	398	-	45,45,45	1.08±0.08	3±1 (6±2%)
3	PX4	A	634	-	45,45,45	1.04±0.10	3±1 (6±3%)
3	PX4	C	355	-	45,45,45	1.04±0.11	3±1 (5±2%)
3	PX4	B	393	-	45,45,45	1.07±0.08	3±1 (7±2%)
3	PX4	A	632	-	45,45,45	1.13±0.14	4±1 (8±2%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	PX4	B	369	-	45,45,45	1.07±0.16	3±2 (6±4%)
3	PX4	B	346	-	45,45,45	1.06±0.08	3±1 (5±2%)
3	PX4	B	312	-	45,45,45	1.09±0.15	3±2 (6±4%)
3	PX4	A	640	-	45,45,45	1.17±0.12	4±1 (8±3%)
3	PX4	C	367	-	45,45,45	1.05±0.09	3±1 (6±2%)
3	PX4	A	604	-	45,45,45	1.07±0.12	3±1 (5±3%)
3	PX4	B	394	-	45,45,45	1.09±0.12	3±1 (5±3%)
3	PX4	A	645	-	45,45,45	1.08±0.09	3±1 (7±2%)
3	PX4	C	310	-	45,45,45	1.06±0.08	3±1 (6±2%)
3	PX4	A	621	-	45,45,45	1.10±0.12	3±2 (7±4%)
3	PX4	A	615	-	45,45,45	1.09±0.12	3±1 (5±3%)
3	PX4	B	384	-	45,45,45	1.05±0.11	3±1 (6±3%)
3	PX4	A	617	-	45,45,45	1.07±0.11	3±1 (6±2%)
3	PX4	A	625	-	45,45,45	1.05±0.13	3±2 (7±4%)
3	PX4	C	368	-	45,45,45	1.13±0.12	4±2 (9±3%)
3	PX4	B	358	-	45,45,45	1.08±0.11	4±2 (8±3%)
3	PX4	C	359	-	45,45,45	1.10±0.13	3±1 (6±2%)
3	PX4	B	343	-	45,45,45	1.04±0.14	3±2 (6±3%)
3	PX4	C	346	-	45,45,45	1.12±0.12	4±1 (8±2%)
3	PX4	A	641	-	45,45,45	1.07±0.11	3±1 (6±2%)
3	PX4	A	636	-	45,45,45	1.07±0.12	3±2 (6±3%)
3	PX4	B	351	-	45,45,45	1.01±0.14	3±2 (6±3%)
3	PX4	A	627	-	45,45,45	1.03±0.09	2±1 (5±2%)
3	PX4	B	378	-	45,45,45	1.02±0.14	3±2 (6±3%)
3	PX4	C	358	-	45,45,45	0.99±0.11	2±1 (5±3%)
3	PX4	A	630	-	45,45,45	1.07±0.16	3±2 (6±3%)
3	PX4	B	335	-	45,45,45	1.09±0.11	3±2 (7±3%)
3	PX4	B	341	-	45,45,45	1.08±0.13	3±2 (7±3%)
3	PX4	B	400	-	45,45,45	1.06±0.15	3±1 (5±2%)
3	PX4	A	648	-	45,45,45	1.10±0.10	4±1 (7±2%)
3	PX4	C	333	-	45,45,45	1.09±0.10	3±1 (7±2%)
3	PX4	C	315	-	45,45,45	1.07±0.11	3±2 (6±3%)
3	PX4	C	349	-	45,45,45	1.10±0.17	3±2 (7±4%)
3	PX4	B	316	-	45,45,45	1.06±0.10	3±2 (6±4%)
3	PX4	A	626	-	45,45,45	1.03±0.09	3±2 (6±3%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	PX4	A	624	-	45,45,45	1.07±0.10	2±1 (5±2%)
3	PX4	C	332	-	45,45,45	1.10±0.09	3±1 (7±2%)
3	PX4	A	605	-	45,45,45	1.09±0.08	3±2 (6±3%)
3	PX4	B	328	-	45,45,45	1.04±0.11	3±1 (5±3%)
3	PX4	C	301	-	45,45,45	1.04±0.09	3±1 (6±2%)
3	PX4	C	328	-	45,45,45	1.03±0.12	3±1 (6±3%)
3	PX4	B	330	-	45,45,45	1.05±0.11	3±2 (7±3%)
3	PX4	B	344	-	45,45,45	1.05±0.10	3±1 (6±2%)
3	PX4	A	613	-	45,45,45	1.04±0.11	3±1 (5±2%)
3	PX4	C	363	-	45,45,45	1.06±0.09	3±2 (6±3%)
3	PX4	C	342	-	45,45,45	1.07±0.13	3±2 (6±3%)
3	PX4	B	305	-	45,45,45	1.06±0.12	3±2 (6±4%)
3	PX4	B	302	-	45,45,45	1.06±0.11	3±1 (6±2%)
3	PX4	C	343	-	45,45,45	1.07±0.10	3±1 (5±2%)
3	PX4	B	318	-	45,45,45	1.09±0.07	3±1 (6±2%)
3	PX4	C	362	-	45,45,45	1.03±0.09	3±1 (6±3%)
3	PX4	B	355	-	45,45,45	1.10±0.10	3±1 (7±3%)

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

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	PX4	C	308	-	51,53,53	0.91±0.12	2±2 (3±2%)
3	PX4	C	306	-	51,53,53	0.97±0.09	2±1 (4±2%)
3	PX4	B	360	-	51,53,53	0.98±0.10	3±1 (5±2%)
3	PX4	B	367	-	51,53,53	0.97±0.09	2±1 (4±2%)
3	PX4	B	338	-	51,53,53	0.89±0.10	2±2 (3±3%)
3	PX4	C	350	-	51,53,53	0.93±0.14	2±1 (4±2%)
3	PX4	C	309	-	51,53,53	0.95±0.09	2±1 (4±2%)
3	PX4	C	339	-	51,53,53	0.94±0.09	2±1 (4±2%)
3	PX4	B	363	-	51,53,53	0.93±0.10	2±2 (4±3%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	PX4	A	639	-	51,53,53	0.91±0.10	2±2 (3±2%)
3	PX4	A	616	-	51,53,53	0.95±0.12	2±1 (4±2%)
3	PX4	B	339	-	51,53,53	0.97±0.13	2±1 (4±2%)
3	PX4	C	361	-	51,53,53	0.93±0.06	2±1 (4±2%)
3	PX4	C	344	-	51,53,53	0.94±0.11	2±1 (4±2%)
3	PX4	B	372	-	51,53,53	0.97±0.11	2±2 (4±2%)
3	PX4	C	324	-	51,53,53	0.99±0.09	3±1 (4±2%)
3	PX4	B	337	-	51,53,53	0.98±0.14	3±2 (5±3%)
3	PX4	C	320	-	51,53,53	0.93±0.11	2±1 (3±1%)
3	PX4	A	629	-	51,53,53	0.95±0.12	2±1 (4±2%)
3	PX4	C	316	-	51,53,53	0.91±0.12	2±1 (3±2%)
3	PX4	B	319	-	51,53,53	0.89±0.08	2±1 (3±2%)
3	PX4	C	327	-	51,53,53	0.92±0.11	2±1 (3±2%)
3	PX4	B	364	-	51,53,53	0.95±0.10	2±1 (4±1%)
3	PX4	A	606	-	51,53,53	0.98±0.07	2±1 (4±1%)
3	PX4	C	337	-	51,53,53	0.98±0.12	2±2 (4±3%)
3	PX4	B	342	-	51,53,53	0.94±0.10	2±1 (4±2%)
3	PX4	B	321	-	51,53,53	0.87±0.14	1±1 (2±1%)
3	PX4	C	369	-	51,53,53	0.90±0.13	2±1 (3±2%)
3	PX4	B	324	-	51,53,53	0.92±0.12	2±1 (3±2%)
3	PX4	B	332	-	51,53,53	0.96±0.14	2±2 (4±3%)
3	PX4	C	323	-	51,53,53	0.98±0.11	3±2 (5±3%)
3	PX4	B	340	-	51,53,53	0.97±0.06	2±1 (4±2%)
3	PX4	C	304	-	51,53,53	0.97±0.13	2±2 (4±3%)
3	PX4	B	387	-	51,53,53	0.94±0.11	2±1 (4±2%)
3	PX4	B	373	-	51,53,53	0.97±0.09	3±1 (4±2%)
3	PX4	C	334	-	51,53,53	0.91±0.07	2±1 (3±1%)
3	PX4	A	614	-	51,53,53	0.99±0.15	3±2 (5±3%)
3	PX4	C	364	-	51,53,53	0.97±0.10	2±1 (4±2%)
3	PX4	C	326	-	51,53,53	1.01±0.12	3±1 (5±2%)
3	PX4	B	395	-	51,53,53	0.97±0.08	3±2 (5±3%)
3	PX4	B	325	-	51,53,53	0.95±0.08	2±1 (4±2%)
3	PX4	A	620	-	51,53,53	0.96±0.09	2±1 (4±2%)
3	PX4	B	390	-	51,53,53	0.93±0.09	2±1 (3±2%)
3	PX4	B	391	-	51,53,53	0.94±0.12	2±1 (3±2%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	PX4	B	350	-	51,53,53	0.96±0.08	2±2 (4±3%)
3	PX4	C	348	-	51,53,53	0.94±0.11	2±1 (3±2%)
3	PX4	C	356	-	51,53,53	0.99±0.15	2±2 (4±3%)
3	PX4	A	642	-	51,53,53	0.95±0.13	2±1 (4±2%)
3	PX4	B	381	-	51,53,53	0.91±0.13	2±1 (3±2%)
3	PX4	B	345	-	51,53,53	0.99±0.10	3±1 (5±2%)
3	PX4	C	322	-	51,53,53	0.95±0.13	3±1 (4±2%)
3	PX4	B	320	-	51,53,53	0.92±0.13	2±2 (4±3%)
3	PX4	B	307	-	51,53,53	0.91±0.09	2±1 (3±2%)
3	PX4	C	307	-	51,53,53	0.96±0.08	2±1 (3±2%)
3	PX4	C	340	-	51,53,53	0.96±0.12	2±1 (3±2%)
3	PX4	C	347	-	51,53,53	0.94±0.12	2±1 (3±2%)
3	PX4	B	366	-	51,53,53	0.96±0.10	2±1 (4±2%)
3	PX4	C	314	-	51,53,53	1.01±0.08	3±1 (6±2%)
3	PX4	B	311	-	51,53,53	0.96±0.13	2±2 (4±4%)
3	PX4	B	308	-	51,53,53	0.96±0.12	3±1 (5±2%)
3	PX4	A	638	-	51,53,53	0.88±0.10	1±1 (2±2%)
3	PX4	B	349	-	51,53,53	0.88±0.09	2±1 (3±1%)
3	PX4	B	388	-	51,53,53	0.92±0.10	2±1 (3±2%)
3	PX4	B	361	-	51,53,53	0.91±0.07	1±1 (2±2%)
3	PX4	B	304	-	51,53,53	0.97±0.09	2±1 (4±2%)
3	PX4	B	333	-	51,53,53	0.92±0.13	2±2 (3±3%)
3	PX4	C	336	-	51,53,53	0.97±0.14	2±2 (3±3%)
3	PX4	B	326	-	51,53,53	0.96±0.09	2±1 (4±2%)
3	PX4	C	366	-	51,53,53	0.93±0.08	2±1 (3±2%)
3	PX4	B	334	-	51,53,53	0.96±0.14	3±2 (5±3%)
3	PX4	A	637	-	51,53,53	0.94±0.12	2±1 (3±2%)
3	PX4	B	368	-	51,53,53	0.92±0.09	2±1 (4±1%)
3	PX4	A	646	-	51,53,53	0.96±0.11	2±1 (3±2%)
3	PX4	B	392	-	51,53,53	0.94±0.11	2±1 (3±2%)
3	PX4	C	354	-	51,53,53	0.94±0.09	2±1 (4±2%)
3	PX4	B	306	-	51,53,53	0.93±0.12	2±2 (3±3%)
3	PX4	B	336	-	51,53,53	0.94±0.11	2±1 (3±2%)
3	PX4	B	313	-	51,53,53	0.91±0.11	2±1 (4±2%)
3	PX4	B	383	-	51,53,53	0.91±0.10	2±1 (3±2%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	PX4	A	631	-	51,53,53	0.95±0.10	2±1 (4±2%)
3	PX4	B	317	-	51,53,53	0.93±0.10	2±2 (4±3%)
3	PX4	B	385	-	51,53,53	0.93±0.10	2±1 (3±2%)
3	PX4	B	389	-	51,53,53	0.88±0.13	1±1 (2±2%)
3	PX4	B	359	-	51,53,53	0.96±0.08	2±1 (4±2%)
3	PX4	C	338	-	51,53,53	0.92±0.09	2±1 (3±2%)
3	PX4	C	321	-	51,53,53	0.96±0.08	2±1 (4±1%)
3	PX4	A	608	-	51,53,53	0.94±0.11	2±1 (3±1%)
3	PX4	A	628	-	51,53,53	0.94±0.10	2±1 (3±2%)
3	PX4	C	345	-	51,53,53	0.97±0.12	3±2 (5±3%)
3	PX4	B	374	-	51,53,53	0.93±0.11	2±2 (4±3%)
3	PX4	B	382	-	51,53,53	0.95±0.10	2±1 (4±2%)
3	PX4	A	618	-	51,53,53	0.94±0.17	2±2 (4±3%)
3	PX4	C	357	-	51,53,53	0.95±0.12	2±2 (4±3%)
3	PX4	B	397	-	51,53,53	0.93±0.13	2±2 (4±3%)
3	PX4	B	301	-	51,53,53	0.95±0.08	2±1 (4±2%)
3	PX4	B	362	-	51,53,53	0.96±0.13	2±2 (3±3%)
3	PX4	A	610	-	51,53,53	0.98±0.10	3±1 (5±2%)
3	PX4	A	619	-	51,53,53	0.93±0.15	2±1 (4±2%)
3	PX4	B	315	-	51,53,53	0.95±0.13	3±2 (5±3%)
3	PX4	A	602	-	51,53,53	0.98±0.10	3±2 (5±3%)
3	PX4	B	309	-	51,53,53	1.00±0.11	3±2 (5±3%)
3	PX4	C	318	-	51,53,53	0.90±0.08	2±1 (3±2%)
3	PX4	A	647	-	51,53,53	0.97±0.13	3±2 (4±3%)
3	PX4	B	348	-	51,53,53	0.97±0.09	2±1 (4±1%)
3	PX4	A	611	-	51,53,53	0.91±0.15	2±2 (3±3%)
3	PX4	A	635	-	51,53,53	0.93±0.12	2±1 (3±2%)
3	PX4	C	331	-	51,53,53	0.96±0.09	3±1 (5±2%)
3	PX4	B	399	-	51,53,53	0.96±0.11	2±2 (4±3%)
3	PX4	A	622	-	51,53,53	1.00±0.11	2±2 (4±3%)
3	PX4	C	352	-	51,53,53	0.93±0.10	2±1 (3±2%)
3	PX4	B	379	-	51,53,53	0.98±0.12	2±2 (4±3%)
3	PX4	A	603	-	51,53,53	0.97±0.12	2±1 (4±2%)
3	PX4	B	327	-	51,53,53	0.98±0.15	2±2 (4±3%)
3	PX4	C	341	-	51,53,53	0.96±0.12	3±2 (4±3%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	PX4	B	353	-	51,53,53	0.94±0.06	2±1 (4±2%)
3	PX4	B	354	-	51,53,53	0.89±0.08	2±2 (4±3%)
3	PX4	B	371	-	51,53,53	0.94±0.09	2±1 (3±2%)
3	PX4	B	314	-	51,53,53	0.96±0.09	2±1 (4±2%)
3	PX4	B	310	-	51,53,53	0.91±0.11	2±1 (3±2%)
3	PX4	C	330	-	51,53,53	0.92±0.12	2±2 (4±3%)
3	PX4	C	325	-	51,53,53	0.93±0.12	2±2 (4±2%)
3	PX4	B	323	-	51,53,53	0.97±0.11	2±2 (4±3%)
3	PX4	B	386	-	51,53,53	0.95±0.12	3±2 (5±3%)
3	PX4	B	370	-	51,53,53	0.95±0.10	3±1 (5±2%)
3	PX4	A	644	-	51,53,53	0.94±0.13	2±1 (4±2%)
3	PX4	A	607	-	51,53,53	0.93±0.10	2±1 (3±2%)
3	PX4	C	365	-	51,53,53	0.98±0.11	2±1 (4±2%)
3	PX4	C	303	-	51,53,53	1.00±0.07	3±1 (6±2%)
3	PX4	A	601	-	51,53,53	0.98±0.10	2±1 (4±2%)
3	PX4	B	352	-	51,53,53	0.95±0.12	2±1 (3±2%)
3	PX4	B	322	-	51,53,53	0.96±0.11	2±1 (3±2%)
3	PX4	B	365	-	51,53,53	0.96±0.13	2±1 (4±2%)
3	PX4	C	353	-	51,53,53	0.92±0.10	2±1 (3±2%)
3	PX4	B	356	-	51,53,53	0.94±0.09	2±1 (3±2%)
3	PX4	B	357	-	51,53,53	1.01±0.11	3±2 (5±3%)
3	PX4	B	396	-	51,53,53	0.96±0.14	2±1 (4±2%)
3	PX4	C	319	-	51,53,53	0.92±0.07	2±1 (3±1%)
3	PX4	A	623	-	51,53,53	0.98±0.09	2±1 (4±2%)
3	PX4	A	643	-	51,53,53	0.95±0.12	2±1 (4±2%)
3	PX4	C	302	-	51,53,53	0.97±0.08	2±1 (4±2%)
3	PX4	B	331	-	51,53,53	0.96±0.11	2±1 (4±2%)
3	PX4	B	329	-	51,53,53	0.93±0.09	2±1 (4±2%)
3	PX4	C	317	-	51,53,53	0.95±0.10	3±1 (5±2%)
3	PX4	C	329	-	51,53,53	0.96±0.14	2±2 (4±3%)
3	PX4	C	370	-	51,53,53	1.04±0.10	3±1 (5±2%)
3	PX4	B	375	-	51,53,53	0.91±0.11	2±1 (3±2%)
3	PX4	A	633	-	51,53,53	0.99±0.11	3±1 (5±2%)
3	PX4	C	311	-	51,53,53	0.94±0.09	2±1 (3±2%)
3	PX4	A	609	-	51,53,53	0.94±0.12	2±2 (4±3%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	PX4	B	303	-	51,53,53	0.96±0.11	3±1 (5±2%)
3	PX4	C	335	-	51,53,53	0.93±0.11	2±2 (4±3%)
3	PX4	B	347	-	51,53,53	0.95±0.12	2±1 (3±2%)
3	PX4	C	351	-	51,53,53	0.94±0.10	2±1 (4±2%)
3	PX4	C	360	-	51,53,53	1.03±0.14	3±2 (5±2%)
3	PX4	B	376	-	51,53,53	0.97±0.12	2±1 (4±2%)
3	PX4	A	612	-	51,53,53	0.94±0.10	2±1 (3±2%)
3	PX4	C	312	-	51,53,53	1.03±0.10	3±2 (5±3%)
3	PX4	B	380	-	51,53,53	0.92±0.13	2±1 (4±2%)
3	PX4	B	377	-	51,53,53	0.95±0.13	2±1 (4±2%)
3	PX4	C	313	-	51,53,53	0.94±0.13	2±1 (3±2%)
3	PX4	C	305	-	51,53,53	0.92±0.12	2±1 (3±2%)
3	PX4	B	398	-	51,53,53	0.98±0.11	2±1 (4±2%)
3	PX4	A	634	-	51,53,53	0.98±0.10	3±1 (4±2%)
3	PX4	C	355	-	51,53,53	0.93±0.12	2±1 (3±2%)
3	PX4	B	393	-	51,53,53	0.96±0.13	3±1 (5±2%)
3	PX4	A	632	-	51,53,53	0.92±0.10	2±1 (4±2%)
3	PX4	B	369	-	51,53,53	1.02±0.14	3±2 (5±3%)
3	PX4	B	346	-	51,53,53	0.93±0.11	2±1 (4±1%)
3	PX4	B	312	-	51,53,53	0.95±0.11	2±1 (4±2%)
3	PX4	A	640	-	51,53,53	0.93±0.13	2±1 (3±2%)
3	PX4	C	367	-	51,53,53	0.91±0.12	2±1 (3±2%)
3	PX4	A	604	-	51,53,53	0.89±0.11	1±1 (2±2%)
3	PX4	B	394	-	51,53,53	1.01±0.14	2±2 (4±3%)
3	PX4	A	645	-	51,53,53	0.93±0.11	2±1 (3±2%)
3	PX4	C	310	-	51,53,53	0.91±0.10	2±1 (3±2%)
3	PX4	A	621	-	51,53,53	0.90±0.09	2±1 (3±1%)
3	PX4	A	615	-	51,53,53	0.95±0.08	2±1 (4±2%)
3	PX4	B	384	-	51,53,53	0.95±0.14	3±2 (5±3%)
3	PX4	A	617	-	51,53,53	0.93±0.10	2±1 (4±1%)
3	PX4	A	625	-	51,53,53	0.87±0.10	1±1 (2±2%)
3	PX4	C	368	-	51,53,53	0.97±0.14	2±2 (4±3%)
3	PX4	B	358	-	51,53,53	0.93±0.11	2±1 (4±2%)
3	PX4	C	359	-	51,53,53	0.95±0.11	2±1 (4±2%)
3	PX4	B	343	-	51,53,53	1.00±0.14	2±2 (4±3%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	PX4	C	346	-	51,53,53	0.99±0.11	2±1 (4±2%)
3	PX4	A	641	-	51,53,53	0.95±0.10	2±1 (3±2%)
3	PX4	A	636	-	51,53,53	0.97±0.12	2±1 (4±2%)
3	PX4	B	351	-	51,53,53	0.96±0.11	3±2 (5±3%)
3	PX4	A	627	-	51,53,53	0.93±0.08	2±1 (4±2%)
3	PX4	B	378	-	51,53,53	0.95±0.09	3±1 (5±2%)
3	PX4	C	358	-	51,53,53	0.97±0.13	2±1 (4±2%)
3	PX4	A	630	-	51,53,53	0.95±0.09	2±1 (4±1%)
3	PX4	B	335	-	51,53,53	0.97±0.15	2±2 (4±4%)
3	PX4	B	341	-	51,53,53	0.89±0.11	2±1 (3±2%)
3	PX4	B	400	-	51,53,53	0.97±0.11	3±1 (5±2%)
3	PX4	A	648	-	51,53,53	1.02±0.12	3±1 (6±1%)
3	PX4	C	333	-	51,53,53	0.95±0.08	2±1 (4±1%)
3	PX4	C	315	-	51,53,53	0.96±0.14	2±1 (4±2%)
3	PX4	C	349	-	51,53,53	0.89±0.15	2±1 (3±2%)
3	PX4	B	316	-	51,53,53	0.92±0.12	2±1 (3±2%)
3	PX4	A	626	-	51,53,53	0.97±0.14	2±2 (4±3%)
3	PX4	A	624	-	51,53,53	0.94±0.09	2±1 (4±2%)
3	PX4	C	332	-	51,53,53	0.92±0.12	2±2 (3±3%)
3	PX4	A	605	-	51,53,53	1.00±0.10	2±1 (4±1%)
3	PX4	B	328	-	51,53,53	0.95±0.14	2±1 (4±2%)
3	PX4	C	301	-	51,53,53	0.92±0.10	2±2 (4±3%)
3	PX4	C	328	-	51,53,53	0.93±0.11	2±1 (3±2%)
3	PX4	B	330	-	51,53,53	0.93±0.11	2±1 (4±2%)
3	PX4	B	344	-	51,53,53	0.93±0.13	2±1 (3±2%)
3	PX4	A	613	-	51,53,53	0.95±0.10	2±1 (4±2%)
3	PX4	C	363	-	51,53,53	0.91±0.15	2±1 (4±2%)
3	PX4	C	342	-	51,53,53	0.98±0.15	3±1 (5±2%)
3	PX4	B	305	-	51,53,53	0.98±0.11	3±2 (5±3%)
3	PX4	B	302	-	51,53,53	0.92±0.12	2±1 (3±2%)
3	PX4	C	343	-	51,53,53	0.93±0.11	2±2 (4±3%)
3	PX4	B	318	-	51,53,53	0.94±0.09	2±1 (3±2%)
3	PX4	C	362	-	51,53,53	0.96±0.11	2±1 (4±2%)
3	PX4	B	355	-	51,53,53	0.98±0.10	2±1 (4±2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PX4	C	350	-	-	0±0,49,49,49	-
3	PX4	C	324	-	-	0±0,49,49,49	-
3	PX4	C	316	-	-	0±0,49,49,49	-
3	PX4	B	332	-	-	0±0,49,49,49	-
3	PX4	B	340	-	-	0±0,49,49,49	-
3	PX4	A	620	-	-	0±0,49,49,49	-
3	PX4	B	390	-	-	0±0,49,49,49	-
3	PX4	B	304	-	-	0±0,49,49,49	-
3	PX4	C	354	-	-	0±0,49,49,49	-
3	PX4	C	361	-	-	0±0,49,49,49	-
3	PX4	C	337	-	-	0±0,49,49,49	-
3	PX4	C	309	-	-	0±0,49,49,49	-
3	PX4	B	321	-	-	0±0,49,49,49	-
3	PX4	B	382	-	-	0±0,49,49,49	-
3	PX4	C	303	-	-	0±0,49,49,49	-
3	PX4	C	353	-	-	0±0,49,49,49	-
3	PX4	B	379	-	-	0±0,49,49,49	-
3	PX4	C	351	-	-	0±0,49,49,49	-
3	PX4	B	352	-	-	0±0,49,49,49	-
3	PX4	B	375	-	-	0±0,49,49,49	-
3	PX4	C	356	-	-	0±0,49,49,49	-
3	PX4	B	398	-	-	0±0,49,49,49	-
3	PX4	B	383	-	-	0±0,49,49,49	-
3	PX4	A	612	-	-	0±0,49,49,49	-
3	PX4	C	346	-	-	0±0,49,49,49	-
3	PX4	A	623	-	-	0±0,49,49,49	-
3	PX4	C	338	-	-	0±0,49,49,49	-
3	PX4	B	339	-	-	0±0,49,49,49	-
3	PX4	B	345	-	-	0±0,49,49,49	-
3	PX4	C	358	-	-	0±0,49,49,49	-
3	PX4	C	357	-	-	0±0,49,49,49	-
3	PX4	A	601	-	-	0±0,49,49,49	-
3	PX4	B	349	-	-	0±0,49,49,49	-
3	PX4	A	632	-	-	0±0,49,49,49	-
3	PX4	B	384	-	-	0±0,49,49,49	-
3	PX4	C	331	-	-	0±0,49,49,49	-
3	PX4	C	325	-	-	0±0,49,49,49	-
3	PX4	B	334	-	-	0±0,49,49,49	-
3	PX4	A	636	-	-	0±0,49,49,49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PX4	B	372	-	-	0±0,49,49,49	-
3	PX4	B	360	-	-	0±0,49,49,49	-
3	PX4	B	326	-	-	0±0,49,49,49	-
3	PX4	A	633	-	-	0±0,49,49,49	-
3	PX4	C	330	-	-	0±0,49,49,49	-
3	PX4	B	328	-	-	0±0,49,49,49	-
3	PX4	B	358	-	-	0±0,49,49,49	-
3	PX4	B	386	-	-	0±0,49,49,49	-
3	PX4	C	341	-	-	0±0,49,49,49	-
3	PX4	B	303	-	-	0±0,49,49,49	-
3	PX4	B	323	-	-	0±0,49,49,49	-
3	PX4	B	392	-	-	0±0,49,49,49	-
3	PX4	A	609	-	-	0±0,49,49,49	-
3	PX4	B	310	-	-	0±0,49,49,49	-
3	PX4	B	368	-	-	0±0,49,49,49	-
3	PX4	B	351	-	-	0±0,49,49,49	-
3	PX4	A	631	-	-	0±0,49,49,49	-
3	PX4	B	313	-	-	0±0,49,49,49	-
3	PX4	A	629	-	-	0±0,49,49,49	-
3	PX4	C	314	-	-	0±0,49,49,49	-
3	PX4	B	376	-	-	0±0,49,49,49	-
3	PX4	C	362	-	-	0±0,49,49,49	-
3	PX4	C	344	-	-	0±0,49,49,49	-
3	PX4	A	613	-	-	0±0,49,49,49	-
3	PX4	B	318	-	-	0±0,49,49,49	-
3	PX4	C	340	-	-	0±0,49,49,49	-
3	PX4	A	648	-	-	0±0,49,49,49	-
3	PX4	B	355	-	-	0±0,49,49,49	-
3	PX4	C	342	-	-	0±0,49,49,49	-
3	PX4	A	630	-	-	0±0,49,49,49	-
3	PX4	C	349	-	-	0±0,49,49,49	-
3	PX4	C	319	-	-	0±0,49,49,49	-
3	PX4	B	374	-	-	0±0,49,49,49	-
3	PX4	A	611	-	-	0±0,49,49,49	-
3	PX4	C	315	-	-	0±0,49,49,49	-
3	PX4	A	640	-	-	0±0,49,49,49	-
3	PX4	C	326	-	-	0±0,49,49,49	-
3	PX4	B	343	-	-	0±0,49,49,49	-
3	PX4	B	302	-	-	0±0,49,49,49	-
3	PX4	C	312	-	-	0±0,49,49,49	-
3	PX4	C	366	-	-	0±0,49,49,49	-
3	PX4	B	378	-	-	0±0,49,49,49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PX4	C	318	-	-	0±0,49,49,49	-
3	PX4	A	634	-	-	0±0,49,49,49	-
3	PX4	B	373	-	-	0±0,49,49,49	-
3	PX4	B	387	-	-	0±0,49,49,49	-
3	PX4	B	362	-	-	0±0,49,49,49	-
3	PX4	B	320	-	-	0±0,49,49,49	-
3	PX4	C	355	-	-	0±0,49,49,49	-
3	PX4	B	364	-	-	0±0,49,49,49	-
3	PX4	A	610	-	-	0±0,49,49,49	-
3	PX4	A	618	-	-	0±0,49,49,49	-
3	PX4	B	391	-	-	0±0,49,49,49	-
3	PX4	B	305	-	-	0±0,49,49,49	-
3	PX4	C	343	-	-	0±0,49,49,49	-
3	PX4	C	370	-	-	0±0,49,49,49	-
3	PX4	C	321	-	-	0±0,49,49,49	-
3	PX4	A	625	-	-	0±0,49,49,49	-
3	PX4	A	605	-	-	0±0,49,49,49	-
3	PX4	B	354	-	-	0±0,49,49,49	-
3	PX4	B	308	-	-	0±0,49,49,49	-
3	PX4	B	338	-	-	0±0,49,49,49	-
3	PX4	B	361	-	-	0±0,49,49,49	-
3	PX4	C	348	-	-	0±0,49,49,49	-
3	PX4	A	621	-	-	0±0,49,49,49	-
3	PX4	C	336	-	-	0±0,49,49,49	-
3	PX4	A	606	-	-	0±0,49,49,49	-
3	PX4	A	646	-	-	0±0,49,49,49	-
3	PX4	A	637	-	-	0±0,49,49,49	-
3	PX4	C	367	-	-	0±0,49,49,49	-
3	PX4	B	363	-	-	0±0,49,49,49	-
3	PX4	A	639	-	-	0±0,49,49,49	-
3	PX4	A	603	-	-	0±0,49,49,49	-
3	PX4	B	369	-	-	0±0,49,49,49	-
3	PX4	B	365	-	-	0±0,49,49,49	-
3	PX4	A	626	-	-	0±0,49,49,49	-
3	PX4	A	624	-	-	0±0,49,49,49	-
3	PX4	A	628	-	-	0±0,49,49,49	-
3	PX4	B	317	-	-	0±0,49,49,49	-
3	PX4	C	334	-	-	0±0,49,49,49	-
3	PX4	B	389	-	-	0±0,49,49,49	-
3	PX4	A	614	-	-	0±0,49,49,49	-
3	PX4	C	347	-	-	0±0,49,49,49	-
3	PX4	C	327	-	-	0±0,49,49,49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PX4	B	380	-	-	0±0,49,49,49	-
3	PX4	C	322	-	-	0±0,49,49,49	-
3	PX4	B	331	-	-	0±0,49,49,49	-
3	PX4	B	325	-	-	0±0,49,49,49	-
3	PX4	C	364	-	-	0±0,49,49,49	-
3	PX4	B	307	-	-	0±0,49,49,49	-
3	PX4	C	304	-	-	0±0,49,49,49	-
3	PX4	B	324	-	-	0±0,49,49,49	-
3	PX4	B	311	-	-	0±0,49,49,49	-
3	PX4	A	644	-	-	0±0,49,49,49	-
3	PX4	B	350	-	-	0±0,49,49,49	-
3	PX4	B	316	-	-	0±0,49,49,49	-
3	PX4	B	359	-	-	0±0,49,49,49	-
3	PX4	B	330	-	-	0±0,49,49,49	-
3	PX4	B	337	-	-	0±0,49,49,49	-
3	PX4	C	323	-	-	0±0,49,49,49	-
3	PX4	A	619	-	-	0±0,49,49,49	-
3	PX4	B	347	-	-	0±0,49,49,49	-
3	PX4	B	353	-	-	0±0,49,49,49	-
3	PX4	C	360	-	-	0±0,49,49,49	-
3	PX4	B	341	-	-	0±0,49,49,49	-
3	PX4	C	332	-	-	0±0,49,49,49	-
3	PX4	C	311	-	-	0±0,49,49,49	-
3	PX4	B	312	-	-	0±0,49,49,49	-
3	PX4	A	635	-	-	0±0,49,49,49	-
3	PX4	A	643	-	-	0±0,49,49,49	-
3	PX4	C	339	-	-	0±0,49,49,49	-
3	PX4	C	363	-	-	0±0,49,49,49	-
3	PX4	B	322	-	-	0±0,49,49,49	-
3	PX4	C	328	-	-	0±0,49,49,49	-
3	PX4	B	395	-	-	0±0,49,49,49	-
3	PX4	C	335	-	-	0±0,49,49,49	-
3	PX4	B	377	-	-	0±0,49,49,49	-
3	PX4	B	344	-	-	0±0,49,49,49	-
3	PX4	C	301	-	-	0±0,49,49,49	-
3	PX4	C	302	-	-	0±0,49,49,49	-
3	PX4	A	616	-	-	0±0,49,49,49	-
3	PX4	B	400	-	-	0±0,49,49,49	-
3	PX4	C	310	-	-	0±0,49,49,49	-
3	PX4	B	319	-	-	0±0,49,49,49	-
3	PX4	B	306	-	-	0±0,49,49,49	-
3	PX4	C	352	-	-	0±0,49,49,49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PX4	B	399	-	-	0±0,49,49,49	-
3	PX4	B	348	-	-	0±0,49,49,49	-
3	PX4	B	329	-	-	0±0,49,49,49	-
3	PX4	A	604	-	-	0±0,49,49,49	-
3	PX4	A	641	-	-	0±0,49,49,49	-
3	PX4	C	345	-	-	0±0,49,49,49	-
3	PX4	A	615	-	-	0±0,49,49,49	-
3	PX4	A	642	-	-	0±0,49,49,49	-
3	PX4	B	335	-	-	0±0,49,49,49	-
3	PX4	A	638	-	-	0±0,49,49,49	-
3	PX4	C	359	-	-	0±0,49,49,49	-
3	PX4	B	301	-	-	0±0,49,49,49	-
3	PX4	A	622	-	-	0±0,49,49,49	-
3	PX4	A	645	-	-	0±0,49,49,49	-
3	PX4	B	366	-	-	0±0,49,49,49	-
3	PX4	B	394	-	-	0±0,49,49,49	-
3	PX4	C	313	-	-	0±0,49,49,49	-
3	PX4	B	336	-	-	0±0,49,49,49	-
3	PX4	B	333	-	-	0±0,49,49,49	-
3	PX4	B	315	-	-	0±0,49,49,49	-
3	PX4	A	647	-	-	0±0,49,49,49	-
3	PX4	A	602	-	-	0±0,49,49,49	-
3	PX4	C	305	-	-	0±0,49,49,49	-
3	PX4	A	608	-	-	0±0,49,49,49	-
3	PX4	B	381	-	-	0±0,49,49,49	-
3	PX4	A	607	-	-	0±0,49,49,49	-
3	PX4	B	370	-	-	0±0,49,49,49	-
3	PX4	C	307	-	-	0±0,49,49,49	-
3	PX4	B	314	-	-	0±0,49,49,49	-
3	PX4	C	365	-	-	0±0,49,49,49	-
3	PX4	C	369	-	-	0±0,49,49,49	-
3	PX4	A	617	-	-	0±0,49,49,49	-
3	PX4	B	371	-	-	0±0,49,49,49	-
3	PX4	B	367	-	-	0±0,49,49,49	-
3	PX4	B	357	-	-	0±0,49,49,49	-
3	PX4	C	333	-	-	0±0,49,49,49	-
3	PX4	C	368	-	-	0±0,49,49,49	-
3	PX4	B	393	-	-	0±0,49,49,49	-
3	PX4	C	317	-	-	0±0,49,49,49	-
3	PX4	B	342	-	-	0±0,49,49,49	-
3	PX4	B	356	-	-	0±0,49,49,49	-
3	PX4	C	329	-	-	0±0,49,49,49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PX4	B	385	-	-	0±0,49,49,49	-
3	PX4	B	397	-	-	0±0,49,49,49	-
3	PX4	C	306	-	-	0±0,49,49,49	-
3	PX4	B	346	-	-	0±0,49,49,49	-
3	PX4	C	320	-	-	0±0,49,49,49	-
3	PX4	C	308	-	-	0±0,49,49,49	-
3	PX4	B	388	-	-	0±0,49,49,49	-
3	PX4	B	396	-	-	0±0,49,49,49	-
3	PX4	B	309	-	-	0±0,49,49,49	-
3	PX4	A	627	-	-	0±0,49,49,49	-
3	PX4	B	327	-	-	0±0,49,49,49	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	307	PX4	C8-C7	5.57	1.68	1.50	9	8
3	A	629	PX4	C6-C7	5.39	1.67	1.50	9	5
3	B	379	PX4	O7-C7	5.26	1.34	1.46	7	3
3	A	609	PX4	C6-C7	5.17	1.67	1.50	15	9
3	C	325	PX4	O7-C7	5.16	1.34	1.46	9	1
3	A	622	PX4	C6-C7	5.14	1.66	1.50	3	7
3	A	613	PX4	C2-C1	5.13	1.66	1.51	2	5
3	B	304	PX4	C2-C1	5.10	1.66	1.51	6	6
3	C	309	PX4	O5-C9	5.06	1.18	1.33	10	1
3	C	330	PX4	C2-C1	5.06	1.66	1.51	15	6
3	A	637	PX4	C2-C1	5.05	1.66	1.51	13	7
3	C	349	PX4	C10-C9	5.02	1.65	1.50	3	3
3	C	338	PX4	C6-C7	5.00	1.66	1.50	3	7
3	C	340	PX4	C6-C7	4.99	1.66	1.50	9	9
3	B	324	PX4	C24-C23	4.99	1.65	1.50	8	2
3	C	351	PX4	C8-C7	4.98	1.66	1.50	5	8
3	C	346	PX4	C8-C7	4.96	1.66	1.50	12	7
3	B	350	PX4	C8-C7	4.94	1.66	1.50	1	7
3	B	324	PX4	C6-C7	4.93	1.66	1.50	5	6
3	C	316	PX4	C10-C9	4.90	1.64	1.50	4	3
3	A	630	PX4	O7-C7	4.88	1.35	1.46	7	3
3	B	339	PX4	C8-C7	4.88	1.66	1.50	13	10
3	B	331	PX4	C2-C1	4.86	1.66	1.51	8	5
3	C	335	PX4	O5-C9	4.86	1.19	1.33	11	2
3	C	325	PX4	C10-C9	4.86	1.64	1.50	4	4
3	C	338	PX4	C2-C1	4.86	1.66	1.51	10	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	635	PX4	O5-C8	4.85	1.56	1.45	11	2
3	B	355	PX4	C8-C7	4.85	1.66	1.50	3	7
3	B	301	PX4	C6-C7	4.84	1.65	1.50	3	8
3	B	376	PX4	O7-C7	4.82	1.35	1.46	13	4
3	B	387	PX4	O7-C7	4.82	1.35	1.46	3	3
3	B	350	PX4	C10-C9	4.82	1.64	1.50	1	7
3	C	357	PX4	C6-C7	4.81	1.65	1.50	14	3
3	C	329	PX4	C8-C7	4.79	1.65	1.50	7	6
3	B	358	PX4	O7-C7	4.77	1.35	1.46	6	5
3	C	350	PX4	C8-C7	4.77	1.65	1.50	1	8
3	B	312	PX4	O5-C8	4.76	1.55	1.45	3	1
3	B	333	PX4	O7-C7	4.75	1.35	1.46	4	3
3	B	305	PX4	C6-C7	4.75	1.65	1.50	13	5
3	B	311	PX4	O7-C7	4.75	1.35	1.46	12	5
3	C	318	PX4	C6-C7	4.74	1.65	1.50	10	3
3	C	312	PX4	C10-C9	4.74	1.64	1.50	10	4
3	A	638	PX4	C8-C7	4.70	1.65	1.50	9	5
3	C	308	PX4	O5-C8	4.70	1.55	1.45	2	2
3	C	303	PX4	C8-C7	4.70	1.65	1.50	11	7
3	B	310	PX4	C10-C9	4.69	1.64	1.50	6	5
3	C	354	PX4	C2-C1	4.69	1.65	1.51	4	5
3	B	387	PX4	O7-C23	4.68	1.21	1.34	15	3
3	B	344	PX4	C2-C1	4.67	1.65	1.51	5	7
3	B	354	PX4	C6-C7	4.66	1.65	1.50	3	5
3	B	303	PX4	C6-C7	4.65	1.65	1.50	5	7
3	A	620	PX4	C8-C7	4.64	1.65	1.50	3	8
3	B	375	PX4	C8-C7	4.63	1.65	1.50	10	7
3	A	640	PX4	C24-C23	4.63	1.64	1.50	11	4
3	B	354	PX4	C8-C7	4.62	1.65	1.50	7	9
3	C	341	PX4	C8-C7	4.62	1.65	1.50	8	6
3	B	306	PX4	O7-C23	4.61	1.21	1.34	12	2
3	A	609	PX4	C2-C1	4.59	1.65	1.51	15	4
3	C	336	PX4	C8-C7	4.59	1.65	1.50	10	7
3	C	313	PX4	C6-C7	4.58	1.65	1.50	4	6
3	C	354	PX4	C6-C7	4.58	1.65	1.50	5	3
3	C	302	PX4	O7-C7	4.57	1.35	1.46	3	3
3	C	317	PX4	C2-C1	4.56	1.65	1.51	5	7
3	B	314	PX4	C6-C7	4.56	1.65	1.50	7	5
3	B	385	PX4	C8-C7	4.56	1.65	1.50	1	5
3	B	400	PX4	C6-C7	4.56	1.65	1.50	5	5
3	A	636	PX4	C8-C7	4.54	1.65	1.50	8	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	620	PX4	C6-C7	4.54	1.65	1.50	8	7
3	B	353	PX4	C24-C23	4.54	1.63	1.50	4	2
3	C	327	PX4	C8-C7	4.53	1.65	1.50	6	8
3	B	336	PX4	C8-C7	4.53	1.65	1.50	7	4
3	B	312	PX4	C2-C1	4.52	1.65	1.51	6	4
3	A	611	PX4	C6-C7	4.51	1.64	1.50	11	9
3	A	640	PX4	C8-C7	4.51	1.64	1.50	15	11
3	B	395	PX4	C10-C9	4.51	1.63	1.50	13	5
3	C	321	PX4	C8-C7	4.50	1.64	1.50	14	12
3	C	315	PX4	C2-C1	4.50	1.64	1.51	15	7
3	B	383	PX4	C8-C7	4.50	1.64	1.50	5	9
3	B	365	PX4	C8-C7	4.49	1.64	1.50	5	8
3	B	360	PX4	C6-C7	4.49	1.64	1.50	1	4
3	C	346	PX4	C6-C7	4.46	1.64	1.50	7	8
3	A	608	PX4	C8-C7	4.46	1.64	1.50	7	5
3	A	624	PX4	O7-C7	4.46	1.36	1.46	6	2
3	B	331	PX4	C24-C23	4.45	1.63	1.50	5	3
3	B	328	PX4	C2-C1	4.44	1.64	1.51	9	3
3	B	338	PX4	C2-C1	4.44	1.64	1.51	2	5
3	A	645	PX4	C6-C7	4.44	1.64	1.50	1	7
3	A	646	PX4	C2-C1	4.44	1.64	1.51	2	4
3	A	614	PX4	O7-C7	4.43	1.36	1.46	3	5
3	B	307	PX4	C2-C1	4.43	1.64	1.51	3	5
3	A	632	PX4	C8-C7	4.43	1.64	1.50	13	9
3	B	317	PX4	C6-C7	4.42	1.64	1.50	11	7
3	B	333	PX4	C6-C7	4.39	1.64	1.50	2	6
3	B	345	PX4	C2-C1	4.39	1.64	1.51	6	7
3	B	396	PX4	O7-C7	4.38	1.36	1.46	2	4
3	C	347	PX4	C6-C7	4.38	1.64	1.50	4	7
3	C	325	PX4	C2-C1	4.38	1.64	1.51	12	7
3	B	357	PX4	C24-C23	4.37	1.63	1.50	15	2
3	B	336	PX4	C6-C7	4.37	1.64	1.50	10	8
3	B	352	PX4	C8-C7	4.37	1.64	1.50	10	7
3	B	352	PX4	O7-C7	4.37	1.36	1.46	13	2
3	B	333	PX4	O5-C8	4.36	1.35	1.45	15	6
3	B	333	PX4	C8-C7	4.35	1.64	1.50	4	7
3	B	354	PX4	O7-C7	4.35	1.36	1.46	2	3
3	C	360	PX4	C8-C7	4.35	1.64	1.50	1	4
3	B	372	PX4	O7-C7	4.34	1.36	1.46	4	4
3	B	384	PX4	C8-C7	4.34	1.64	1.50	13	5
3	B	348	PX4	C6-C7	4.34	1.64	1.50	4	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	617	PX4	C6-C7	4.33	1.64	1.50	13	7
3	A	622	PX4	C2-C1	4.33	1.64	1.51	2	6
3	B	372	PX4	C8-C7	4.32	1.64	1.50	4	5
3	B	338	PX4	C24-C23	4.32	1.63	1.50	4	4
3	B	367	PX4	C6-C7	4.32	1.64	1.50	10	8
3	B	312	PX4	C8-C7	4.31	1.64	1.50	1	10
3	A	615	PX4	C6-C7	4.31	1.64	1.50	14	4
3	C	321	PX4	C2-C1	4.31	1.64	1.51	14	5
3	B	336	PX4	O7-C7	4.30	1.36	1.46	11	6
3	A	635	PX4	C6-C7	4.30	1.64	1.50	7	6
3	B	301	PX4	O7-C7	4.30	1.36	1.46	7	3
3	A	604	PX4	C24-C23	4.29	1.63	1.50	7	1
3	C	317	PX4	C8-C7	4.29	1.64	1.50	6	6
3	C	318	PX4	C2-C1	4.29	1.64	1.51	3	4
3	B	315	PX4	C8-C7	4.29	1.64	1.50	3	10
3	B	346	PX4	C6-C7	4.29	1.64	1.50	9	9
3	B	392	PX4	C6-C7	4.29	1.64	1.50	4	7
3	C	370	PX4	C24-C23	4.29	1.63	1.50	13	5
3	C	302	PX4	C6-C7	4.28	1.64	1.50	12	6
3	B	355	PX4	C2-C1	4.28	1.64	1.51	4	5
3	B	350	PX4	C2-N1	4.28	1.64	1.51	12	1
3	A	621	PX4	C8-C7	4.28	1.64	1.50	12	6
3	B	341	PX4	C2-C1	4.27	1.64	1.51	1	6
3	C	314	PX4	C8-C7	4.27	1.64	1.50	13	6
3	A	615	PX4	C8-C7	4.27	1.64	1.50	3	6
3	C	308	PX4	C6-C7	4.27	1.64	1.50	4	7
3	B	374	PX4	C6-C7	4.27	1.64	1.50	11	8
3	B	386	PX4	C8-C7	4.27	1.64	1.50	14	7
3	B	324	PX4	C8-C7	4.26	1.64	1.50	2	6
3	B	393	PX4	C10-C9	4.26	1.63	1.50	4	8
3	B	317	PX4	O7-C7	4.26	1.36	1.46	2	2
3	C	327	PX4	O7-C23	4.26	1.22	1.34	4	3
3	B	394	PX4	C11-C10	4.26	1.67	1.52	5	2
3	A	635	PX4	C8-C7	4.25	1.64	1.50	5	7
3	B	388	PX4	O7-C7	4.24	1.36	1.46	2	4
3	B	353	PX4	C6-C7	4.23	1.64	1.50	9	6
3	B	389	PX4	O5-C8	4.23	1.35	1.45	2	3
3	B	325	PX4	C6-C7	4.22	1.64	1.50	11	4
3	C	305	PX4	C8-C7	4.22	1.64	1.50	3	6
3	B	331	PX4	C8-C7	4.22	1.64	1.50	3	7
3	B	334	PX4	C8-C7	4.22	1.64	1.50	11	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	391	PX4	C8-C7	4.22	1.64	1.50	5	6
3	B	304	PX4	O7-C7	4.21	1.36	1.46	8	4
3	C	349	PX4	C6-C7	4.21	1.64	1.50	5	5
3	B	391	PX4	O7-C7	4.21	1.36	1.46	3	3
3	A	624	PX4	C2-C1	4.20	1.64	1.51	10	5
3	B	395	PX4	C6-C7	4.20	1.63	1.50	12	8
3	B	390	PX4	O7-C23	4.19	1.22	1.34	15	4
3	A	633	PX4	C8-C7	4.18	1.63	1.50	11	3
3	C	316	PX4	C8-C7	4.18	1.63	1.50	14	5
3	A	613	PX4	C8-C7	4.18	1.63	1.50	13	6
3	A	610	PX4	C8-C7	4.18	1.63	1.50	2	6
3	B	321	PX4	C6-C7	4.18	1.63	1.50	1	6
3	A	644	PX4	C24-C23	4.17	1.62	1.50	9	4
3	B	382	PX4	C2-C1	4.16	1.63	1.51	9	2
3	B	365	PX4	C2-C1	4.16	1.63	1.51	10	6
3	B	387	PX4	C6-C7	4.16	1.63	1.50	8	8
3	C	345	PX4	C6-C7	4.15	1.63	1.50	2	8
3	A	615	PX4	C24-C23	4.15	1.62	1.50	13	2
3	B	332	PX4	C6-C7	4.15	1.63	1.50	11	7
3	B	345	PX4	C6-C7	4.15	1.63	1.50	2	8
3	C	344	PX4	C6-C7	4.14	1.63	1.50	8	7
3	B	347	PX4	C2-C1	4.14	1.63	1.51	2	8
3	A	619	PX4	C6-C7	4.14	1.63	1.50	15	7
3	B	309	PX4	O5-C8	4.14	1.35	1.45	14	3
3	B	319	PX4	C10-C9	4.13	1.62	1.50	14	7
3	C	364	PX4	C2-C1	4.13	1.63	1.51	4	7
3	A	647	PX4	C8-C7	4.12	1.63	1.50	11	6
3	A	636	PX4	C24-C23	4.12	1.62	1.50	3	5
3	B	301	PX4	C10-C9	4.12	1.62	1.50	13	4
3	C	340	PX4	C2-C1	4.11	1.63	1.51	11	6
3	C	337	PX4	C8-C7	4.11	1.63	1.50	9	6
3	A	624	PX4	C8-C7	4.10	1.63	1.50	6	7
3	C	323	PX4	C24-C23	4.10	1.62	1.50	11	3
3	B	325	PX4	C8-C7	4.09	1.63	1.50	9	7
3	B	327	PX4	O7-C23	4.09	1.45	1.34	11	3
3	C	334	PX4	C8-C7	4.09	1.63	1.50	6	3
3	A	617	PX4	C8-C7	4.09	1.63	1.50	3	8
3	A	646	PX4	C6-C7	4.09	1.63	1.50	4	6
3	C	339	PX4	C2-C1	4.08	1.63	1.51	14	4
3	C	350	PX4	C24-C23	4.08	1.62	1.50	1	3
3	B	314	PX4	C8-C7	4.08	1.63	1.50	3	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	394	PX4	C8-C7	4.08	1.63	1.50	10	8
3	C	330	PX4	O5-C8	4.08	1.36	1.45	12	5
3	C	368	PX4	C6-C7	4.07	1.63	1.50	7	8
3	B	369	PX4	C2-C1	4.07	1.63	1.51	9	4
3	C	307	PX4	C2-C1	4.07	1.63	1.51	10	5
3	B	388	PX4	C6-C7	4.07	1.63	1.50	3	6
3	A	632	PX4	C6-C7	4.06	1.63	1.50	7	5
3	B	365	PX4	O5-C8	4.06	1.36	1.45	6	4
3	A	619	PX4	C2-C1	4.06	1.63	1.51	4	4
3	B	371	PX4	C6-C7	4.06	1.63	1.50	6	3
3	A	621	PX4	O7-C7	4.06	1.37	1.46	14	2
3	A	607	PX4	C24-C23	4.05	1.62	1.50	13	3
3	A	616	PX4	O7-C7	4.05	1.37	1.46	7	2
3	B	388	PX4	C8-C7	4.05	1.63	1.50	1	6
3	B	320	PX4	C2-C1	4.05	1.63	1.51	3	5
3	B	377	PX4	C6-C7	4.05	1.63	1.50	1	9
3	A	628	PX4	O7-C7	4.05	1.37	1.46	6	4
3	A	646	PX4	C8-C7	4.05	1.63	1.50	15	6
3	B	352	PX4	O5-C9	4.05	1.45	1.33	14	1
3	B	392	PX4	C2-C1	4.05	1.63	1.51	8	6
3	A	606	PX4	C8-C7	4.04	1.63	1.50	4	9
3	B	399	PX4	C10-C9	4.04	1.62	1.50	15	3
3	A	618	PX4	C2-N1	4.04	1.63	1.51	4	2
3	C	364	PX4	C8-C7	4.04	1.63	1.50	3	7
3	C	361	PX4	C8-C7	4.04	1.63	1.50	15	6
3	B	394	PX4	O7-C7	4.04	1.37	1.46	7	3
3	A	624	PX4	C5-N1	4.03	1.61	1.50	3	2
3	B	400	PX4	C8-C7	4.03	1.63	1.50	13	6
3	A	641	PX4	C6-C7	4.03	1.63	1.50	2	7
3	B	366	PX4	C6-C7	4.03	1.63	1.50	11	9
3	C	310	PX4	C8-C7	4.02	1.63	1.50	10	8
3	C	349	PX4	O5-C8	4.02	1.54	1.45	8	3
3	A	626	PX4	C2-C1	4.02	1.63	1.51	3	5
3	C	354	PX4	O7-C7	4.02	1.37	1.46	2	4
3	B	341	PX4	C6-C7	4.01	1.63	1.50	2	6
3	B	357	PX4	C8-C7	4.01	1.63	1.50	13	6
3	B	361	PX4	C8-C7	4.01	1.63	1.50	2	7
3	B	317	PX4	C2-N1	4.01	1.63	1.51	7	2
3	B	352	PX4	C2-C1	4.00	1.63	1.51	9	5
3	C	320	PX4	C8-C7	4.01	1.63	1.50	4	5
3	A	613	PX4	O7-C7	4.00	1.37	1.46	7	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	329	PX4	O5-C8	4.00	1.54	1.45	1	3
3	C	322	PX4	O7-C23	4.00	1.23	1.34	1	3
3	C	352	PX4	C2-C1	4.00	1.63	1.51	12	4
3	C	354	PX4	C8-C7	4.00	1.63	1.50	13	9
3	B	378	PX4	C6-C7	4.00	1.63	1.50	5	8
3	B	392	PX4	O7-C7	4.00	1.37	1.46	10	3
3	C	367	PX4	C2-C1	3.99	1.63	1.51	13	7
3	A	642	PX4	O5-C8	3.99	1.54	1.45	12	1
3	C	339	PX4	C8-C7	3.99	1.63	1.50	15	7
3	C	342	PX4	C24-C23	3.99	1.62	1.50	5	3
3	C	366	PX4	O5-C9	3.99	1.21	1.33	11	3
3	A	608	PX4	C6-C7	3.98	1.63	1.50	4	7
3	B	338	PX4	C8-C7	3.98	1.63	1.50	15	5
3	B	349	PX4	O5-C8	3.98	1.36	1.45	4	2
3	C	334	PX4	C6-C7	3.97	1.63	1.50	3	7
3	C	366	PX4	C8-C7	3.97	1.63	1.50	14	4
3	B	336	PX4	C2-C1	3.97	1.63	1.51	13	4
3	B	383	PX4	O7-C23	3.97	1.23	1.34	9	3
3	C	323	PX4	C6-C7	3.96	1.63	1.50	4	7
3	B	397	PX4	C6-C7	3.96	1.63	1.50	11	7
3	B	318	PX4	C24-C23	3.96	1.62	1.50	12	4
3	C	314	PX4	C2-C1	3.96	1.63	1.51	15	8
3	C	344	PX4	C10-C9	3.96	1.62	1.50	2	3
3	C	327	PX4	C2-C1	3.96	1.63	1.51	14	6
3	C	370	PX4	C10-C9	3.96	1.62	1.50	13	4
3	B	352	PX4	C6-C7	3.95	1.63	1.50	1	8
3	C	338	PX4	C8-C7	3.95	1.63	1.50	10	8
3	A	626	PX4	C10-C9	3.95	1.62	1.50	8	4
3	B	329	PX4	O5-C9	3.95	1.44	1.33	1	2
3	B	363	PX4	C8-C7	3.95	1.63	1.50	2	6
3	A	642	PX4	C6-C7	3.95	1.63	1.50	11	6
3	B	373	PX4	C6-C7	3.95	1.63	1.50	6	6
3	C	320	PX4	C6-C7	3.95	1.63	1.50	1	6
3	B	376	PX4	O7-C23	3.94	1.23	1.34	8	4
3	B	379	PX4	C2-C1	3.93	1.63	1.51	13	4
3	B	384	PX4	O7-C23	3.92	1.23	1.34	4	3
3	C	306	PX4	C2-C1	3.92	1.63	1.51	4	5
3	B	356	PX4	C2-C1	3.92	1.63	1.51	7	6
3	A	619	PX4	C8-C7	3.92	1.63	1.50	9	5
3	C	349	PX4	C24-C23	3.92	1.62	1.50	3	2
3	B	396	PX4	C2-C1	3.91	1.63	1.51	15	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	638	PX4	C6-C7	3.91	1.63	1.50	4	7
3	C	329	PX4	C10-C9	3.91	1.62	1.50	7	2
3	C	360	PX4	C6-C7	3.91	1.63	1.50	10	10
3	B	327	PX4	C2-C1	3.91	1.63	1.51	1	2
3	B	398	PX4	C24-C23	3.91	1.62	1.50	11	1
3	C	302	PX4	C24-C23	3.91	1.62	1.50	10	4
3	B	360	PX4	O5-C9	3.91	1.22	1.33	13	2
3	B	311	PX4	C24-C23	3.90	1.62	1.50	2	2
3	B	355	PX4	O7-C23	3.90	1.23	1.34	15	2
3	C	347	PX4	O5-C9	3.90	1.22	1.33	7	1
3	A	643	PX4	O7-C23	3.90	1.23	1.34	1	2
3	C	314	PX4	C6-C7	3.90	1.63	1.50	7	6
3	A	615	PX4	O5-C8	3.89	1.36	1.45	15	2
3	A	616	PX4	C2-C1	3.89	1.63	1.51	13	5
3	A	648	PX4	C8-C7	3.89	1.63	1.50	7	8
3	C	348	PX4	C24-C23	3.89	1.62	1.50	5	6
3	B	337	PX4	C6-C7	3.89	1.63	1.50	2	8
3	B	329	PX4	C6-C7	3.89	1.63	1.50	2	4
3	B	396	PX4	C8-C7	3.89	1.63	1.50	7	8
3	A	640	PX4	C4-N1	3.89	1.61	1.50	8	4
3	B	363	PX4	C2-C1	3.88	1.63	1.51	6	5
3	C	350	PX4	O5-C9	3.88	1.22	1.33	8	4
3	B	366	PX4	C8-C7	3.88	1.63	1.50	5	8
3	C	365	PX4	C24-C23	3.88	1.62	1.50	12	4
3	B	310	PX4	C8-C7	3.88	1.62	1.50	12	8
3	A	640	PX4	O5-C8	3.88	1.36	1.45	8	5
3	B	318	PX4	C8-C7	3.87	1.62	1.50	12	9
3	B	343	PX4	O5-C8	3.87	1.53	1.45	13	3
3	C	332	PX4	C8-C7	3.87	1.62	1.50	12	5
3	B	329	PX4	C2-N1	3.87	1.63	1.51	7	4
3	B	323	PX4	C24-C23	3.86	1.61	1.50	8	1
3	C	310	PX4	C6-C7	3.86	1.62	1.50	1	6
3	C	313	PX4	C8-C7	3.86	1.62	1.50	14	8
3	C	330	PX4	C8-C7	3.86	1.62	1.50	14	9
3	A	648	PX4	O7-C7	3.85	1.37	1.46	9	6
3	B	318	PX4	O7-C23	3.85	1.23	1.34	5	1
3	C	345	PX4	O7-C7	3.85	1.37	1.46	5	3
3	C	359	PX4	O7-C7	3.85	1.37	1.46	7	6
3	B	396	PX4	C6-C7	3.85	1.62	1.50	4	4
3	C	308	PX4	C8-C7	3.85	1.62	1.50	12	6
3	C	328	PX4	C24-C23	3.85	1.39	1.50	15	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	323	PX4	C8-C7	3.85	1.62	1.50	12	8
3	C	350	PX4	O7-C7	3.85	1.37	1.46	12	3
3	C	326	PX4	C2-C1	3.85	1.63	1.51	1	3
3	B	359	PX4	C6-C7	3.84	1.62	1.50	1	9
3	B	384	PX4	C6-C7	3.84	1.62	1.50	2	5
3	C	344	PX4	C8-C7	3.84	1.62	1.50	2	6
3	A	602	PX4	C2-C1	3.84	1.62	1.51	15	6
3	A	643	PX4	C2-C1	3.84	1.62	1.51	3	4
3	B	306	PX4	C10-C9	3.84	1.61	1.50	6	4
3	A	602	PX4	O7-C7	3.84	1.37	1.46	13	3
3	B	309	PX4	C8-C7	3.84	1.62	1.50	9	6
3	C	323	PX4	O5-C8	3.84	1.36	1.45	12	3
3	C	316	PX4	O7-C7	3.83	1.55	1.46	11	1
3	C	336	PX4	C2-C1	3.84	1.62	1.51	9	6
3	B	328	PX4	C6-C7	3.83	1.62	1.50	9	6
3	A	631	PX4	C24-C23	3.83	1.61	1.50	1	1
3	B	343	PX4	C2-C1	3.82	1.62	1.51	3	5
3	B	343	PX4	C8-C7	3.82	1.62	1.50	11	8
3	B	353	PX4	C8-C7	3.82	1.62	1.50	7	6
3	B	354	PX4	C4-N1	3.82	1.61	1.50	11	1
3	B	364	PX4	C24-C23	3.82	1.61	1.50	14	3
3	B	375	PX4	C2-C1	3.82	1.62	1.51	6	5
3	B	397	PX4	O7-C7	3.82	1.37	1.46	11	4
3	A	617	PX4	C4-N1	3.82	1.38	1.50	13	3
3	C	321	PX4	O5-C9	3.82	1.44	1.33	6	2
3	B	340	PX4	O5-C9	3.81	1.44	1.33	6	3
3	C	359	PX4	C6-C7	3.81	1.62	1.50	10	6
3	C	307	PX4	C8-C7	3.81	1.62	1.50	5	6
3	C	343	PX4	O7-C7	3.81	1.37	1.46	3	2
3	A	614	PX4	C6-C7	3.81	1.62	1.50	12	9
3	B	376	PX4	C8-C7	3.80	1.62	1.50	14	7
3	B	399	PX4	O5-C8	3.80	1.36	1.45	8	4
3	A	603	PX4	C8-C7	3.80	1.62	1.50	1	7
3	B	306	PX4	C6-C7	3.80	1.62	1.50	12	8
3	B	368	PX4	C8-C7	3.79	1.62	1.50	3	11
3	A	626	PX4	C8-C7	3.79	1.62	1.50	12	5
3	A	601	PX4	C10-C9	3.79	1.61	1.50	12	5
3	B	331	PX4	C6-C7	3.79	1.62	1.50	7	7
3	C	328	PX4	C8-C7	3.79	1.62	1.50	6	9
3	C	337	PX4	C6-C7	3.79	1.62	1.50	5	4
3	C	301	PX4	C2-C1	3.79	1.62	1.51	9	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	366	PX4	C2-N1	3.79	1.39	1.51	2	4
3	B	381	PX4	C2-C1	3.79	1.62	1.51	6	5
3	C	349	PX4	C2-C1	3.79	1.62	1.51	13	6
3	A	608	PX4	C24-C23	3.78	1.61	1.50	13	5
3	B	380	PX4	C6-C7	3.78	1.62	1.50	11	11
3	B	373	PX4	C8-C7	3.78	1.62	1.50	12	7
3	B	327	PX4	O7-C7	3.78	1.37	1.46	8	3
3	C	355	PX4	C8-C7	3.78	1.62	1.50	14	8
3	B	381	PX4	C4-N1	3.77	1.39	1.50	1	3
3	B	304	PX4	O5-C9	3.77	1.44	1.33	1	4
3	B	340	PX4	C10-C9	3.77	1.61	1.50	3	4
3	B	366	PX4	O7-C7	3.77	1.37	1.46	4	2
3	B	390	PX4	O5-C9	3.77	1.44	1.33	2	2
3	C	345	PX4	C8-C7	3.76	1.62	1.50	3	8
3	C	355	PX4	O7-C23	3.76	1.23	1.34	7	1
3	A	636	PX4	C6-C7	3.76	1.62	1.50	10	5
3	B	340	PX4	C2-C1	3.76	1.62	1.51	8	4
3	B	306	PX4	C8-C7	3.76	1.62	1.50	8	6
3	B	335	PX4	C8-C7	3.76	1.62	1.50	11	6
3	B	366	PX4	C24-C23	3.76	1.61	1.50	15	3
3	B	312	PX4	C10-C9	3.75	1.61	1.50	14	5
3	B	349	PX4	C2-C1	3.75	1.62	1.51	14	4
3	A	629	PX4	C8-C7	3.75	1.62	1.50	13	8
3	C	345	PX4	C2-C1	3.75	1.62	1.51	9	7
3	C	370	PX4	C8-C7	3.75	1.62	1.50	14	7
3	B	363	PX4	O7-C7	3.75	1.37	1.46	2	2
3	B	380	PX4	O5-C8	3.75	1.53	1.45	15	2
3	C	320	PX4	O5-C8	3.74	1.36	1.45	7	4
3	B	328	PX4	C10-C9	3.74	1.61	1.50	8	2
3	B	332	PX4	C8-C7	3.74	1.62	1.50	12	4
3	C	320	PX4	C2-N1	3.74	1.62	1.51	6	3
3	A	643	PX4	C6-C7	3.74	1.62	1.50	12	4
3	B	308	PX4	O5-C9	3.74	1.22	1.33	11	2
3	B	363	PX4	C24-C23	3.73	1.61	1.50	8	7
3	B	380	PX4	C2-C1	3.73	1.62	1.51	1	4
3	A	643	PX4	C8-C7	3.73	1.62	1.50	8	5
3	A	612	PX4	C8-C7	3.73	1.62	1.50	14	7
3	A	621	PX4	C11-C10	3.73	1.65	1.52	8	2
3	A	640	PX4	C2-C1	3.73	1.62	1.51	15	3
3	A	619	PX4	O7-C7	3.72	1.37	1.46	13	7
3	B	359	PX4	C10-C9	3.72	1.61	1.50	3	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	370	PX4	C8-C7	3.72	1.62	1.50	1	5
3	C	304	PX4	C6-C7	3.72	1.62	1.50	1	7
3	B	392	PX4	O5-C8	3.72	1.53	1.45	11	3
3	A	606	PX4	C6-C7	3.72	1.62	1.50	8	6
3	A	638	PX4	C25-C24	3.72	1.65	1.52	13	3
3	C	327	PX4	C6-C7	3.71	1.62	1.50	9	4
3	B	356	PX4	C8-C7	3.71	1.62	1.50	5	8
3	B	316	PX4	C6-C7	3.71	1.62	1.50	4	7
3	C	321	PX4	C10-C9	3.71	1.61	1.50	11	3
3	A	635	PX4	O7-C7	3.71	1.37	1.46	6	4
3	B	351	PX4	C6-C7	3.71	1.62	1.50	10	5
3	B	364	PX4	C2-C1	3.71	1.62	1.51	13	6
3	A	605	PX4	O7-C7	3.70	1.37	1.46	5	5
3	A	610	PX4	O5-C8	3.70	1.36	1.45	11	2
3	B	313	PX4	C8-C7	3.70	1.62	1.50	13	6
3	C	344	PX4	O7-C23	3.70	1.23	1.34	11	3
3	B	345	PX4	C8-C7	3.70	1.62	1.50	13	6
3	C	350	PX4	C6-C7	3.70	1.62	1.50	5	6
3	B	330	PX4	C2-N1	3.70	1.62	1.51	6	1
3	C	357	PX4	O7-C7	3.70	1.37	1.46	14	3
3	A	628	PX4	C24-C23	3.69	1.61	1.50	2	4
3	A	639	PX4	O5-C8	3.69	1.36	1.45	13	4
3	B	321	PX4	C8-C7	3.69	1.62	1.50	15	7
3	B	355	PX4	C6-C7	3.69	1.62	1.50	2	6
3	C	331	PX4	C6-C7	3.69	1.62	1.50	3	7
3	B	319	PX4	C6-C7	3.69	1.62	1.50	8	6
3	C	367	PX4	C8-C7	3.69	1.62	1.50	9	6
3	A	630	PX4	C8-C7	3.69	1.62	1.50	8	9
3	A	603	PX4	O7-C23	3.68	1.23	1.34	10	4
3	C	349	PX4	O5-C9	3.68	1.22	1.33	3	5
3	C	331	PX4	C25-C24	3.68	1.65	1.52	15	2
3	C	369	PX4	C10-C9	3.68	1.61	1.50	13	6
3	B	381	PX4	C8-C7	3.68	1.62	1.50	12	6
3	C	352	PX4	C8-C7	3.68	1.62	1.50	14	7
3	B	339	PX4	C6-C7	3.67	1.62	1.50	11	8
3	B	391	PX4	C10-C9	3.67	1.61	1.50	1	6
3	A	616	PX4	C10-C9	3.67	1.61	1.50	13	3
3	B	313	PX4	C6-C7	3.67	1.62	1.50	11	8
3	B	320	PX4	C8-C7	3.67	1.62	1.50	13	7
3	C	369	PX4	O7-C23	3.67	1.23	1.34	3	3
3	C	310	PX4	C10-C9	3.67	1.61	1.50	8	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	387	PX4	C2-N1	3.66	1.62	1.51	12	3
3	C	302	PX4	C8-C7	3.66	1.62	1.50	8	8
3	C	305	PX4	O5-C8	3.66	1.53	1.45	9	1
3	C	362	PX4	O5-C8	3.66	1.37	1.45	4	3
3	A	618	PX4	C8-C7	3.66	1.62	1.50	14	5
3	A	643	PX4	O7-C7	3.66	1.38	1.46	3	3
3	C	340	PX4	C10-C9	3.66	1.61	1.50	6	3
3	B	302	PX4	C2-C1	3.65	1.62	1.51	11	4
3	B	334	PX4	C6-C7	3.65	1.62	1.50	6	5
3	B	313	PX4	C10-C9	3.65	1.61	1.50	10	2
3	B	373	PX4	C2-C1	3.65	1.62	1.51	8	8
3	A	640	PX4	O7-C7	3.65	1.38	1.46	4	4
3	C	348	PX4	C2-C1	3.65	1.62	1.51	1	6
3	B	371	PX4	C2-C1	3.64	1.62	1.51	12	3
3	B	384	PX4	C2-C1	3.64	1.62	1.51	10	6
3	B	336	PX4	C24-C23	3.64	1.61	1.50	15	4
3	C	328	PX4	C2-C1	3.64	1.62	1.51	10	4
3	C	357	PX4	C8-C7	3.64	1.62	1.50	11	10
3	C	320	PX4	C2-C1	3.63	1.62	1.51	1	3
3	B	390	PX4	C8-C7	3.63	1.62	1.50	10	7
3	C	332	PX4	O7-C23	3.63	1.24	1.34	5	1
3	C	342	PX4	O7-C7	3.63	1.38	1.46	5	4
3	B	335	PX4	C2-C1	3.63	1.62	1.51	4	5
3	C	346	PX4	C2-C1	3.63	1.62	1.51	7	6
3	A	617	PX4	C24-C23	3.62	1.61	1.50	15	4
3	B	301	PX4	C8-C7	3.62	1.62	1.50	6	7
3	B	382	PX4	C6-C7	3.63	1.62	1.50	2	3
3	B	391	PX4	C2-C1	3.62	1.62	1.51	2	5
3	C	311	PX4	C8-C7	3.62	1.62	1.50	8	7
3	C	366	PX4	C6-C7	3.62	1.62	1.50	2	7
3	B	367	PX4	C2-C1	3.62	1.62	1.51	1	6
3	C	319	PX4	C24-C23	3.62	1.61	1.50	9	2
3	A	647	PX4	C10-C9	3.62	1.61	1.50	1	4
3	A	625	PX4	C6-C7	3.62	1.62	1.50	15	8
3	A	631	PX4	C8-C7	3.62	1.62	1.50	10	7
3	B	314	PX4	C10-C9	3.62	1.61	1.50	14	3
3	C	332	PX4	C6-C7	3.62	1.62	1.50	14	10
3	B	334	PX4	C2-C1	3.61	1.62	1.51	8	3
3	C	370	PX4	C6-C7	3.62	1.62	1.50	1	5
3	B	371	PX4	C24-C23	3.61	1.61	1.50	10	3
3	B	398	PX4	C6-C7	3.61	1.62	1.50	9	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	308	PX4	O7-C7	3.61	1.38	1.46	11	4
3	A	646	PX4	C24-C23	3.61	1.61	1.50	1	5
3	C	343	PX4	C8-C7	3.61	1.62	1.50	5	6
3	B	394	PX4	C6-C7	3.61	1.62	1.50	15	3
3	C	353	PX4	O5-C9	3.61	1.43	1.33	4	3
3	A	605	PX4	C6-C7	3.60	1.62	1.50	3	6
3	C	360	PX4	O5-C8	3.60	1.37	1.45	13	2
3	B	335	PX4	C10-C9	3.60	1.61	1.50	6	3
3	C	311	PX4	O5-C8	3.60	1.37	1.45	3	1
3	C	339	PX4	O7-C7	3.60	1.55	1.46	11	4
3	B	357	PX4	O5-C8	3.60	1.37	1.45	12	2
3	B	315	PX4	C10-C9	3.59	1.61	1.50	14	1
3	A	604	PX4	O7-C23	3.59	1.24	1.34	4	1
3	B	315	PX4	C2-C1	3.59	1.62	1.51	12	6
3	B	400	PX4	C2-C1	3.59	1.62	1.51	11	5
3	C	369	PX4	C8-C7	3.59	1.62	1.50	10	5
3	B	310	PX4	C6-C7	3.59	1.62	1.50	4	8
3	A	648	PX4	C6-C7	3.58	1.62	1.50	2	6
3	B	359	PX4	C2-C1	3.58	1.62	1.51	15	7
3	A	641	PX4	C4-N1	3.58	1.60	1.50	8	1
3	C	314	PX4	C2-N1	3.58	1.62	1.51	8	2
3	B	312	PX4	C6-C7	3.58	1.62	1.50	4	6
3	B	314	PX4	P1-O4	3.58	1.45	1.59	6	1
3	C	363	PX4	O7-C7	3.58	1.38	1.46	5	2
3	A	601	PX4	C6-C7	3.58	1.62	1.50	7	4
3	B	352	PX4	C5-N1	3.57	1.60	1.50	8	2
3	A	604	PX4	C8-C7	3.57	1.62	1.50	7	4
3	A	630	PX4	C6-C7	3.57	1.62	1.50	4	6
3	A	644	PX4	C8-C7	3.57	1.62	1.50	1	7
3	B	397	PX4	C2-C1	3.57	1.62	1.51	14	7
3	C	337	PX4	O7-C23	3.57	1.24	1.34	15	2
3	A	611	PX4	O7-C23	3.57	1.24	1.34	3	1
3	A	643	PX4	C24-C23	3.57	1.61	1.50	6	3
3	B	307	PX4	C6-C7	3.57	1.62	1.50	8	7
3	C	313	PX4	C10-C9	3.57	1.61	1.50	15	6
3	A	648	PX4	C2-C1	3.56	1.62	1.51	14	4
3	A	617	PX4	O7-C23	3.56	1.24	1.34	1	2
3	C	305	PX4	C10-C9	3.56	1.61	1.50	4	4
3	C	325	PX4	C6-C7	3.56	1.61	1.50	10	9
3	C	341	PX4	C6-C7	3.56	1.61	1.50	13	5
3	A	614	PX4	C8-C7	3.56	1.61	1.50	13	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	318	PX4	C2-C1	3.56	1.62	1.51	6	5
3	C	332	PX4	O5-C8	3.56	1.37	1.45	15	3
3	B	376	PX4	C6-C7	3.55	1.61	1.50	4	6
3	B	380	PX4	O7-C7	3.55	1.38	1.46	1	2
3	B	367	PX4	C24-C23	3.55	1.61	1.50	12	3
3	C	312	PX4	C8-C7	3.55	1.61	1.50	13	8
3	B	314	PX4	C2-C1	3.55	1.62	1.51	8	8
3	B	333	PX4	C2-C1	3.55	1.62	1.51	12	5
3	B	398	PX4	O7-C7	3.55	1.38	1.46	7	3
3	C	309	PX4	C8-C7	3.55	1.61	1.50	6	7
3	C	325	PX4	C24-C23	3.55	1.61	1.50	7	4
3	B	316	PX4	C10-C9	3.54	1.61	1.50	6	5
3	A	639	PX4	C6-C7	3.54	1.61	1.50	4	4
3	C	331	PX4	O7-C7	3.54	1.38	1.46	7	2
3	C	323	PX4	C2-C1	3.54	1.62	1.51	3	5
3	B	320	PX4	C6-C7	3.54	1.61	1.50	3	5
3	B	327	PX4	C24-C23	3.53	1.61	1.50	15	5
3	C	333	PX4	C8-C7	3.53	1.61	1.50	2	12
3	C	335	PX4	C8-C7	3.53	1.61	1.50	15	7
3	A	633	PX4	O7-C7	3.53	1.38	1.46	14	3
3	C	365	PX4	C2-C1	3.53	1.62	1.51	9	4
3	B	328	PX4	C8-C7	3.52	1.61	1.50	3	8
3	C	323	PX4	C10-C9	3.52	1.60	1.50	7	4
3	B	379	PX4	C6-C7	3.52	1.61	1.50	3	7
3	A	612	PX4	C24-C23	3.52	1.60	1.50	14	2
3	B	359	PX4	C24-C23	3.52	1.60	1.50	15	3
3	C	353	PX4	C2-C1	3.52	1.62	1.51	15	4
3	A	634	PX4	C6-C7	3.51	1.61	1.50	13	5
3	C	301	PX4	C24-C23	3.51	1.60	1.50	11	4
3	B	305	PX4	O5-C8	3.51	1.37	1.45	1	1
3	B	327	PX4	C6-C7	3.51	1.61	1.50	6	7
3	B	309	PX4	C6-C7	3.51	1.61	1.50	6	4
3	B	330	PX4	C6-C7	3.51	1.61	1.50	15	6
3	C	346	PX4	C2-N1	3.51	1.62	1.51	2	5
3	B	323	PX4	C8-C7	3.50	1.61	1.50	8	7
3	A	616	PX4	C8-C7	3.50	1.61	1.50	6	8
3	B	337	PX4	C4-N1	3.50	1.39	1.50	5	2
3	B	369	PX4	O5-C8	3.50	1.37	1.45	9	5
3	A	610	PX4	C5-N1	3.50	1.39	1.50	2	2
3	C	350	PX4	C2-C1	3.50	1.61	1.51	9	5
3	B	346	PX4	C3-N1	3.50	1.39	1.50	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	618	PX4	C10-C9	3.49	1.60	1.50	14	2
3	B	358	PX4	C8-C7	3.49	1.61	1.50	8	4
3	B	377	PX4	C2-C1	3.49	1.61	1.51	10	6
3	B	311	PX4	C8-C7	3.49	1.61	1.50	15	6
3	B	323	PX4	C10-C9	3.49	1.60	1.50	10	2
3	B	332	PX4	C2-C1	3.49	1.61	1.51	9	6
3	B	367	PX4	C10-C9	3.49	1.60	1.50	2	3
3	B	361	PX4	C10-C9	3.49	1.60	1.50	1	3
3	C	301	PX4	C8-C7	3.49	1.61	1.50	5	7
3	B	322	PX4	C8-C7	3.48	1.61	1.50	6	2
3	B	376	PX4	O5-C9	3.48	1.43	1.33	2	2
3	C	328	PX4	C10-C9	3.48	1.60	1.50	8	1
3	B	387	PX4	C10-C9	3.48	1.60	1.50	6	2
3	B	384	PX4	O7-C7	3.48	1.38	1.46	14	2
3	C	339	PX4	O5-C8	3.48	1.37	1.45	10	3
3	B	337	PX4	C8-C7	3.48	1.61	1.50	10	8
3	B	369	PX4	O7-C23	3.48	1.24	1.34	4	2
3	A	633	PX4	O7-C23	3.47	1.24	1.34	6	2
3	B	358	PX4	C6-C7	3.47	1.61	1.50	1	7
3	C	341	PX4	C10-C9	3.47	1.60	1.50	3	7
3	B	350	PX4	C6-C7	3.47	1.61	1.50	9	6
3	B	351	PX4	C10-C9	3.47	1.60	1.50	10	4
3	C	321	PX4	O7-C7	3.47	1.38	1.46	12	1
3	A	633	PX4	C11-C10	3.47	1.64	1.52	2	2
3	B	394	PX4	C10-C9	3.46	1.60	1.50	15	2
3	B	304	PX4	C24-C23	3.46	1.60	1.50	6	5
3	C	319	PX4	C6-C7	3.46	1.61	1.50	14	6
3	A	614	PX4	C2-C1	3.46	1.61	1.51	15	4
3	B	311	PX4	C2-C1	3.46	1.61	1.51	1	4
3	C	356	PX4	C2-C1	3.46	1.61	1.51	3	7
3	A	628	PX4	C8-C7	3.46	1.61	1.50	8	6
3	B	339	PX4	C2-N1	3.46	1.62	1.51	6	1
3	B	340	PX4	O7-C23	3.46	1.24	1.34	9	2
3	B	395	PX4	C8-C7	3.46	1.61	1.50	3	5
3	C	363	PX4	O7-C23	3.46	1.24	1.34	2	2
3	B	397	PX4	C10-C9	3.45	1.60	1.50	9	5
3	B	367	PX4	C8-C7	3.45	1.61	1.50	6	7
3	A	632	PX4	C2-N1	3.45	1.62	1.51	8	2
3	A	633	PX4	O5-C9	3.45	1.23	1.33	4	5
3	A	639	PX4	C3-N1	3.45	1.40	1.50	10	1
3	A	641	PX4	C2-C1	3.45	1.61	1.51	11	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	603	PX4	O7-C7	3.44	1.38	1.46	4	4
3	C	353	PX4	C18-C17	3.44	1.68	1.51	4	1
3	B	338	PX4	C10-C9	3.44	1.60	1.50	7	4
3	C	317	PX4	C24-C23	3.44	1.60	1.50	3	3
3	A	614	PX4	C25-C24	3.44	1.64	1.52	11	2
3	C	363	PX4	C24-C23	3.43	1.60	1.50	7	4
3	C	349	PX4	C25-C24	3.43	1.64	1.52	2	4
3	B	399	PX4	C24-C23	3.43	1.60	1.50	6	3
3	C	323	PX4	O7-C7	3.43	1.38	1.46	12	3
3	B	334	PX4	C10-C9	3.43	1.60	1.50	6	4
3	B	323	PX4	O5-C9	3.43	1.23	1.33	10	2
3	B	357	PX4	C2-C1	3.43	1.61	1.51	11	3
3	B	365	PX4	C24-C23	3.42	1.60	1.50	11	3
3	B	378	PX4	C8-C7	3.42	1.61	1.50	6	2
3	C	315	PX4	O7-C7	3.42	1.38	1.46	11	3
3	C	321	PX4	C2-N1	3.42	1.61	1.51	14	1
3	C	334	PX4	C10-C9	3.42	1.60	1.50	4	2
3	A	602	PX4	O5-C8	3.42	1.52	1.45	1	3
3	A	620	PX4	O5-C8	3.42	1.52	1.45	11	2
3	B	326	PX4	C8-C7	3.42	1.61	1.50	1	8
3	B	346	PX4	O7-C7	3.42	1.38	1.46	3	4
3	C	335	PX4	O5-C8	3.42	1.52	1.45	6	4
3	B	342	PX4	C6-C7	3.42	1.61	1.50	3	3
3	C	312	PX4	O5-C8	3.41	1.52	1.45	3	4
3	A	637	PX4	O7-C7	3.41	1.54	1.46	7	5
3	B	361	PX4	C4-N1	3.41	1.40	1.50	11	1
3	A	627	PX4	C8-C7	3.41	1.61	1.50	7	7
3	C	318	PX4	C8-C7	3.41	1.61	1.50	14	6
3	C	329	PX4	C24-C23	3.41	1.60	1.50	13	2
3	B	370	PX4	C2-C1	3.41	1.61	1.51	11	7
3	C	304	PX4	C24-C23	3.41	1.60	1.50	15	4
3	A	607	PX4	C10-C9	3.40	1.60	1.50	10	3
3	B	344	PX4	O7-C23	3.40	1.24	1.34	8	3
3	C	362	PX4	O7-C7	3.40	1.38	1.46	13	2
3	A	625	PX4	C8-C7	3.40	1.61	1.50	8	7
3	A	644	PX4	C3-N1	3.40	1.40	1.50	9	2
3	C	303	PX4	C24-C23	3.40	1.60	1.50	12	3
3	C	356	PX4	C8-C7	3.40	1.61	1.50	8	7
3	A	633	PX4	C24-C23	3.40	1.60	1.50	12	4
3	A	635	PX4	C3-N1	3.40	1.40	1.50	13	1
3	A	645	PX4	C2-C1	3.40	1.61	1.51	1	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	612	PX4	C6-C7	3.40	1.61	1.50	2	5
3	B	323	PX4	C25-C24	3.39	1.64	1.52	11	1
3	C	303	PX4	C2-C1	3.39	1.61	1.51	5	7
3	B	372	PX4	C10-C9	3.39	1.60	1.50	3	1
3	B	380	PX4	C5-N1	3.39	1.59	1.50	7	3
3	B	351	PX4	C24-C23	3.39	1.60	1.50	9	4
3	C	301	PX4	O7-C23	3.39	1.24	1.34	5	3
3	B	383	PX4	O7-C7	3.39	1.38	1.46	10	1
3	B	390	PX4	C6-C7	3.39	1.61	1.50	7	8
3	C	350	PX4	C25-C24	3.39	1.64	1.52	11	4
3	C	311	PX4	C24-C23	3.39	1.60	1.50	10	2
3	A	605	PX4	O5-C8	3.38	1.52	1.45	5	2
3	A	608	PX4	C10-C9	3.38	1.60	1.50	12	3
3	B	356	PX4	C10-C9	3.38	1.60	1.50	13	2
3	B	374	PX4	C10-C9	3.38	1.60	1.50	4	3
3	C	342	PX4	C6-C7	3.38	1.61	1.50	4	6
3	B	377	PX4	C8-C7	3.38	1.61	1.50	8	7
3	A	641	PX4	C10-C9	3.38	1.60	1.50	13	2
3	B	322	PX4	C24-C23	3.38	1.60	1.50	14	5
3	C	317	PX4	C10-C9	3.38	1.60	1.50	13	2
3	B	371	PX4	C8-C7	3.38	1.61	1.50	11	7
3	C	322	PX4	C8-C7	3.38	1.61	1.50	1	7
3	A	637	PX4	O5-C8	3.37	1.37	1.45	6	1
3	C	337	PX4	O5-C9	3.37	1.23	1.33	13	2
3	C	353	PX4	O7-C23	3.37	1.24	1.34	1	3
3	A	621	PX4	C2-C1	3.37	1.61	1.51	5	7
3	A	602	PX4	C24-C23	3.37	1.60	1.50	5	1
3	B	308	PX4	C8-C7	3.37	1.61	1.50	2	6
3	C	351	PX4	O7-C7	3.37	1.38	1.46	4	4
3	B	336	PX4	C5-N1	3.37	1.40	1.50	15	2
3	B	346	PX4	O5-C9	3.37	1.43	1.33	4	2
3	C	321	PX4	C6-C7	3.37	1.61	1.50	8	5
3	A	604	PX4	C6-C7	3.37	1.61	1.50	12	6
3	C	352	PX4	C24-C23	3.37	1.60	1.50	9	4
3	C	366	PX4	C2-C1	3.37	1.61	1.51	11	2
3	B	349	PX4	C24-C23	3.37	1.60	1.50	3	5
3	B	349	PX4	O7-C7	3.37	1.38	1.46	11	3
3	B	387	PX4	C8-C7	3.36	1.61	1.50	14	11
3	A	620	PX4	O5-C9	3.36	1.43	1.33	8	2
3	A	627	PX4	C25-C24	3.36	1.64	1.52	3	1
3	B	324	PX4	O7-C23	3.36	1.24	1.34	10	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	333	PX4	C10-C9	3.36	1.60	1.50	7	4
3	B	303	PX4	O7-C7	3.36	1.38	1.46	11	2
3	B	342	PX4	C10-C9	3.36	1.60	1.50	9	2
3	B	307	PX4	O5-C9	3.35	1.23	1.33	1	1
3	C	339	PX4	C11-C10	3.35	1.64	1.52	8	3
3	B	326	PX4	C2-C1	3.35	1.61	1.51	8	5
3	B	358	PX4	C2-C1	3.35	1.61	1.51	14	9
3	B	385	PX4	C6-C7	3.35	1.61	1.50	7	4
3	C	315	PX4	C4-N1	3.35	1.59	1.50	14	1
3	C	356	PX4	O7-C23	3.35	1.24	1.34	1	2
3	C	358	PX4	O7-C23	3.35	1.24	1.34	1	4
3	B	375	PX4	O5-C8	3.35	1.52	1.45	7	3
3	C	324	PX4	C6-C7	3.35	1.61	1.50	4	4
3	B	308	PX4	C6-C7	3.34	1.61	1.50	12	4
3	B	393	PX4	C2-C1	3.34	1.61	1.51	11	5
3	B	388	PX4	C11-C10	3.34	1.64	1.52	8	2
3	A	617	PX4	C10-C9	3.34	1.60	1.50	5	3
3	B	397	PX4	C24-C23	3.34	1.60	1.50	11	5
3	A	645	PX4	O7-C7	3.34	1.38	1.46	6	2
3	B	396	PX4	O7-C23	3.34	1.24	1.34	13	1
3	C	304	PX4	C2-C1	3.34	1.61	1.51	9	6
3	C	335	PX4	C2-C1	3.34	1.61	1.51	6	5
3	B	369	PX4	C10-C9	3.34	1.60	1.50	10	4
3	A	621	PX4	O5-C9	3.33	1.23	1.33	13	4
3	A	645	PX4	O5-C9	3.33	1.43	1.33	8	1
3	C	307	PX4	C11-C10	3.33	1.64	1.52	13	2
3	C	359	PX4	C24-C23	3.33	1.60	1.50	9	1
3	B	399	PX4	C6-C7	3.33	1.61	1.50	9	7
3	C	334	PX4	C2-C1	3.33	1.61	1.51	5	6
3	B	381	PX4	O7-C7	3.33	1.38	1.46	2	2
3	C	320	PX4	C10-C9	3.33	1.60	1.50	9	3
3	C	362	PX4	C2-C1	3.33	1.61	1.51	6	6
3	C	368	PX4	C10-C9	3.33	1.60	1.50	7	7
3	C	324	PX4	C2-C1	3.33	1.61	1.51	13	3
3	C	348	PX4	C6-C7	3.33	1.61	1.50	4	4
3	C	325	PX4	C8-C7	3.32	1.61	1.50	2	7
3	A	631	PX4	O5-C8	3.32	1.37	1.45	3	1
3	B	319	PX4	C5-N1	3.32	1.40	1.50	3	3
3	C	329	PX4	C6-C7	3.32	1.61	1.50	6	7
3	C	335	PX4	C25-C24	3.32	1.64	1.52	5	3
3	C	352	PX4	O7-C7	3.32	1.38	1.46	7	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	332	PX4	O7-C23	3.32	1.24	1.34	14	4
3	B	315	PX4	C6-C7	3.32	1.61	1.50	11	3
3	B	341	PX4	O5-C9	3.32	1.23	1.33	6	3
3	C	350	PX4	C10-C9	3.32	1.60	1.50	12	4
3	A	642	PX4	C19-C18	3.32	1.68	1.51	1	1
3	C	349	PX4	C8-C7	3.32	1.61	1.50	11	6
3	B	323	PX4	C2-C1	3.31	1.61	1.51	4	3
3	B	381	PX4	C6-C7	3.31	1.61	1.50	4	4
3	B	314	PX4	C3-N1	3.31	1.59	1.50	9	1
3	C	325	PX4	C25-C24	3.31	1.64	1.52	10	1
3	A	611	PX4	C8-C7	3.31	1.61	1.50	11	6
3	B	302	PX4	C2-N1	3.31	1.61	1.51	8	2
3	C	309	PX4	O7-C7	3.31	1.38	1.46	1	1
3	C	327	PX4	C3-N1	3.31	1.59	1.50	15	3
3	C	359	PX4	C2-N1	3.31	1.61	1.51	1	2
3	A	632	PX4	C10-C9	3.31	1.60	1.50	13	7
3	B	349	PX4	C8-C7	3.31	1.61	1.50	14	4
3	C	327	PX4	C5-N1	3.31	1.40	1.50	2	2
3	A	607	PX4	C6-C7	3.31	1.61	1.50	10	10
3	B	337	PX4	C24-C23	3.31	1.60	1.50	2	4
3	B	394	PX4	C24-C23	3.31	1.60	1.50	12	3
3	B	304	PX4	C5-N1	3.31	1.59	1.50	14	2
3	B	334	PX4	C24-C23	3.30	1.60	1.50	7	3
3	B	303	PX4	C2-C1	3.30	1.61	1.51	14	5
3	C	321	PX4	C4-N1	3.30	1.40	1.50	13	3
3	C	361	PX4	C6-C7	3.30	1.61	1.50	10	5
3	B	368	PX4	C6-C7	3.30	1.61	1.50	15	5
3	C	346	PX4	O5-C8	3.30	1.37	1.45	12	5
3	B	351	PX4	C8-C7	3.30	1.61	1.50	3	3
3	B	391	PX4	O7-C23	3.30	1.24	1.34	11	2
3	B	399	PX4	C8-C7	3.30	1.61	1.50	1	8
3	A	629	PX4	O7-C23	3.30	1.24	1.34	11	1
3	C	346	PX4	C10-C9	3.30	1.60	1.50	2	2
3	A	611	PX4	C10-C9	3.29	1.60	1.50	13	1
3	B	382	PX4	O7-C23	3.29	1.25	1.34	11	3
3	C	338	PX4	C10-C9	3.29	1.60	1.50	7	3
3	B	394	PX4	C2-C1	3.29	1.61	1.51	15	6
3	A	620	PX4	C4-N1	3.29	1.40	1.50	11	2
3	A	622	PX4	C8-C7	3.29	1.61	1.50	11	2
3	C	343	PX4	C25-C24	3.29	1.64	1.52	1	2
3	B	354	PX4	C2-N1	3.29	1.41	1.51	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	342	PX4	C8-C7	3.29	1.61	1.50	15	4
3	B	361	PX4	C2-C1	3.29	1.61	1.51	15	6
3	B	382	PX4	C8-C7	3.29	1.61	1.50	8	8
3	C	331	PX4	C8-C7	3.29	1.61	1.50	11	4
3	A	608	PX4	O5-C8	3.29	1.52	1.45	12	3
3	A	620	PX4	C2-C1	3.28	1.61	1.51	13	4
3	C	329	PX4	O5-C8	3.29	1.37	1.45	2	2
3	C	331	PX4	C2-C1	3.28	1.61	1.51	7	5
3	B	323	PX4	O7-C7	3.28	1.38	1.46	12	3
3	A	642	PX4	C8-C7	3.28	1.61	1.50	13	9
3	B	307	PX4	O7-C7	3.28	1.38	1.46	6	3
3	A	604	PX4	C2-C1	3.28	1.61	1.51	7	8
3	B	378	PX4	C25-C24	3.28	1.64	1.52	5	2
3	A	625	PX4	O7-C23	3.28	1.25	1.34	11	2
3	B	386	PX4	O5-C8	3.28	1.52	1.45	2	2
3	C	368	PX4	C2-N1	3.28	1.61	1.51	8	4
3	C	305	PX4	C24-C23	3.28	1.60	1.50	7	3
3	C	324	PX4	C10-C9	3.27	1.60	1.50	6	3
3	A	617	PX4	C28-C27	3.27	1.68	1.51	14	1
3	B	315	PX4	C11-C10	3.27	1.64	1.52	12	6
3	B	332	PX4	C24-C23	3.27	1.60	1.50	10	3
3	B	304	PX4	C6-C7	3.27	1.61	1.50	7	7
3	B	319	PX4	C2-C1	3.27	1.61	1.51	14	6
3	A	624	PX4	C6-C7	3.27	1.61	1.50	12	5
3	A	647	PX4	C2-C1	3.27	1.61	1.51	11	5
3	B	302	PX4	O7-C23	3.27	1.25	1.34	9	3
3	B	321	PX4	C28-C27	3.27	1.68	1.51	13	1
3	C	362	PX4	C8-C7	3.27	1.61	1.50	6	7
3	A	633	PX4	C2-C1	3.27	1.61	1.51	9	3
3	B	362	PX4	C8-C7	3.27	1.61	1.50	9	5
3	B	365	PX4	C6-C7	3.27	1.61	1.50	2	4
3	A	625	PX4	C2-C1	3.26	1.61	1.51	9	6
3	B	342	PX4	C8-C7	3.26	1.61	1.50	10	7
3	C	341	PX4	O5-C8	3.26	1.52	1.45	14	2
3	A	623	PX4	C25-C24	3.26	1.64	1.52	11	4
3	A	640	PX4	O5-C9	3.26	1.23	1.33	10	1
3	A	647	PX4	C6-C7	3.26	1.61	1.50	4	8
3	C	351	PX4	C10-C9	3.26	1.60	1.50	13	5
3	C	360	PX4	C2-C1	3.26	1.61	1.51	13	4
3	B	322	PX4	C2-C1	3.25	1.61	1.51	7	7
3	C	317	PX4	C4-N1	3.25	1.59	1.50	5	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	341	PX4	O7-C7	3.25	1.38	1.46	14	5
3	A	609	PX4	O5-C9	3.25	1.23	1.33	1	1
3	A	642	PX4	C2-C1	3.25	1.61	1.51	12	2
3	B	350	PX4	C24-C23	3.25	1.60	1.50	12	2
3	C	347	PX4	C24-C23	3.25	1.41	1.50	1	4
3	C	366	PX4	C10-C9	3.24	1.60	1.50	13	5
3	C	370	PX4	C25-C24	3.24	1.64	1.52	9	3
3	A	608	PX4	C2-C1	3.24	1.61	1.51	8	4
3	B	324	PX4	O7-C7	3.24	1.39	1.46	1	2
3	A	601	PX4	C2-C1	3.24	1.61	1.51	5	6
3	B	379	PX4	C11-C10	3.24	1.64	1.52	3	1
3	C	353	PX4	C8-C7	3.24	1.60	1.50	4	4
3	A	601	PX4	C8-C7	3.24	1.60	1.50	12	7
3	A	639	PX4	C2-C1	3.24	1.61	1.51	12	6
3	A	644	PX4	C6-C7	3.24	1.60	1.50	10	3
3	B	326	PX4	C25-C24	3.24	1.64	1.52	14	1
3	B	330	PX4	O7-C23	3.24	1.25	1.34	3	4
3	B	302	PX4	O7-C7	3.23	1.39	1.46	1	3
3	B	359	PX4	C8-C7	3.23	1.60	1.50	11	6
3	C	353	PX4	C24-C23	3.23	1.60	1.50	11	3
3	C	319	PX4	C8-C7	3.23	1.60	1.50	7	5
3	C	359	PX4	C8-C7	3.23	1.60	1.50	11	5
3	B	371	PX4	O7-C7	3.23	1.39	1.46	6	1
3	B	389	PX4	C2-C1	3.23	1.61	1.51	10	5
3	B	345	PX4	C11-C10	3.23	1.64	1.52	14	1
3	B	348	PX4	C24-C23	3.23	1.60	1.50	13	6
3	A	616	PX4	C6-C7	3.23	1.60	1.50	9	5
3	A	641	PX4	O7-C7	3.22	1.39	1.46	5	1
3	B	362	PX4	O5-C8	3.22	1.38	1.45	7	3
3	B	368	PX4	C2-C1	3.23	1.61	1.51	8	4
3	C	359	PX4	O7-C23	3.23	1.25	1.34	2	2
3	B	322	PX4	C6-C7	3.22	1.60	1.50	3	6
3	C	312	PX4	O7-C7	3.22	1.39	1.46	1	2
3	C	359	PX4	C10-C9	3.22	1.60	1.50	5	4
3	C	328	PX4	O7-C7	3.22	1.39	1.46	14	5
3	A	645	PX4	O7-C23	3.22	1.25	1.34	11	2
3	B	336	PX4	C10-C9	3.22	1.60	1.50	11	3
3	B	380	PX4	C8-C7	3.22	1.60	1.50	6	3
3	C	347	PX4	C10-C9	3.22	1.60	1.50	14	3
3	B	345	PX4	O7-C7	3.22	1.39	1.46	1	4
3	C	305	PX4	C2-C1	3.22	1.61	1.51	1	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	351	PX4	C6-C7	3.22	1.60	1.50	12	4
3	A	634	PX4	C8-C7	3.21	1.60	1.50	4	5
3	C	322	PX4	O7-C7	3.21	1.54	1.46	12	2
3	A	623	PX4	C10-C9	3.21	1.60	1.50	5	4
3	B	388	PX4	C25-C24	3.21	1.64	1.52	13	3
3	C	324	PX4	C3-N1	3.21	1.59	1.50	2	2
3	A	627	PX4	C6-C7	3.21	1.60	1.50	11	8
3	B	313	PX4	O7-C23	3.21	1.43	1.34	10	1
3	B	327	PX4	C8-C7	3.21	1.60	1.50	5	12
3	C	355	PX4	C2-C1	3.21	1.61	1.51	1	6
3	B	338	PX4	O5-C8	3.21	1.38	1.45	4	2
3	B	400	PX4	O7-C7	3.21	1.39	1.46	5	3
3	C	317	PX4	C6-C7	3.21	1.60	1.50	7	5
3	C	322	PX4	C10-C9	3.21	1.60	1.50	6	4
3	B	331	PX4	C10-C9	3.20	1.60	1.50	2	2
3	A	619	PX4	C10-C9	3.20	1.60	1.50	11	1
3	B	330	PX4	C10-C9	3.20	1.60	1.50	6	5
3	C	303	PX4	C10-C9	3.20	1.60	1.50	9	3
3	A	632	PX4	O5-C9	3.20	1.24	1.33	15	1
3	B	311	PX4	C6-C7	3.20	1.60	1.50	12	6
3	C	319	PX4	C10-C9	3.20	1.60	1.50	14	1
3	B	324	PX4	C2-C1	3.20	1.61	1.51	8	7
3	C	356	PX4	C6-C7	3.20	1.60	1.50	11	5
3	B	308	PX4	C24-C23	3.20	1.60	1.50	10	3
3	C	362	PX4	C24-C23	3.20	1.60	1.50	12	4
3	A	636	PX4	C2-C1	3.19	1.61	1.51	14	3
3	A	644	PX4	C2-C1	3.19	1.61	1.51	14	5
3	B	309	PX4	C2-C1	3.19	1.61	1.51	11	4
3	C	361	PX4	C2-C1	3.19	1.61	1.51	7	2
3	B	332	PX4	O7-C7	3.19	1.39	1.46	13	3
3	B	340	PX4	C11-C10	3.19	1.63	1.52	3	5
3	B	393	PX4	C6-C7	3.19	1.60	1.50	9	5
3	A	605	PX4	C8-C7	3.19	1.60	1.50	1	8
3	A	607	PX4	C8-C7	3.19	1.60	1.50	14	5
3	B	321	PX4	O5-C8	3.19	1.38	1.45	12	3
3	C	358	PX4	C2-C1	3.19	1.61	1.51	3	1
3	B	353	PX4	C2-C1	3.19	1.61	1.51	2	3
3	B	380	PX4	C24-C23	3.19	1.60	1.50	2	2
3	C	316	PX4	C2-C1	3.19	1.61	1.51	9	6
3	B	379	PX4	C10-C9	3.18	1.59	1.50	10	2
3	A	608	PX4	O5-C9	3.18	1.24	1.33	15	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	312	PX4	C2-C1	3.18	1.61	1.51	10	5
3	A	606	PX4	C11-C10	3.18	1.63	1.52	8	3
3	B	313	PX4	O7-C7	3.18	1.39	1.46	4	2
3	B	343	PX4	C6-C7	3.18	1.60	1.50	13	4
3	B	343	PX4	O5-C9	3.18	1.42	1.33	10	2
3	B	350	PX4	P1-O3	3.18	1.46	1.59	11	2
3	C	311	PX4	C2-C1	3.18	1.60	1.51	12	5
3	A	637	PX4	C8-C7	3.18	1.60	1.50	14	6
3	A	603	PX4	O5-C8	3.18	1.52	1.45	11	1
3	A	645	PX4	C8-C7	3.18	1.60	1.50	13	6
3	B	396	PX4	C4-N1	3.17	1.59	1.50	6	1
3	C	337	PX4	C11-C10	3.17	1.63	1.52	4	2
3	A	625	PX4	C2-N1	3.17	1.61	1.51	11	1
3	B	385	PX4	O5-C8	3.17	1.52	1.45	14	1
3	B	320	PX4	O7-C7	3.17	1.39	1.46	7	2
3	B	330	PX4	C2-C1	3.17	1.60	1.51	2	3
3	B	333	PX4	C4-N1	3.17	1.59	1.50	14	2
3	B	302	PX4	C8-C7	3.17	1.60	1.50	8	6
3	B	375	PX4	O7-C23	3.17	1.25	1.34	6	5
3	A	630	PX4	O7-C23	3.17	1.25	1.34	2	3
3	B	310	PX4	O5-C8	3.17	1.52	1.45	4	1
3	B	389	PX4	C10-C9	3.17	1.59	1.50	15	7
3	C	363	PX4	P1-O4	3.16	1.47	1.59	7	1
3	A	615	PX4	O7-C23	3.16	1.25	1.34	5	3
3	B	347	PX4	C10-C9	3.16	1.59	1.50	2	4
3	B	362	PX4	O7-C23	3.16	1.25	1.34	3	2
3	C	332	PX4	C24-C23	3.16	1.59	1.50	2	4
3	C	346	PX4	C5-N1	3.16	1.59	1.50	2	2
3	C	366	PX4	O5-C8	3.16	1.38	1.45	5	3
3	A	635	PX4	C10-C9	3.16	1.59	1.50	11	3
3	C	306	PX4	C24-C23	3.16	1.59	1.50	13	3
3	C	351	PX4	O5-C8	3.16	1.52	1.45	2	4
3	A	632	PX4	O5-C8	3.15	1.38	1.45	13	4
3	B	302	PX4	O5-C8	3.16	1.38	1.45	2	3
3	B	379	PX4	C24-C23	3.15	1.59	1.50	11	5
3	C	307	PX4	C6-C7	3.15	1.60	1.50	3	4
3	C	355	PX4	O5-C8	3.16	1.38	1.45	10	2
3	B	341	PX4	C8-C7	3.15	1.60	1.50	12	7
3	B	350	PX4	C2-C1	3.15	1.60	1.51	4	4
3	C	309	PX4	C6-C7	3.15	1.60	1.50	8	8
3	C	363	PX4	C2-C1	3.15	1.60	1.51	4	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	325	PX4	C5-N1	3.15	1.40	1.50	8	2
3	B	377	PX4	C5-N1	3.15	1.40	1.50	2	1
3	A	627	PX4	C11-C10	3.15	1.63	1.52	10	3
3	A	628	PX4	C6-C7	3.15	1.60	1.50	3	3
3	A	642	PX4	O7-C7	3.15	1.39	1.46	8	5
3	B	344	PX4	C8-C7	3.15	1.60	1.50	15	6
3	B	348	PX4	O5-C8	3.15	1.38	1.45	2	2
3	B	378	PX4	C5-N1	3.15	1.59	1.50	5	2
3	C	366	PX4	O7-C7	3.15	1.39	1.46	8	3
3	C	370	PX4	O7-C7	3.15	1.39	1.46	13	4
3	B	303	PX4	O7-C23	3.14	1.25	1.34	3	2
3	B	396	PX4	C11-C10	3.14	1.63	1.52	10	2
3	C	312	PX4	P1-O3	3.14	1.47	1.59	12	1
3	B	327	PX4	C4-N1	3.14	1.40	1.50	11	4
3	C	337	PX4	C10-C9	3.14	1.59	1.50	3	2
3	C	336	PX4	O5-C9	3.14	1.24	1.33	6	2
3	A	638	PX4	C2-C1	3.14	1.60	1.51	5	3
3	B	312	PX4	O7-C23	3.14	1.25	1.34	2	1
3	B	317	PX4	C8-C7	3.14	1.60	1.50	4	7
3	C	306	PX4	C8-C7	3.14	1.60	1.50	4	8
3	C	316	PX4	C24-C23	3.14	1.59	1.50	1	5
3	A	602	PX4	C6-C7	3.14	1.60	1.50	13	6
3	A	619	PX4	O5-C8	3.13	1.52	1.45	4	2
3	B	329	PX4	C2-C1	3.14	1.60	1.51	8	7
3	B	356	PX4	C6-C7	3.14	1.60	1.50	11	3
3	C	306	PX4	O7-C7	3.14	1.39	1.46	4	3
3	B	379	PX4	C8-C7	3.13	1.60	1.50	7	7
3	C	304	PX4	C10-C9	3.13	1.59	1.50	9	3
3	C	309	PX4	O5-C8	3.13	1.52	1.45	3	1
3	C	343	PX4	C2-C1	3.13	1.60	1.51	5	2
3	C	355	PX4	C3-N1	3.13	1.59	1.50	4	1
3	A	606	PX4	C3-N1	3.13	1.59	1.50	15	2
3	A	613	PX4	O5-C9	3.13	1.24	1.33	6	2
3	A	635	PX4	C2-C1	3.13	1.60	1.51	10	4
3	C	364	PX4	C24-C23	3.13	1.59	1.50	1	2
3	B	341	PX4	O7-C7	3.13	1.39	1.46	2	3
3	B	358	PX4	C10-C9	3.13	1.59	1.50	2	4
3	A	647	PX4	C11-C10	3.12	1.63	1.52	10	2
3	B	323	PX4	C6-C7	3.12	1.60	1.50	6	5
3	A	609	PX4	C8-C7	3.12	1.60	1.50	4	8
3	A	615	PX4	C2-C1	3.12	1.60	1.51	15	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	374	PX4	C8-C7	3.12	1.60	1.50	12	4
3	C	303	PX4	O7-C23	3.12	1.25	1.34	12	2
3	C	305	PX4	O7-C7	3.12	1.39	1.46	7	2
3	B	340	PX4	C6-C7	3.12	1.60	1.50	14	4
3	A	614	PX4	C24-C23	3.11	1.59	1.50	8	6
3	B	321	PX4	O7-C7	3.11	1.39	1.46	15	3
3	B	397	PX4	C5-N1	3.11	1.41	1.50	7	4
3	C	326	PX4	C8-C7	3.11	1.60	1.50	3	3
3	B	322	PX4	C10-C9	3.11	1.59	1.50	11	3
3	B	319	PX4	O7-C7	3.11	1.39	1.46	13	2
3	C	326	PX4	C6-C7	3.11	1.60	1.50	14	7
3	C	367	PX4	C24-C23	3.11	1.59	1.50	11	6
3	B	390	PX4	O5-C8	3.11	1.38	1.45	10	2
3	A	634	PX4	C2-C1	3.10	1.60	1.51	7	8
3	B	305	PX4	C24-C23	3.11	1.59	1.50	15	4
3	B	371	PX4	O5-C8	3.11	1.52	1.45	10	4
3	C	339	PX4	C6-C7	3.11	1.60	1.50	7	6
3	B	321	PX4	C2-C1	3.11	1.60	1.51	3	6
3	B	398	PX4	C10-C9	3.11	1.59	1.50	15	2
3	A	645	PX4	C10-C9	3.10	1.59	1.50	3	6
3	B	311	PX4	C10-C9	3.10	1.59	1.50	6	2
3	B	315	PX4	C3-N1	3.10	1.41	1.50	11	1
3	C	307	PX4	C10-C9	3.10	1.59	1.50	13	5
3	C	302	PX4	O5-C8	3.10	1.52	1.45	10	1
3	C	357	PX4	C25-C24	3.10	1.63	1.52	8	2
3	A	614	PX4	C10-C9	3.10	1.59	1.50	6	1
3	A	608	PX4	O7-C7	3.10	1.39	1.46	8	2
3	A	629	PX4	O5-C9	3.10	1.24	1.33	2	5
3	B	321	PX4	C3-N1	3.10	1.41	1.50	11	3
3	B	356	PX4	C25-C24	3.10	1.63	1.52	1	2
3	C	325	PX4	C3-N1	3.10	1.41	1.50	14	2
3	A	640	PX4	C5-N1	3.10	1.41	1.50	12	2
3	B	314	PX4	O5-C8	3.10	1.38	1.45	4	2
3	C	355	PX4	P1-O1	3.10	1.41	1.55	15	3
3	B	372	PX4	C2-N1	3.09	1.60	1.51	14	3
3	C	336	PX4	C11-C10	3.10	1.63	1.52	9	3
3	A	603	PX4	C2-C1	3.09	1.60	1.51	3	5
3	B	345	PX4	C24-C23	3.09	1.59	1.50	13	1
3	B	365	PX4	C10-C9	3.09	1.59	1.50	11	2
3	B	317	PX4	C10-C9	3.09	1.59	1.50	11	5
3	C	301	PX4	C6-C7	3.09	1.60	1.50	12	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	368	PX4	C2-C1	3.09	1.60	1.51	6	8
3	A	630	PX4	C25-C24	3.09	1.63	1.52	9	2
3	B	322	PX4	O5-C8	3.09	1.38	1.45	9	2
3	B	316	PX4	C8-C7	3.09	1.60	1.50	4	4
3	B	324	PX4	C10-C9	3.09	1.59	1.50	6	3
3	B	341	PX4	O5-C8	3.09	1.52	1.45	9	2
3	B	336	PX4	O5-C8	3.09	1.52	1.45	10	1
3	B	341	PX4	O7-C23	3.09	1.25	1.34	8	2
3	B	394	PX4	O5-C8	3.09	1.52	1.45	1	2
3	B	315	PX4	C24-C23	3.09	1.59	1.50	15	3
3	B	362	PX4	C25-C24	3.09	1.63	1.52	2	3
3	B	400	PX4	O5-C8	3.09	1.38	1.45	6	2
3	B	369	PX4	C8-C7	3.09	1.60	1.50	12	8
3	C	348	PX4	O5-C8	3.08	1.38	1.45	2	3
3	A	624	PX4	C11-C10	3.08	1.63	1.52	15	3
3	A	633	PX4	C10-C9	3.08	1.59	1.50	11	3
3	C	321	PX4	C24-C23	3.08	1.59	1.50	5	4
3	C	365	PX4	C11-C10	3.08	1.63	1.52	2	1
3	A	636	PX4	O7-C23	3.08	1.43	1.34	5	2
3	C	322	PX4	C24-C23	3.08	1.59	1.50	7	4
3	C	336	PX4	C3-N1	3.08	1.41	1.50	6	4
3	C	358	PX4	O7-C7	3.08	1.39	1.46	8	2
3	B	318	PX4	O5-C9	3.08	1.42	1.33	8	5
3	B	334	PX4	C25-C24	3.08	1.63	1.52	6	3
3	B	391	PX4	O5-C9	3.08	1.42	1.33	11	4
3	B	392	PX4	O7-C23	3.08	1.25	1.34	15	2
3	C	327	PX4	C2-N1	3.08	1.60	1.51	5	1
3	B	331	PX4	O5-C9	3.07	1.42	1.33	13	3
3	B	344	PX4	C24-C23	3.07	1.59	1.50	7	2
3	B	370	PX4	C6-C7	3.07	1.60	1.50	3	4
3	B	308	PX4	C5-N1	3.07	1.41	1.50	1	1
3	B	329	PX4	C8-C7	3.07	1.60	1.50	13	7
3	B	361	PX4	C3-N1	3.07	1.41	1.50	7	1
3	A	621	PX4	C10-C9	3.07	1.59	1.50	15	5
3	B	360	PX4	C10-C9	3.07	1.59	1.50	12	4
3	C	345	PX4	C3-N1	3.07	1.58	1.50	5	1
3	A	607	PX4	O7-C23	3.07	1.25	1.34	11	2
3	A	611	PX4	C24-C23	3.06	1.59	1.50	13	2
3	B	310	PX4	P1-O4	3.07	1.47	1.59	2	1
3	A	637	PX4	C24-C23	3.06	1.59	1.50	14	2
3	B	312	PX4	C24-C23	3.06	1.59	1.50	14	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	337	PX4	C2-C1	3.07	1.60	1.51	7	5
3	B	366	PX4	C10-C9	3.06	1.59	1.50	1	4
3	C	321	PX4	P1-O4	3.06	1.47	1.59	13	1
3	C	330	PX4	C6-C7	3.06	1.60	1.50	8	6
3	B	306	PX4	C2-C1	3.06	1.60	1.51	11	3
3	B	337	PX4	C25-C24	3.06	1.63	1.52	12	2
3	B	364	PX4	C8-C7	3.06	1.60	1.50	1	4
3	B	396	PX4	C24-C23	3.06	1.59	1.50	11	3
3	A	610	PX4	C4-N1	3.06	1.41	1.50	13	4
3	B	398	PX4	C8-C7	3.06	1.60	1.50	7	5
3	A	631	PX4	C2-C1	3.06	1.60	1.51	14	3
3	C	319	PX4	C13-C12	3.06	1.67	1.51	1	1
3	B	325	PX4	O5-C8	3.06	1.52	1.45	14	3
3	B	334	PX4	O7-C7	3.06	1.39	1.46	13	3
3	B	372	PX4	C3-N1	3.06	1.58	1.50	5	2
3	A	608	PX4	C4-N1	3.06	1.41	1.50	14	3
3	A	628	PX4	C10-C9	3.06	1.59	1.50	11	2
3	A	629	PX4	C3-N1	3.06	1.58	1.50	6	1
3	A	634	PX4	O7-C7	3.06	1.39	1.46	2	1
3	A	645	PX4	P1-O2	3.06	1.40	1.50	1	2
3	B	316	PX4	C2-C1	3.06	1.60	1.51	9	5
3	B	318	PX4	O7-C7	3.06	1.39	1.46	14	4
3	B	367	PX4	O7-C7	3.06	1.39	1.46	8	3
3	C	358	PX4	C24-C23	3.06	1.59	1.50	2	4
3	A	621	PX4	O7-C23	3.05	1.25	1.34	5	1
3	A	631	PX4	C6-C7	3.05	1.60	1.50	9	7
3	B	363	PX4	C6-C7	3.05	1.60	1.50	2	4
3	C	311	PX4	C5-N1	3.05	1.58	1.50	4	4
3	B	303	PX4	C24-C23	3.05	1.59	1.50	3	4
3	B	340	PX4	C8-C7	3.05	1.60	1.50	15	8
3	B	348	PX4	C8-C7	3.05	1.60	1.50	8	8
3	B	317	PX4	O7-C23	3.05	1.25	1.34	15	1
3	B	336	PX4	O5-C9	3.05	1.24	1.33	10	3
3	B	355	PX4	O3-C1	3.05	1.32	1.44	3	1
3	B	356	PX4	O7-C7	3.05	1.39	1.46	15	2
3	C	317	PX4	O7-C7	3.05	1.39	1.46	13	5
3	B	400	PX4	C10-C9	3.05	1.59	1.50	6	4
3	C	333	PX4	O7-C7	3.05	1.39	1.46	6	1
3	B	320	PX4	C10-C9	3.04	1.59	1.50	8	5
3	B	373	PX4	C24-C23	3.04	1.59	1.50	4	4
3	C	333	PX4	C6-C7	3.04	1.60	1.50	8	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	338	PX4	C2-N1	3.04	1.60	1.51	2	3
3	C	314	PX4	C10-C9	3.04	1.59	1.50	6	4
3	C	369	PX4	C6-C7	3.04	1.60	1.50	11	7
3	A	613	PX4	C6-C7	3.04	1.60	1.50	3	8
3	A	625	PX4	O4-C6	3.04	1.56	1.44	10	1
3	B	303	PX4	C10-C9	3.04	1.59	1.50	1	3
3	C	337	PX4	C2-N1	3.04	1.60	1.51	2	1
3	C	320	PX4	O7-C23	3.03	1.25	1.34	9	4
3	C	352	PX4	C6-C7	3.03	1.60	1.50	12	3
3	A	633	PX4	C4-N1	3.03	1.58	1.50	1	1
3	B	381	PX4	C3-N1	3.03	1.58	1.50	1	2
3	A	630	PX4	O5-C8	3.03	1.38	1.45	9	5
3	B	350	PX4	C11-C10	3.03	1.63	1.52	1	4
3	B	377	PX4	O5-C9	3.03	1.24	1.33	11	5
3	C	329	PX4	C2-C1	3.03	1.60	1.51	4	7
3	C	301	PX4	C10-C9	3.03	1.59	1.50	5	2
3	C	352	PX4	C5-N1	3.03	1.58	1.50	4	1
3	C	355	PX4	C24-C23	3.03	1.59	1.50	7	4
3	C	358	PX4	C5-N1	3.03	1.58	1.50	2	2
3	B	359	PX4	C2-N1	3.03	1.60	1.51	13	1
3	B	382	PX4	C25-C24	3.03	1.63	1.52	9	2
3	B	387	PX4	C24-C23	3.03	1.59	1.50	2	3
3	C	329	PX4	O7-C7	3.03	1.39	1.46	4	1
3	A	619	PX4	C5-N1	3.03	1.58	1.50	3	3
3	B	320	PX4	O7-C23	3.03	1.25	1.34	9	4
3	A	641	PX4	C3-N1	3.02	1.41	1.50	11	4
3	A	618	PX4	C6-C7	3.02	1.60	1.50	14	4
3	B	339	PX4	C3-N1	3.02	1.58	1.50	11	2
3	B	348	PX4	C2-C1	3.02	1.60	1.51	7	6
3	C	341	PX4	C2-C1	3.02	1.60	1.51	7	7
3	C	367	PX4	C6-C7	3.02	1.60	1.50	9	5
3	C	370	PX4	C2-C1	3.02	1.60	1.51	12	3
3	A	636	PX4	C10-C9	3.02	1.59	1.50	8	2
3	B	386	PX4	C6-C7	3.02	1.60	1.50	7	5
3	C	331	PX4	C2-N1	3.02	1.60	1.51	6	2
3	B	318	PX4	C10-C9	3.02	1.59	1.50	1	1
3	A	622	PX4	P1-O1	3.02	1.41	1.55	14	3
3	C	312	PX4	O7-C23	3.02	1.25	1.34	9	2
3	C	363	PX4	C8-C7	3.02	1.60	1.50	5	8
3	B	399	PX4	O5-C9	3.02	1.24	1.33	2	2
3	B	313	PX4	C32-C31	3.02	1.66	1.51	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	640	PX4	C10-C9	3.01	1.59	1.50	9	5
3	A	647	PX4	C2-N1	3.01	1.60	1.51	15	1
3	B	397	PX4	C8-C7	3.01	1.60	1.50	13	4
3	B	399	PX4	C11-C10	3.01	1.63	1.52	6	3
3	C	365	PX4	O5-C8	3.02	1.38	1.45	5	2
3	B	375	PX4	C24-C23	3.01	1.59	1.50	14	2
3	C	341	PX4	C25-C24	3.01	1.63	1.52	11	1
3	A	606	PX4	O7-C7	3.01	1.39	1.46	10	4
3	A	641	PX4	O5-C9	3.01	1.42	1.33	14	2
3	B	305	PX4	C8-C7	3.01	1.60	1.50	6	6
3	C	317	PX4	O5-C9	3.01	1.24	1.33	6	3
3	B	365	PX4	O7-C7	3.01	1.39	1.46	11	5
3	C	365	PX4	C6-C7	3.01	1.60	1.50	13	5
3	A	609	PX4	O7-C23	3.01	1.25	1.34	11	3
3	A	627	PX4	C2-C1	3.01	1.60	1.51	11	4
3	C	302	PX4	C11-C10	3.01	1.63	1.52	8	4
3	C	336	PX4	C25-C24	3.01	1.63	1.52	10	2
3	A	607	PX4	C11-C10	3.01	1.63	1.52	1	1
3	A	610	PX4	C2-C1	3.00	1.60	1.51	8	6
3	B	335	PX4	C25-C24	3.00	1.63	1.52	4	1
3	B	393	PX4	O7-C23	3.00	1.25	1.34	1	5
3	C	357	PX4	C2-C1	3.00	1.60	1.51	8	6
3	C	368	PX4	C8-C7	3.00	1.60	1.50	8	8
3	A	615	PX4	C25-C24	3.00	1.63	1.52	8	1
3	A	623	PX4	C2-C1	3.00	1.60	1.51	2	8
3	A	601	PX4	C24-C23	3.00	1.59	1.50	12	3
3	A	605	PX4	C2-C1	3.00	1.60	1.51	10	6
3	C	307	PX4	O7-C7	3.00	1.39	1.46	11	5
3	C	332	PX4	C2-C1	3.00	1.60	1.51	2	3
3	B	383	PX4	C4-N1	3.00	1.58	1.50	5	1
3	B	390	PX4	O7-C7	3.00	1.39	1.46	1	5
3	C	342	PX4	C2-C1	3.00	1.60	1.51	3	3
3	B	313	PX4	C24-C23	3.00	1.59	1.50	8	4
3	C	348	PX4	O7-C23	3.00	1.42	1.34	13	5
3	A	607	PX4	C3-N1	3.00	1.58	1.50	12	3
3	B	374	PX4	C2-N1	3.00	1.60	1.51	5	1
3	B	397	PX4	O5-C9	2.99	1.24	1.33	10	2
3	C	315	PX4	C8-C7	2.99	1.60	1.50	4	8
3	A	633	PX4	P1-O1	2.99	1.41	1.55	1	2
3	B	389	PX4	C6-C7	2.99	1.60	1.50	10	4
3	B	398	PX4	C2-C1	2.99	1.60	1.51	11	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	626	PX4	O7-C7	2.99	1.39	1.46	9	3
3	B	346	PX4	C4-N1	2.99	1.58	1.50	6	2
3	B	373	PX4	O3-C1	2.99	1.32	1.44	8	2
3	A	618	PX4	O7-C7	2.99	1.39	1.46	6	4
3	B	388	PX4	O5-C9	2.98	1.42	1.33	11	1
3	B	390	PX4	C2-C1	2.98	1.60	1.51	11	5
3	C	303	PX4	O5-C8	2.98	1.38	1.45	5	1
3	C	338	PX4	O5-C8	2.98	1.38	1.45	15	2
3	C	355	PX4	P1-O3	2.98	1.47	1.59	6	1
3	C	323	PX4	C2-N1	2.98	1.60	1.51	13	3
3	C	368	PX4	C25-C24	2.98	1.63	1.52	7	3
3	B	308	PX4	C10-C9	2.98	1.59	1.50	5	2
3	B	309	PX4	O7-C7	2.98	1.39	1.46	13	5
3	B	362	PX4	C2-C1	2.98	1.60	1.51	7	4
3	B	369	PX4	C24-C23	2.98	1.59	1.50	4	3
3	B	399	PX4	C2-C1	2.98	1.60	1.51	9	3
3	A	622	PX4	C24-C23	2.98	1.59	1.50	11	2
3	B	317	PX4	C2-C1	2.98	1.60	1.51	2	5
3	B	317	PX4	O5-C8	2.98	1.38	1.45	11	4
3	B	335	PX4	O5-C8	2.97	1.51	1.45	9	2
3	C	318	PX4	P1-O4	2.97	1.47	1.59	5	1
3	C	330	PX4	C10-C9	2.97	1.59	1.50	11	4
3	B	304	PX4	O5-C8	2.97	1.51	1.45	7	2
3	B	343	PX4	C10-C9	2.97	1.59	1.50	10	1
3	A	608	PX4	C25-C24	2.97	1.63	1.52	5	1
3	B	344	PX4	O7-C7	2.97	1.39	1.46	3	2
3	B	390	PX4	C3-N1	2.97	1.41	1.50	14	3
3	C	332	PX4	C4-N1	2.97	1.41	1.50	1	1
3	C	335	PX4	C11-C10	2.97	1.63	1.52	3	2
3	C	370	PX4	O5-C8	2.97	1.38	1.45	7	4
3	B	363	PX4	C17-C16	2.97	1.66	1.51	15	1
3	B	386	PX4	C11-C10	2.97	1.63	1.52	10	2
3	C	304	PX4	C8-C7	2.97	1.60	1.50	5	7
3	C	314	PX4	O7-C7	2.97	1.39	1.46	11	4
3	B	355	PX4	C24-C23	2.97	1.59	1.50	9	5
3	C	322	PX4	C6-C7	2.97	1.60	1.50	5	7
3	C	358	PX4	C6-C7	2.97	1.60	1.50	2	5
3	A	630	PX4	C10-C9	2.96	1.59	1.50	3	5
3	B	360	PX4	C8-C7	2.97	1.60	1.50	2	6
3	C	313	PX4	O5-C8	2.97	1.51	1.45	4	2
3	C	359	PX4	C25-C24	2.97	1.63	1.52	1	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	361	PX4	C6-C7	2.96	1.60	1.50	10	7
3	B	376	PX4	C2-C1	2.96	1.60	1.51	4	5
3	A	620	PX4	C24-C23	2.96	1.59	1.50	13	1
3	B	344	PX4	C6-C7	2.96	1.60	1.50	14	5
3	C	302	PX4	C10-C9	2.96	1.59	1.50	1	3
3	B	357	PX4	C10-C9	2.96	1.59	1.50	15	4
3	A	604	PX4	C10-C9	2.96	1.59	1.50	14	2
3	B	343	PX4	O7-C7	2.96	1.39	1.46	11	2
3	C	334	PX4	C4-N1	2.96	1.58	1.50	3	3
3	C	348	PX4	C8-C7	2.96	1.60	1.50	13	8
3	A	606	PX4	C10-C9	2.96	1.59	1.50	14	4
3	B	369	PX4	C6-C7	2.96	1.60	1.50	15	4
3	C	308	PX4	C24-C23	2.96	1.59	1.50	5	3
3	A	606	PX4	C2-C1	2.96	1.60	1.51	2	5
3	B	311	PX4	O5-C8	2.96	1.51	1.45	3	3
3	B	356	PX4	C11-C10	2.96	1.63	1.52	7	3
3	C	348	PX4	C25-C24	2.96	1.63	1.52	15	2
3	A	612	PX4	C2-C1	2.96	1.60	1.51	6	4
3	A	614	PX4	C11-C10	2.95	1.63	1.52	14	2
3	A	622	PX4	O5-C8	2.95	1.51	1.45	9	1
3	B	304	PX4	C11-C10	2.95	1.63	1.52	7	4
3	B	312	PX4	P1-O4	2.95	1.47	1.59	2	1
3	C	316	PX4	O5-C8	2.95	1.38	1.45	1	2
3	B	390	PX4	C10-C9	2.95	1.59	1.50	11	1
3	A	623	PX4	C2-N1	2.95	1.60	1.51	5	3
3	B	351	PX4	O5-C8	2.95	1.38	1.45	3	2
3	B	399	PX4	C5-N1	2.95	1.58	1.50	12	2
3	C	316	PX4	C6-C7	2.95	1.60	1.50	1	6
3	A	612	PX4	C11-C10	2.95	1.63	1.52	11	2
3	B	342	PX4	O7-C7	2.95	1.39	1.46	3	2
3	B	360	PX4	O7-C23	2.95	1.25	1.34	6	2
3	C	332	PX4	C33-C32	2.95	1.66	1.51	13	1
3	C	333	PX4	O5-C9	2.95	1.24	1.33	6	2
3	B	341	PX4	C10-C9	2.95	1.59	1.50	1	5
3	B	354	PX4	O5-C8	2.95	1.51	1.45	9	3
3	B	374	PX4	C11-C10	2.95	1.63	1.52	15	4
3	B	380	PX4	O7-C23	2.95	1.25	1.34	13	3
3	C	307	PX4	C3-N1	2.95	1.41	1.50	11	3
3	C	339	PX4	C28-C27	2.95	1.66	1.51	10	1
3	C	334	PX4	C11-C10	2.95	1.63	1.52	5	2
3	C	301	PX4	C25-C24	2.95	1.63	1.52	12	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	310	PX4	C24-C23	2.94	1.59	1.50	15	5
3	C	360	PX4	C5-N1	2.94	1.58	1.50	8	1
3	C	340	PX4	C24-C23	2.94	1.59	1.50	10	1
3	C	344	PX4	C2-C1	2.94	1.60	1.51	9	6
3	B	307	PX4	C10-C9	2.94	1.59	1.50	2	5
3	C	314	PX4	O5-C8	2.94	1.51	1.45	5	2
3	C	365	PX4	C8-C7	2.94	1.60	1.50	4	6
3	A	618	PX4	O7-C23	2.93	1.26	1.34	8	1
3	B	314	PX4	C5-N1	2.93	1.41	1.50	14	1
3	C	306	PX4	C5-N1	2.93	1.58	1.50	4	1
3	B	368	PX4	O7-C7	2.93	1.39	1.46	14	5
3	B	384	PX4	P1-O3	2.93	1.47	1.59	12	1
3	C	321	PX4	O7-C23	2.93	1.26	1.34	5	2
3	B	307	PX4	C11-C10	2.93	1.62	1.52	5	2
3	B	378	PX4	O7-C7	2.93	1.39	1.46	6	4
3	C	342	PX4	O5-C9	2.93	1.41	1.33	11	1
3	C	362	PX4	O5-C9	2.93	1.24	1.33	8	2
3	A	603	PX4	C6-C7	2.93	1.60	1.50	5	6
3	A	622	PX4	O7-C23	2.92	1.26	1.34	6	1
3	B	371	PX4	C25-C24	2.92	1.62	1.52	12	3
3	C	323	PX4	P1-O3	2.93	1.70	1.59	15	3
3	B	304	PX4	C10-C9	2.92	1.59	1.50	1	6
3	B	315	PX4	P1-O2	2.92	1.40	1.50	12	1
3	C	345	PX4	C24-C23	2.92	1.59	1.50	8	4
3	B	389	PX4	O5-C9	2.92	1.41	1.33	12	3
3	B	360	PX4	C2-C1	2.92	1.60	1.51	10	2
3	B	362	PX4	C6-C7	2.92	1.59	1.50	10	5
3	B	395	PX4	O7-C7	2.92	1.39	1.46	7	2
3	B	398	PX4	O5-C8	2.92	1.51	1.45	8	2
3	C	365	PX4	C2-N1	2.92	1.42	1.51	8	1
3	A	648	PX4	C25-C24	2.92	1.62	1.52	8	3
3	B	331	PX4	O7-C7	2.92	1.39	1.46	3	4
3	B	335	PX4	C24-C23	2.92	1.59	1.50	1	2
3	A	628	PX4	C11-C10	2.92	1.62	1.52	14	3
3	C	338	PX4	C24-C23	2.92	1.59	1.50	14	2
3	B	326	PX4	C6-C7	2.92	1.59	1.50	14	4
3	A	620	PX4	O7-C7	2.91	1.39	1.46	11	2
3	A	632	PX4	C2-C1	2.91	1.60	1.51	9	6
3	C	348	PX4	C18-C17	2.92	1.66	1.51	13	1
3	C	365	PX4	O7-C7	2.92	1.39	1.46	6	3
3	B	320	PX4	O5-C9	2.91	1.41	1.33	9	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	310	PX4	C2-C1	2.91	1.60	1.51	2	5
3	B	330	PX4	C8-C7	2.91	1.59	1.50	1	5
3	B	303	PX4	C25-C24	2.91	1.62	1.52	7	2
3	C	322	PX4	C2-N1	2.91	1.60	1.51	6	3
3	C	333	PX4	C2-C1	2.91	1.60	1.51	4	6
3	A	602	PX4	C25-C24	2.91	1.62	1.52	7	2
3	A	610	PX4	P1-O3	2.91	1.48	1.59	12	1
3	A	643	PX4	C10-C9	2.91	1.59	1.50	5	6
3	B	305	PX4	C2-N1	2.91	1.42	1.51	12	4
3	B	310	PX4	P1-O1	2.91	1.41	1.55	3	6
3	B	313	PX4	C2-N1	2.91	1.60	1.51	9	2
3	B	338	PX4	O7-C7	2.91	1.39	1.46	7	3
3	B	382	PX4	C24-C23	2.91	1.59	1.50	6	2
3	C	341	PX4	O5-C9	2.91	1.41	1.33	9	3
3	A	615	PX4	C4-N1	2.90	1.58	1.50	5	3
3	B	365	PX4	O7-C23	2.90	1.26	1.34	7	3
3	C	315	PX4	C10-C9	2.90	1.59	1.50	4	3
3	C	347	PX4	O7-C23	2.90	1.26	1.34	5	1
3	C	357	PX4	O5-C8	2.90	1.51	1.45	9	1
3	A	637	PX4	O5-C9	2.90	1.41	1.33	12	1
3	B	355	PX4	C10-C9	2.90	1.59	1.50	7	3
3	B	397	PX4	C4-N1	2.90	1.41	1.50	14	2
3	C	305	PX4	P1-O1	2.90	1.41	1.55	8	4
3	A	602	PX4	C10-C9	2.90	1.59	1.50	14	3
3	A	635	PX4	C5-N1	2.90	1.58	1.50	1	2
3	B	341	PX4	C24-C23	2.90	1.59	1.50	8	3
3	C	345	PX4	C10-C9	2.90	1.59	1.50	14	5
3	A	607	PX4	O7-C7	2.89	1.39	1.46	7	6
3	C	306	PX4	C6-C7	2.89	1.59	1.50	14	5
3	A	617	PX4	C3-N1	2.89	1.41	1.50	14	2
3	A	632	PX4	C24-C23	2.89	1.59	1.50	2	5
3	B	339	PX4	O5-C9	2.89	1.41	1.33	12	1
3	A	633	PX4	P1-O4	2.89	1.48	1.59	12	1
3	A	641	PX4	O5-C8	2.89	1.38	1.45	5	2
3	B	364	PX4	C6-C7	2.89	1.59	1.50	15	2
3	B	389	PX4	C8-C7	2.89	1.59	1.50	1	1
3	B	378	PX4	O7-C23	2.89	1.26	1.34	14	2
3	C	368	PX4	O5-C8	2.89	1.38	1.45	1	2
3	A	635	PX4	P1-O1	2.89	1.42	1.55	3	5
3	C	313	PX4	C25-C24	2.89	1.62	1.52	8	1
3	B	347	PX4	C11-C10	2.89	1.62	1.52	9	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	352	PX4	O3-C1	2.89	1.33	1.44	6	1
3	B	396	PX4	O5-C9	2.89	1.25	1.33	4	5
3	C	358	PX4	C10-C9	2.89	1.59	1.50	9	4
3	B	365	PX4	C25-C24	2.89	1.62	1.52	7	1
3	B	400	PX4	O7-C23	2.89	1.42	1.34	5	2
3	C	316	PX4	O5-C9	2.89	1.41	1.33	9	4
3	A	644	PX4	C11-C10	2.89	1.62	1.52	1	1
3	B	309	PX4	O7-C23	2.89	1.26	1.34	11	1
3	B	371	PX4	C10-C9	2.89	1.59	1.50	13	4
3	C	353	PX4	C3-N1	2.89	1.58	1.50	14	1
3	C	324	PX4	C8-C7	2.89	1.59	1.50	2	4
3	C	345	PX4	C5-N1	2.89	1.58	1.50	7	1
3	A	621	PX4	C24-C23	2.88	1.59	1.50	7	3
3	B	324	PX4	C3-N1	2.88	1.41	1.50	11	3
3	A	621	PX4	P1-O1	2.88	1.42	1.55	12	5
3	A	638	PX4	O5-C8	2.88	1.38	1.45	14	2
3	B	385	PX4	C3-N1	2.88	1.41	1.50	1	1
3	B	344	PX4	C10-C9	2.88	1.59	1.50	10	4
3	A	616	PX4	C3-N1	2.88	1.41	1.50	6	1
3	B	364	PX4	C25-C24	2.88	1.62	1.52	2	1
3	C	353	PX4	C10-C9	2.88	1.59	1.50	15	2
3	C	366	PX4	O7-C23	2.88	1.26	1.34	10	2
3	A	648	PX4	C10-C9	2.88	1.59	1.50	5	5
3	C	354	PX4	P1-O1	2.88	1.42	1.55	4	3
3	C	358	PX4	C8-C7	2.88	1.59	1.50	12	6
3	A	601	PX4	C2-N1	2.88	1.42	1.51	15	2
3	A	605	PX4	C10-C9	2.88	1.59	1.50	14	1
3	B	356	PX4	O5-C9	2.88	1.41	1.33	11	3
3	A	609	PX4	C10-C9	2.87	1.59	1.50	12	1
3	A	633	PX4	C6-C7	2.87	1.59	1.50	11	5
3	B	303	PX4	C8-C7	2.87	1.59	1.50	7	7
3	B	307	PX4	C24-C23	2.87	1.59	1.50	11	3
3	B	325	PX4	C2-C1	2.87	1.60	1.51	11	6
3	B	335	PX4	C11-C10	2.87	1.62	1.52	9	3
3	C	315	PX4	O5-C8	2.87	1.38	1.45	6	2
3	A	617	PX4	O7-C7	2.87	1.39	1.46	2	2
3	A	617	PX4	C2-C1	2.87	1.60	1.51	8	4
3	B	372	PX4	C11-C10	2.87	1.62	1.52	9	2
3	B	385	PX4	C10-C9	2.87	1.59	1.50	7	3
3	B	324	PX4	C4-N1	2.87	1.58	1.50	11	3
3	C	310	PX4	C24-C23	2.87	1.59	1.50	2	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	385	PX4	O7-C7	2.87	1.39	1.46	7	4
3	C	333	PX4	C10-C9	2.87	1.59	1.50	6	3
3	A	611	PX4	C2-C1	2.87	1.60	1.51	7	5
3	B	386	PX4	C4-N1	2.87	1.58	1.50	3	1
3	C	340	PX4	O5-C8	2.87	1.38	1.45	15	2
3	A	625	PX4	C19-C18	2.86	1.66	1.51	10	2
3	B	352	PX4	C10-C9	2.86	1.59	1.50	10	4
3	B	395	PX4	C11-C10	2.86	1.62	1.52	15	2
3	C	304	PX4	O7-C7	2.86	1.39	1.46	4	4
3	A	644	PX4	O7-C23	2.86	1.26	1.34	1	3
3	A	642	PX4	C25-C24	2.86	1.62	1.52	1	1
3	B	321	PX4	C4-N1	2.86	1.41	1.50	1	3
3	B	332	PX4	O5-C9	2.86	1.25	1.33	13	3
3	B	400	PX4	C24-C23	2.86	1.59	1.50	12	2
3	C	333	PX4	C24-C23	2.86	1.59	1.50	6	1
3	B	318	PX4	O5-C8	2.86	1.38	1.45	11	1
3	A	622	PX4	C10-C9	2.86	1.42	1.50	12	2
3	B	359	PX4	O5-C9	2.85	1.25	1.33	7	2
3	B	380	PX4	C10-C9	2.85	1.59	1.50	6	3
3	C	368	PX4	C24-C23	2.85	1.59	1.50	14	4
3	B	318	PX4	C6-C7	2.85	1.59	1.50	15	8
3	A	629	PX4	O7-C7	2.85	1.39	1.46	14	1
3	A	640	PX4	C6-C7	2.85	1.59	1.50	9	4
3	B	367	PX4	C11-C10	2.85	1.62	1.52	15	4
3	A	641	PX4	C8-C7	2.85	1.59	1.50	3	6
3	B	385	PX4	C2-C1	2.85	1.59	1.51	3	4
3	B	381	PX4	C11-C10	2.85	1.62	1.52	13	2
3	B	359	PX4	C3-N1	2.85	1.41	1.50	12	2
3	A	610	PX4	C6-C7	2.84	1.59	1.50	7	4
3	C	313	PX4	C24-C23	2.84	1.59	1.50	8	3
3	B	335	PX4	C6-C7	2.84	1.59	1.50	8	6
3	A	616	PX4	C5-N1	2.84	1.41	1.50	10	3
3	B	369	PX4	C25-C24	2.84	1.62	1.52	3	1
3	A	615	PX4	C2-N1	2.84	1.60	1.51	11	1
3	B	339	PX4	C24-C23	2.84	1.58	1.50	12	4
3	B	316	PX4	C24-C23	2.84	1.58	1.50	12	2
3	C	349	PX4	C11-C10	2.84	1.62	1.52	8	4
3	B	339	PX4	C10-C9	2.84	1.58	1.50	12	2
3	B	301	PX4	C2-C1	2.84	1.59	1.51	9	5
3	B	389	PX4	C11-C10	2.84	1.62	1.52	3	2
3	C	330	PX4	O7-C23	2.84	1.26	1.34	10	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	336	PX4	C24-C23	2.84	1.58	1.50	8	3
3	B	329	PX4	C24-C23	2.84	1.58	1.50	11	1
3	B	361	PX4	O5-C8	2.83	1.38	1.45	6	1
3	C	331	PX4	C10-C9	2.83	1.58	1.50	15	2
3	C	303	PX4	C25-C24	2.83	1.62	1.52	4	3
3	B	364	PX4	C4-N1	2.83	1.58	1.50	15	3
3	C	344	PX4	O7-C7	2.83	1.39	1.46	15	4
3	B	380	PX4	O5-C9	2.83	1.41	1.33	1	5
3	C	351	PX4	C2-C1	2.83	1.59	1.51	2	5
3	A	602	PX4	C8-C7	2.83	1.59	1.50	4	2
3	B	378	PX4	C10-C9	2.83	1.58	1.50	6	4
3	C	351	PX4	C24-C23	2.83	1.58	1.50	6	1
3	B	304	PX4	O7-C23	2.83	1.42	1.34	8	2
3	B	359	PX4	P1-O1	2.83	1.42	1.55	9	2
3	C	339	PX4	O5-C9	2.83	1.25	1.33	15	1
3	A	629	PX4	C4-N1	2.82	1.41	1.50	10	3
3	A	645	PX4	C4-N1	2.82	1.58	1.50	9	2
3	B	328	PX4	O7-C23	2.82	1.26	1.34	8	2
3	B	359	PX4	O7-C23	2.82	1.26	1.34	4	3
3	C	355	PX4	C10-C9	2.82	1.58	1.50	7	2
3	C	349	PX4	O7-C7	2.82	1.40	1.46	5	4
3	C	354	PX4	O7-C23	2.82	1.26	1.34	5	5
3	B	301	PX4	O7-C23	2.82	1.42	1.34	1	4
3	B	354	PX4	C24-C23	2.82	1.58	1.50	12	5
3	A	610	PX4	C27-C26	2.82	1.65	1.51	14	1
3	A	631	PX4	C5-N1	2.82	1.58	1.50	2	1
3	A	640	PX4	C11-C10	2.82	1.62	1.52	6	1
3	B	367	PX4	P1-O2	2.82	1.41	1.50	14	1
3	C	328	PX4	C11-C10	2.82	1.62	1.52	4	2
3	C	337	PX4	C3-N1	2.82	1.41	1.50	14	4
3	A	605	PX4	C25-C24	2.82	1.62	1.52	11	3
3	A	622	PX4	C3-N1	2.82	1.58	1.50	9	1
3	A	629	PX4	C31-C30	2.82	1.65	1.51	4	1
3	B	384	PX4	O5-C8	2.82	1.38	1.45	6	1
3	B	384	PX4	C25-C24	2.82	1.62	1.52	12	3
3	C	331	PX4	C11-C10	2.82	1.62	1.52	10	6
3	C	363	PX4	C6-C7	2.82	1.59	1.50	7	3
3	A	606	PX4	C5-N1	2.82	1.58	1.50	4	1
3	B	321	PX4	P1-O4	2.82	1.48	1.59	5	2
3	B	347	PX4	C25-C24	2.82	1.62	1.52	8	3
3	B	351	PX4	C2-C1	2.82	1.59	1.51	14	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	310	PX4	C25-C24	2.82	1.62	1.52	15	1
3	C	361	PX4	O5-C9	2.82	1.41	1.33	6	5
3	A	612	PX4	P1-O1	2.81	1.42	1.55	4	3
3	B	325	PX4	C24-C23	2.81	1.58	1.50	7	2
3	B	328	PX4	C24-C23	2.81	1.58	1.50	10	3
3	B	392	PX4	C3-N1	2.81	1.58	1.50	4	3
3	A	638	PX4	C10-C9	2.81	1.58	1.50	3	1
3	B	313	PX4	C3-N1	2.81	1.58	1.50	11	1
3	C	319	PX4	C3-N1	2.81	1.58	1.50	6	1
3	C	322	PX4	O5-C9	2.81	1.25	1.33	11	1
3	C	369	PX4	O5-C8	2.81	1.51	1.45	12	3
3	B	372	PX4	C6-C7	2.81	1.59	1.50	4	3
3	A	621	PX4	C3-N1	2.81	1.58	1.50	3	4
3	B	333	PX4	C24-C23	2.81	1.58	1.50	1	2
3	C	361	PX4	C4-N1	2.81	1.41	1.50	12	1
3	B	306	PX4	O7-C7	2.81	1.40	1.46	11	5
3	C	351	PX4	C5-N1	2.81	1.58	1.50	3	2
3	B	323	PX4	C5-N1	2.81	1.41	1.50	2	1
3	C	367	PX4	C25-C24	2.81	1.62	1.52	3	2
3	A	631	PX4	O7-C7	2.80	1.40	1.46	14	3
3	C	349	PX4	C3-N1	2.80	1.58	1.50	15	1
3	A	621	PX4	C6-C7	2.80	1.59	1.50	6	4
3	B	320	PX4	P1-O1	2.80	1.42	1.55	14	3
3	B	317	PX4	C11-C10	2.80	1.62	1.52	7	2
3	B	377	PX4	O7-C23	2.80	1.26	1.34	5	2
3	C	314	PX4	O7-C23	2.80	1.26	1.34	13	5
3	C	340	PX4	C8-C7	2.80	1.59	1.50	2	2
3	C	362	PX4	C6-C7	2.80	1.59	1.50	2	4
3	B	385	PX4	C4-N1	2.79	1.41	1.50	6	1
3	C	361	PX4	C11-C10	2.79	1.42	1.52	8	3
3	C	364	PX4	C4-N1	2.79	1.41	1.50	7	1
3	B	395	PX4	O7-C23	2.79	1.26	1.34	6	1
3	B	395	PX4	O5-C9	2.79	1.41	1.33	1	2
3	C	316	PX4	O7-C23	2.79	1.26	1.34	3	2
3	B	351	PX4	C3-N1	2.79	1.58	1.50	9	3
3	C	323	PX4	C25-C24	2.79	1.62	1.52	13	2
3	B	394	PX4	O7-C23	2.79	1.26	1.34	14	1
3	A	611	PX4	O5-C9	2.79	1.41	1.33	1	1
3	B	328	PX4	O7-C7	2.79	1.40	1.46	3	4
3	B	329	PX4	C12-C11	2.79	1.65	1.51	5	1
3	C	326	PX4	O7-C7	2.79	1.40	1.46	8	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	352	PX4	P1-O1	2.79	1.42	1.55	14	4
3	B	357	PX4	O7-C7	2.79	1.40	1.46	10	3
3	B	310	PX4	O7-C7	2.78	1.40	1.46	14	3
3	B	320	PX4	C2-N1	2.78	1.60	1.51	8	1
3	A	622	PX4	C11-C10	2.78	1.62	1.52	13	1
3	B	360	PX4	C24-C23	2.78	1.58	1.50	6	4
3	C	313	PX4	O7-C7	2.78	1.40	1.46	4	4
3	B	302	PX4	C15-C14	2.78	1.65	1.51	6	1
3	B	354	PX4	P1-O2	2.78	1.41	1.50	2	1
3	B	363	PX4	O7-C23	2.78	1.26	1.34	3	3
3	C	324	PX4	O5-C9	2.78	1.25	1.33	6	2
3	C	359	PX4	C2-C1	2.78	1.59	1.51	10	4
3	A	647	PX4	O7-C7	2.78	1.40	1.46	14	3
3	A	628	PX4	C3-N1	2.78	1.58	1.50	7	1
3	B	325	PX4	C10-C9	2.78	1.58	1.50	9	2
3	B	377	PX4	C10-C9	2.78	1.58	1.50	15	5
3	B	388	PX4	C24-C23	2.78	1.58	1.50	10	4
3	C	351	PX4	P1-O1	2.78	1.42	1.55	11	3
3	B	342	PX4	O3-C1	2.78	1.33	1.44	9	1
3	C	361	PX4	C10-C9	2.78	1.58	1.50	3	1
3	C	345	PX4	P1-O1	2.77	1.42	1.55	13	3
3	B	349	PX4	C6-C7	2.77	1.59	1.50	4	7
3	B	378	PX4	O5-C9	2.77	1.25	1.33	4	1
3	B	340	PX4	C24-C23	2.77	1.58	1.50	15	7
3	B	358	PX4	C3-N1	2.77	1.42	1.50	13	2
3	C	338	PX4	O7-C23	2.77	1.26	1.34	6	3
3	C	347	PX4	P1-O1	2.77	1.42	1.55	8	3
3	B	344	PX4	O5-C8	2.77	1.51	1.45	2	4
3	B	396	PX4	C10-C9	2.77	1.58	1.50	5	3
3	C	304	PX4	O7-C23	2.77	1.26	1.34	5	1
3	B	305	PX4	C2-C1	2.77	1.59	1.51	2	2
3	B	348	PX4	P1-O1	2.77	1.42	1.55	14	2
3	C	308	PX4	C2-C1	2.77	1.59	1.51	7	5
3	C	334	PX4	C3-N1	2.77	1.58	1.50	2	3
3	C	334	PX4	O7-C23	2.77	1.26	1.34	2	1
3	C	357	PX4	O7-C23	2.77	1.26	1.34	2	4
3	C	357	PX4	C24-C23	2.77	1.58	1.50	7	4
3	C	364	PX4	O7-C7	2.77	1.40	1.46	8	5
3	C	367	PX4	C10-C9	2.77	1.58	1.50	13	4
3	B	339	PX4	C28-C27	2.77	1.65	1.51	10	1
3	A	612	PX4	C10-C9	2.77	1.58	1.50	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	630	PX4	C2-C1	2.77	1.59	1.51	14	4
3	B	332	PX4	C2-N1	2.77	1.59	1.51	3	2
3	B	343	PX4	C25-C24	2.77	1.62	1.52	3	4
3	B	347	PX4	C6-C7	2.77	1.59	1.50	4	7
3	B	399	PX4	C2-N1	2.77	1.43	1.51	3	3
3	B	354	PX4	C3-N1	2.76	1.58	1.50	12	2
3	B	391	PX4	C24-C23	2.76	1.58	1.50	4	2
3	C	366	PX4	C5-N1	2.76	1.58	1.50	12	2
3	A	648	PX4	O7-C23	2.76	1.26	1.34	6	1
3	B	304	PX4	C8-C7	2.76	1.59	1.50	13	7
3	B	375	PX4	C6-C7	2.76	1.59	1.50	12	4
3	A	618	PX4	O5-C9	2.76	1.41	1.33	3	3
3	B	358	PX4	C25-C24	2.76	1.62	1.52	9	3
3	C	330	PX4	C24-C23	2.76	1.58	1.50	13	4
3	B	306	PX4	C11-C10	2.76	1.62	1.52	11	2
3	B	308	PX4	O7-C23	2.76	1.26	1.34	14	2
3	C	309	PX4	O7-C23	2.76	1.26	1.34	8	1
3	B	384	PX4	P1-O1	2.76	1.42	1.55	14	4
3	C	317	PX4	C5-N1	2.76	1.58	1.50	6	4
3	C	317	PX4	C13-C12	2.76	1.65	1.51	15	1
3	C	340	PX4	C25-C24	2.76	1.62	1.52	1	1
3	C	345	PX4	C4-N1	2.76	1.42	1.50	8	1
3	B	329	PX4	C10-C9	2.76	1.58	1.50	15	5
3	B	354	PX4	C25-C24	2.75	1.62	1.52	8	2
3	A	623	PX4	O5-C9	2.75	1.41	1.33	1	2
3	A	640	PX4	O7-C23	2.75	1.26	1.34	8	4
3	B	301	PX4	C5-N1	2.75	1.42	1.50	6	3
3	B	378	PX4	P1-O3	2.75	1.48	1.59	6	1
3	C	337	PX4	O7-C7	2.75	1.40	1.46	8	2
3	A	617	PX4	P1-O4	2.75	1.48	1.59	6	1
3	A	647	PX4	C24-C23	2.75	1.58	1.50	9	4
3	B	327	PX4	C25-C24	2.75	1.62	1.52	4	1
3	B	330	PX4	C33-C32	2.75	1.65	1.51	14	1
3	B	348	PX4	O7-C7	2.75	1.40	1.46	8	2
3	B	397	PX4	C11-C10	2.75	1.62	1.52	4	1
3	A	606	PX4	C2-N1	2.75	1.59	1.51	11	3
3	A	619	PX4	C4-N1	2.75	1.58	1.50	3	3
3	A	639	PX4	C8-C7	2.75	1.59	1.50	6	4
3	B	342	PX4	C24-C23	2.75	1.58	1.50	6	2
3	B	345	PX4	P1-O1	2.75	1.42	1.55	15	1
3	B	376	PX4	C2-N1	2.75	1.59	1.51	11	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	359	PX4	C17-C16	2.75	1.65	1.51	7	1
3	B	362	PX4	C3-N1	2.75	1.42	1.50	5	1
3	C	328	PX4	O5-C9	2.75	1.25	1.33	4	4
3	B	383	PX4	C25-C24	2.74	1.62	1.52	1	5
3	C	357	PX4	O5-C9	2.74	1.41	1.33	11	1
3	B	334	PX4	O5-C9	2.74	1.25	1.33	2	3
3	B	393	PX4	C11-C10	2.74	1.62	1.52	6	3
3	C	310	PX4	O5-C8	2.74	1.39	1.45	10	2
3	C	324	PX4	O7-C7	2.74	1.40	1.46	3	1
3	A	638	PX4	O7-C7	2.74	1.40	1.46	15	5
3	B	370	PX4	C4-N1	2.74	1.42	1.50	6	2
3	B	375	PX4	P1-O4	2.74	1.48	1.59	6	1
3	B	383	PX4	C3-N1	2.74	1.58	1.50	14	1
3	C	303	PX4	C6-C7	2.74	1.59	1.50	2	5
3	B	314	PX4	O7-C7	2.74	1.40	1.46	1	2
3	B	386	PX4	C2-C1	2.74	1.59	1.51	11	4
3	C	336	PX4	O7-C23	2.74	1.26	1.34	5	4
3	A	614	PX4	O5-C9	2.73	1.41	1.33	13	4
3	B	361	PX4	O7-C23	2.73	1.26	1.34	7	3
3	C	363	PX4	C25-C24	2.74	1.62	1.52	11	2
3	B	350	PX4	C3-N1	2.73	1.57	1.50	9	2
3	B	362	PX4	C2-N1	2.73	1.59	1.51	12	2
3	C	346	PX4	P1-O1	2.73	1.42	1.55	2	4
3	C	352	PX4	P1-O1	2.73	1.42	1.55	3	1
3	B	367	PX4	O7-C23	2.73	1.26	1.34	12	3
3	B	375	PX4	C4-N1	2.73	1.57	1.50	3	3
3	B	384	PX4	C24-C23	2.73	1.58	1.50	3	4
3	A	619	PX4	C24-C23	2.73	1.58	1.50	11	2
3	B	363	PX4	C10-C9	2.73	1.58	1.50	1	3
3	C	312	PX4	C29-C28	2.73	1.65	1.51	4	1
3	C	312	PX4	O5-C9	2.73	1.25	1.33	8	2
3	A	602	PX4	C4-N1	2.73	1.57	1.50	15	2
3	B	316	PX4	O5-C8	2.73	1.51	1.45	1	2
3	B	372	PX4	P1-O1	2.73	1.42	1.55	4	5
3	B	389	PX4	P1-O1	2.73	1.42	1.55	2	3
3	A	631	PX4	O5-C9	2.72	1.41	1.33	7	1
3	C	347	PX4	O7-C7	2.72	1.40	1.46	10	4
3	B	342	PX4	O5-C9	2.72	1.41	1.33	8	1
3	A	646	PX4	O5-C8	2.72	1.39	1.45	2	1
3	B	374	PX4	C2-C1	2.72	1.59	1.51	8	4
3	C	301	PX4	O7-C7	2.72	1.40	1.46	14	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	626	PX4	P1-O1	2.72	1.42	1.55	7	5
3	B	358	PX4	O5-C8	2.72	1.51	1.45	13	3
3	B	305	PX4	C4-N1	2.72	1.42	1.50	2	1
3	B	358	PX4	C11-C10	2.72	1.62	1.52	9	5
3	A	619	PX4	O7-C23	2.72	1.41	1.34	15	4
3	C	315	PX4	C6-C7	2.72	1.59	1.50	10	4
3	B	305	PX4	O5-C9	2.71	1.25	1.33	15	4
3	B	317	PX4	C3-N1	2.71	1.57	1.50	9	3
3	B	309	PX4	C3-N1	2.71	1.57	1.50	7	2
3	B	325	PX4	C25-C24	2.71	1.62	1.52	11	3
3	C	333	PX4	C16-C15	2.71	1.65	1.51	10	1
3	C	347	PX4	C13-C12	2.71	1.65	1.51	13	1
3	B	375	PX4	C25-C24	2.71	1.62	1.52	13	1
3	B	391	PX4	C2-N1	2.71	1.43	1.51	8	2
3	C	350	PX4	C11-C10	2.71	1.62	1.52	12	2
3	A	634	PX4	C30-C29	2.71	1.65	1.51	9	1
3	B	309	PX4	C4-N1	2.71	1.57	1.50	3	1
3	B	395	PX4	O5-C8	2.71	1.51	1.45	11	2
3	A	637	PX4	C6-C7	2.71	1.59	1.50	7	4
3	B	342	PX4	C5-N1	2.71	1.42	1.50	10	2
3	C	329	PX4	C4-N1	2.71	1.57	1.50	3	1
3	B	318	PX4	C4-N1	2.71	1.57	1.50	3	2
3	B	379	PX4	O5-C9	2.71	1.41	1.33	2	3
3	C	313	PX4	C4-N1	2.71	1.57	1.50	12	1
3	A	636	PX4	O5-C8	2.71	1.39	1.45	15	3
3	A	642	PX4	C10-C9	2.71	1.58	1.50	4	5
3	B	315	PX4	C2-N1	2.71	1.59	1.51	11	2
3	B	319	PX4	C8-C7	2.70	1.59	1.50	4	7
3	B	377	PX4	O7-C7	2.70	1.40	1.46	15	1
3	B	320	PX4	P1-O4	2.70	1.48	1.59	10	1
3	B	347	PX4	C4-N1	2.70	1.42	1.50	3	2
3	C	338	PX4	C20-C19	2.70	1.65	1.51	11	1
3	A	603	PX4	C10-C9	2.70	1.58	1.50	6	2
3	B	308	PX4	C2-C1	2.70	1.59	1.51	8	4
3	B	321	PX4	C11-C10	2.70	1.62	1.52	14	1
3	A	626	PX4	C24-C23	2.70	1.58	1.50	15	4
3	A	626	PX4	O7-C23	2.70	1.26	1.34	7	3
3	B	353	PX4	C25-C24	2.70	1.62	1.52	5	1
3	C	320	PX4	C33-C32	2.70	1.65	1.51	3	2
3	C	335	PX4	C6-C7	2.70	1.59	1.50	6	4
3	C	347	PX4	C8-C7	2.70	1.59	1.50	10	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	365	PX4	O5-C9	2.70	1.25	1.33	2	3
3	C	306	PX4	C10-C9	2.70	1.58	1.50	8	3
3	C	309	PX4	C24-C23	2.70	1.58	1.50	6	2
3	C	357	PX4	P1-O4	2.70	1.70	1.59	14	1
3	B	321	PX4	P1-O2	2.70	1.41	1.50	3	1
3	B	334	PX4	C4-N1	2.69	1.57	1.50	13	1
3	B	342	PX4	C2-C1	2.69	1.59	1.51	10	5
3	B	344	PX4	C4-N1	2.70	1.42	1.50	11	2
3	B	388	PX4	C10-C9	2.70	1.58	1.50	1	2
3	C	302	PX4	O7-C23	2.70	1.26	1.34	7	3
3	C	326	PX4	O7-C23	2.69	1.26	1.34	10	1
3	A	602	PX4	C2-N1	2.69	1.43	1.51	13	2
3	A	636	PX4	C11-C10	2.69	1.62	1.52	1	2
3	C	343	PX4	C6-C7	2.69	1.59	1.50	9	9
3	A	612	PX4	O7-C7	2.69	1.40	1.46	12	3
3	A	635	PX4	C2-N1	2.69	1.59	1.51	14	2
3	B	307	PX4	O5-C8	2.69	1.39	1.45	7	5
3	A	620	PX4	O7-C23	2.69	1.26	1.34	3	1
3	B	336	PX4	C11-C10	2.69	1.62	1.52	9	1
3	C	325	PX4	P1-O1	2.69	1.42	1.55	11	4
3	A	628	PX4	C2-C1	2.69	1.59	1.51	10	2
3	B	308	PX4	O7-C7	2.69	1.40	1.46	9	2
3	B	376	PX4	C4-N1	2.69	1.42	1.50	1	1
3	B	321	PX4	C10-C9	2.69	1.58	1.50	5	3
3	B	326	PX4	O7-C7	2.69	1.40	1.46	2	4
3	B	366	PX4	C2-C1	2.69	1.59	1.51	13	3
3	B	370	PX4	C11-C10	2.69	1.62	1.52	11	1
3	B	372	PX4	C25-C24	2.69	1.62	1.52	5	1
3	C	311	PX4	O3-C1	2.69	1.34	1.44	6	1
3	B	375	PX4	C10-C9	2.69	1.58	1.50	9	1
3	B	382	PX4	O7-C7	2.69	1.40	1.46	9	2
3	A	628	PX4	O5-C8	2.68	1.39	1.45	12	1
3	B	327	PX4	P1-O1	2.68	1.42	1.55	2	2
3	B	337	PX4	C10-C9	2.68	1.58	1.50	13	3
3	B	391	PX4	C30-C29	2.68	1.65	1.51	1	1
3	B	392	PX4	C11-C10	2.68	1.62	1.52	12	1
3	C	324	PX4	P1-O1	2.68	1.42	1.55	5	3
3	C	334	PX4	P1-O1	2.68	1.42	1.55	5	4
3	C	336	PX4	C6-C7	2.68	1.59	1.50	15	6
3	C	354	PX4	C12-C11	2.68	1.65	1.51	3	1
3	B	311	PX4	C29-C28	2.68	1.65	1.51	15	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	345	PX4	C5-N1	2.68	1.57	1.50	2	1
3	B	385	PX4	P1-O1	2.68	1.42	1.55	15	5
3	B	364	PX4	C11-C10	2.68	1.62	1.52	1	2
3	B	373	PX4	C27-C26	2.68	1.65	1.51	4	2
3	A	604	PX4	C11-C10	2.68	1.62	1.52	3	2
3	A	644	PX4	C25-C24	2.68	1.62	1.52	1	3
3	B	313	PX4	C4-N1	2.68	1.57	1.50	3	2
3	A	601	PX4	C11-C10	2.67	1.62	1.52	9	2
3	B	326	PX4	C10-C9	2.67	1.58	1.50	5	2
3	B	328	PX4	O5-C9	2.67	1.25	1.33	11	2
3	A	621	PX4	O3-C1	2.67	1.34	1.44	10	1
3	B	373	PX4	C2-N1	2.67	1.59	1.51	1	2
3	C	312	PX4	C11-C10	2.67	1.62	1.52	11	3
3	A	602	PX4	O5-C9	2.67	1.25	1.33	9	1
3	A	638	PX4	C24-C23	2.67	1.58	1.50	2	3
3	B	316	PX4	C4-N1	2.67	1.57	1.50	4	1
3	B	392	PX4	C25-C24	2.67	1.62	1.52	5	2
3	C	361	PX4	C3-N1	2.67	1.57	1.50	2	2
3	C	322	PX4	C19-C18	2.67	1.65	1.51	9	1
3	C	360	PX4	O7-C7	2.67	1.40	1.46	8	1
3	C	335	PX4	P1-O3	2.67	1.48	1.59	12	1
3	B	381	PX4	O5-C8	2.67	1.51	1.45	10	2
3	C	319	PX4	O7-C7	2.67	1.40	1.46	6	3
3	A	615	PX4	C10-C9	2.67	1.58	1.50	12	4
3	C	331	PX4	O5-C8	2.67	1.39	1.45	3	2
3	C	321	PX4	C5-N1	2.66	1.57	1.50	4	2
3	C	327	PX4	C24-C23	2.67	1.58	1.50	7	2
3	C	362	PX4	C25-C24	2.67	1.62	1.52	14	2
3	C	368	PX4	O7-C23	2.67	1.26	1.34	1	3
3	B	381	PX4	C10-C9	2.66	1.58	1.50	8	2
3	C	326	PX4	C25-C24	2.66	1.61	1.52	1	2
3	A	604	PX4	O5-C8	2.66	1.51	1.45	14	2
3	A	633	PX4	O5-C8	2.66	1.51	1.45	5	2
3	A	638	PX4	C28-C27	2.66	1.65	1.51	1	1
3	B	319	PX4	C11-C10	2.66	1.61	1.52	8	3
3	B	326	PX4	C5-N1	2.66	1.57	1.50	9	1
3	B	330	PX4	C5-N1	2.66	1.42	1.50	4	1
3	B	378	PX4	C29-C28	2.66	1.65	1.51	7	2
3	C	330	PX4	C18-C17	2.66	1.65	1.51	15	2
3	C	335	PX4	C24-C23	2.66	1.58	1.50	7	1
3	B	397	PX4	O5-C8	2.66	1.39	1.45	5	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	343	PX4	C11-C10	2.66	1.61	1.52	3	2
3	A	625	PX4	C24-C23	2.66	1.58	1.50	10	2
3	B	354	PX4	C10-C9	2.66	1.58	1.50	4	5
3	C	346	PX4	C11-C10	2.66	1.61	1.52	13	3
3	C	361	PX4	C12-C11	2.66	1.65	1.51	3	1
3	B	304	PX4	C25-C24	2.66	1.61	1.52	8	3
3	A	602	PX4	C11-C10	2.66	1.61	1.52	13	1
3	B	302	PX4	C10-C9	2.66	1.58	1.50	6	4
3	B	357	PX4	C6-C7	2.66	1.59	1.50	2	5
3	B	393	PX4	C24-C23	2.66	1.58	1.50	12	6
3	B	358	PX4	P1-O1	2.66	1.43	1.55	3	1
3	B	363	PX4	O5-C8	2.66	1.51	1.45	6	2
3	C	315	PX4	C25-C24	2.66	1.61	1.52	1	1
3	C	323	PX4	O7-C23	2.66	1.26	1.34	12	1
3	A	629	PX4	C10-C9	2.65	1.58	1.50	2	4
3	B	322	PX4	C25-C24	2.65	1.61	1.52	15	2
3	B	337	PX4	P1-O1	2.65	1.43	1.55	7	3
3	A	607	PX4	O5-C8	2.65	1.51	1.45	8	1
3	A	639	PX4	P1-O3	2.65	1.49	1.59	15	4
3	C	301	PX4	C29-C28	2.65	1.65	1.51	12	1
3	A	619	PX4	C11-C10	2.65	1.61	1.52	10	1
3	A	629	PX4	C2-N1	2.65	1.59	1.51	4	2
3	A	641	PX4	C24-C23	2.65	1.58	1.50	2	2
3	B	387	PX4	C5-N1	2.65	1.42	1.50	4	1
3	C	334	PX4	C24-C23	2.65	1.58	1.50	11	4
3	A	632	PX4	C11-C10	2.65	1.61	1.52	10	2
3	B	324	PX4	C12-C11	2.65	1.65	1.51	13	1
3	B	346	PX4	C8-C7	2.65	1.59	1.50	6	3
3	B	310	PX4	C3-N1	2.65	1.57	1.50	7	1
3	B	314	PX4	C28-C27	2.65	1.65	1.51	5	1
3	B	328	PX4	O5-C8	2.65	1.51	1.45	4	1
3	B	338	PX4	C6-C7	2.65	1.59	1.50	15	4
3	B	311	PX4	P1-O2	2.65	1.41	1.50	6	2
3	B	347	PX4	C8-C7	2.65	1.59	1.50	12	5
3	B	400	PX4	O5-C9	2.65	1.41	1.33	11	1
3	A	629	PX4	C11-C10	2.65	1.61	1.52	9	1
3	B	350	PX4	C25-C24	2.65	1.61	1.52	3	3
3	B	352	PX4	C25-C24	2.65	1.61	1.52	15	2
3	B	355	PX4	C25-C24	2.65	1.61	1.52	2	1
3	C	360	PX4	C4-N1	2.65	1.57	1.50	1	1
3	B	331	PX4	C3-N1	2.64	1.57	1.50	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	631	PX4	C20-C19	2.64	1.64	1.51	8	1
3	B	342	PX4	C27-C26	2.64	1.64	1.51	1	1
3	B	345	PX4	O7-C23	2.64	1.26	1.34	15	3
3	B	373	PX4	C11-C10	2.64	1.61	1.52	8	2
3	B	388	PX4	C2-C1	2.64	1.59	1.51	14	3
3	C	366	PX4	C24-C23	2.64	1.58	1.50	14	2
3	B	314	PX4	O5-C9	2.64	1.41	1.33	8	2
3	B	400	PX4	C2-N1	2.64	1.59	1.51	2	2
3	A	624	PX4	P1-O1	2.64	1.43	1.55	5	4
3	A	645	PX4	O5-C8	2.64	1.39	1.45	10	2
3	B	320	PX4	O5-C8	2.64	1.39	1.45	12	3
3	C	338	PX4	C11-C10	2.64	1.61	1.52	11	3
3	C	327	PX4	C10-C9	2.64	1.58	1.50	8	3
3	C	344	PX4	O5-C8	2.64	1.51	1.45	5	1
3	A	626	PX4	C6-C7	2.64	1.59	1.50	1	3
3	B	336	PX4	P1-O1	2.64	1.43	1.55	13	8
3	C	344	PX4	C25-C24	2.64	1.61	1.52	7	3
3	A	603	PX4	C25-C24	2.64	1.61	1.52	12	2
3	B	303	PX4	C5-N1	2.64	1.57	1.50	9	1
3	B	389	PX4	C3-N1	2.64	1.42	1.50	14	2
3	C	369	PX4	C2-C1	2.64	1.59	1.51	5	8
3	B	301	PX4	O5-C8	2.63	1.51	1.45	7	2
3	B	339	PX4	P1-O1	2.63	1.43	1.55	13	5
3	A	626	PX4	C5-N1	2.63	1.57	1.50	10	1
3	A	632	PX4	C4-N1	2.63	1.42	1.50	10	1
3	C	305	PX4	C4-N1	2.63	1.57	1.50	11	1
3	C	360	PX4	C24-C23	2.63	1.58	1.50	15	2
3	A	646	PX4	C25-C24	2.63	1.61	1.52	3	3
3	C	334	PX4	C2-N1	2.63	1.59	1.51	8	1
3	B	309	PX4	C20-C19	2.63	1.64	1.51	2	1
3	A	642	PX4	O3-C1	2.63	1.34	1.44	14	1
3	C	320	PX4	O3-C1	2.63	1.34	1.44	6	1
3	C	339	PX4	C10-C9	2.63	1.58	1.50	4	5
3	C	347	PX4	C2-C1	2.63	1.59	1.51	10	6
3	B	305	PX4	C27-C26	2.63	1.64	1.51	4	1
3	C	344	PX4	C24-C23	2.63	1.58	1.50	3	4
3	C	345	PX4	O7-C23	2.63	1.41	1.34	2	2
3	C	348	PX4	O7-C7	2.63	1.40	1.46	6	3
3	B	390	PX4	P1-O1	2.63	1.43	1.55	12	4
3	A	601	PX4	C25-C24	2.62	1.61	1.52	14	1
3	B	400	PX4	P1-O3	2.62	1.49	1.59	12	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	353	PX4	C14-C13	2.62	1.64	1.51	9	1
3	A	646	PX4	P1-O1	2.62	1.43	1.55	7	5
3	B	393	PX4	P1-O1	2.62	1.43	1.55	13	7
3	A	647	PX4	P1-O4	2.62	1.49	1.59	6	1
3	B	307	PX4	O7-C23	2.62	1.26	1.34	1	3
3	B	307	PX4	P1-O1	2.62	1.43	1.55	2	3
3	C	318	PX4	C11-C10	2.62	1.61	1.52	10	1
3	C	353	PX4	C11-C10	2.62	1.61	1.52	7	2
3	B	392	PX4	C4-N1	2.62	1.57	1.50	1	1
3	A	613	PX4	C25-C24	2.62	1.61	1.52	10	2
3	B	375	PX4	P1-O2	2.62	1.41	1.50	12	1
3	B	367	PX4	O5-C9	2.61	1.41	1.33	14	2
3	B	348	PX4	O7-C23	2.61	1.41	1.34	5	2
3	A	610	PX4	C15-C14	2.61	1.64	1.51	7	1
3	C	321	PX4	P1-O1	2.61	1.43	1.55	6	3
3	C	316	PX4	P1-O4	2.61	1.49	1.59	10	1
3	C	328	PX4	C6-C7	2.61	1.59	1.50	3	3
3	B	310	PX4	C11-C10	2.61	1.61	1.52	3	1
3	B	316	PX4	C3-N1	2.61	1.57	1.50	9	2
3	C	311	PX4	O4-C6	2.61	1.34	1.44	1	1
3	C	342	PX4	C18-C17	2.61	1.64	1.51	11	1
3	A	639	PX4	C10-C9	2.61	1.58	1.50	11	3
3	B	344	PX4	C25-C24	2.61	1.61	1.52	7	1
3	C	317	PX4	C25-C24	2.61	1.61	1.52	14	3
3	B	383	PX4	O5-C9	2.61	1.41	1.33	3	2
3	C	356	PX4	C24-C23	2.61	1.58	1.50	8	2
3	A	602	PX4	P1-O1	2.61	1.43	1.55	8	4
3	A	609	PX4	C2-N1	2.61	1.59	1.51	5	1
3	A	620	PX4	C11-C10	2.61	1.61	1.52	11	4
3	A	623	PX4	O3-C1	2.61	1.34	1.44	4	1
3	A	627	PX4	C4-N1	2.61	1.57	1.50	6	1
3	A	627	PX4	C15-C14	2.61	1.38	1.51	7	2
3	A	633	PX4	C5-N1	2.61	1.42	1.50	13	2
3	C	334	PX4	O5-C8	2.61	1.51	1.45	5	1
3	C	350	PX4	O7-C23	2.61	1.26	1.34	5	3
3	B	325	PX4	O7-C7	2.60	1.40	1.46	14	1
3	B	326	PX4	C29-C28	2.60	1.64	1.51	3	2
3	B	341	PX4	C28-C27	2.60	1.64	1.51	8	1
3	B	371	PX4	C3-N1	2.60	1.42	1.50	13	2
3	C	345	PX4	O5-C8	2.60	1.51	1.45	3	2
3	C	311	PX4	O5-C9	2.60	1.40	1.33	6	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	627	PX4	C10-C9	2.60	1.58	1.50	11	1
3	C	306	PX4	C4-N1	2.60	1.42	1.50	14	2
3	C	347	PX4	O5-C8	2.60	1.51	1.45	9	3
3	C	348	PX4	C2-N1	2.60	1.59	1.51	2	2
3	C	356	PX4	C11-C10	2.60	1.61	1.52	9	3
3	C	303	PX4	C3-N1	2.60	1.57	1.50	14	4
3	C	303	PX4	C28-C27	2.60	1.64	1.51	14	1
3	B	386	PX4	O7-C7	2.60	1.40	1.46	15	2
3	C	306	PX4	C3-N1	2.60	1.42	1.50	4	1
3	A	624	PX4	C10-C9	2.60	1.58	1.50	2	3
3	A	647	PX4	C20-C19	2.60	1.64	1.51	1	2
3	B	383	PX4	C6-C7	2.60	1.58	1.50	6	3
3	B	390	PX4	C25-C24	2.60	1.61	1.52	15	3
3	C	339	PX4	C24-C23	2.60	1.58	1.50	12	3
3	C	367	PX4	C2-N1	2.60	1.59	1.51	3	1
3	B	325	PX4	O7-C23	2.59	1.26	1.34	14	3
3	B	330	PX4	C25-C24	2.59	1.61	1.52	12	3
3	B	335	PX4	O7-C7	2.59	1.40	1.46	13	4
3	A	617	PX4	O5-C9	2.59	1.25	1.33	4	2
3	A	632	PX4	P1-O1	2.59	1.43	1.55	5	3
3	A	608	PX4	O4-C6	2.59	1.34	1.44	11	1
3	B	391	PX4	P1-O3	2.59	1.49	1.59	15	1
3	C	326	PX4	C10-C9	2.59	1.58	1.50	11	1
3	A	628	PX4	P1-O1	2.59	1.43	1.55	8	3
3	A	640	PX4	C3-N1	2.59	1.57	1.50	5	1
3	B	310	PX4	C25-C24	2.59	1.61	1.52	11	1
3	B	358	PX4	C24-C23	2.59	1.58	1.50	6	3
3	C	364	PX4	C5-N1	2.59	1.42	1.50	1	1
3	B	386	PX4	C16-C15	2.59	1.64	1.51	13	1
3	A	632	PX4	P1-O2	2.59	1.41	1.50	1	1
3	A	639	PX4	O5-C9	2.59	1.40	1.33	11	1
3	B	330	PX4	C24-C23	2.59	1.58	1.50	10	2
3	B	377	PX4	C3-N1	2.59	1.57	1.50	9	1
3	B	387	PX4	C3-N1	2.59	1.42	1.50	12	1
3	C	333	PX4	C28-C27	2.59	1.64	1.51	5	1
3	B	332	PX4	C26-C25	2.59	1.64	1.51	12	1
3	B	356	PX4	C2-N1	2.59	1.59	1.51	7	1
3	C	349	PX4	C30-C29	2.59	1.64	1.51	4	2
3	C	340	PX4	C11-C10	2.58	1.61	1.52	4	2
3	C	347	PX4	C29-C28	2.58	1.64	1.51	9	1
3	A	645	PX4	C5-N1	2.58	1.42	1.50	13	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	345	PX4	C25-C24	2.58	1.61	1.52	11	3
3	C	348	PX4	P1-O1	2.58	1.43	1.55	4	2
3	A	637	PX4	C3-N1	2.58	1.57	1.50	9	3
3	A	648	PX4	C24-C23	2.58	1.58	1.50	1	3
3	B	341	PX4	C16-C15	2.58	1.64	1.51	2	1
3	C	311	PX4	C4-N1	2.58	1.42	1.50	15	5
3	B	384	PX4	C2-N1	2.58	1.59	1.51	13	1
3	C	310	PX4	C5-N1	2.58	1.57	1.50	12	1
3	A	623	PX4	O7-C23	2.58	1.27	1.34	8	4
3	A	646	PX4	C20-C19	2.58	1.64	1.51	9	2
3	B	311	PX4	C25-C24	2.57	1.61	1.52	12	1
3	B	335	PX4	O7-C23	2.57	1.27	1.34	11	4
3	C	360	PX4	C31-C30	2.58	1.64	1.51	7	1
3	B	339	PX4	C11-C10	2.57	1.61	1.52	5	1
3	B	362	PX4	C24-C23	2.57	1.58	1.50	2	3
3	C	307	PX4	C24-C23	2.57	1.58	1.50	3	1
3	A	636	PX4	O7-C7	2.57	1.40	1.46	10	1
3	B	374	PX4	O5-C9	2.57	1.40	1.33	5	2
3	B	384	PX4	C26-C25	2.57	1.64	1.51	15	1
3	C	323	PX4	C5-N1	2.57	1.57	1.50	11	2
3	C	326	PX4	O5-C8	2.57	1.50	1.45	12	4
3	C	331	PX4	O7-C23	2.57	1.27	1.34	15	1
3	C	363	PX4	C10-C9	2.57	1.58	1.50	4	3
3	C	368	PX4	C4-N1	2.57	1.42	1.50	7	2
3	B	373	PX4	O5-C9	2.57	1.40	1.33	14	2
3	B	392	PX4	C8-C7	2.57	1.58	1.50	14	3
3	C	303	PX4	C33-C32	2.57	1.64	1.51	7	1
3	B	340	PX4	C25-C24	2.57	1.61	1.52	10	2
3	B	350	PX4	P1-O4	2.57	1.49	1.59	1	1
3	C	320	PX4	C11-C10	2.57	1.61	1.52	14	1
3	B	314	PX4	C33-C32	2.57	1.64	1.51	2	1
3	C	349	PX4	P1-O1	2.57	1.43	1.55	7	2
3	A	634	PX4	C2-N1	2.57	1.59	1.51	10	1
3	B	335	PX4	P1-O2	2.57	1.41	1.50	10	2
3	C	353	PX4	C6-C7	2.57	1.58	1.50	5	3
3	A	631	PX4	P1-O1	2.56	1.43	1.55	8	4
3	C	303	PX4	O7-C7	2.56	1.40	1.46	1	7
3	C	367	PX4	C33-C32	2.56	1.64	1.51	15	1
3	A	604	PX4	O7-C7	2.56	1.40	1.46	4	2
3	B	343	PX4	C5-N1	2.56	1.42	1.50	9	1
3	A	644	PX4	C18-C17	2.56	1.64	1.51	13	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	318	PX4	C10-C9	2.56	1.58	1.50	2	2
3	C	348	PX4	C10-C9	2.56	1.58	1.50	4	1
3	B	387	PX4	P1-O1	2.56	1.43	1.55	1	4
3	C	368	PX4	C19-C18	2.56	1.64	1.51	11	1
3	B	309	PX4	C11-C10	2.56	1.61	1.52	7	1
3	A	603	PX4	P1-O1	2.56	1.43	1.55	7	4
3	A	610	PX4	C11-C10	2.56	1.61	1.52	10	3
3	A	634	PX4	O5-C8	2.56	1.39	1.45	15	2
3	B	314	PX4	P1-O2	2.56	1.41	1.50	7	1
3	B	370	PX4	C24-C23	2.56	1.58	1.50	7	4
3	C	332	PX4	C2-N1	2.56	1.59	1.51	15	1
3	C	305	PX4	C25-C24	2.56	1.61	1.52	9	3
3	C	311	PX4	C10-C9	2.56	1.58	1.50	7	2
3	C	360	PX4	C10-C9	2.56	1.58	1.50	6	2
3	B	306	PX4	C4-N1	2.56	1.57	1.50	8	1
3	B	358	PX4	C2-N1	2.56	1.59	1.51	11	2
3	C	326	PX4	C24-C23	2.56	1.58	1.50	1	1
3	A	609	PX4	O5-C8	2.56	1.50	1.45	14	5
3	A	648	PX4	C11-C10	2.56	1.61	1.52	8	3
3	C	359	PX4	O3-C1	2.56	1.34	1.44	14	1
3	A	626	PX4	O5-C8	2.55	1.39	1.45	14	1
3	B	303	PX4	C11-C10	2.55	1.61	1.52	14	1
3	B	337	PX4	C11-C10	2.55	1.61	1.52	6	2
3	B	389	PX4	C25-C24	2.55	1.61	1.52	12	1
3	C	330	PX4	P1-O1	2.55	1.43	1.55	4	2
3	A	605	PX4	P1-O1	2.55	1.43	1.55	9	3
3	A	631	PX4	C2-N1	2.55	1.43	1.51	2	1
3	B	356	PX4	O7-C23	2.55	1.27	1.34	3	2
3	A	613	PX4	C10-C9	2.55	1.58	1.50	7	1
3	A	636	PX4	P1-O1	2.55	1.43	1.55	1	5
3	C	351	PX4	C27-C26	2.55	1.64	1.51	4	1
3	C	367	PX4	O7-C23	2.55	1.27	1.34	5	1
3	B	319	PX4	O5-C8	2.55	1.50	1.45	9	3
3	B	378	PX4	C24-C23	2.55	1.58	1.50	9	1
3	B	339	PX4	O7-C23	2.55	1.27	1.34	2	2
3	B	367	PX4	O5-C8	2.55	1.39	1.45	5	1
3	B	374	PX4	O7-C7	2.55	1.40	1.46	10	1
3	C	354	PX4	O5-C9	2.55	1.40	1.33	1	1
3	A	602	PX4	C3-N1	2.55	1.57	1.50	11	2
3	B	342	PX4	O7-C23	2.55	1.27	1.34	2	3
3	B	362	PX4	C10-C9	2.55	1.43	1.50	15	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	366	PX4	P1-O1	2.55	1.43	1.55	13	4
3	A	621	PX4	C5-N1	2.55	1.42	1.50	9	1
3	A	625	PX4	C11-C10	2.55	1.61	1.52	15	2
3	B	307	PX4	C25-C24	2.55	1.61	1.52	13	3
3	B	378	PX4	P1-O1	2.54	1.43	1.55	15	4
3	B	390	PX4	C2-N1	2.54	1.59	1.51	15	3
3	C	332	PX4	C25-C24	2.54	1.61	1.52	5	3
3	C	354	PX4	C25-C24	2.55	1.61	1.52	1	2
3	B	375	PX4	P1-O1	2.54	1.43	1.55	4	2
3	B	395	PX4	C25-C24	2.54	1.61	1.52	7	1
3	C	304	PX4	C25-C24	2.54	1.61	1.52	10	2
3	C	311	PX4	P1-O1	2.54	1.43	1.55	5	3
3	C	340	PX4	O5-C9	2.54	1.40	1.33	11	1
3	B	318	PX4	C5-N1	2.54	1.42	1.50	3	1
3	B	352	PX4	C24-C23	2.54	1.58	1.50	1	2
3	B	317	PX4	C4-N1	2.54	1.57	1.50	5	2
3	C	315	PX4	P1-O1	2.54	1.43	1.55	13	6
3	C	336	PX4	C31-C30	2.54	1.64	1.51	14	1
3	A	606	PX4	O4-C6	2.54	1.35	1.44	15	1
3	B	382	PX4	P1-O1	2.54	1.43	1.55	15	2
3	C	328	PX4	O5-C8	2.54	1.39	1.45	9	3
3	A	603	PX4	C11-C10	2.54	1.61	1.52	1	3
3	B	384	PX4	P1-O2	2.54	1.42	1.50	9	1
3	C	311	PX4	C6-C7	2.54	1.58	1.50	11	6
3	C	341	PX4	P1-O1	2.54	1.43	1.55	4	5
3	B	301	PX4	C11-C10	2.54	1.61	1.52	15	2
3	B	322	PX4	C5-N1	2.54	1.57	1.50	11	1
3	B	314	PX4	C25-C24	2.54	1.61	1.52	3	6
3	A	644	PX4	P1-O1	2.53	1.43	1.55	13	3
3	B	353	PX4	O7-C7	2.53	1.40	1.46	7	1
3	B	375	PX4	O3-C1	2.53	1.34	1.44	5	1
3	C	334	PX4	O7-C7	2.54	1.40	1.46	9	2
3	C	356	PX4	C10-C9	2.53	1.58	1.50	9	1
3	C	365	PX4	O5-C9	2.53	1.40	1.33	11	4
3	A	605	PX4	C4-N1	2.53	1.42	1.50	6	2
3	B	326	PX4	O5-C8	2.53	1.50	1.45	7	1
3	B	383	PX4	C2-N1	2.53	1.59	1.51	12	2
3	A	618	PX4	C2-C1	2.53	1.59	1.51	11	1
3	B	361	PX4	C2-N1	2.53	1.43	1.51	2	1
3	B	363	PX4	C5-N1	2.53	1.57	1.50	5	2
3	B	388	PX4	C3-N1	2.53	1.57	1.50	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	372	PX4	C2-C1	2.53	1.59	1.51	15	3
3	B	391	PX4	O5-C8	2.53	1.39	1.45	15	2
3	C	346	PX4	C24-C23	2.53	1.58	1.50	15	2
3	A	623	PX4	C24-C23	2.53	1.43	1.50	8	1
3	B	314	PX4	P1-O1	2.53	1.43	1.55	10	5
3	B	329	PX4	C15-C14	2.53	1.64	1.51	6	1
3	C	342	PX4	C2-N1	2.53	1.59	1.51	10	1
3	B	329	PX4	P1-O1	2.53	1.43	1.55	12	3
3	B	349	PX4	C3-N1	2.52	1.42	1.50	11	1
3	B	382	PX4	C10-C9	2.52	1.58	1.50	10	2
3	C	314	PX4	C25-C24	2.52	1.61	1.52	3	1
3	A	612	PX4	O5-C8	2.52	1.50	1.45	2	1
3	A	613	PX4	C2-N1	2.52	1.59	1.51	13	1
3	C	317	PX4	P1-O1	2.52	1.43	1.55	1	3
3	A	646	PX4	O7-C23	2.52	1.27	1.34	7	1
3	B	339	PX4	O5-C8	2.52	1.39	1.45	11	1
3	B	382	PX4	C5-N1	2.52	1.57	1.50	15	1
3	B	398	PX4	P1-O4	2.52	1.49	1.59	5	2
3	C	312	PX4	C25-C24	2.52	1.61	1.52	15	1
3	C	354	PX4	C3-N1	2.52	1.57	1.50	4	2
3	C	369	PX4	O5-C9	2.52	1.26	1.33	15	3
3	B	330	PX4	C11-C10	2.52	1.61	1.52	2	2
3	C	336	PX4	O5-C8	2.52	1.50	1.45	10	2
3	C	311	PX4	O7-C23	2.52	1.27	1.34	11	2
3	A	610	PX4	C18-C17	2.52	1.64	1.51	7	1
3	C	319	PX4	O7-C23	2.52	1.27	1.34	1	3
3	C	338	PX4	C2-N1	2.52	1.59	1.51	9	4
3	C	368	PX4	O5-C9	2.52	1.40	1.33	5	1
3	B	316	PX4	C11-C10	2.52	1.61	1.52	2	1
3	A	619	PX4	C2-N1	2.51	1.59	1.51	7	4
3	B	341	PX4	P1-O1	2.51	1.43	1.55	11	4
3	B	342	PX4	C11-C10	2.51	1.61	1.52	4	2
3	B	360	PX4	C11-C10	2.51	1.61	1.52	8	1
3	B	385	PX4	C24-C23	2.51	1.58	1.50	1	2
3	C	359	PX4	C31-C30	2.51	1.64	1.51	7	1
3	A	625	PX4	O5-C9	2.51	1.40	1.33	10	3
3	B	327	PX4	P1-O4	2.51	1.49	1.59	10	1
3	C	364	PX4	C6-C7	2.51	1.58	1.50	15	3
3	A	646	PX4	P1-O4	2.51	1.49	1.59	12	1
3	B	348	PX4	C10-C9	2.51	1.58	1.50	8	3
3	C	310	PX4	C2-C1	2.51	1.58	1.51	13	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	608	PX4	O7-C23	2.51	1.27	1.34	13	2
3	B	316	PX4	O7-C7	2.51	1.52	1.46	14	4
3	B	355	PX4	P1-O1	2.51	1.43	1.55	6	2
3	C	343	PX4	C10-C9	2.51	1.58	1.50	10	1
3	C	344	PX4	C2-N1	2.51	1.59	1.51	13	3
3	A	623	PX4	C11-C10	2.51	1.61	1.52	5	1
3	A	629	PX4	C24-C23	2.51	1.58	1.50	5	1
3	C	314	PX4	C5-N1	2.51	1.42	1.50	8	1
3	B	316	PX4	C25-C24	2.51	1.61	1.52	4	4
3	B	353	PX4	C3-N1	2.51	1.42	1.50	6	1
3	B	361	PX4	P1-O1	2.51	1.43	1.55	13	3
3	C	355	PX4	O5-C9	2.51	1.40	1.33	14	1
3	A	608	PX4	O3-C1	2.50	1.34	1.44	14	1
3	A	615	PX4	C31-C30	2.50	1.64	1.51	15	1
3	A	636	PX4	P1-O4	2.50	1.49	1.59	11	1
3	B	366	PX4	O7-C23	2.50	1.27	1.34	14	4
3	B	389	PX4	O7-C7	2.50	1.40	1.46	14	4
3	C	330	PX4	C25-C24	2.50	1.61	1.52	14	2
3	B	314	PX4	C4-N1	2.50	1.57	1.50	4	2
3	B	338	PX4	C25-C24	2.50	1.61	1.52	15	3
3	B	325	PX4	P1-O1	2.50	1.43	1.55	6	2
3	C	328	PX4	P1-O2	2.50	1.42	1.50	15	2
3	C	357	PX4	P1-O1	2.50	1.43	1.55	8	4
3	A	601	PX4	C26-C25	2.50	1.64	1.51	14	1
3	A	633	PX4	C3-N1	2.50	1.57	1.50	1	1
3	B	364	PX4	O7-C23	2.50	1.27	1.34	4	2
3	C	340	PX4	P1-O1	2.50	1.43	1.55	5	3
3	C	345	PX4	C30-C29	2.50	1.64	1.51	5	1
3	A	645	PX4	P1-O1	2.50	1.43	1.55	3	1
3	B	348	PX4	C25-C24	2.50	1.61	1.52	12	1
3	B	373	PX4	C28-C27	2.50	1.64	1.51	1	1
3	C	367	PX4	C5-N1	2.50	1.57	1.50	2	2
3	C	361	PX4	C2-N1	2.50	1.59	1.51	7	1
3	A	632	PX4	O7-C7	2.50	1.40	1.46	12	3
3	B	303	PX4	C3-N1	2.50	1.42	1.50	4	1
3	B	384	PX4	C3-N1	2.50	1.57	1.50	15	1
3	C	304	PX4	C11-C10	2.50	1.61	1.52	15	1
3	C	364	PX4	O5-C8	2.50	1.50	1.45	9	2
3	B	302	PX4	C11-C10	2.49	1.61	1.52	10	1
3	B	399	PX4	O7-C23	2.50	1.27	1.34	11	2
3	B	351	PX4	O7-C7	2.49	1.52	1.46	14	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	395	PX4	C2-C1	2.49	1.58	1.51	9	2
3	A	634	PX4	C25-C24	2.49	1.61	1.52	5	2
3	B	385	PX4	C11-C10	2.49	1.61	1.52	9	1
3	C	362	PX4	C2-N1	2.49	1.59	1.51	8	1
3	A	637	PX4	C10-C9	2.49	1.57	1.50	15	2
3	B	307	PX4	C5-N1	2.49	1.42	1.50	15	3
3	B	317	PX4	P1-O1	2.49	1.43	1.55	5	4
3	B	377	PX4	C31-C30	2.49	1.64	1.51	8	1
3	B	380	PX4	C25-C24	2.49	1.61	1.52	2	1
3	C	304	PX4	O5-C9	2.49	1.26	1.33	1	1
3	C	341	PX4	C24-C23	2.49	1.57	1.50	8	3
3	B	302	PX4	C6-C7	2.49	1.58	1.50	2	7
3	B	331	PX4	C11-C10	2.49	1.61	1.52	8	1
3	C	369	PX4	C25-C24	2.49	1.61	1.52	10	4
3	B	392	PX4	P1-O1	2.49	1.43	1.55	8	6
3	C	311	PX4	C11-C10	2.49	1.61	1.52	3	1
3	B	388	PX4	C4-N1	2.49	1.42	1.50	3	1
3	C	303	PX4	P1-O1	2.49	1.43	1.55	7	2
3	C	366	PX4	C2-N1	2.49	1.43	1.51	3	1
3	C	367	PX4	P1-O1	2.49	1.43	1.55	10	4
3	B	346	PX4	C10-C9	2.49	1.43	1.50	10	1
3	B	362	PX4	P1-O1	2.48	1.43	1.55	7	2
3	C	323	PX4	O5-C9	2.49	1.26	1.33	6	1
3	C	332	PX4	C11-C10	2.48	1.61	1.52	1	2
3	C	357	PX4	C10-C9	2.48	1.57	1.50	8	2
3	B	347	PX4	P1-O1	2.48	1.43	1.55	5	3
3	B	356	PX4	P1-O1	2.48	1.43	1.55	2	2
3	C	316	PX4	C11-C10	2.48	1.61	1.52	11	2
3	B	302	PX4	C4-N1	2.48	1.42	1.50	8	1
3	C	335	PX4	O3-C1	2.48	1.34	1.44	13	1
3	C	343	PX4	O5-C8	2.48	1.39	1.45	5	2
3	B	324	PX4	P1-O4	2.48	1.49	1.59	4	2
3	B	359	PX4	C34-C33	2.48	1.64	1.51	3	1
3	C	343	PX4	C24-C23	2.48	1.57	1.50	11	2
3	A	635	PX4	C25-C24	2.48	1.61	1.52	13	1
3	A	642	PX4	O5-C9	2.48	1.40	1.33	15	3
3	B	306	PX4	C5-N1	2.48	1.42	1.50	9	1
3	B	340	PX4	O4-C6	2.48	1.35	1.44	2	1
3	B	383	PX4	C2-C1	2.48	1.58	1.51	12	3
3	C	342	PX4	C10-C9	2.48	1.57	1.50	15	2
3	C	353	PX4	O7-C7	2.48	1.40	1.46	13	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	627	PX4	P1-O4	2.48	1.49	1.59	15	1
3	A	637	PX4	P1-O2	2.48	1.42	1.50	7	3
3	B	302	PX4	P1-O1	2.48	1.43	1.55	6	1
3	A	618	PX4	P1-O3	2.47	1.49	1.59	8	1
3	B	302	PX4	O5-C9	2.47	1.40	1.33	11	1
3	B	307	PX4	C4-N1	2.48	1.57	1.50	9	2
3	C	341	PX4	O7-C23	2.48	1.27	1.34	10	4
3	A	630	PX4	C24-C23	2.47	1.57	1.50	15	1
3	A	637	PX4	C2-N1	2.47	1.59	1.51	8	2
3	B	372	PX4	C24-C23	2.47	1.57	1.50	11	2
3	B	399	PX4	O7-C7	2.47	1.40	1.46	12	2
3	A	623	PX4	C8-C7	2.47	1.58	1.50	15	4
3	A	642	PX4	C24-C23	2.47	1.57	1.50	13	3
3	B	378	PX4	C11-C10	2.47	1.61	1.52	2	3
3	B	389	PX4	O7-C23	2.47	1.27	1.34	14	1
3	C	354	PX4	C11-C10	2.47	1.61	1.52	3	4
3	A	627	PX4	C24-C23	2.47	1.57	1.50	9	1
3	A	610	PX4	C25-C24	2.47	1.61	1.52	11	1
3	B	301	PX4	O5-C9	2.47	1.40	1.33	2	2
3	B	311	PX4	C4-N1	2.47	1.42	1.50	2	4
3	C	304	PX4	P1-O1	2.47	1.43	1.55	7	2
3	B	364	PX4	C31-C30	2.47	1.64	1.51	7	1
3	B	393	PX4	C30-C29	2.47	1.64	1.51	9	1
3	C	302	PX4	O5-C9	2.47	1.40	1.33	10	1
3	C	335	PX4	O7-C23	2.47	1.27	1.34	4	4
3	C	335	PX4	P1-O2	2.47	1.42	1.50	9	1
3	A	607	PX4	C2-C1	2.47	1.58	1.51	12	6
3	B	322	PX4	C11-C10	2.47	1.61	1.52	6	3
3	B	361	PX4	C25-C24	2.47	1.61	1.52	12	2
3	C	359	PX4	C26-C25	2.47	1.64	1.51	9	2
3	B	374	PX4	P1-O1	2.46	1.43	1.55	9	1
3	B	379	PX4	C5-N1	2.47	1.57	1.50	10	1
3	B	333	PX4	P1-O3	2.46	1.49	1.59	10	2
3	C	324	PX4	P1-O2	2.46	1.42	1.50	3	2
3	C	341	PX4	P1-O3	2.46	1.49	1.59	14	1
3	C	357	PX4	P1-O2	2.46	1.42	1.50	15	1
3	A	610	PX4	C10-C9	2.46	1.57	1.50	6	4
3	C	347	PX4	P1-O3	2.46	1.49	1.59	1	1
3	C	359	PX4	P1-O1	2.46	1.43	1.55	14	4
3	A	619	PX4	P1-O1	2.46	1.43	1.55	15	1
3	B	330	PX4	P1-O1	2.46	1.43	1.55	9	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	604	PX4	P1-O2	2.46	1.42	1.50	4	1
3	A	616	PX4	C31-C30	2.46	1.64	1.51	15	1
3	B	305	PX4	C3-N1	2.46	1.57	1.50	10	1
3	B	375	PX4	C2-N1	2.46	1.59	1.51	5	2
3	C	329	PX4	O7-C23	2.46	1.41	1.34	1	1
3	C	332	PX4	P1-O1	2.46	1.44	1.55	15	3
3	A	609	PX4	O3-C1	2.46	1.34	1.44	10	2
3	A	629	PX4	P1-O2	2.46	1.42	1.50	8	1
3	A	631	PX4	C10-C9	2.46	1.57	1.50	6	2
3	A	634	PX4	C3-N1	2.45	1.57	1.50	13	1
3	B	337	PX4	O7-C7	2.45	1.40	1.46	2	2
3	B	349	PX4	O7-C23	2.45	1.27	1.34	15	1
3	B	372	PX4	P1-O4	2.46	1.49	1.59	1	1
3	B	376	PX4	C11-C10	2.45	1.61	1.52	8	2
3	B	389	PX4	C24-C23	2.46	1.57	1.50	3	1
3	C	369	PX4	C24-C23	2.46	1.57	1.50	13	2
3	B	382	PX4	C3-N1	2.45	1.57	1.50	11	1
3	C	325	PX4	O5-C9	2.45	1.40	1.33	3	1
3	C	334	PX4	P1-O4	2.45	1.49	1.59	2	2
3	C	348	PX4	C33-C32	2.45	1.64	1.51	2	1
3	C	355	PX4	O7-C7	2.45	1.40	1.46	14	2
3	B	369	PX4	O7-C7	2.45	1.40	1.46	4	2
3	B	389	PX4	C29-C28	2.45	1.64	1.51	13	1
3	A	645	PX4	C24-C23	2.45	1.57	1.50	7	4
3	B	308	PX4	O5-C8	2.45	1.39	1.45	5	3
3	B	391	PX4	P1-O2	2.45	1.42	1.50	1	1
3	C	305	PX4	C2-N1	2.45	1.58	1.51	4	1
3	C	346	PX4	C4-N1	2.45	1.42	1.50	1	1
3	C	352	PX4	C2-N1	2.45	1.58	1.51	3	1
3	B	304	PX4	C4-N1	2.45	1.57	1.50	7	1
3	B	363	PX4	O5-C9	2.45	1.26	1.33	3	1
3	B	305	PX4	O7-C7	2.45	1.40	1.46	10	5
3	B	345	PX4	O5-C8	2.45	1.50	1.45	2	2
3	A	607	PX4	C5-N1	2.45	1.42	1.50	8	1
3	B	312	PX4	P1-O1	2.45	1.44	1.55	3	3
3	B	330	PX4	O7-C7	2.45	1.40	1.46	2	2
3	B	344	PX4	P1-O4	2.45	1.49	1.59	10	2
3	B	372	PX4	O5-C9	2.45	1.26	1.33	10	1
3	C	363	PX4	P1-O1	2.45	1.44	1.55	2	4
3	A	616	PX4	O5-C9	2.44	1.26	1.33	15	1
3	B	317	PX4	C24-C23	2.44	1.57	1.50	10	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	331	PX4	C4-N1	2.45	1.57	1.50	11	3
3	B	362	PX4	C11-C10	2.44	1.61	1.52	11	4
3	B	386	PX4	C31-C30	2.44	1.63	1.51	3	1
3	C	319	PX4	C2-C1	2.44	1.58	1.51	13	2
3	C	322	PX4	C4-N1	2.44	1.57	1.50	4	1
3	C	330	PX4	O7-C7	2.45	1.40	1.46	2	3
3	A	614	PX4	C3-N1	2.44	1.57	1.50	9	1
3	B	359	PX4	O7-C7	2.44	1.40	1.46	3	1
3	A	622	PX4	C28-C27	2.44	1.63	1.51	6	2
3	A	625	PX4	O5-C8	2.44	1.50	1.45	4	1
3	C	370	PX4	C4-N1	2.44	1.57	1.50	2	1
3	B	366	PX4	P1-O3	2.44	1.49	1.59	4	1
3	B	381	PX4	C5-N1	2.44	1.57	1.50	4	3
3	C	302	PX4	C2-C1	2.44	1.58	1.51	10	3
3	B	309	PX4	C15-C14	2.44	1.63	1.51	12	1
3	A	634	PX4	C26-C25	2.44	1.63	1.51	4	1
3	B	319	PX4	O7-C23	2.44	1.27	1.34	14	3
3	C	335	PX4	C10-C9	2.44	1.57	1.50	10	1
3	C	350	PX4	O5-C8	2.44	1.39	1.45	10	3
3	B	373	PX4	P1-O1	2.44	1.44	1.55	5	2
3	B	374	PX4	C33-C32	2.44	1.63	1.51	13	1
3	C	355	PX4	C5-N1	2.44	1.42	1.50	1	2
3	B	302	PX4	C14-C13	2.44	1.63	1.51	10	1
3	B	313	PX4	C14-C13	2.44	1.63	1.51	2	1
3	A	604	PX4	C28-C27	2.44	1.63	1.51	13	1
3	B	325	PX4	C16-C15	2.44	1.63	1.51	4	1
3	C	323	PX4	C11-C10	2.44	1.61	1.52	12	3
3	C	333	PX4	C25-C24	2.44	1.61	1.52	13	1
3	C	370	PX4	P1-O1	2.44	1.44	1.55	10	2
3	C	365	PX4	C3-N1	2.44	1.57	1.50	9	3
3	C	369	PX4	O7-C7	2.44	1.40	1.46	7	2
3	B	326	PX4	C2-N1	2.43	1.58	1.51	12	3
3	B	337	PX4	C33-C32	2.44	1.63	1.51	15	1
3	B	367	PX4	C29-C28	2.44	1.63	1.51	12	1
3	B	392	PX4	P1-O2	2.44	1.42	1.50	15	1
3	B	362	PX4	O7-C7	2.43	1.40	1.46	15	1
3	C	356	PX4	O7-C7	2.43	1.40	1.46	1	2
3	A	611	PX4	C11-C10	2.43	1.61	1.52	9	2
3	A	634	PX4	C24-C23	2.43	1.57	1.50	5	3
3	A	639	PX4	O7-C7	2.43	1.40	1.46	12	2
3	B	314	PX4	O7-C23	2.43	1.27	1.34	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	354	PX4	O7-C23	2.43	1.27	1.34	15	1
3	B	360	PX4	O7-C7	2.43	1.40	1.46	12	2
3	B	365	PX4	C12-C11	2.43	1.63	1.51	10	1
3	B	386	PX4	C24-C23	2.43	1.57	1.50	12	3
3	B	395	PX4	P1-O3	2.43	1.49	1.59	10	1
3	C	313	PX4	P1-O1	2.43	1.44	1.55	5	7
3	A	610	PX4	P1-O1	2.43	1.44	1.55	5	4
3	A	636	PX4	C26-C25	2.43	1.63	1.51	4	1
3	C	356	PX4	O5-C8	2.43	1.50	1.45	4	2
3	A	620	PX4	C5-N1	2.43	1.43	1.50	14	1
3	B	301	PX4	P1-O1	2.43	1.44	1.55	12	4
3	B	338	PX4	C19-C18	2.43	1.63	1.51	11	1
3	B	351	PX4	C31-C30	2.43	1.63	1.51	6	2
3	B	379	PX4	C17-C16	2.43	1.63	1.51	10	1
3	C	304	PX4	P1-O2	2.43	1.42	1.50	12	1
3	A	625	PX4	O7-C7	2.43	1.40	1.46	4	2
3	C	369	PX4	C3-N1	2.43	1.43	1.50	7	1
3	C	369	PX4	C27-C26	2.43	1.63	1.51	12	1
3	B	323	PX4	O3-C1	2.43	1.35	1.44	9	1
3	B	390	PX4	C24-C23	2.43	1.57	1.50	15	2
3	B	331	PX4	C2-N1	2.42	1.58	1.51	11	3
3	B	388	PX4	C12-C11	2.42	1.63	1.51	8	1
3	B	390	PX4	C32-C31	2.42	1.63	1.51	13	1
3	B	400	PX4	P1-O1	2.42	1.44	1.55	14	3
3	B	320	PX4	C3-N1	2.42	1.57	1.50	10	2
3	B	329	PX4	C25-C24	2.42	1.61	1.52	1	1
3	B	377	PX4	C11-C10	2.42	1.61	1.52	6	3
3	B	387	PX4	C16-C15	2.42	1.63	1.51	15	1
3	B	394	PX4	P1-O1	2.42	1.44	1.55	9	2
3	C	337	PX4	C2-C1	2.42	1.58	1.51	12	3
3	C	348	PX4	C5-N1	2.42	1.43	1.50	11	1
3	B	306	PX4	C2-N1	2.42	1.58	1.51	7	1
3	B	313	PX4	C2-C1	2.42	1.58	1.51	1	4
3	B	321	PX4	C25-C24	2.42	1.61	1.52	4	1
3	C	311	PX4	C25-C24	2.42	1.61	1.52	7	2
3	C	358	PX4	C26-C25	2.42	1.63	1.51	8	1
3	C	319	PX4	C33-C32	2.42	1.63	1.51	10	1
3	A	623	PX4	P1-O1	2.42	1.44	1.55	8	2
3	B	302	PX4	P1-O2	2.42	1.42	1.50	7	1
3	C	327	PX4	C11-C10	2.42	1.61	1.52	15	2
3	B	315	PX4	O5-C9	2.42	1.26	1.33	2	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	319	PX4	C20-C19	2.42	1.63	1.51	1	1
3	B	351	PX4	O7-C23	2.42	1.27	1.34	5	2
3	B	371	PX4	C20-C19	2.42	1.63	1.51	9	1
3	B	382	PX4	O5-C8	2.42	1.50	1.45	14	2
3	C	337	PX4	C24-C23	2.42	1.57	1.50	1	2
3	C	366	PX4	C16-C15	2.42	1.63	1.51	12	1
3	B	327	PX4	O5-C9	2.42	1.40	1.33	7	1
3	C	370	PX4	C11-C10	2.42	1.61	1.52	3	2
3	B	348	PX4	O5-C9	2.42	1.40	1.33	5	1
3	B	340	PX4	C5-N1	2.41	1.57	1.50	5	2
3	B	353	PX4	O5-C8	2.42	1.39	1.45	15	2
3	C	361	PX4	O7-C7	2.42	1.40	1.46	11	2
3	B	376	PX4	C5-N1	2.41	1.57	1.50	1	2
3	B	306	PX4	C25-C24	2.41	1.61	1.52	2	1
3	B	368	PX4	C24-C23	2.41	1.57	1.50	6	2
3	B	369	PX4	C30-C29	2.41	1.63	1.51	12	1
3	B	372	PX4	O4-C6	2.41	1.53	1.44	10	1
3	B	373	PX4	O7-C23	2.41	1.27	1.34	6	3
3	B	379	PX4	P1-O1	2.41	1.44	1.55	11	2
3	C	337	PX4	P1-O1	2.41	1.44	1.55	8	5
3	C	344	PX4	P1-O1	2.41	1.44	1.55	14	2
3	A	632	PX4	O7-C23	2.41	1.27	1.34	13	1
3	B	306	PX4	P1-O1	2.41	1.44	1.55	10	2
3	C	308	PX4	C3-N1	2.41	1.43	1.50	9	2
3	C	344	PX4	C13-C12	2.41	1.63	1.51	10	1
3	C	363	PX4	O5-C8	2.41	1.50	1.45	7	1
3	B	346	PX4	O7-C23	2.41	1.27	1.34	5	2
3	B	349	PX4	P1-O3	2.41	1.50	1.59	7	2
3	B	366	PX4	C26-C25	2.41	1.63	1.51	1	1
3	B	377	PX4	C19-C18	2.41	1.63	1.51	7	1
3	B	382	PX4	C4-N1	2.41	1.57	1.50	4	3
3	C	344	PX4	C4-N1	2.41	1.43	1.50	8	1
3	B	355	PX4	C11-C10	2.41	1.61	1.52	10	2
3	A	626	PX4	C33-C32	2.41	1.63	1.51	14	1
3	A	627	PX4	P1-O1	2.41	1.44	1.55	10	2
3	A	634	PX4	P1-O4	2.41	1.50	1.59	10	1
3	B	335	PX4	C2-N1	2.41	1.58	1.51	4	1
3	C	315	PX4	C2-N1	2.41	1.58	1.51	12	2
3	C	346	PX4	C25-C24	2.41	1.61	1.52	10	2
3	B	319	PX4	C25-C24	2.41	1.61	1.52	6	2
3	B	368	PX4	P1-O2	2.41	1.42	1.50	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	310	PX4	P1-O2	2.41	1.42	1.50	1	2
3	C	334	PX4	C25-C24	2.41	1.61	1.52	1	2
3	B	340	PX4	P1-O2	2.41	1.42	1.50	15	2
3	C	365	PX4	C10-C9	2.41	1.57	1.50	15	2
3	A	625	PX4	P1-O1	2.40	1.44	1.55	3	5
3	A	643	PX4	P1-O1	2.40	1.44	1.55	10	3
3	B	332	PX4	C32-C31	2.40	1.63	1.51	14	1
3	B	365	PX4	P1-O1	2.40	1.44	1.55	14	2
3	B	385	PX4	O7-C23	2.40	1.41	1.34	2	2
3	C	352	PX4	P1-O3	2.40	1.50	1.59	14	2
3	A	622	PX4	O5-C9	2.40	1.26	1.33	3	1
3	A	632	PX4	C28-C27	2.40	1.63	1.51	14	1
3	A	637	PX4	C11-C10	2.40	1.61	1.52	6	1
3	B	347	PX4	O7-C7	2.40	1.41	1.46	12	2
3	B	391	PX4	C3-N1	2.40	1.57	1.50	8	2
3	C	354	PX4	C24-C23	2.40	1.57	1.50	8	1
3	C	354	PX4	C4-N1	2.40	1.57	1.50	10	1
3	B	347	PX4	C18-C17	2.40	1.63	1.51	10	1
3	B	373	PX4	C4-N1	2.40	1.43	1.50	4	2
3	B	347	PX4	O7-C23	2.40	1.27	1.34	12	3
3	B	353	PX4	C10-C9	2.40	1.57	1.50	7	3
3	C	316	PX4	P1-O1	2.40	1.44	1.55	13	1
3	C	314	PX4	O4-C6	2.40	1.35	1.44	9	1
3	C	333	PX4	P1-O2	2.40	1.42	1.50	7	1
3	C	301	PX4	C11-C10	2.40	1.61	1.52	9	2
3	C	321	PX4	C11-C10	2.40	1.61	1.52	4	2
3	C	351	PX4	C3-N1	2.40	1.43	1.50	4	1
3	C	305	PX4	C6-C7	2.40	1.58	1.50	8	4
3	C	351	PX4	C2-N1	2.40	1.58	1.51	13	2
3	A	633	PX4	C2-N1	2.40	1.44	1.51	1	1
3	B	360	PX4	C5-N1	2.40	1.57	1.50	3	3
3	B	335	PX4	P1-O1	2.40	1.44	1.55	15	4
3	B	337	PX4	C5-N1	2.40	1.57	1.50	12	1
3	B	338	PX4	C32-C31	2.39	1.63	1.51	12	1
3	B	340	PX4	O7-C7	2.39	1.41	1.46	10	2
3	B	378	PX4	C4-N1	2.40	1.57	1.50	7	1
3	A	619	PX4	C18-C17	2.39	1.63	1.51	9	1
3	A	635	PX4	O7-C23	2.39	1.27	1.34	4	3
3	B	373	PX4	C12-C11	2.39	1.63	1.51	7	1
3	A	617	PX4	O5-C8	2.39	1.39	1.45	11	1
3	A	636	PX4	C2-N1	2.39	1.58	1.51	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	327	PX4	C11-C10	2.39	1.60	1.52	10	3
3	B	331	PX4	O4-C6	2.39	1.35	1.44	10	1
3	C	360	PX4	C25-C24	2.39	1.61	1.52	14	2
3	B	322	PX4	O7-C7	2.39	1.41	1.46	8	2
3	B	329	PX4	O7-C23	2.39	1.27	1.34	8	1
3	B	333	PX4	C25-C24	2.39	1.60	1.52	8	3
3	B	341	PX4	P1-O3	2.39	1.50	1.59	7	1
3	B	346	PX4	C2-C1	2.39	1.58	1.51	1	3
3	B	365	PX4	C28-C27	2.39	1.63	1.51	2	1
3	C	303	PX4	C2-N1	2.39	1.44	1.51	7	1
3	A	610	PX4	O7-C23	2.39	1.41	1.34	1	3
3	A	620	PX4	P1-O3	2.39	1.50	1.59	5	1
3	A	630	PX4	P1-O4	2.39	1.50	1.59	12	3
3	B	301	PX4	P1-O3	2.39	1.50	1.59	2	1
3	B	322	PX4	C29-C28	2.39	1.63	1.51	10	1
3	C	312	PX4	C18-C17	2.39	1.63	1.51	10	1
3	A	616	PX4	O5-C8	2.38	1.50	1.45	6	4
3	A	626	PX4	O5-C9	2.38	1.26	1.33	13	2
3	C	313	PX4	C2-C1	2.39	1.58	1.51	6	2
3	B	320	PX4	P1-O3	2.38	1.68	1.59	13	1
3	B	322	PX4	P1-O1	2.38	1.44	1.55	8	2
3	B	367	PX4	C18-C17	2.38	1.63	1.51	5	1
3	C	360	PX4	P1-O1	2.38	1.44	1.55	3	2
3	B	308	PX4	C3-N1	2.38	1.56	1.50	14	3
3	A	604	PX4	C15-C14	2.38	1.63	1.51	3	1
3	A	614	PX4	O5-C8	2.38	1.39	1.45	10	1
3	B	370	PX4	C16-C15	2.38	1.63	1.51	11	1
3	B	346	PX4	C11-C10	2.38	1.60	1.52	15	1
3	B	368	PX4	O4-C6	2.38	1.53	1.44	1	1
3	B	395	PX4	C32-C31	2.38	1.63	1.51	13	1
3	C	319	PX4	P1-O4	2.38	1.50	1.59	11	2
3	A	601	PX4	O5-C8	2.38	1.39	1.45	12	2
3	A	643	PX4	C25-C24	2.38	1.60	1.52	1	1
3	B	345	PX4	C13-C12	2.38	1.63	1.51	5	1
3	A	628	PX4	C20-C19	2.38	1.63	1.51	8	1
3	A	640	PX4	C25-C24	2.38	1.60	1.52	6	1
3	B	387	PX4	C29-C28	2.38	1.63	1.51	15	1
3	C	310	PX4	O7-C23	2.38	1.27	1.34	10	2
3	C	313	PX4	O7-C23	2.38	1.27	1.34	13	2
3	C	364	PX4	O7-C23	2.38	1.27	1.34	8	2
3	A	630	PX4	C2-N1	2.38	1.44	1.51	2	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	381	PX4	O5-C9	2.38	1.40	1.33	3	1
3	B	384	PX4	C10-C9	2.38	1.57	1.50	2	2
3	C	329	PX4	C2-N1	2.38	1.58	1.51	10	2
3	C	350	PX4	P1-O1	2.38	1.44	1.55	14	2
3	B	352	PX4	C27-C26	2.37	1.63	1.51	4	1
3	B	356	PX4	O5-C8	2.38	1.39	1.45	10	3
3	B	317	PX4	C16-C15	2.37	1.63	1.51	3	1
3	B	327	PX4	C10-C9	2.37	1.57	1.50	6	2
3	C	342	PX4	P1-O2	2.37	1.42	1.50	1	2
3	C	358	PX4	O5-C9	2.37	1.26	1.33	4	1
3	A	609	PX4	C20-C19	2.37	1.63	1.51	10	1
3	A	629	PX4	P1-O4	2.37	1.68	1.59	12	1
3	A	646	PX4	C2-N1	2.37	1.58	1.51	6	1
3	B	304	PX4	C2-N1	2.37	1.58	1.51	12	1
3	C	353	PX4	C16-C15	2.37	1.63	1.51	8	2
3	B	343	PX4	C12-C11	2.37	1.63	1.51	12	1
3	C	338	PX4	O7-C7	2.37	1.52	1.46	6	2
3	B	319	PX4	C12-C11	2.37	1.63	1.51	3	1
3	B	332	PX4	O5-C8	2.37	1.39	1.45	2	1
3	B	366	PX4	C4-N1	2.37	1.56	1.50	13	1
3	B	368	PX4	O7-C23	2.37	1.27	1.34	12	2
3	B	369	PX4	C3-N1	2.37	1.43	1.50	12	2
3	B	396	PX4	C3-N1	2.37	1.56	1.50	1	2
3	C	302	PX4	P1-O2	2.37	1.42	1.50	11	1
3	C	311	PX4	O7-C7	2.37	1.41	1.46	2	1
3	C	318	PX4	O5-C9	2.37	1.40	1.33	1	2
3	B	333	PX4	O7-C23	2.37	1.27	1.34	15	1
3	B	319	PX4	P1-O1	2.37	1.44	1.55	14	4
3	B	339	PX4	C5-N1	2.37	1.56	1.50	9	1
3	C	322	PX4	C3-N1	2.37	1.43	1.50	5	1
3	B	328	PX4	C4-N1	2.37	1.43	1.50	7	1
3	B	347	PX4	O5-C8	2.37	1.39	1.45	7	1
3	B	370	PX4	C29-C28	2.36	1.63	1.51	2	1
3	C	312	PX4	C2-N1	2.37	1.58	1.51	9	3
3	C	336	PX4	O7-C7	2.37	1.41	1.46	1	4
3	C	346	PX4	P1-O4	2.37	1.68	1.59	6	1
3	A	608	PX4	C11-C10	2.36	1.60	1.52	5	2
3	B	378	PX4	O5-C8	2.36	1.39	1.45	9	1
3	C	332	PX4	C10-C9	2.36	1.57	1.50	14	4
3	A	605	PX4	C24-C23	2.36	1.57	1.50	10	1
3	A	645	PX4	C25-C24	2.36	1.60	1.52	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	305	PX4	C10-C9	2.36	1.57	1.50	10	3
3	B	374	PX4	C30-C29	2.36	1.63	1.51	13	1
3	B	398	PX4	C18-C17	2.36	1.63	1.51	8	1
3	C	347	PX4	C3-N1	2.36	1.56	1.50	8	1
3	B	343	PX4	C2-N1	2.36	1.44	1.51	2	1
3	C	317	PX4	C11-C10	2.36	1.60	1.52	2	3
3	A	643	PX4	P1-O3	2.36	1.50	1.59	13	1
3	B	318	PX4	C15-C14	2.36	1.63	1.51	14	1
3	B	337	PX4	O4-C6	2.36	1.35	1.44	11	1
3	B	353	PX4	C5-N1	2.36	1.56	1.50	2	2
3	C	341	PX4	P1-O4	2.36	1.50	1.59	12	1
3	C	342	PX4	P1-O1	2.36	1.44	1.55	14	4
3	B	334	PX4	O7-C23	2.36	1.27	1.34	2	1
3	B	356	PX4	O3-C1	2.36	1.54	1.44	2	1
3	C	316	PX4	C2-N1	2.36	1.58	1.51	3	1
3	C	309	PX4	C5-N1	2.36	1.56	1.50	3	1
3	C	353	PX4	C4-N1	2.36	1.43	1.50	7	3
3	A	620	PX4	P1-O1	2.36	1.44	1.55	1	2
3	A	637	PX4	C25-C24	2.36	1.60	1.52	5	1
3	A	646	PX4	O7-C7	2.36	1.41	1.46	6	1
3	B	376	PX4	P1-O1	2.36	1.44	1.55	5	2
3	B	394	PX4	C18-C17	2.35	1.63	1.51	12	1
3	B	400	PX4	C16-C15	2.36	1.63	1.51	13	1
3	C	305	PX4	C11-C10	2.36	1.60	1.52	10	3
3	C	314	PX4	C28-C27	2.36	1.63	1.51	9	1
3	C	324	PX4	C25-C24	2.36	1.60	1.52	13	1
3	A	635	PX4	C24-C23	2.35	1.57	1.50	12	1
3	A	637	PX4	P1-O1	2.35	1.44	1.55	7	6
3	A	615	PX4	C28-C27	2.35	1.63	1.51	9	1
3	A	628	PX4	C25-C24	2.35	1.60	1.52	10	1
3	A	638	PX4	P1-O1	2.35	1.44	1.55	13	5
3	B	345	PX4	C25-C24	2.35	1.60	1.52	4	3
3	B	354	PX4	O5-C9	2.35	1.26	1.33	8	1
3	C	360	PX4	P1-O2	2.35	1.42	1.50	2	1
3	B	367	PX4	C13-C12	2.35	1.63	1.51	12	1
3	B	378	PX4	C17-C16	2.35	1.63	1.51	13	3
3	B	368	PX4	C25-C24	2.35	1.60	1.52	9	1
3	C	308	PX4	P1-O1	2.35	1.44	1.55	10	3
3	C	338	PX4	O5-C9	2.35	1.40	1.33	1	1
3	A	631	PX4	C13-C12	2.35	1.63	1.51	15	1
3	B	363	PX4	C25-C24	2.35	1.60	1.52	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	383	PX4	C10-C9	2.35	1.57	1.50	5	1
3	A	602	PX4	C30-C29	2.35	1.63	1.51	2	1
3	A	626	PX4	C12-C11	2.35	1.63	1.51	5	1
3	B	329	PX4	C18-C17	2.35	1.63	1.51	12	1
3	B	352	PX4	P1-O3	2.35	1.50	1.59	15	1
3	B	370	PX4	C10-C9	2.35	1.57	1.50	13	1
3	C	310	PX4	P1-O1	2.35	1.44	1.55	4	3
3	B	363	PX4	C33-C32	2.35	1.63	1.51	2	2
3	C	340	PX4	O7-C7	2.35	1.41	1.46	3	1
3	A	647	PX4	C35-C34	2.35	1.66	1.51	1	1
3	B	396	PX4	C30-C29	2.35	1.63	1.51	8	1
3	C	365	PX4	P1-O1	2.35	1.44	1.55	6	2
3	B	383	PX4	O5-C8	2.35	1.39	1.45	3	2
3	C	318	PX4	C4-N1	2.34	1.43	1.50	9	2
3	C	319	PX4	C25-C24	2.35	1.60	1.52	14	1
3	B	362	PX4	P1-O2	2.34	1.42	1.50	14	1
3	C	307	PX4	C27-C26	2.34	1.63	1.51	10	1
3	C	333	PX4	C19-C18	2.34	1.63	1.51	14	1
3	C	335	PX4	P1-O1	2.34	1.44	1.55	10	3
3	C	361	PX4	C24-C23	2.34	1.57	1.50	2	1
3	C	361	PX4	O5-C8	2.35	1.39	1.45	14	2
3	A	605	PX4	C33-C32	2.34	1.63	1.51	9	1
3	B	309	PX4	C25-C24	2.34	1.60	1.52	15	1
3	B	315	PX4	C5-N1	2.34	1.43	1.50	10	2
3	B	353	PX4	P1-O1	2.34	1.44	1.55	6	3
3	B	398	PX4	O7-C23	2.34	1.27	1.34	1	3
3	C	323	PX4	P1-O1	2.34	1.44	1.55	9	2
3	C	362	PX4	P1-O1	2.34	1.44	1.55	2	2
3	C	363	PX4	C5-N1	2.34	1.43	1.50	10	1
3	A	603	PX4	P1-O3	2.34	1.50	1.59	9	1
3	A	607	PX4	P1-O1	2.34	1.44	1.55	3	4
3	A	625	PX4	C10-C9	2.34	1.57	1.50	6	3
3	B	318	PX4	P1-O1	2.34	1.44	1.55	5	2
3	B	348	PX4	C16-C15	2.34	1.63	1.51	12	1
3	B	366	PX4	C16-C15	2.34	1.63	1.51	7	1
3	B	372	PX4	C15-C14	2.34	1.63	1.51	10	1
3	B	316	PX4	P1-O1	2.34	1.44	1.55	3	3
3	B	346	PX4	C13-C12	2.34	1.63	1.51	13	1
3	B	340	PX4	C4-N1	2.34	1.43	1.50	5	1
3	C	308	PX4	C13-C12	2.34	1.63	1.51	7	1
3	C	309	PX4	C10-C9	2.34	1.57	1.50	2	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	313	PX4	P1-O2	2.34	1.42	1.50	8	2
3	C	335	PX4	C2-N1	2.34	1.58	1.51	6	3
3	C	348	PX4	C11-C10	2.34	1.60	1.52	14	1
3	C	355	PX4	C6-C7	2.34	1.58	1.50	4	2
3	A	604	PX4	C5-N1	2.34	1.43	1.50	2	1
3	A	606	PX4	C4-N1	2.34	1.43	1.50	13	1
3	B	311	PX4	C11-C10	2.34	1.60	1.52	3	2
3	B	313	PX4	O5-C8	2.34	1.50	1.45	15	1
3	B	315	PX4	C17-C16	2.34	1.63	1.51	6	1
3	B	328	PX4	P1-O1	2.34	1.44	1.55	14	3
3	B	332	PX4	P1-O1	2.34	1.44	1.55	12	1
3	B	393	PX4	C5-N1	2.34	1.56	1.50	13	2
3	C	319	PX4	C2-N1	2.34	1.58	1.51	4	1
3	C	354	PX4	C2-N1	2.34	1.58	1.51	12	2
3	C	363	PX4	C3-N1	2.34	1.56	1.50	7	3
3	B	384	PX4	P1-O4	2.34	1.68	1.59	3	1
3	B	386	PX4	C27-C26	2.34	1.63	1.51	15	1
3	A	634	PX4	O5-C9	2.33	1.26	1.33	7	1
3	B	398	PX4	C15-C14	2.33	1.63	1.51	1	1
3	C	316	PX4	C25-C24	2.33	1.60	1.52	9	1
3	C	322	PX4	C5-N1	2.34	1.56	1.50	13	2
3	B	309	PX4	C31-C30	2.33	1.63	1.51	8	1
3	B	328	PX4	O4-C6	2.33	1.35	1.44	15	1
3	A	636	PX4	C20-C19	2.33	1.63	1.51	6	1
3	A	616	PX4	C17-C16	2.33	1.63	1.51	13	1
3	B	334	PX4	O5-C8	2.33	1.50	1.45	5	1
3	B	355	PX4	P1-O2	2.33	1.42	1.50	9	2
3	B	367	PX4	C5-N1	2.33	1.56	1.50	8	2
3	C	306	PX4	P1-O3	2.33	1.50	1.59	6	1
3	C	338	PX4	C17-C16	2.33	1.63	1.51	7	1
3	A	611	PX4	C2-N1	2.33	1.58	1.51	9	1
3	B	309	PX4	P1-O1	2.33	1.44	1.55	14	3
3	C	310	PX4	O5-C9	2.33	1.26	1.33	9	2
3	C	311	PX4	C26-C25	2.33	1.63	1.51	6	1
3	C	351	PX4	C11-C10	2.33	1.60	1.52	6	2
3	B	313	PX4	C18-C17	2.33	1.63	1.51	4	1
3	C	327	PX4	O7-C7	2.33	1.41	1.46	5	1
3	C	360	PX4	C3-N1	2.33	1.56	1.50	8	2
3	B	304	PX4	P1-O1	2.33	1.44	1.55	15	3
3	B	325	PX4	C31-C30	2.33	1.63	1.51	7	1
3	B	333	PX4	P1-O1	2.33	1.44	1.55	6	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	356	PX4	C3-N1	2.33	1.56	1.50	13	1
3	B	336	PX4	C30-C29	2.33	1.63	1.51	11	1
3	C	306	PX4	O7-C23	2.33	1.27	1.34	4	2
3	A	625	PX4	C30-C29	2.33	1.63	1.51	9	2
3	A	639	PX4	C11-C10	2.33	1.60	1.52	9	1
3	A	648	PX4	O5-C9	2.33	1.26	1.33	15	2
3	B	363	PX4	C11-C10	2.33	1.60	1.52	8	1
3	B	371	PX4	C4-N1	2.33	1.43	1.50	1	2
3	B	386	PX4	P1-O3	2.33	1.68	1.59	5	1
3	C	355	PX4	C25-C24	2.33	1.60	1.52	5	1
3	A	613	PX4	P1-O1	2.32	1.44	1.55	15	4
3	A	646	PX4	O5-C9	2.32	1.26	1.33	4	2
3	B	321	PX4	C31-C30	2.33	1.63	1.51	1	1
3	B	371	PX4	C2-N1	2.32	1.44	1.51	1	1
3	B	395	PX4	P1-O1	2.33	1.44	1.55	6	3
3	C	369	PX4	C31-C30	2.32	1.63	1.51	7	1
3	A	646	PX4	C17-C16	2.32	1.63	1.51	14	1
3	B	314	PX4	C24-C23	2.32	1.57	1.50	8	2
3	B	370	PX4	P1-O1	2.32	1.44	1.55	3	2
3	C	307	PX4	O5-C8	2.32	1.40	1.45	12	1
3	A	604	PX4	C33-C32	2.32	1.63	1.51	7	1
3	A	618	PX4	C25-C24	2.32	1.60	1.52	15	1
3	A	647	PX4	P1-O1	2.32	1.44	1.55	1	4
3	B	392	PX4	C10-C9	2.32	1.57	1.50	15	3
3	B	393	PX4	C8-C7	2.32	1.58	1.50	3	3
3	C	333	PX4	C3-N1	2.32	1.43	1.50	13	2
3	C	344	PX4	C12-C11	2.32	1.63	1.51	8	1
3	C	363	PX4	C15-C14	2.32	1.63	1.51	11	1
3	B	349	PX4	C20-C19	2.32	1.63	1.51	15	1
3	B	383	PX4	C5-N1	2.32	1.43	1.50	2	1
3	C	309	PX4	C2-C1	2.32	1.58	1.51	6	4
3	A	629	PX4	C16-C15	2.32	1.63	1.51	8	1
3	C	325	PX4	C32-C31	2.32	1.63	1.51	13	1
3	B	377	PX4	C25-C24	2.32	1.60	1.52	1	1
3	B	390	PX4	C4-N1	2.32	1.56	1.50	11	1
3	C	315	PX4	P1-O4	2.32	1.50	1.59	13	1
3	C	328	PX4	C25-C24	2.32	1.60	1.52	5	2
3	C	368	PX4	C5-N1	2.32	1.56	1.50	3	1
3	A	605	PX4	P1-O4	2.32	1.50	1.59	10	1
3	B	310	PX4	O4-C6	2.32	1.35	1.44	5	1
3	A	607	PX4	P1-O2	2.32	1.42	1.50	3	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	616	PX4	P1-O1	2.32	1.44	1.55	5	2
3	A	636	PX4	C4-N1	2.32	1.56	1.50	13	1
3	A	614	PX4	C2-N1	2.31	1.58	1.51	11	1
3	A	643	PX4	C32-C31	2.32	1.63	1.51	3	1
3	B	344	PX4	C5-N1	2.32	1.56	1.50	10	2
3	C	340	PX4	O7-C23	2.32	1.27	1.34	3	2
3	C	317	PX4	O7-C23	2.31	1.27	1.34	8	1
3	C	323	PX4	C31-C30	2.32	1.63	1.51	3	1
3	A	608	PX4	C12-C11	2.31	1.63	1.51	9	1
3	A	618	PX4	C24-C23	2.31	1.57	1.50	4	3
3	B	309	PX4	C16-C15	2.31	1.63	1.51	14	1
3	C	337	PX4	C5-N1	2.31	1.43	1.50	8	2
3	C	357	PX4	C2-N1	2.31	1.58	1.51	8	1
3	B	310	PX4	O5-C9	2.31	1.40	1.33	9	3
3	A	620	PX4	C25-C24	2.31	1.60	1.52	10	2
3	B	312	PX4	P1-O3	2.31	1.68	1.59	3	2
3	B	321	PX4	C34-C33	2.31	1.63	1.51	6	1
3	B	326	PX4	C24-C23	2.31	1.57	1.50	10	1
3	B	305	PX4	C5-N1	2.31	1.43	1.50	4	1
3	B	375	PX4	C5-N1	2.31	1.43	1.50	7	1
3	B	318	PX4	C32-C31	2.31	1.63	1.51	11	1
3	B	339	PX4	C32-C31	2.31	1.63	1.51	9	1
3	B	357	PX4	C19-C18	2.31	1.63	1.51	8	1
3	B	395	PX4	P1-O2	2.31	1.42	1.50	13	2
3	A	639	PX4	C14-C13	2.31	1.63	1.51	7	1
3	A	624	PX4	C25-C24	2.31	1.60	1.52	12	2
3	A	628	PX4	C19-C18	2.31	1.63	1.51	9	1
3	C	312	PX4	P1-O2	2.31	1.42	1.50	5	1
3	B	368	PX4	P1-O1	2.31	1.44	1.55	13	2
3	B	384	PX4	C11-C10	2.31	1.60	1.52	3	2
3	C	347	PX4	C11-C10	2.31	1.60	1.52	4	2
3	C	366	PX4	O6-C9	2.31	1.29	1.22	2	1
3	A	615	PX4	P1-O1	2.31	1.44	1.55	12	4
3	A	612	PX4	C25-C24	2.30	1.60	1.52	6	2
3	B	324	PX4	C34-C33	2.31	1.63	1.51	3	1
3	B	341	PX4	O4-C6	2.31	1.35	1.44	11	1
3	B	377	PX4	O3-C1	2.31	1.35	1.44	4	1
3	B	387	PX4	C2-C1	2.31	1.58	1.51	15	2
3	B	355	PX4	C2-N1	2.31	1.44	1.51	13	2
3	B	362	PX4	C17-C16	2.31	1.63	1.51	14	1
3	B	383	PX4	C24-C23	2.31	1.57	1.50	1	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	385	PX4	C25-C24	2.31	1.60	1.52	4	2
3	C	314	PX4	P1-O1	2.31	1.44	1.55	8	4
3	C	324	PX4	C24-C23	2.31	1.57	1.50	9	2
3	C	341	PX4	C2-N1	2.31	1.58	1.51	8	2
3	B	366	PX4	C5-N1	2.30	1.43	1.50	11	2
3	B	393	PX4	C2-N1	2.30	1.58	1.51	15	1
3	C	318	PX4	C24-C23	2.30	1.57	1.50	12	2
3	A	618	PX4	C11-C10	2.30	1.60	1.52	10	4
3	C	352	PX4	C3-N1	2.30	1.56	1.50	6	2
3	B	380	PX4	P1-O2	2.30	1.42	1.50	6	2
3	C	346	PX4	C3-N1	2.30	1.43	1.50	8	2
3	C	365	PX4	O7-C23	2.30	1.27	1.34	12	1
3	A	603	PX4	C13-C12	2.30	1.63	1.51	1	1
3	A	608	PX4	C27-C26	2.30	1.63	1.51	9	1
3	A	644	PX4	C2-N1	2.30	1.58	1.51	3	2
3	B	370	PX4	O5-C9	2.30	1.40	1.33	15	1
3	B	376	PX4	C24-C23	2.30	1.57	1.50	10	3
3	A	609	PX4	C24-C23	2.30	1.57	1.50	10	2
3	B	358	PX4	C14-C13	2.30	1.63	1.51	14	2
3	C	321	PX4	C27-C26	2.30	1.63	1.51	5	1
3	B	379	PX4	O5-C8	2.30	1.40	1.45	13	1
3	A	609	PX4	P1-O1	2.30	1.44	1.55	1	2
3	A	618	PX4	P1-O1	2.30	1.44	1.55	3	1
3	B	386	PX4	C29-C28	2.30	1.63	1.51	1	1
3	B	395	PX4	C12-C11	2.30	1.63	1.51	5	1
3	C	303	PX4	C15-C14	2.30	1.63	1.51	9	1
3	C	365	PX4	C28-C27	2.30	1.63	1.51	11	1
3	A	610	PX4	C24-C23	2.30	1.57	1.50	7	1
3	A	621	PX4	C25-C24	2.30	1.60	1.52	2	1
3	A	646	PX4	C10-C9	2.30	1.57	1.50	6	3
3	B	305	PX4	C30-C29	2.30	1.63	1.51	14	1
3	A	616	PX4	O3-C1	2.30	1.53	1.44	11	1
3	B	309	PX4	C10-C9	2.30	1.57	1.50	1	5
3	B	322	PX4	C2-N1	2.30	1.58	1.51	8	3
3	B	340	PX4	C13-C12	2.30	1.63	1.51	2	1
3	A	622	PX4	P1-O3	2.29	1.50	1.59	15	1
3	A	623	PX4	C6-C7	2.29	1.58	1.50	4	5
3	B	331	PX4	C25-C24	2.29	1.60	1.52	10	2
3	B	346	PX4	O5-C8	2.30	1.50	1.45	15	2
3	C	362	PX4	O3-C1	2.30	1.35	1.44	10	1
3	B	395	PX4	C3-N1	2.30	1.43	1.50	13	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	386	PX4	O7-C23	2.29	1.27	1.34	1	2
3	C	366	PX4	C33-C32	2.30	1.63	1.51	10	1
3	A	648	PX4	O5-C8	2.29	1.50	1.45	6	3
3	B	301	PX4	C32-C31	2.29	1.63	1.51	11	1
3	B	335	PX4	C5-N1	2.29	1.43	1.50	8	3
3	C	333	PX4	O7-C23	2.29	1.27	1.34	10	4
3	B	397	PX4	C31-C30	2.29	1.63	1.51	12	1
3	A	604	PX4	P1-O3	2.29	1.50	1.59	7	1
3	B	333	PX4	C17-C16	2.29	1.63	1.51	9	1
3	B	340	PX4	C2-N1	2.29	1.44	1.51	8	4
3	B	342	PX4	C2-N1	2.29	1.58	1.51	10	2
3	C	315	PX4	C11-C10	2.29	1.60	1.52	10	1
3	C	336	PX4	C32-C31	2.29	1.63	1.51	5	1
3	C	366	PX4	P1-O1	2.29	1.44	1.55	10	1
3	B	375	PX4	C3-N1	2.29	1.56	1.50	5	1
3	B	399	PX4	P1-O1	2.29	1.44	1.55	1	2
3	C	303	PX4	C18-C17	2.29	1.63	1.51	5	1
3	C	303	PX4	C32-C31	2.29	1.63	1.51	15	1
3	C	367	PX4	O5-C9	2.29	1.40	1.33	3	1
3	C	370	PX4	C3-N1	2.29	1.43	1.50	15	1
3	A	603	PX4	C33-C32	2.29	1.63	1.51	14	1
3	B	351	PX4	C25-C24	2.29	1.60	1.52	11	1
3	B	373	PX4	O7-C7	2.28	1.41	1.46	4	2
3	B	385	PX4	C31-C30	2.29	1.63	1.51	12	1
3	C	334	PX4	C33-C32	2.29	1.63	1.51	15	1
3	C	345	PX4	O3-C1	2.29	1.35	1.44	15	3
3	B	346	PX4	P1-O1	2.28	1.44	1.55	11	2
3	B	371	PX4	P1-O2	2.28	1.42	1.50	3	1
3	B	377	PX4	O5-C8	2.28	1.50	1.45	1	2
3	C	320	PX4	O7-C7	2.28	1.41	1.46	8	1
3	C	330	PX4	C3-N1	2.28	1.43	1.50	6	2
3	C	351	PX4	O7-C23	2.28	1.27	1.34	7	1
3	B	339	PX4	P1-O3	2.28	1.50	1.59	8	1
3	A	602	PX4	P1-O3	2.28	1.50	1.59	4	1
3	A	645	PX4	C11-C10	2.28	1.60	1.52	13	3
3	B	393	PX4	O5-C9	2.28	1.26	1.33	13	1
3	C	326	PX4	P1-O2	2.28	1.42	1.50	6	1
3	A	628	PX4	C13-C12	2.28	1.63	1.51	14	1
3	A	608	PX4	P1-O2	2.28	1.42	1.50	12	1
3	B	314	PX4	C32-C31	2.28	1.63	1.51	5	1
3	B	324	PX4	C25-C24	2.28	1.60	1.52	1	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	368	PX4	C15-C14	2.28	1.63	1.51	10	1
3	B	383	PX4	C11-C10	2.28	1.60	1.52	9	2
3	C	327	PX4	C26-C25	2.28	1.63	1.51	14	1
3	B	356	PX4	P1-O2	2.28	1.42	1.50	10	1
3	C	308	PX4	P1-O2	2.28	1.42	1.50	15	1
3	C	331	PX4	P1-O4	2.28	1.50	1.59	11	1
3	B	368	PX4	O5-C8	2.28	1.50	1.45	5	2
3	C	333	PX4	P1-O1	2.28	1.44	1.55	4	3
3	A	629	PX4	C2-C1	2.28	1.58	1.51	7	2
3	B	393	PX4	C4-N1	2.28	1.56	1.50	4	1
3	B	364	PX4	O4-C6	2.28	1.36	1.44	15	1
3	C	308	PX4	C25-C24	2.28	1.60	1.52	8	3
3	C	342	PX4	C3-N1	2.28	1.43	1.50	1	3
3	C	362	PX4	C5-N1	2.28	1.56	1.50	15	2
3	A	631	PX4	C28-C27	2.27	1.63	1.51	8	2
3	B	311	PX4	C30-C29	2.28	1.63	1.51	14	1
3	B	360	PX4	O5-C8	2.28	1.50	1.45	10	2
3	B	377	PX4	P1-O4	2.27	1.68	1.59	12	1
3	B	391	PX4	C16-C15	2.27	1.63	1.51	10	1
3	C	315	PX4	C13-C12	2.28	1.63	1.51	11	1
3	C	326	PX4	P1-O1	2.28	1.44	1.55	10	2
3	C	360	PX4	C14-C13	2.28	1.63	1.51	15	1
3	B	310	PX4	C2-N1	2.27	1.58	1.51	8	1
3	B	319	PX4	C24-C23	2.27	1.57	1.50	14	1
3	B	329	PX4	C4-N1	2.27	1.56	1.50	2	1
3	B	329	PX4	C5-N1	2.27	1.56	1.50	6	1
3	B	335	PX4	C33-C32	2.27	1.63	1.51	11	2
3	B	342	PX4	C25-C24	2.27	1.60	1.52	10	1
3	B	379	PX4	C4-N1	2.27	1.43	1.50	3	1
3	C	305	PX4	P1-O4	2.27	1.50	1.59	1	1
3	A	620	PX4	O3-C1	2.27	1.35	1.44	15	1
3	B	373	PX4	C25-C24	2.27	1.60	1.52	6	3
3	B	377	PX4	P1-O1	2.27	1.44	1.55	13	4
3	B	386	PX4	P1-O1	2.27	1.44	1.55	3	3
3	B	359	PX4	C25-C24	2.27	1.60	1.52	6	1
3	B	379	PX4	O7-C23	2.27	1.27	1.34	10	4
3	B	398	PX4	P1-O1	2.27	1.44	1.55	14	3
3	C	301	PX4	C5-N1	2.27	1.56	1.50	14	3
3	C	302	PX4	C2-N1	2.27	1.58	1.51	11	1
3	B	323	PX4	C11-C10	2.27	1.60	1.52	8	2
3	B	343	PX4	P1-O1	2.27	1.44	1.55	7	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	369	PX4	P1-O1	2.27	1.44	1.55	14	3
3	B	393	PX4	O7-C7	2.27	1.41	1.46	13	1
3	C	355	PX4	O4-C6	2.27	1.36	1.44	4	1
3	B	349	PX4	C10-C9	2.27	1.57	1.50	6	3
3	C	356	PX4	P1-O1	2.27	1.44	1.55	4	2
3	B	315	PX4	P1-O1	2.26	1.44	1.55	8	1
3	B	337	PX4	P1-O2	2.26	1.43	1.50	13	1
3	B	340	PX4	P1-O1	2.26	1.44	1.55	10	1
3	B	361	PX4	C5-N1	2.27	1.56	1.50	13	1
3	C	307	PX4	O5-C9	2.27	1.26	1.33	1	1
3	C	348	PX4	P1-O2	2.27	1.43	1.50	5	2
3	C	351	PX4	C34-C33	2.26	1.63	1.51	3	1
3	C	362	PX4	C10-C9	2.27	1.57	1.50	6	1
3	B	340	PX4	O5-C8	2.26	1.50	1.45	4	2
3	C	306	PX4	O5-C9	2.26	1.40	1.33	3	2
3	C	309	PX4	C4-N1	2.26	1.43	1.50	7	2
3	A	604	PX4	C25-C24	2.26	1.60	1.52	4	2
3	A	611	PX4	P1-O1	2.26	1.44	1.55	5	3
3	A	648	PX4	C28-C27	2.26	1.63	1.51	12	2
3	A	628	PX4	P1-O4	2.26	1.50	1.59	14	1
3	A	644	PX4	C16-C15	2.26	1.63	1.51	7	2
3	B	302	PX4	C24-C23	2.26	1.57	1.50	5	1
3	B	316	PX4	C5-N1	2.26	1.56	1.50	7	1
3	B	395	PX4	C24-C23	2.26	1.57	1.50	2	1
3	B	355	PX4	C33-C32	2.26	1.63	1.51	5	1
3	B	377	PX4	C4-N1	2.26	1.43	1.50	8	1
3	B	381	PX4	C24-C23	2.26	1.57	1.50	13	1
3	B	399	PX4	C30-C29	2.26	1.63	1.51	10	1
3	C	368	PX4	C31-C30	2.26	1.63	1.51	1	2
3	B	329	PX4	C30-C29	2.26	1.63	1.51	5	1
3	B	363	PX4	C3-N1	2.26	1.43	1.50	5	3
3	C	339	PX4	C13-C12	2.26	1.63	1.51	12	1
3	A	612	PX4	O7-C23	2.26	1.27	1.34	1	1
3	A	619	PX4	P1-O4	2.26	1.68	1.59	1	2
3	B	307	PX4	C14-C13	2.26	1.63	1.51	8	1
3	B	386	PX4	C17-C16	2.26	1.63	1.51	6	1
3	B	392	PX4	C2-N1	2.26	1.58	1.51	7	1
3	B	397	PX4	C13-C12	2.26	1.63	1.51	12	1
3	C	343	PX4	C3-N1	2.26	1.56	1.50	4	2
3	B	319	PX4	C4-N1	2.26	1.43	1.50	9	1
3	A	616	PX4	C24-C23	2.25	1.57	1.50	10	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	317	PX4	P1-O2	2.25	1.43	1.50	4	1
3	B	386	PX4	C3-N1	2.25	1.56	1.50	1	2
3	C	353	PX4	C5-N1	2.25	1.43	1.50	3	2
3	A	613	PX4	C32-C31	2.25	1.63	1.51	14	1
3	A	631	PX4	C30-C29	2.25	1.63	1.51	15	1
3	A	634	PX4	O7-C23	2.25	1.27	1.34	14	3
3	A	611	PX4	C29-C28	2.25	1.63	1.51	3	1
3	B	309	PX4	P1-O3	2.25	1.50	1.59	5	1
3	B	312	PX4	P1-O2	2.25	1.43	1.50	6	1
3	B	339	PX4	C2-C1	2.25	1.58	1.51	15	1
3	B	371	PX4	O5-C9	2.25	1.39	1.33	5	1
3	C	312	PX4	C14-C13	2.25	1.63	1.51	5	1
3	C	337	PX4	C4-N1	2.25	1.56	1.50	9	1
3	B	348	PX4	P1-O3	2.25	1.50	1.59	14	3
3	C	329	PX4	C25-C24	2.25	1.60	1.52	9	2
3	C	359	PX4	C4-N1	2.25	1.43	1.50	6	1
3	A	632	PX4	C3-N1	2.25	1.56	1.50	12	1
3	A	648	PX4	P1-O1	2.25	1.44	1.55	9	1
3	B	367	PX4	C4-N1	2.25	1.56	1.50	3	1
3	B	315	PX4	O7-C23	2.25	1.27	1.34	8	1
3	B	330	PX4	C4-N1	2.25	1.56	1.50	13	2
3	C	367	PX4	C13-C12	2.25	1.63	1.51	12	1
3	B	367	PX4	P1-O1	2.25	1.44	1.55	3	4
3	C	316	PX4	C13-C12	2.25	1.63	1.51	10	1
3	A	615	PX4	C34-C33	2.25	1.63	1.51	5	2
3	B	311	PX4	O7-C23	2.25	1.40	1.34	3	2
3	B	316	PX4	O7-C23	2.25	1.40	1.34	3	2
3	B	371	PX4	P1-O1	2.25	1.44	1.55	11	2
3	B	338	PX4	O7-C23	2.24	1.27	1.34	3	1
3	C	302	PX4	C13-C12	2.25	1.63	1.51	13	1
3	B	390	PX4	P1-O4	2.24	1.50	1.59	5	1
3	A	621	PX4	C20-C19	2.24	1.62	1.51	7	1
3	A	606	PX4	O7-C23	2.24	1.27	1.34	8	1
3	B	322	PX4	O7-C23	2.24	1.27	1.34	12	1
3	B	313	PX4	P1-O1	2.24	1.45	1.55	2	2
3	B	337	PX4	C27-C26	2.24	1.62	1.51	13	1
3	B	369	PX4	C11-C10	2.24	1.60	1.52	14	2
3	B	380	PX4	C2-N1	2.24	1.58	1.51	8	2
3	B	383	PX4	P1-O3	2.24	1.50	1.59	11	1
3	C	302	PX4	C17-C16	2.24	1.62	1.51	11	1
3	C	357	PX4	C5-N1	2.24	1.43	1.50	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	361	PX4	C26-C25	2.24	1.62	1.51	12	1
3	B	322	PX4	C3-N1	2.24	1.56	1.50	7	1
3	C	312	PX4	P1-O1	2.24	1.45	1.55	9	3
3	C	324	PX4	C2-N1	2.24	1.58	1.51	1	3
3	C	325	PX4	C5-N1	2.24	1.56	1.50	8	3
3	C	350	PX4	C31-C30	2.24	1.62	1.51	2	1
3	A	634	PX4	C11-C10	2.24	1.60	1.52	1	2
3	B	301	PX4	C2-N1	2.24	1.58	1.51	9	2
3	B	370	PX4	O7-C7	2.24	1.41	1.46	13	1
3	B	386	PX4	C10-C9	2.24	1.57	1.50	4	2
3	B	392	PX4	C34-C33	2.24	1.62	1.51	5	1
3	A	619	PX4	C15-C14	2.24	1.62	1.51	2	1
3	B	335	PX4	O5-C9	2.24	1.39	1.33	2	1
3	C	309	PX4	P1-O1	2.24	1.45	1.55	8	1
3	C	318	PX4	O7-C7	2.24	1.41	1.46	5	1
3	C	318	PX4	C2-N1	2.24	1.44	1.51	12	1
3	B	316	PX4	C19-C18	2.23	1.62	1.51	9	1
3	B	355	PX4	O5-C9	2.23	1.26	1.33	10	1
3	B	368	PX4	O5-C9	2.23	1.26	1.33	2	1
3	B	380	PX4	C3-N1	2.24	1.43	1.50	1	1
3	B	369	PX4	C2-N1	2.23	1.58	1.51	12	2
3	B	389	PX4	C5-N1	2.23	1.43	1.50	14	1
3	B	391	PX4	C28-C27	2.23	1.62	1.51	12	1
3	C	315	PX4	C5-N1	2.23	1.56	1.50	15	1
3	C	316	PX4	C29-C28	2.23	1.62	1.51	1	1
3	C	325	PX4	C18-C17	2.23	1.62	1.51	13	1
3	A	631	PX4	C32-C31	2.23	1.62	1.51	12	2
3	B	330	PX4	O5-C8	2.23	1.40	1.45	7	3
3	B	333	PX4	C13-C12	2.23	1.62	1.51	14	2
3	C	361	PX4	O7-C23	2.23	1.28	1.34	6	1
3	C	366	PX4	C25-C24	2.23	1.60	1.52	8	3
3	B	360	PX4	C3-N1	2.23	1.56	1.50	9	2
3	B	370	PX4	P1-O3	2.23	1.50	1.59	6	1
3	B	371	PX4	C27-C26	2.23	1.62	1.51	9	1
3	B	379	PX4	C34-C33	2.23	1.62	1.51	1	1
3	C	327	PX4	O5-C8	2.23	1.50	1.45	13	1
3	B	343	PX4	C24-C23	2.23	1.44	1.50	7	2
3	B	396	PX4	C20-C19	2.23	1.62	1.51	5	1
3	C	333	PX4	C11-C10	2.23	1.60	1.52	3	3
3	B	325	PX4	C4-N1	2.23	1.43	1.50	1	3
3	C	340	PX4	C3-N1	2.23	1.43	1.50	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	605	PX4	C30-C29	2.23	1.62	1.51	3	1
3	A	634	PX4	P1-O1	2.23	1.45	1.55	11	4
3	A	623	PX4	P1-O3	2.23	1.50	1.59	8	1
3	B	348	PX4	C19-C18	2.23	1.62	1.51	12	1
3	A	622	PX4	C25-C24	2.23	1.60	1.52	12	1
3	B	338	PX4	C11-C10	2.23	1.60	1.52	4	2
3	B	340	PX4	C33-C32	2.23	1.62	1.51	2	1
3	B	362	PX4	C26-C25	2.23	1.62	1.51	13	1
3	B	310	PX4	P1-O2	2.23	1.43	1.50	12	2
3	B	361	PX4	C24-C23	2.23	1.57	1.50	1	1
3	B	380	PX4	C28-C27	2.23	1.62	1.51	15	1
3	C	304	PX4	C2-N1	2.23	1.58	1.51	7	1
3	C	304	PX4	O3-C1	2.23	1.35	1.44	9	2
3	C	318	PX4	P1-O1	2.23	1.45	1.55	5	2
3	C	332	PX4	O3-C1	2.23	1.35	1.44	2	1
3	C	323	PX4	C33-C32	2.23	1.62	1.51	11	1
3	C	335	PX4	C32-C31	2.23	1.62	1.51	10	1
3	B	348	PX4	C33-C32	2.23	1.62	1.51	3	1
3	C	337	PX4	P1-O2	2.23	1.43	1.50	1	1
3	C	339	PX4	P1-O1	2.22	1.45	1.55	13	2
3	A	622	PX4	C20-C19	2.22	1.62	1.51	10	1
3	B	385	PX4	C28-C27	2.22	1.62	1.51	8	1
3	A	612	PX4	C2-N1	2.22	1.58	1.51	9	1
3	A	642	PX4	C11-C10	2.22	1.60	1.52	12	1
3	A	644	PX4	O7-C7	2.22	1.41	1.46	14	3
3	A	614	PX4	O7-C23	2.22	1.28	1.34	11	1
3	B	315	PX4	C25-C24	2.22	1.60	1.52	3	1
3	B	344	PX4	C16-C15	2.22	1.62	1.51	8	1
3	C	313	PX4	C12-C11	2.22	1.62	1.51	8	1
3	C	332	PX4	C19-C18	2.22	1.62	1.51	12	1
3	B	396	PX4	P1-O1	2.22	1.45	1.55	10	1
3	C	327	PX4	C12-C11	2.22	1.62	1.51	1	1
3	C	352	PX4	C10-C9	2.22	1.57	1.50	12	1
3	A	627	PX4	P1-O2	2.22	1.43	1.50	11	1
3	A	630	PX4	O5-C9	2.22	1.26	1.33	13	1
3	A	646	PX4	P1-O2	2.22	1.43	1.50	2	1
3	B	320	PX4	C27-C26	2.22	1.62	1.51	9	1
3	B	345	PX4	C10-C9	2.22	1.57	1.50	1	1
3	B	351	PX4	C16-C15	2.22	1.62	1.51	5	1
3	B	357	PX4	C25-C24	2.22	1.60	1.52	6	1
3	C	332	PX4	C13-C12	2.22	1.62	1.51	10	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	357	PX4	C17-C16	2.22	1.62	1.51	5	2
3	A	644	PX4	C10-C9	2.22	1.57	1.50	13	1
3	C	303	PX4	C4-N1	2.22	1.56	1.50	9	1
3	C	359	PX4	O5-C8	2.22	1.50	1.45	9	2
3	A	629	PX4	C25-C24	2.21	1.60	1.52	12	2
3	B	331	PX4	P1-O2	2.21	1.43	1.50	1	1
3	A	629	PX4	C17-C16	2.21	1.62	1.51	11	1
3	B	330	PX4	O4-C6	2.21	1.36	1.44	3	1
3	B	363	PX4	C4-N1	2.21	1.56	1.50	8	2
3	B	371	PX4	C11-C10	2.21	1.60	1.52	5	2
3	B	382	PX4	P1-O3	2.21	1.50	1.59	3	1
3	B	386	PX4	O5-C9	2.21	1.26	1.33	7	1
3	C	342	PX4	C14-C13	2.21	1.62	1.51	13	1
3	B	372	PX4	C13-C12	2.21	1.62	1.51	14	1
3	B	400	PX4	C5-N1	2.21	1.56	1.50	2	1
3	C	305	PX4	O4-C6	2.21	1.36	1.44	5	1
3	C	346	PX4	O5-C9	2.21	1.26	1.33	13	3
3	A	609	PX4	C28-C27	2.21	1.62	1.51	15	1
3	A	609	PX4	C11-C10	2.21	1.60	1.52	2	1
3	B	326	PX4	O5-C9	2.21	1.26	1.33	11	1
3	B	338	PX4	C12-C11	2.21	1.62	1.51	12	1
3	C	332	PX4	O4-C6	2.21	1.36	1.44	9	1
3	C	345	PX4	O5-C9	2.21	1.39	1.33	10	3
3	B	355	PX4	C31-C30	2.21	1.62	1.51	11	1
3	C	339	PX4	O7-C23	2.21	1.28	1.34	2	2
3	C	355	PX4	C18-C17	2.21	1.62	1.51	2	1
3	A	609	PX4	O7-C7	2.21	1.41	1.46	12	1
3	A	646	PX4	P1-O3	2.21	1.50	1.59	5	1
3	B	374	PX4	C31-C30	2.21	1.62	1.51	3	1
3	B	381	PX4	C30-C29	2.21	1.62	1.51	3	1
3	C	302	PX4	C5-N1	2.21	1.56	1.50	13	1
3	C	358	PX4	C30-C29	2.21	1.62	1.51	10	1
3	C	370	PX4	O7-C23	2.21	1.28	1.34	6	1
3	B	321	PX4	C24-C23	2.21	1.44	1.50	15	1
3	C	329	PX4	P1-O4	2.21	1.68	1.59	2	1
3	B	312	PX4	C15-C14	2.21	1.62	1.51	1	1
3	A	606	PX4	O5-C9	2.21	1.26	1.33	7	1
3	B	336	PX4	C2-N1	2.21	1.58	1.51	6	2
3	B	388	PX4	C13-C12	2.21	1.62	1.51	13	1
3	B	391	PX4	C6-C7	2.21	1.57	1.50	5	3
3	B	337	PX4	O5-C9	2.20	1.26	1.33	1	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	333	PX4	C5-N1	2.21	1.43	1.50	7	1
3	A	625	PX4	C28-C27	2.20	1.62	1.51	15	1
3	B	310	PX4	C12-C11	2.20	1.62	1.51	6	1
3	B	320	PX4	C25-C24	2.20	1.60	1.52	2	1
3	B	329	PX4	O7-C7	2.20	1.41	1.46	9	1
3	B	330	PX4	C20-C19	2.20	1.62	1.51	1	1
3	B	342	PX4	P1-O1	2.20	1.45	1.55	15	3
3	B	345	PX4	C30-C29	2.20	1.62	1.51	3	1
3	B	368	PX4	C10-C9	2.20	1.57	1.50	14	1
3	C	326	PX4	C29-C28	2.20	1.62	1.51	4	1
3	C	342	PX4	C33-C32	2.20	1.62	1.51	9	1
3	A	617	PX4	C5-N1	2.20	1.56	1.50	12	1
3	B	341	PX4	C5-N1	2.20	1.56	1.50	15	2
3	B	351	PX4	C26-C25	2.20	1.62	1.51	9	1
3	B	325	PX4	C28-C27	2.20	1.62	1.51	3	1
3	C	317	PX4	P1-O3	2.20	1.50	1.59	13	1
3	C	349	PX4	C4-N1	2.20	1.56	1.50	1	1
3	C	368	PX4	P1-O1	2.20	1.45	1.55	11	3
3	C	369	PX4	P1-O1	2.20	1.45	1.55	5	4
3	A	612	PX4	C5-N1	2.20	1.56	1.50	12	1
3	B	313	PX4	C25-C24	2.20	1.60	1.52	13	1
3	B	316	PX4	P1-O4	2.20	1.50	1.59	8	1
3	A	648	PX4	C3-N1	2.20	1.43	1.50	7	1
3	B	338	PX4	P1-O1	2.20	1.45	1.55	9	3
3	B	364	PX4	O5-C8	2.20	1.50	1.45	10	1
3	C	327	PX4	P1-O2	2.20	1.43	1.50	11	1
3	C	360	PX4	C26-C25	2.20	1.62	1.51	13	2
3	A	605	PX4	C28-C27	2.20	1.62	1.51	5	1
3	A	612	PX4	P1-O4	2.19	1.50	1.59	2	1
3	A	612	PX4	O4-C6	2.19	1.36	1.44	10	1
3	A	612	PX4	C4-N1	2.20	1.56	1.50	12	1
3	A	633	PX4	P1-O3	2.20	1.50	1.59	1	1
3	B	372	PX4	C29-C28	2.20	1.62	1.51	11	1
3	B	374	PX4	P1-O3	2.19	1.50	1.59	10	1
3	C	306	PX4	O5-C8	2.20	1.40	1.45	6	4
3	A	609	PX4	C17-C16	2.19	1.62	1.51	1	1
3	B	308	PX4	P1-O1	2.19	1.45	1.55	11	4
3	C	313	PX4	C27-C26	2.19	1.62	1.51	1	1
3	C	324	PX4	C14-C13	2.19	1.62	1.51	2	1
3	A	606	PX4	C24-C23	2.19	1.57	1.50	12	2
3	B	348	PX4	C11-C10	2.19	1.60	1.52	11	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	305	PX4	P1-O4	2.19	1.50	1.59	2	1
3	B	364	PX4	C10-C9	2.19	1.57	1.50	4	2
3	B	386	PX4	C15-C14	2.19	1.62	1.51	5	1
3	C	314	PX4	C11-C10	2.19	1.60	1.52	8	1
3	C	341	PX4	C13-C12	2.19	1.62	1.51	14	1
3	C	342	PX4	C5-N1	2.19	1.43	1.50	10	1
3	C	351	PX4	P1-O3	2.19	1.50	1.59	15	1
3	B	301	PX4	C15-C14	2.19	1.62	1.51	15	1
3	B	311	PX4	C14-C13	2.19	1.62	1.51	1	1
3	A	624	PX4	C3-N1	2.19	1.43	1.50	13	1
3	B	330	PX4	O5-C9	2.19	1.39	1.33	7	1
3	B	337	PX4	O5-C8	2.19	1.40	1.45	10	1
3	B	365	PX4	C2-N1	2.19	1.44	1.51	8	2
3	C	322	PX4	C2-C1	2.19	1.57	1.51	6	2
3	C	329	PX4	O5-C9	2.19	1.39	1.33	6	2
3	B	353	PX4	O4-C6	2.19	1.36	1.44	13	1
3	B	310	PX4	C4-N1	2.19	1.56	1.50	15	2
3	B	336	PX4	C4-N1	2.19	1.56	1.50	13	1
3	B	355	PX4	C5-N1	2.19	1.56	1.50	15	1
3	B	366	PX4	O5-C8	2.19	1.50	1.45	1	2
3	B	367	PX4	C26-C25	2.19	1.62	1.51	13	1
3	B	374	PX4	C3-N1	2.19	1.43	1.50	10	1
3	B	394	PX4	C33-C32	2.19	1.62	1.51	10	1
3	B	396	PX4	C15-C14	2.19	1.62	1.51	9	1
3	C	318	PX4	C25-C24	2.19	1.60	1.52	13	2
3	C	320	PX4	C3-N1	2.19	1.43	1.50	10	2
3	C	332	PX4	O7-C7	2.19	1.41	1.46	13	1
3	C	352	PX4	O5-C9	2.19	1.27	1.33	4	1
3	C	331	PX4	O5-C9	2.19	1.27	1.33	5	1
3	C	364	PX4	P1-O1	2.19	1.45	1.55	1	2
3	A	601	PX4	C4-N1	2.19	1.43	1.50	12	1
3	A	605	PX4	P1-O2	2.19	1.43	1.50	3	1
3	A	633	PX4	C25-C24	2.19	1.60	1.52	6	1
3	B	323	PX4	C28-C27	2.19	1.62	1.51	7	1
3	B	349	PX4	P1-O1	2.19	1.45	1.55	15	3
3	B	366	PX4	C25-C24	2.19	1.60	1.52	15	3
3	B	370	PX4	O7-C23	2.19	1.28	1.34	14	2
3	B	387	PX4	C4-N1	2.19	1.56	1.50	10	1
3	B	398	PX4	C27-C26	2.19	1.62	1.51	12	2
3	C	307	PX4	C2-N1	2.19	1.58	1.51	1	1
3	C	309	PX4	C3-N1	2.19	1.43	1.50	13	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	332	PX4	C3-N1	2.19	1.43	1.50	14	1
3	C	329	PX4	C3-N1	2.19	1.43	1.50	8	1
3	C	361	PX4	C30-C29	2.18	1.62	1.51	5	1
3	C	364	PX4	C33-C32	2.19	1.62	1.51	11	1
3	A	641	PX4	O7-C23	2.18	1.40	1.34	6	1
3	A	629	PX4	P1-O3	2.18	1.67	1.59	15	1
3	A	641	PX4	C13-C12	2.18	1.62	1.51	13	1
3	A	647	PX4	O7-C23	2.18	1.28	1.34	10	1
3	B	314	PX4	C2-N1	2.18	1.58	1.51	10	1
3	B	321	PX4	P1-O1	2.18	1.45	1.55	2	1
3	B	333	PX4	C12-C11	2.18	1.62	1.51	15	1
3	B	356	PX4	C4-N1	2.18	1.43	1.50	4	2
3	C	313	PX4	O5-C9	2.18	1.39	1.33	9	1
3	B	323	PX4	C4-N1	2.18	1.56	1.50	4	1
3	B	394	PX4	C25-C24	2.18	1.60	1.52	8	1
3	A	607	PX4	C25-C24	2.18	1.60	1.52	6	1
3	A	610	PX4	O7-C7	2.18	1.41	1.46	8	2
3	A	616	PX4	O8-C23	2.18	1.29	1.22	1	1
3	A	647	PX4	O5-C9	2.18	1.27	1.33	6	2
3	C	347	PX4	C5-N1	2.18	1.56	1.50	11	1
3	C	365	PX4	C4-N1	2.18	1.56	1.50	2	1
3	B	315	PX4	C32-C31	2.18	1.62	1.51	12	1
3	A	628	PX4	C27-C26	2.18	1.62	1.51	10	1
3	B	304	PX4	C3-N1	2.18	1.56	1.50	4	1
3	A	648	PX4	C13-C12	2.18	1.62	1.51	14	1
3	A	608	PX4	P1-O1	2.18	1.45	1.55	12	3
3	B	305	PX4	P1-O1	2.18	1.45	1.55	6	1
3	B	330	PX4	C15-C14	2.18	1.62	1.51	7	1
3	B	331	PX4	P1-O1	2.18	1.45	1.55	3	1
3	B	331	PX4	O7-C23	2.18	1.28	1.34	7	1
3	B	332	PX4	P1-O4	2.18	1.50	1.59	8	1
3	C	307	PX4	C5-N1	2.18	1.56	1.50	9	1
3	C	342	PX4	C4-N1	2.18	1.56	1.50	8	1
3	C	359	PX4	P1-O3	2.18	1.50	1.59	3	2
3	B	354	PX4	P1-O3	2.18	1.50	1.59	7	1
3	C	313	PX4	C31-C30	2.18	1.62	1.51	1	1
3	C	351	PX4	C32-C31	2.18	1.62	1.51	14	1
3	C	361	PX4	C28-C27	2.18	1.62	1.51	6	1
3	C	323	PX4	C34-C33	2.18	1.62	1.51	11	1
3	B	357	PX4	C32-C31	2.17	1.62	1.51	15	2
3	B	350	PX4	O3-C1	2.17	1.36	1.44	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	307	PX4	P1-O3	2.17	1.50	1.59	15	1
3	A	601	PX4	O5-C9	2.17	1.39	1.33	3	1
3	A	604	PX4	C34-C33	2.17	1.62	1.51	6	1
3	C	335	PX4	C3-N1	2.17	1.56	1.50	6	1
3	C	353	PX4	O5-C8	2.17	1.50	1.45	13	1
3	A	642	PX4	P1-O1	2.17	1.45	1.55	9	1
3	B	361	PX4	O5-C9	2.17	1.27	1.33	6	1
3	B	399	PX4	O3-C1	2.17	1.36	1.44	1	1
3	C	338	PX4	C3-N1	2.17	1.43	1.50	11	1
3	C	318	PX4	O5-C8	2.17	1.40	1.45	14	2
3	C	321	PX4	P1-O2	2.17	1.43	1.50	11	1
3	B	312	PX4	C5-N1	2.17	1.56	1.50	2	1
3	B	338	PX4	O5-C9	2.17	1.39	1.33	9	1
3	B	314	PX4	C12-C11	2.17	1.62	1.51	8	1
3	B	319	PX4	C3-N1	2.17	1.56	1.50	12	1
3	B	326	PX4	P1-O1	2.17	1.45	1.55	12	3
3	B	329	PX4	O3-C1	2.17	1.36	1.44	7	1
3	B	352	PX4	C2-N1	2.17	1.58	1.51	4	1
3	B	391	PX4	P1-O1	2.17	1.45	1.55	13	2
3	A	621	PX4	C4-N1	2.17	1.43	1.50	9	1
3	B	341	PX4	C11-C10	2.17	1.60	1.52	8	1
3	B	348	PX4	C4-N1	2.17	1.56	1.50	9	1
3	A	601	PX4	O3-C1	2.17	1.36	1.44	4	1
3	A	632	PX4	C29-C28	2.17	1.62	1.51	15	1
3	B	303	PX4	P1-O1	2.17	1.45	1.55	10	2
3	B	307	PX4	P1-O3	2.17	1.50	1.59	4	1
3	C	303	PX4	C31-C30	2.17	1.62	1.51	7	1
3	C	319	PX4	O5-C9	2.17	1.39	1.33	15	1
3	C	347	PX4	C14-C13	2.17	1.62	1.51	14	1
3	C	356	PX4	C19-C18	2.17	1.62	1.51	15	1
3	A	630	PX4	C4-N1	2.17	1.56	1.50	9	1
3	B	364	PX4	P1-O1	2.17	1.45	1.55	11	2
3	C	346	PX4	O7-C7	2.17	1.41	1.46	13	2
3	C	353	PX4	P1-O1	2.17	1.45	1.55	7	4
3	B	322	PX4	O5-C9	2.17	1.27	1.33	2	1
3	B	324	PX4	C17-C16	2.17	1.62	1.51	11	1
3	B	358	PX4	C18-C17	2.17	1.62	1.51	12	1
3	A	604	PX4	C3-N1	2.16	1.56	1.50	8	1
3	A	619	PX4	C25-C24	2.16	1.60	1.52	5	2
3	B	355	PX4	C17-C16	2.16	1.62	1.51	7	1
3	B	358	PX4	O7-C23	2.17	1.40	1.34	13	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	605	PX4	C3-N1	2.16	1.56	1.50	9	1
3	B	325	PX4	O5-C9	2.16	1.27	1.33	14	1
3	B	335	PX4	P1-O3	2.16	1.50	1.59	1	1
3	B	355	PX4	P1-O4	2.16	1.50	1.59	1	1
3	C	331	PX4	C27-C26	2.16	1.62	1.51	6	1
3	C	345	PX4	P1-O2	2.16	1.43	1.50	10	2
3	C	364	PX4	C10-C9	2.16	1.57	1.50	1	1
3	A	608	PX4	C30-C29	2.16	1.62	1.51	9	1
3	B	318	PX4	C11-C10	2.16	1.60	1.52	10	2
3	B	354	PX4	C2-C1	2.16	1.57	1.51	13	2
3	C	316	PX4	P1-O2	2.16	1.43	1.50	3	1
3	B	376	PX4	C32-C31	2.16	1.62	1.51	12	1
3	C	327	PX4	C18-C17	2.16	1.62	1.51	10	1
3	A	611	PX4	C35-C34	2.16	1.65	1.51	6	1
3	A	644	PX4	C5-N1	2.16	1.56	1.50	13	1
3	B	312	PX4	C3-N1	2.16	1.56	1.50	7	1
3	B	392	PX4	C30-C29	2.16	1.62	1.51	15	1
3	B	370	PX4	C27-C26	2.16	1.62	1.51	11	1
3	B	397	PX4	C18-C17	2.16	1.62	1.51	13	2
3	C	307	PX4	C13-C12	2.16	1.62	1.51	4	1
3	A	627	PX4	C31-C30	2.16	1.62	1.51	9	1
3	B	391	PX4	C20-C19	2.16	1.62	1.51	1	1
3	C	336	PX4	C13-C12	2.16	1.62	1.51	9	1
3	C	338	PX4	C4-N1	2.16	1.43	1.50	12	1
3	C	343	PX4	P1-O4	2.16	1.50	1.59	12	2
3	B	336	PX4	C25-C24	2.16	1.60	1.52	4	1
3	C	348	PX4	C3-N1	2.16	1.43	1.50	8	2
3	A	641	PX4	P1-O1	2.16	1.45	1.55	8	2
3	A	633	PX4	C15-C14	2.16	1.62	1.51	8	1
3	B	329	PX4	C11-C10	2.16	1.60	1.52	14	2
3	B	352	PX4	C14-C13	2.16	1.62	1.51	10	1
3	C	305	PX4	C31-C30	2.16	1.62	1.51	8	1
3	C	353	PX4	C34-C33	2.16	1.62	1.51	7	1
3	B	388	PX4	P1-O1	2.16	1.45	1.55	10	1
3	C	333	PX4	O4-C6	2.16	1.36	1.44	5	1
3	B	313	PX4	C5-N1	2.15	1.56	1.50	10	2
3	A	614	PX4	C13-C12	2.15	1.62	1.51	3	1
3	A	620	PX4	C2-N1	2.15	1.58	1.51	12	1
3	B	337	PX4	P1-O4	2.15	1.51	1.59	8	1
3	C	313	PX4	O4-C6	2.15	1.36	1.44	15	1
3	C	329	PX4	C11-C10	2.15	1.60	1.52	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	336	PX4	C4-N1	2.15	1.43	1.50	8	2
3	C	344	PX4	C32-C31	2.15	1.62	1.51	6	1
3	A	603	PX4	C2-N1	2.15	1.58	1.51	1	1
3	A	614	PX4	C4-N1	2.15	1.56	1.50	14	1
3	A	627	PX4	O7-C7	2.15	1.41	1.46	1	2
3	A	634	PX4	C10-C9	2.15	1.57	1.50	12	2
3	B	362	PX4	C34-C33	2.15	1.62	1.51	10	1
3	B	395	PX4	C19-C18	2.15	1.62	1.51	13	1
3	C	357	PX4	C11-C10	2.15	1.60	1.52	10	1
3	A	637	PX4	O7-C23	2.15	1.40	1.34	10	1
3	A	601	PX4	C5-N1	2.15	1.56	1.50	12	2
3	A	602	PX4	C16-C15	2.15	1.62	1.51	12	1
3	A	628	PX4	O3-C1	2.15	1.36	1.44	14	1
3	A	640	PX4	C2-N1	2.15	1.44	1.51	2	1
3	A	646	PX4	C4-N1	2.15	1.56	1.50	7	1
3	B	319	PX4	P1-O3	2.15	1.51	1.59	6	1
3	B	326	PX4	P1-O3	2.15	1.67	1.59	9	1
3	B	349	PX4	C11-C10	2.15	1.60	1.52	1	1
3	B	379	PX4	C13-C12	2.15	1.62	1.51	4	1
3	B	399	PX4	P1-O3	2.15	1.51	1.59	10	1
3	C	316	PX4	C28-C27	2.15	1.62	1.51	12	1
3	C	324	PX4	O7-C23	2.15	1.28	1.34	14	2
3	C	369	PX4	C20-C19	2.15	1.62	1.51	10	1
3	C	370	PX4	C20-C19	2.15	1.62	1.51	1	1
3	A	601	PX4	P1-O1	2.15	1.45	1.55	15	3
3	B	367	PX4	C25-C24	2.15	1.60	1.52	8	1
3	B	392	PX4	P1-O4	2.15	1.51	1.59	9	1
3	B	379	PX4	P1-O2	2.15	1.43	1.50	5	1
3	B	389	PX4	P1-O2	2.15	1.43	1.50	15	1
3	C	362	PX4	C26-C25	2.15	1.62	1.51	2	1
3	A	602	PX4	O3-C1	2.15	1.36	1.44	15	1
3	A	608	PX4	C2-N1	2.15	1.44	1.51	10	1
3	A	640	PX4	C28-C27	2.15	1.62	1.51	3	1
3	B	382	PX4	C11-C10	2.15	1.60	1.52	3	2
3	B	398	PX4	C12-C11	2.15	1.62	1.51	5	1
3	B	312	PX4	O7-C7	2.15	1.41	1.46	14	1
3	A	602	PX4	O4-C6	2.15	1.36	1.44	9	1
3	A	645	PX4	C29-C28	2.15	1.62	1.51	3	1
3	B	306	PX4	C13-C12	2.15	1.62	1.51	5	1
3	B	327	PX4	C3-N1	2.15	1.56	1.50	13	1
3	B	338	PX4	C5-N1	2.14	1.43	1.50	12	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	341	PX4	C2-N1	2.15	1.44	1.51	11	1
3	B	370	PX4	C3-N1	2.15	1.56	1.50	9	1
3	B	380	PX4	C26-C25	2.15	1.62	1.51	12	1
3	B	387	PX4	C32-C31	2.14	1.62	1.51	11	1
3	B	376	PX4	C25-C24	2.14	1.60	1.52	13	2
3	B	392	PX4	C32-C31	2.14	1.62	1.51	5	1
3	C	320	PX4	C25-C24	2.14	1.60	1.52	15	1
3	C	365	PX4	C25-C24	2.14	1.60	1.52	7	2
3	B	309	PX4	C24-C23	2.14	1.56	1.50	2	1
3	B	350	PX4	O5-C9	2.14	1.39	1.33	13	1
3	B	355	PX4	P1-O3	2.14	1.51	1.59	14	1
3	C	361	PX4	C27-C26	2.14	1.62	1.51	5	1
3	C	366	PX4	C26-C25	2.14	1.62	1.51	12	1
3	B	301	PX4	C24-C23	2.14	1.56	1.50	10	4
3	B	323	PX4	C13-C12	2.14	1.62	1.51	13	1
3	B	381	PX4	P1-O2	2.14	1.43	1.50	8	1
3	B	355	PX4	C12-C11	2.14	1.62	1.51	15	1
3	C	364	PX4	C31-C30	2.14	1.62	1.51	6	1
3	C	314	PX4	C24-C23	2.14	1.56	1.50	10	2
3	C	318	PX4	C5-N1	2.14	1.56	1.50	4	1
3	C	319	PX4	O5-C8	2.14	1.49	1.45	12	1
3	C	342	PX4	C19-C18	2.14	1.62	1.51	13	1
3	C	359	PX4	C11-C10	2.14	1.60	1.52	3	1
3	A	643	PX4	C3-N1	2.14	1.56	1.50	2	1
3	C	352	PX4	O5-C8	2.14	1.49	1.45	10	2
3	C	361	PX4	O4-C6	2.14	1.36	1.44	7	1
3	C	363	PX4	O5-C9	2.14	1.39	1.33	10	1
3	B	309	PX4	C33-C32	2.14	1.62	1.51	13	1
3	B	372	PX4	C28-C27	2.14	1.62	1.51	9	1
3	C	343	PX4	C5-N1	2.14	1.56	1.50	13	1
3	C	354	PX4	O5-C8	2.14	1.40	1.45	13	2
3	B	352	PX4	C31-C30	2.14	1.62	1.51	2	1
3	A	615	PX4	C5-N1	2.14	1.56	1.50	7	2
3	A	616	PX4	C25-C24	2.14	1.44	1.52	12	2
3	B	394	PX4	C4-N1	2.14	1.56	1.50	8	1
3	C	310	PX4	O7-C7	2.14	1.41	1.46	7	1
3	C	333	PX4	C33-C32	2.14	1.62	1.51	14	1
3	B	379	PX4	C25-C24	2.14	1.60	1.52	4	3
3	C	308	PX4	C31-C30	2.14	1.62	1.51	5	1
3	C	318	PX4	P1-O3	2.14	1.67	1.59	13	1
3	C	343	PX4	C14-C13	2.14	1.62	1.51	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	602	PX4	O7-C23	2.13	1.28	1.34	6	1
3	A	644	PX4	C32-C31	2.13	1.62	1.51	11	1
3	B	399	PX4	C12-C11	2.13	1.62	1.51	8	1
3	C	301	PX4	P1-O2	2.13	1.43	1.50	9	1
3	B	323	PX4	C15-C14	2.13	1.62	1.51	8	1
3	C	302	PX4	P1-O1	2.13	1.45	1.55	14	2
3	C	329	PX4	P1-O1	2.13	1.45	1.55	2	1
3	C	349	PX4	P1-O2	2.13	1.43	1.50	10	1
3	C	367	PX4	O7-C7	2.13	1.41	1.46	12	2
3	A	605	PX4	C16-C15	2.13	1.62	1.51	8	1
3	A	606	PX4	P1-O1	2.13	1.45	1.55	10	1
3	B	307	PX4	C3-N1	2.13	1.56	1.50	4	1
3	A	635	PX4	O4-C6	2.13	1.52	1.44	3	1
3	B	320	PX4	C33-C32	2.13	1.62	1.51	11	1
3	B	321	PX4	C16-C15	2.13	1.62	1.51	4	1
3	B	331	PX4	O5-C8	2.13	1.49	1.45	15	2
3	B	351	PX4	P1-O1	2.13	1.45	1.55	12	2
3	B	353	PX4	C34-C33	2.13	1.62	1.51	11	1
3	B	395	PX4	C4-N1	2.13	1.56	1.50	5	1
3	C	347	PX4	C2-N1	2.13	1.58	1.51	12	1
3	C	370	PX4	O5-C9	2.13	1.39	1.33	4	1
3	B	353	PX4	O7-C23	2.13	1.28	1.34	2	1
3	A	603	PX4	C24-C23	2.13	1.56	1.50	2	1
3	A	626	PX4	C16-C15	2.13	1.62	1.51	10	1
3	C	301	PX4	O5-C8	2.13	1.49	1.45	11	1
3	A	630	PX4	P1-O1	2.13	1.45	1.55	10	1
3	A	637	PX4	P1-O4	2.13	1.67	1.59	3	2
3	A	638	PX4	C31-C30	2.13	1.62	1.51	10	1
3	B	360	PX4	C2-N1	2.13	1.58	1.51	15	1
3	C	324	PX4	C27-C26	2.13	1.62	1.51	2	1
3	A	616	PX4	C27-C26	2.13	1.62	1.51	12	2
3	A	616	PX4	C28-C27	2.13	1.62	1.51	15	1
3	A	627	PX4	C12-C11	2.13	1.62	1.51	13	1
3	A	647	PX4	C4-N1	2.13	1.43	1.50	15	2
3	B	375	PX4	C14-C13	2.13	1.62	1.51	13	1
3	B	398	PX4	C33-C32	2.13	1.62	1.51	11	2
3	C	315	PX4	P1-O3	2.13	1.51	1.59	4	1
3	C	355	PX4	P1-O4	2.13	1.51	1.59	9	1
3	C	358	PX4	O4-C6	2.13	1.36	1.44	2	1
3	C	365	PX4	C15-C14	2.13	1.62	1.51	2	1
3	B	322	PX4	C16-C15	2.13	1.41	1.51	13	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	325	PX4	C27-C26	2.13	1.62	1.51	2	1
3	A	626	PX4	C2-N1	2.12	1.57	1.51	15	2
3	B	303	PX4	C2-N1	2.13	1.57	1.51	11	2
3	B	311	PX4	O5-C9	2.12	1.39	1.33	1	1
3	B	344	PX4	O4-C6	2.13	1.36	1.44	5	1
3	B	355	PX4	O5-C8	2.13	1.40	1.45	14	1
3	B	359	PX4	C14-C13	2.13	1.62	1.51	12	1
3	B	360	PX4	P1-O1	2.13	1.45	1.55	1	1
3	B	372	PX4	C33-C32	2.13	1.62	1.51	11	1
3	C	331	PX4	C3-N1	2.13	1.56	1.50	1	1
3	B	387	PX4	O5-C9	2.12	1.27	1.33	4	1
3	C	321	PX4	O5-C8	2.13	1.40	1.45	1	1
3	A	636	PX4	O4-C6	2.12	1.36	1.44	15	1
3	A	645	PX4	C2-N1	2.12	1.57	1.51	2	1
3	C	302	PX4	P1-O3	2.12	1.51	1.59	5	1
3	C	347	PX4	O3-C1	2.12	1.36	1.44	7	1
3	C	356	PX4	C28-C27	2.12	1.62	1.51	6	1
3	A	614	PX4	C5-N1	2.12	1.56	1.50	11	2
3	B	392	PX4	C14-C13	2.12	1.62	1.51	4	1
3	B	397	PX4	C25-C24	2.12	1.60	1.52	11	1
3	C	304	PX4	C3-N1	2.12	1.56	1.50	2	1
3	C	304	PX4	O5-C8	2.12	1.40	1.45	7	2
3	C	305	PX4	C34-C33	2.12	1.62	1.51	11	1
3	C	309	PX4	C13-C12	2.12	1.62	1.51	6	1
3	A	601	PX4	C14-C13	2.12	1.62	1.51	6	1
3	A	623	PX4	C15-C14	2.12	1.62	1.51	6	1
3	A	642	PX4	C20-C19	2.12	1.62	1.51	14	2
3	C	324	PX4	P1-O4	2.12	1.51	1.59	1	1
3	C	331	PX4	C24-C23	2.12	1.44	1.50	2	1
3	C	354	PX4	C33-C32	2.12	1.62	1.51	6	1
3	A	632	PX4	C27-C26	2.12	1.62	1.51	7	2
3	B	337	PX4	C14-C13	2.12	1.62	1.51	7	1
3	A	637	PX4	C29-C28	2.12	1.62	1.51	5	1
3	B	344	PX4	P1-O2	2.12	1.43	1.50	2	1
3	B	354	PX4	C29-C28	2.12	1.62	1.51	6	1
3	C	310	PX4	O4-C6	2.12	1.36	1.44	3	1
3	C	313	PX4	C29-C28	2.12	1.62	1.51	8	2
3	C	341	PX4	C3-N1	2.12	1.56	1.50	11	1
3	C	352	PX4	C19-C18	2.12	1.62	1.51	13	1
3	B	311	PX4	C5-N1	2.12	1.43	1.50	14	1
3	B	326	PX4	C31-C30	2.12	1.62	1.51	1	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	340	PX4	C3-N1	2.12	1.56	1.50	7	2
3	A	608	PX4	C3-N1	2.12	1.43	1.50	12	1
3	A	613	PX4	C4-N1	2.12	1.56	1.50	6	1
3	A	647	PX4	O5-C8	2.12	1.40	1.45	15	2
3	B	335	PX4	C13-C12	2.12	1.62	1.51	3	1
3	B	357	PX4	O7-C23	2.12	1.28	1.34	9	1
3	B	374	PX4	C12-C11	2.12	1.62	1.51	15	1
3	C	308	PX4	C4-N1	2.12	1.43	1.50	10	1
3	A	611	PX4	C26-C25	2.11	1.62	1.51	15	1
3	C	351	PX4	O5-C9	2.12	1.39	1.33	3	2
3	A	636	PX4	C15-C14	2.11	1.62	1.51	14	1
3	A	642	PX4	C3-N1	2.11	1.56	1.50	8	2
3	B	354	PX4	C27-C26	2.11	1.62	1.51	11	1
3	C	339	PX4	C5-N1	2.11	1.56	1.50	5	1
3	B	397	PX4	P1-O4	2.11	1.51	1.59	3	1
3	C	310	PX4	C4-N1	2.11	1.56	1.50	11	1
3	C	360	PX4	C18-C17	2.11	1.62	1.51	8	1
3	A	609	PX4	C25-C24	2.11	1.59	1.52	7	1
3	A	619	PX4	P1-O3	2.11	1.51	1.59	14	1
3	B	317	PX4	C32-C31	2.11	1.62	1.51	14	1
3	C	365	PX4	C13-C12	2.11	1.62	1.51	3	1
3	B	312	PX4	C27-C26	2.11	1.62	1.51	1	1
3	B	340	PX4	C27-C26	2.11	1.62	1.51	5	1
3	B	343	PX4	O7-C23	2.11	1.40	1.34	1	1
3	B	385	PX4	P1-O2	2.11	1.43	1.50	12	1
3	B	390	PX4	C20-C19	2.11	1.62	1.51	1	1
3	B	391	PX4	C5-N1	2.11	1.56	1.50	5	1
3	C	315	PX4	O7-C23	2.11	1.40	1.34	1	1
3	C	336	PX4	C2-N1	2.11	1.45	1.51	5	1
3	C	354	PX4	C18-C17	2.11	1.62	1.51	2	1
3	A	646	PX4	O4-C6	2.11	1.36	1.44	2	1
3	B	301	PX4	C3-N1	2.11	1.56	1.50	6	3
3	B	334	PX4	C2-N1	2.11	1.57	1.51	4	1
3	A	613	PX4	O4-C6	2.11	1.52	1.44	8	1
3	A	614	PX4	C16-C15	2.11	1.62	1.51	15	1
3	A	636	PX4	C16-C15	2.11	1.62	1.51	15	1
3	B	312	PX4	O4-C6	2.11	1.36	1.44	2	1
3	B	343	PX4	C4-N1	2.11	1.56	1.50	12	1
3	C	349	PX4	C5-N1	2.11	1.43	1.50	2	1
3	A	641	PX4	C5-N1	2.11	1.56	1.50	13	1
3	B	337	PX4	C16-C15	2.10	1.62	1.51	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	338	PX4	C28-C27	2.10	1.62	1.51	14	1
3	B	350	PX4	P1-O1	2.11	1.45	1.55	3	4
3	B	359	PX4	C27-C26	2.11	1.62	1.51	10	1
3	B	362	PX4	C4-N1	2.11	1.56	1.50	13	1
3	B	367	PX4	C2-N1	2.11	1.57	1.51	7	1
3	B	398	PX4	C28-C27	2.10	1.62	1.51	6	1
3	C	342	PX4	C25-C24	2.11	1.59	1.52	5	3
3	B	306	PX4	C26-C25	2.10	1.62	1.51	12	1
3	B	350	PX4	O7-C23	2.10	1.40	1.34	1	1
3	B	357	PX4	C30-C29	2.10	1.62	1.51	4	1
3	B	358	PX4	C4-N1	2.10	1.43	1.50	8	1
3	B	395	PX4	C34-C33	2.10	1.62	1.51	8	1
3	B	368	PX4	C31-C30	2.10	1.62	1.51	12	1
3	B	389	PX4	C20-C19	2.10	1.62	1.51	12	1
3	C	326	PX4	C11-C10	2.10	1.59	1.52	15	1
3	B	397	PX4	C12-C11	2.10	1.62	1.51	13	1
3	C	308	PX4	C2-N1	2.10	1.57	1.51	4	2
3	A	631	PX4	O6-C9	2.10	1.16	1.22	2	1
3	B	319	PX4	C13-C12	2.10	1.62	1.51	2	1
3	B	326	PX4	O7-C23	2.10	1.28	1.34	9	1
3	C	321	PX4	C19-C18	2.10	1.62	1.51	6	1
3	C	367	PX4	P1-O3	2.10	1.51	1.59	7	1
3	A	618	PX4	C20-C19	2.10	1.62	1.51	15	1
3	A	624	PX4	O5-C8	2.10	1.49	1.45	8	1
3	B	306	PX4	O8-C23	2.10	1.28	1.22	12	1
3	B	328	PX4	C11-C10	2.10	1.59	1.52	4	2
3	B	368	PX4	C17-C16	2.10	1.62	1.51	4	1
3	C	316	PX4	C32-C31	2.10	1.62	1.51	12	1
3	C	328	PX4	P1-O1	2.10	1.45	1.55	11	1
3	C	317	PX4	O5-C8	2.10	1.49	1.45	9	1
3	C	364	PX4	C25-C24	2.10	1.59	1.52	7	1
3	C	369	PX4	C33-C32	2.10	1.62	1.51	14	1
3	B	301	PX4	C25-C24	2.10	1.59	1.52	3	1
3	B	302	PX4	C36-C35	2.10	1.65	1.50	8	1
3	B	323	PX4	P1-O1	2.10	1.45	1.55	6	1
3	B	327	PX4	C17-C16	2.10	1.62	1.51	10	1
3	B	370	PX4	C13-C12	2.10	1.62	1.51	13	1
3	C	341	PX4	C26-C25	2.10	1.62	1.51	12	1
3	B	340	PX4	P1-O4	2.10	1.51	1.59	11	1
3	C	321	PX4	C18-C17	2.10	1.62	1.51	1	1
3	C	335	PX4	C27-C26	2.09	1.62	1.51	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	342	PX4	C31-C30	2.10	1.62	1.51	12	1
3	C	368	PX4	P1-O3	2.10	1.51	1.59	9	1
3	A	647	PX4	C3-N1	2.09	1.56	1.50	13	2
3	A	633	PX4	C34-C33	2.09	1.62	1.51	12	1
3	B	310	PX4	O7-C23	2.09	1.28	1.34	10	1
3	B	364	PX4	P1-O4	2.09	1.67	1.59	15	1
3	B	376	PX4	C28-C27	2.09	1.62	1.51	2	1
3	C	319	PX4	C4-N1	2.09	1.56	1.50	4	1
3	C	368	PX4	C33-C32	2.09	1.62	1.51	10	1
3	B	355	PX4	C27-C26	2.09	1.62	1.51	1	1
3	B	362	PX4	O5-C9	2.09	1.39	1.33	7	1
3	B	381	PX4	O7-C23	2.09	1.28	1.34	2	1
3	B	387	PX4	P1-O2	2.09	1.43	1.50	3	1
3	A	614	PX4	P1-O1	2.09	1.45	1.55	10	2
3	C	352	PX4	C29-C28	2.09	1.62	1.51	14	1
3	A	621	PX4	O5-C8	2.09	1.40	1.45	15	1
3	B	353	PX4	P1-O2	2.09	1.43	1.50	11	1
3	B	382	PX4	C15-C14	2.09	1.62	1.51	6	1
3	C	309	PX4	C11-C10	2.09	1.59	1.52	7	1
3	C	327	PX4	C16-C15	2.09	1.62	1.51	8	1
3	A	639	PX4	P1-O1	2.09	1.45	1.55	9	2
3	B	372	PX4	O7-C23	2.09	1.28	1.34	8	2
3	B	384	PX4	C16-C15	2.09	1.62	1.51	5	1
3	B	394	PX4	C32-C31	2.09	1.62	1.51	11	1
3	C	327	PX4	P1-O4	2.09	1.51	1.59	9	1
3	B	361	PX4	O7-C7	2.09	1.41	1.46	9	1
3	A	601	PX4	C30-C29	2.09	1.62	1.51	3	1
3	A	631	PX4	O3-C1	2.09	1.36	1.44	15	1
3	C	362	PX4	C18-C17	2.09	1.62	1.51	7	1
3	B	319	PX4	C30-C29	2.09	1.62	1.51	15	1
3	B	323	PX4	O4-C6	2.09	1.52	1.44	2	2
3	C	306	PX4	C26-C25	2.09	1.62	1.51	3	1
3	C	322	PX4	C11-C10	2.09	1.59	1.52	12	1
3	A	608	PX4	C31-C30	2.08	1.62	1.51	12	1
3	A	605	PX4	P1-O3	2.08	1.67	1.59	8	1
3	A	640	PX4	P1-O1	2.08	1.45	1.55	13	1
3	B	303	PX4	C27-C26	2.08	1.62	1.51	13	1
3	B	321	PX4	C2-N1	2.08	1.57	1.51	10	1
3	B	391	PX4	C11-C10	2.09	1.59	1.52	7	1
3	B	306	PX4	C24-C23	2.08	1.56	1.50	4	2
3	C	322	PX4	P1-O2	2.08	1.43	1.50	13	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	318	PX4	O3-C1	2.08	1.36	1.44	4	1
3	C	356	PX4	C31-C30	2.08	1.62	1.51	6	1
3	B	342	PX4	C31-C30	2.08	1.62	1.51	11	1
3	A	603	PX4	C12-C11	2.08	1.62	1.51	11	1
3	A	628	PX4	P1-O2	2.08	1.43	1.50	13	2
3	A	609	PX4	P1-O2	2.08	1.43	1.50	14	2
3	A	631	PX4	C25-C24	2.08	1.59	1.52	1	1
3	B	312	PX4	C11-C10	2.08	1.59	1.52	14	1
3	B	322	PX4	C17-C16	2.08	1.62	1.51	7	1
3	A	606	PX4	P1-O2	2.08	1.43	1.50	8	1
3	B	303	PX4	C4-N1	2.08	1.56	1.50	8	1
3	B	308	PX4	C2-N1	2.08	1.57	1.51	6	2
3	B	324	PX4	C11-C10	2.08	1.59	1.52	10	1
3	B	357	PX4	C2-N1	2.08	1.57	1.51	8	1
3	C	363	PX4	P1-O2	2.08	1.43	1.50	12	1
3	C	322	PX4	O4-C6	2.08	1.36	1.44	15	1
3	C	343	PX4	O5-C9	2.08	1.27	1.33	3	2
3	C	368	PX4	C11-C10	2.08	1.59	1.52	11	1
3	A	644	PX4	C31-C30	2.08	1.62	1.51	2	1
3	C	353	PX4	P1-O2	2.08	1.43	1.50	7	1
3	B	376	PX4	O4-C6	2.08	1.36	1.44	12	1
3	C	303	PX4	C11-C10	2.08	1.59	1.52	4	1
3	C	311	PX4	C16-C15	2.08	1.62	1.51	10	1
3	A	639	PX4	C28-C27	2.08	1.62	1.51	5	1
3	C	316	PX4	C3-N1	2.08	1.44	1.50	12	1
3	C	318	PX4	C16-C15	2.08	1.62	1.51	14	1
3	A	608	PX4	C5-N1	2.07	1.44	1.50	2	1
3	B	334	PX4	C11-C10	2.07	1.59	1.52	5	1
3	B	339	PX4	C19-C18	2.07	1.62	1.51	4	1
3	A	634	PX4	C29-C28	2.07	1.62	1.51	6	1
3	A	647	PX4	P1-O2	2.07	1.43	1.50	7	1
3	B	361	PX4	C11-C10	2.07	1.59	1.52	14	1
3	B	370	PX4	P1-O4	2.07	1.51	1.59	8	1
3	B	372	PX4	C32-C31	2.07	1.62	1.51	3	2
3	C	343	PX4	P1-O1	2.07	1.45	1.55	2	1
3	C	369	PX4	C32-C31	2.07	1.62	1.51	12	1
3	A	635	PX4	C30-C29	2.07	1.62	1.51	13	1
3	A	638	PX4	C15-C14	2.07	1.62	1.51	5	1
3	A	639	PX4	C19-C18	2.07	1.62	1.51	10	1
3	B	305	PX4	P1-O2	2.07	1.43	1.50	5	1
3	B	330	PX4	C12-C11	2.07	1.62	1.51	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	352	PX4	P1-O2	2.07	1.43	1.50	14	1
3	B	360	PX4	C32-C31	2.07	1.62	1.51	14	1
3	C	323	PX4	C16-C15	2.07	1.62	1.51	13	1
3	A	605	PX4	C27-C26	2.07	1.62	1.51	2	1
3	A	613	PX4	O5-C8	2.07	1.40	1.45	1	1
3	A	618	PX4	C31-C30	2.07	1.62	1.51	4	1
3	B	311	PX4	O4-C6	2.07	1.36	1.44	11	1
3	C	332	PX4	C20-C19	2.07	1.62	1.51	3	1
3	C	370	PX4	O4-C6	2.07	1.36	1.44	8	1
3	B	324	PX4	C20-C19	2.07	1.62	1.51	10	1
3	B	328	PX4	C25-C24	2.07	1.59	1.52	10	1
3	A	641	PX4	O4-C6	2.07	1.36	1.44	15	1
3	A	647	PX4	C5-N1	2.07	1.56	1.50	10	2
3	B	317	PX4	C25-C24	2.07	1.59	1.52	8	1
3	B	332	PX4	C18-C17	2.07	1.62	1.51	3	1
3	B	334	PX4	P1-O2	2.07	1.43	1.50	14	2
3	B	361	PX4	C26-C25	2.07	1.62	1.51	7	1
3	B	398	PX4	C13-C12	2.07	1.62	1.51	2	1
3	C	334	PX4	O5-C9	2.07	1.27	1.33	1	1
3	C	348	PX4	O3-C1	2.07	1.36	1.44	4	1
3	C	361	PX4	C25-C24	2.07	1.59	1.52	2	1
3	C	309	PX4	P1-O2	2.07	1.43	1.50	11	1
3	C	309	PX4	C12-C11	2.07	1.62	1.51	12	1
3	A	631	PX4	C3-N1	2.06	1.56	1.50	3	1
3	B	315	PX4	C4-N1	2.06	1.56	1.50	2	2
3	C	315	PX4	P1-O2	2.07	1.43	1.50	11	1
3	B	332	PX4	O8-C23	2.06	1.28	1.22	8	1
3	C	360	PX4	O5-C9	2.07	1.39	1.33	5	1
3	A	601	PX4	C3-N1	2.06	1.56	1.50	15	1
3	A	648	PX4	P1-O2	2.06	1.43	1.50	2	1
3	B	333	PX4	C11-C10	2.06	1.59	1.52	2	1
3	B	357	PX4	C11-C10	2.06	1.59	1.52	8	1
3	B	372	PX4	C30-C29	2.06	1.62	1.51	14	1
3	B	394	PX4	O5-C9	2.06	1.39	1.33	8	2
3	B	399	PX4	C4-N1	2.06	1.56	1.50	9	2
3	C	307	PX4	O7-C23	2.06	1.28	1.34	1	1
3	C	344	PX4	C3-N1	2.06	1.44	1.50	8	2
3	C	356	PX4	C25-C24	2.06	1.59	1.52	1	2
3	A	602	PX4	C5-N1	2.06	1.44	1.50	9	1
3	A	607	PX4	C4-N1	2.06	1.44	1.50	11	1
3	A	632	PX4	O4-C6	2.06	1.52	1.44	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	332	PX4	C12-C11	2.06	1.62	1.51	15	1
3	B	353	PX4	C20-C19	2.06	1.62	1.51	8	1
3	C	334	PX4	C20-C19	2.06	1.62	1.51	7	1
3	C	338	PX4	P1-O1	2.06	1.45	1.55	5	2
3	B	367	PX4	C31-C30	2.06	1.62	1.51	3	1
3	B	398	PX4	C19-C18	2.06	1.62	1.51	13	1
3	C	358	PX4	P1-O1	2.06	1.45	1.55	5	1
3	A	621	PX4	P1-O4	2.06	1.51	1.59	15	1
3	B	339	PX4	C16-C15	2.06	1.62	1.51	7	1
3	C	340	PX4	C17-C16	2.06	1.62	1.51	14	1
3	C	342	PX4	C34-C33	2.06	1.62	1.51	12	1
3	C	325	PX4	O5-C8	2.06	1.49	1.45	15	1
3	C	330	PX4	C30-C29	2.06	1.62	1.51	7	1
3	C	330	PX4	C4-N1	2.06	1.56	1.50	12	1
3	B	354	PX4	P1-O4	2.06	1.51	1.59	4	1
3	B	377	PX4	C2-N1	2.06	1.45	1.51	4	1
3	B	395	PX4	C14-C13	2.06	1.62	1.51	7	1
3	C	350	PX4	P1-O3	2.06	1.51	1.59	14	1
3	A	609	PX4	P1-O4	2.06	1.51	1.59	6	1
3	A	648	PX4	C2-N1	2.06	1.57	1.51	3	1
3	B	354	PX4	C14-C13	2.06	1.62	1.51	13	1
3	B	359	PX4	C16-C15	2.06	1.62	1.51	1	1
3	B	362	PX4	P1-O4	2.06	1.51	1.59	14	1
3	C	301	PX4	C3-N1	2.06	1.56	1.50	2	1
3	C	318	PX4	C31-C30	2.06	1.62	1.51	4	1
3	C	321	PX4	C26-C25	2.06	1.62	1.51	8	1
3	C	341	PX4	C31-C30	2.06	1.62	1.51	4	1
3	A	625	PX4	C31-C30	2.06	1.62	1.51	2	1
3	A	626	PX4	C11-C10	2.06	1.59	1.52	4	1
3	A	639	PX4	C4-N1	2.06	1.44	1.50	2	1
3	B	302	PX4	C28-C27	2.05	1.62	1.51	1	1
3	B	335	PX4	C18-C17	2.05	1.62	1.51	4	1
3	C	313	PX4	C3-N1	2.06	1.44	1.50	1	1
3	C	328	PX4	C31-C30	2.06	1.62	1.51	2	1
3	B	362	PX4	C29-C28	2.05	1.62	1.51	8	1
3	C	345	PX4	C19-C18	2.06	1.62	1.51	12	1
3	B	339	PX4	C13-C12	2.05	1.62	1.51	13	2
3	B	341	PX4	C25-C24	2.05	1.59	1.52	10	1
3	B	353	PX4	C2-N1	2.05	1.57	1.51	8	1
3	B	363	PX4	P1-O4	2.05	1.51	1.59	14	1
3	B	380	PX4	O3-C1	2.05	1.36	1.44	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	359	PX4	O3-C1	2.05	1.36	1.44	9	1
3	B	380	PX4	C34-C33	2.05	1.62	1.51	13	1
3	B	392	PX4	C5-N1	2.05	1.56	1.50	2	1
3	B	368	PX4	C26-C25	2.05	1.62	1.51	9	1
3	B	373	PX4	O5-C8	2.05	1.40	1.45	14	1
3	B	385	PX4	C5-N1	2.05	1.44	1.50	1	1
3	C	338	PX4	C33-C32	2.05	1.62	1.51	3	1
3	B	374	PX4	C28-C27	2.05	1.62	1.51	14	1
3	C	306	PX4	C11-C10	2.05	1.59	1.52	9	1
3	C	309	PX4	C33-C32	2.05	1.62	1.51	12	1
3	C	343	PX4	O7-C23	2.05	1.28	1.34	8	1
3	B	320	PX4	C11-C10	2.05	1.59	1.52	11	1
3	B	338	PX4	C34-C33	2.05	1.62	1.51	2	1
3	B	360	PX4	C14-C13	2.05	1.62	1.51	15	1
3	A	608	PX4	C14-C13	2.05	1.62	1.51	10	1
3	C	312	PX4	O4-C6	2.05	1.36	1.44	12	1
3	C	337	PX4	C27-C26	2.05	1.62	1.51	7	1
3	B	321	PX4	C33-C32	2.05	1.62	1.51	12	1
3	B	331	PX4	C29-C28	2.05	1.62	1.51	8	2
3	B	373	PX4	C13-C12	2.05	1.62	1.51	15	1
3	C	311	PX4	C31-C30	2.05	1.62	1.51	15	1
3	A	615	PX4	O7-C7	2.05	1.41	1.46	4	1
3	B	399	PX4	P1-O4	2.05	1.67	1.59	4	1
3	B	399	PX4	C32-C31	2.05	1.62	1.51	12	1
3	C	342	PX4	C13-C12	2.05	1.62	1.51	8	1
3	A	629	PX4	C13-C12	2.04	1.62	1.51	10	1
3	A	635	PX4	C11-C10	2.05	1.59	1.52	9	2
3	A	639	PX4	C16-C15	2.04	1.61	1.51	4	1
3	A	644	PX4	C28-C27	2.04	1.62	1.51	1	1
3	B	314	PX4	C11-C10	2.04	1.59	1.52	11	3
3	B	334	PX4	C3-N1	2.05	1.44	1.50	2	1
3	C	344	PX4	C19-C18	2.05	1.62	1.51	12	1
3	B	337	PX4	O7-C23	2.04	1.28	1.34	12	1
3	B	346	PX4	C15-C14	2.05	1.62	1.51	3	1
3	B	320	PX4	C5-N1	2.04	1.55	1.50	1	2
3	B	358	PX4	C33-C32	2.04	1.62	1.51	15	1
3	C	322	PX4	C33-C32	2.04	1.62	1.51	3	1
3	C	364	PX4	C14-C13	2.05	1.62	1.51	2	1
3	A	607	PX4	P1-O4	2.04	1.51	1.59	15	1
3	A	609	PX4	C3-N1	2.04	1.44	1.50	15	1
3	A	620	PX4	P1-O2	2.04	1.43	1.50	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	336	PX4	O7-C23	2.04	1.28	1.34	2	1
3	B	399	PX4	O6-C9	2.04	1.28	1.22	9	1
3	C	311	PX4	C35-C34	2.04	1.64	1.51	15	1
3	B	360	PX4	C16-C15	2.04	1.61	1.51	5	1
3	C	319	PX4	P1-O1	2.04	1.45	1.55	6	1
3	C	320	PX4	P1-O1	2.04	1.45	1.55	2	1
3	A	606	PX4	O5-C8	2.04	1.49	1.45	11	1
3	A	627	PX4	O7-C23	2.04	1.28	1.34	6	1
3	C	328	PX4	C3-N1	2.04	1.44	1.50	9	1
3	A	607	PX4	C15-C14	2.04	1.61	1.51	1	1
3	A	607	PX4	C14-C13	2.04	1.61	1.51	13	1
3	B	309	PX4	C18-C17	2.04	1.61	1.51	3	1
3	B	340	PX4	C30-C29	2.04	1.61	1.51	3	1
3	B	364	PX4	O5-C9	2.04	1.39	1.33	3	1
3	C	350	PX4	C29-C28	2.04	1.61	1.51	2	1
3	B	324	PX4	O5-C8	2.04	1.40	1.45	9	1
3	B	339	PX4	C25-C24	2.04	1.59	1.52	3	1
3	B	346	PX4	C34-C33	2.04	1.61	1.51	13	1
3	B	351	PX4	C2-N1	2.04	1.45	1.51	9	1
3	C	325	PX4	O8-C23	2.04	1.28	1.22	12	1
3	A	601	PX4	P1-O4	2.04	1.67	1.59	5	1
3	A	644	PX4	C29-C28	2.04	1.61	1.51	3	1
3	B	303	PX4	P1-O2	2.04	1.43	1.50	6	1
3	B	375	PX4	O7-C7	2.04	1.51	1.46	12	1
3	C	353	PX4	C30-C29	2.04	1.61	1.51	8	1
3	B	357	PX4	P1-O1	2.03	1.45	1.55	3	2
3	B	389	PX4	C12-C11	2.03	1.61	1.51	1	1
3	B	391	PX4	C4-N1	2.03	1.44	1.50	15	1
3	C	368	PX4	O4-C6	2.03	1.36	1.44	13	1
3	A	609	PX4	C27-C26	2.03	1.61	1.51	11	1
3	A	614	PX4	C34-C33	2.03	1.61	1.51	7	1
3	A	631	PX4	O8-C23	2.03	1.28	1.22	6	1
3	A	643	PX4	P1-O2	2.03	1.43	1.50	12	1
3	A	645	PX4	C26-C25	2.03	1.61	1.51	11	1
3	A	619	PX4	C27-C26	2.03	1.61	1.51	8	1
3	A	641	PX4	C11-C10	2.03	1.59	1.52	9	1
3	A	625	PX4	C5-N1	2.03	1.55	1.50	14	1
3	A	643	PX4	O5-C8	2.03	1.40	1.45	15	1
3	B	317	PX4	C33-C32	2.03	1.61	1.51	14	1
3	B	327	PX4	C30-C29	2.03	1.61	1.51	6	1
3	B	394	PX4	C35-C34	2.03	1.64	1.51	14	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	310	PX4	C2-N1	2.03	1.45	1.51	7	1
3	C	313	PX4	C34-C33	2.03	1.61	1.51	11	1
3	C	354	PX4	C17-C16	2.03	1.61	1.51	11	2
3	C	358	PX4	O3-C1	2.03	1.36	1.44	14	1
3	B	363	PX4	P1-O3	2.03	1.51	1.59	2	1
3	B	378	PX4	C2-N1	2.03	1.57	1.51	15	1
3	C	328	PX4	P1-O3	2.03	1.51	1.59	11	1
3	C	350	PX4	C4-N1	2.03	1.55	1.50	5	1
3	B	369	PX4	O5-C9	2.03	1.39	1.33	9	1
3	B	383	PX4	P1-O1	2.03	1.45	1.55	10	1
3	C	315	PX4	C32-C31	2.03	1.61	1.51	15	1
3	B	352	PX4	C11-C10	2.03	1.59	1.52	11	1
3	B	399	PX4	C26-C25	2.03	1.61	1.51	8	1
3	C	305	PX4	C18-C17	2.03	1.61	1.51	11	1
3	C	320	PX4	O5-C9	2.03	1.39	1.33	3	1
3	C	320	PX4	C26-C25	2.03	1.61	1.51	11	1
3	C	348	PX4	O5-C9	2.03	1.27	1.33	3	1
3	B	398	PX4	C20-C19	2.03	1.61	1.51	12	1
3	C	308	PX4	C10-C9	2.03	1.56	1.50	2	1
3	C	322	PX4	C20-C19	2.03	1.41	1.51	8	1
3	C	336	PX4	C10-C9	2.03	1.56	1.50	8	1
3	C	361	PX4	O6-C9	2.03	1.28	1.22	5	1
3	A	605	PX4	C11-C10	2.03	1.59	1.52	15	1
3	A	618	PX4	C3-N1	2.03	1.55	1.50	4	1
3	B	321	PX4	C21-C20	2.03	1.64	1.51	10	1
3	B	339	PX4	P1-O4	2.03	1.51	1.59	12	1
3	A	629	PX4	C5-N1	2.03	1.55	1.50	1	1
3	A	632	PX4	O3-C1	2.03	1.36	1.44	12	1
3	A	642	PX4	C4-N1	2.03	1.55	1.50	14	1
3	B	311	PX4	P1-O1	2.03	1.46	1.55	1	1
3	A	610	PX4	C3-N1	2.02	1.55	1.50	15	1
3	A	622	PX4	C14-C13	2.02	1.61	1.51	6	1
3	B	317	PX4	C30-C29	2.02	1.61	1.51	10	1
3	B	319	PX4	P1-O4	2.03	1.51	1.59	12	1
3	B	329	PX4	P1-O2	2.03	1.43	1.50	12	1
3	B	329	PX4	C26-C25	2.03	1.61	1.51	14	1
3	B	344	PX4	P1-O1	2.03	1.46	1.55	12	1
3	B	349	PX4	C5-N1	2.03	1.55	1.50	10	1
3	B	385	PX4	C2-N1	2.03	1.45	1.51	5	1
3	C	308	PX4	O5-C9	2.03	1.27	1.33	4	1
3	C	315	PX4	O5-C9	2.03	1.27	1.33	15	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	331	PX4	C4-N1	2.03	1.55	1.50	5	1
3	C	334	PX4	C30-C29	2.03	1.61	1.51	3	1
3	C	361	PX4	C32-C31	2.03	1.61	1.51	14	1
3	B	331	PX4	C31-C30	2.02	1.61	1.51	8	1
3	B	333	PX4	C3-N1	2.02	1.44	1.50	5	1
3	B	310	PX4	C5-N1	2.02	1.44	1.50	15	1
3	B	321	PX4	C20-C19	2.02	1.61	1.51	5	1
3	B	337	PX4	C20-C19	2.02	1.61	1.51	9	1
3	C	306	PX4	C27-C26	2.02	1.61	1.51	14	1
3	C	318	PX4	C19-C18	2.02	1.61	1.51	8	1
3	C	360	PX4	C27-C26	2.02	1.61	1.51	9	1
3	B	363	PX4	C32-C31	2.02	1.61	1.51	13	1
3	C	302	PX4	C25-C24	2.02	1.59	1.52	8	1
3	C	362	PX4	C20-C19	2.02	1.61	1.51	1	1
3	B	369	PX4	C33-C32	2.02	1.61	1.51	7	1
3	B	398	PX4	C4-N1	2.02	1.44	1.50	14	1
3	C	307	PX4	C4-N1	2.02	1.44	1.50	2	1
3	C	313	PX4	C13-C12	2.02	1.61	1.51	15	1
3	A	624	PX4	C16-C15	2.02	1.61	1.51	8	1
3	A	638	PX4	C33-C32	2.02	1.61	1.51	8	1
3	B	327	PX4	O5-C8	2.02	1.49	1.45	6	1
3	B	331	PX4	C26-C25	2.02	1.61	1.51	8	1
3	B	355	PX4	O7-C7	2.02	1.41	1.46	9	1
3	C	351	PX4	C16-C15	2.02	1.61	1.51	11	1
3	A	628	PX4	C4-N1	2.02	1.55	1.50	10	2
3	B	302	PX4	C34-C33	2.02	1.61	1.51	7	1
3	B	305	PX4	O7-C23	2.02	1.28	1.34	14	1
3	B	314	PX4	C16-C15	2.02	1.61	1.51	1	1
3	A	607	PX4	C27-C26	2.02	1.61	1.51	4	1
3	B	315	PX4	C18-C17	2.02	1.61	1.51	9	1
3	B	322	PX4	C27-C26	2.02	1.61	1.51	4	1
3	B	346	PX4	O8-C23	2.02	1.28	1.22	8	1
3	B	351	PX4	C27-C26	2.02	1.61	1.51	11	1
3	B	366	PX4	C34-C33	2.02	1.61	1.51	13	1
3	C	304	PX4	C4-N1	2.02	1.44	1.50	7	1
3	C	310	PX4	C11-C10	2.02	1.59	1.52	2	1
3	C	356	PX4	C26-C25	2.02	1.61	1.51	10	1
3	B	373	PX4	C10-C9	2.02	1.56	1.50	11	1
3	B	374	PX4	O7-C23	2.02	1.28	1.34	10	1
3	B	400	PX4	C25-C24	2.02	1.59	1.52	15	1
3	C	308	PX4	C14-C13	2.02	1.61	1.51	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	314	PX4	C3-N1	2.02	1.55	1.50	2	1
3	B	306	PX4	P1-O4	2.02	1.51	1.59	8	1
3	A	635	PX4	P1-O4	2.01	1.51	1.59	10	1
3	A	648	PX4	O3-C1	2.01	1.52	1.44	14	1
3	B	302	PX4	C18-C17	2.01	1.61	1.51	10	1
3	B	304	PX4	C15-C14	2.01	1.61	1.51	14	1
3	B	309	PX4	C17-C16	2.01	1.61	1.51	8	1
3	B	351	PX4	O5-C9	2.01	1.39	1.33	13	1
3	B	352	PX4	O4-C6	2.01	1.37	1.44	4	1
3	C	369	PX4	O3-C1	2.02	1.36	1.44	2	1
3	A	643	PX4	C5-N1	2.01	1.55	1.50	4	1
3	A	623	PX4	C5-N1	2.01	1.44	1.50	5	1
3	B	307	PX4	C20-C19	2.01	1.61	1.51	6	1
3	B	312	PX4	C2-N1	2.01	1.57	1.51	11	1
3	B	313	PX4	O5-C9	2.01	1.39	1.33	14	1
3	B	347	PX4	O4-C6	2.01	1.37	1.44	4	1
3	B	370	PX4	C2-N1	2.01	1.57	1.51	12	1
3	B	381	PX4	P1-O4	2.01	1.51	1.59	9	1
3	B	400	PX4	C33-C32	2.01	1.61	1.51	4	1
3	C	314	PX4	C34-C33	2.01	1.61	1.51	9	1
3	C	367	PX4	P1-O4	2.01	1.51	1.59	15	1
3	B	391	PX4	C17-C16	2.01	1.61	1.51	14	1
3	B	322	PX4	C19-C18	2.01	1.61	1.51	3	1
3	B	336	PX4	C34-C33	2.01	1.61	1.51	10	1
3	C	310	PX4	C28-C27	2.01	1.61	1.51	8	1
3	B	363	PX4	P1-O1	2.01	1.46	1.55	9	1
3	B	387	PX4	C13-C12	2.01	1.61	1.51	1	1
3	C	316	PX4	P1-O3	2.01	1.51	1.59	3	1
3	C	319	PX4	C11-C10	2.01	1.59	1.52	8	1
3	C	329	PX4	C33-C32	2.01	1.61	1.51	13	1
3	C	362	PX4	C11-C10	2.01	1.59	1.52	10	1
3	B	320	PX4	C31-C30	2.01	1.61	1.51	10	1
3	B	346	PX4	C2-N1	2.01	1.45	1.51	9	1
3	B	373	PX4	C29-C28	2.01	1.61	1.51	3	1
3	B	373	PX4	C32-C31	2.01	1.61	1.51	15	1
3	C	322	PX4	C16-C15	2.01	1.61	1.51	1	1
3	C	369	PX4	P1-O2	2.01	1.43	1.50	10	1
3	A	647	PX4	O3-C1	2.01	1.36	1.44	1	1
3	B	308	PX4	P1-O3	2.01	1.51	1.59	4	1
3	C	323	PX4	C19-C18	2.01	1.61	1.51	7	1
3	C	358	PX4	O5-C8	2.01	1.40	1.45	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	360	PX4	C11-C10	2.01	1.59	1.52	1	1
3	A	636	PX4	C3-N1	2.01	1.44	1.50	11	1
3	B	340	PX4	C26-C25	2.01	1.61	1.51	12	1
3	C	321	PX4	C25-C24	2.01	1.59	1.52	6	1
3	C	325	PX4	P1-O4	2.01	1.67	1.59	15	1
3	A	641	PX4	C25-C24	2.01	1.59	1.52	13	1
3	A	642	PX4	P1-O2	2.00	1.43	1.50	12	1
3	B	332	PX4	P1-O3	2.00	1.67	1.59	7	1
3	A	640	PX4	C12-C11	2.00	1.61	1.51	4	1
3	A	643	PX4	C30-C29	2.00	1.61	1.51	13	1
3	B	343	PX4	C32-C31	2.00	1.61	1.51	14	1
3	B	370	PX4	O5-C8	2.00	1.40	1.45	3	1
3	B	350	PX4	O7-C7	2.00	1.41	1.46	1	1
3	C	319	PX4	C28-C27	2.00	1.61	1.51	1	1
3	A	644	PX4	C14-C13	2.00	1.61	1.51	14	1
3	B	373	PX4	P1-O3	2.00	1.51	1.59	14	1
3	A	613	PX4	C24-C23	2.00	1.56	1.50	3	1
3	A	621	PX4	C18-C17	2.00	1.61	1.51	12	1
3	A	622	PX4	C5-N1	2.00	1.44	1.50	4	1
3	A	631	PX4	C34-C33	2.00	1.61	1.51	5	1
3	A	648	PX4	O6-C9	2.00	1.28	1.22	15	1
3	B	364	PX4	C3-N1	2.00	1.55	1.50	15	1
3	C	332	PX4	C34-C33	2.00	1.61	1.51	10	1
3	C	342	PX4	P1-O4	2.00	1.51	1.59	2	1
3	C	367	PX4	C30-C29	2.00	1.61	1.51	2	1
3	B	346	PX4	C24-C23	2.00	1.56	1.50	4	1
3	C	312	PX4	C6-C7	2.00	1.57	1.50	1	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	394	PX4	O7-C23-C24	6.26	97.94	111.48	7	4
3	B	343	PX4	C8-C7-C6	5.82	125.35	111.78	3	4
3	C	346	PX4	O5-C8-C7	5.77	125.03	108.40	12	5
3	B	396	PX4	C7-O7-C23	5.70	104.16	117.80	11	5
3	B	327	PX4	C7-O7-C23	5.64	104.30	117.80	1	7
3	B	316	PX4	C7-O7-C23	5.56	104.48	117.80	10	4
3	B	322	PX4	C7-O7-C23	5.47	104.69	117.80	10	3
3	B	347	PX4	C7-O7-C23	5.24	105.26	117.80	15	5
3	C	365	PX4	O7-C23-C24	5.24	100.15	111.48	2	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	618	PX4	O7-C23-C24	5.19	100.26	111.48	15	5
3	C	348	PX4	O7-C23-C24	5.16	100.31	111.48	11	2
3	B	348	PX4	O5-C8-C7	5.10	123.11	108.40	3	4
3	B	376	PX4	O7-C23-C24	5.08	100.49	111.48	10	3
3	C	362	PX4	O5-C8-C7	5.08	123.03	108.40	15	5
3	C	356	PX4	C8-C7-C6	5.06	99.98	111.78	8	5
3	A	629	PX4	C7-O7-C23	5.06	105.69	117.80	8	6
3	C	312	PX4	C7-O7-C23	5.06	105.69	117.80	13	3
3	A	630	PX4	O5-C8-C7	5.05	122.97	108.40	12	6
3	A	614	PX4	C7-O7-C23	4.96	105.92	117.80	4	4
3	C	342	PX4	C7-O7-C23	4.89	106.09	117.80	2	4
3	B	352	PX4	C7-O7-C23	4.88	106.11	117.80	3	2
3	C	368	PX4	O7-C23-C24	4.84	101.01	111.48	8	4
3	C	369	PX4	O5-C8-C7	4.82	122.29	108.40	15	8
3	A	613	PX4	O5-C8-C7	4.81	122.27	108.40	9	4
3	B	394	PX4	O5-C8-C7	4.81	122.26	108.40	2	7
3	C	305	PX4	O5-C8-C7	4.76	122.12	108.40	3	7
3	A	606	PX4	O5-C8-C7	4.76	122.10	108.40	10	3
3	C	313	PX4	C7-O7-C23	4.74	106.45	117.80	7	4
3	B	323	PX4	C8-C7-C6	4.72	122.79	111.78	14	7
3	B	302	PX4	C7-O7-C23	4.71	106.52	117.80	5	2
3	A	637	PX4	C4-N1-C3	4.71	96.61	108.98	12	2
3	B	368	PX4	O7-C23-O8	4.71	134.71	123.70	4	2
3	B	328	PX4	O5-C8-C7	4.69	121.93	108.40	3	4
3	B	331	PX4	C8-C7-C6	4.69	100.85	111.78	12	3
3	C	337	PX4	O7-C23-O8	4.68	134.65	123.70	15	4
3	B	381	PX4	C7-O7-C23	4.65	106.67	117.80	11	2
3	A	622	PX4	C5-N1-C3	4.63	96.82	108.98	3	4
3	B	377	PX4	O7-C23-C24	4.63	101.47	111.48	12	3
3	B	392	PX4	O5-C8-C7	4.60	121.67	108.40	5	2
3	C	316	PX4	C7-O7-C23	4.59	106.81	117.80	11	2
3	C	315	PX4	C7-O7-C23	4.57	106.87	117.80	10	4
3	B	396	PX4	O7-C23-C24	4.54	101.66	111.48	6	2
3	B	353	PX4	C7-O7-C23	4.53	106.96	117.80	11	2
3	B	373	PX4	C4-N1-C3	4.52	120.85	108.98	5	2
3	C	325	PX4	C7-O7-C23	4.51	106.99	117.80	14	5
3	B	358	PX4	C7-O7-C23	4.50	107.02	117.80	1	6
3	C	316	PX4	O5-C8-C7	4.50	121.37	108.40	13	4
3	C	322	PX4	O7-C23-C24	4.49	101.77	111.48	3	4
3	B	369	PX4	C7-O7-C23	4.49	107.06	117.80	5	8
3	A	616	PX4	O7-C23-C24	4.48	101.79	111.48	15	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	640	PX4	C5-N1-C3	4.47	97.23	108.98	7	3
3	C	312	PX4	O7-C23-C24	4.47	101.82	111.48	6	5
3	C	301	PX4	O7-C23-C24	4.46	101.83	111.48	12	4
3	B	362	PX4	C8-C7-C6	4.44	101.43	111.78	11	3
3	A	612	PX4	C7-O7-C23	4.43	107.19	117.80	11	2
3	C	309	PX4	O5-C8-C7	4.43	121.16	108.40	8	4
3	C	324	PX4	O7-C23-C24	4.42	101.92	111.48	9	6
3	B	331	PX4	O7-C23-C24	4.40	101.95	111.48	5	4
3	B	362	PX4	O5-C9-C10	4.39	98.44	111.83	9	4
3	B	316	PX4	C8-C7-C6	4.39	101.55	111.78	9	3
3	A	634	PX4	O7-C23-C24	4.38	102.00	111.48	11	2
3	B	367	PX4	O7-C23-C24	4.38	120.95	111.48	9	7
3	C	310	PX4	C7-O7-C23	4.37	107.34	117.80	13	3
3	C	356	PX4	C7-O7-C23	4.34	107.42	117.80	13	5
3	C	363	PX4	O7-C23-C24	4.32	102.13	111.48	7	4
3	A	641	PX4	C7-O7-C23	4.31	107.47	117.80	9	7
3	C	360	PX4	O7-C23-C24	4.31	102.15	111.48	4	4
3	B	350	PX4	C7-O7-C23	4.31	107.49	117.80	14	4
3	A	604	PX4	C7-O7-C23	4.29	107.52	117.80	6	6
3	B	330	PX4	C7-O7-C23	4.29	107.53	117.80	13	5
3	B	392	PX4	C7-O7-C23	4.29	107.53	117.80	13	1
3	C	310	PX4	O5-C8-C7	4.29	120.76	108.40	1	5
3	B	351	PX4	C7-O7-C23	4.28	107.55	117.80	1	7
3	C	337	PX4	O7-C23-C24	4.28	102.22	111.48	1	6
3	C	331	PX4	O5-C8-C7	4.28	120.72	108.40	6	4
3	A	617	PX4	C4-N1-C3	4.26	97.78	108.98	13	3
3	C	359	PX4	O7-C23-C24	4.26	102.27	111.48	15	4
3	B	305	PX4	C7-O7-C23	4.25	107.62	117.80	13	8
3	B	385	PX4	C7-O7-C23	4.25	107.63	117.80	11	4
3	B	359	PX4	C5-N1-C3	4.24	97.84	108.98	6	2
3	B	360	PX4	O7-C23-C24	4.24	102.31	111.48	13	7
3	C	320	PX4	C7-O7-C23	4.24	107.66	117.80	13	3
3	B	337	PX4	C7-O7-C23	4.23	107.66	117.80	4	7
3	B	370	PX4	O7-C23-C24	4.23	102.32	111.48	10	5
3	B	342	PX4	O7-C23-C24	4.22	102.35	111.48	4	6
3	B	398	PX4	C8-C7-C6	4.21	101.96	111.78	4	1
3	C	334	PX4	O7-C23-C24	4.21	102.37	111.48	11	2
3	B	371	PX4	O7-C23-C24	4.21	102.38	111.48	6	3
3	A	642	PX4	O7-C23-C24	4.20	102.40	111.48	2	6
3	B	400	PX4	C7-O7-C23	4.20	107.75	117.80	14	7
3	B	347	PX4	O7-C23-C24	4.19	102.42	111.48	2	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	C	315	PX4	O5-C8-C7	4.18	120.45	108.40	12	7
3	A	603	PX4	O7-C23-C24	4.18	102.44	111.48	6	7
3	A	647	PX4	O5-C8-C7	4.18	120.44	108.40	12	3
3	B	389	PX4	O7-C23-O8	4.17	133.46	123.70	15	2
3	A	609	PX4	C7-O7-C23	4.17	107.81	117.80	15	4
3	B	320	PX4	C7-O7-C23	4.17	107.81	117.80	8	4
3	C	326	PX4	C7-O7-C23	4.17	127.78	117.80	11	8
3	C	337	PX4	O5-C8-C7	4.17	120.42	108.40	1	5
3	A	646	PX4	O7-C23-C24	4.17	102.47	111.48	5	2
3	B	384	PX4	O7-C23-C24	4.16	102.48	111.48	4	4
3	A	640	PX4	O7-C23-C24	4.16	102.49	111.48	7	2
3	C	306	PX4	O7-C23-C24	4.16	102.49	111.48	15	6
3	B	321	PX4	C7-O7-C23	4.15	107.87	117.80	13	5
3	C	370	PX4	O7-C23-C24	4.13	102.55	111.48	5	2
3	B	339	PX4	C7-O7-C23	4.13	107.92	117.80	4	8
3	C	340	PX4	C7-O7-C23	4.13	107.92	117.80	7	4
3	B	366	PX4	C7-O7-C23	4.12	107.95	117.80	1	6
3	B	398	PX4	O7-C23-C24	4.11	102.58	111.48	11	8
3	A	645	PX4	O5-C8-C7	4.10	120.23	108.40	10	2
3	B	351	PX4	O7-C23-C24	4.10	102.61	111.48	11	3
3	A	610	PX4	O7-C23-C24	4.09	102.62	111.48	8	3
3	C	323	PX4	O7-C23-C24	4.09	102.62	111.48	9	3
3	C	352	PX4	C8-C7-C6	4.09	102.25	111.78	9	3
3	A	643	PX4	O7-C23-C24	4.08	102.66	111.48	6	5
3	C	313	PX4	O5-C8-C7	4.08	120.14	108.40	14	5
3	C	329	PX4	C4-N1-C3	4.07	98.28	108.98	13	2
3	A	636	PX4	C7-O7-C23	4.07	108.06	117.80	11	4
3	B	334	PX4	O7-C23-C24	4.07	102.68	111.48	12	3
3	C	324	PX4	C7-O7-C23	4.07	108.06	117.80	12	4
3	B	310	PX4	C7-O7-C23	4.07	108.06	117.80	8	3
3	C	301	PX4	O5-C8-C7	4.07	120.12	108.40	10	6
3	C	307	PX4	C7-O7-C23	4.06	108.08	117.80	8	2
3	A	620	PX4	C8-O5-C9	4.05	102.30	117.12	15	1
3	A	647	PX4	C7-O7-C23	4.04	108.12	117.80	1	7
3	C	360	PX4	C8-C7-C6	4.04	102.37	111.78	4	5
3	B	364	PX4	O7-C23-C24	4.04	102.75	111.48	1	2
3	A	631	PX4	C7-O7-C23	4.03	108.14	117.80	12	5
3	A	642	PX4	C7-O7-C23	4.03	108.14	117.80	10	4
3	A	633	PX4	C7-O7-C23	4.03	108.16	117.80	3	6
3	B	377	PX4	C7-O7-C23	4.02	108.19	117.80	14	2
3	A	608	PX4	C7-O7-C23	4.01	127.40	117.80	1	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	618	PX4	C8-C7-C6	4.01	102.44	111.78	10	2
3	A	608	PX4	C8-C7-C6	4.01	102.44	111.78	12	3
3	B	355	PX4	C7-O7-C23	4.00	108.21	117.80	5	5
3	C	354	PX4	O5-C8-C7	4.00	119.92	108.40	6	6
3	C	362	PX4	C7-O7-C23	4.00	108.22	117.80	2	3
3	B	326	PX4	C7-O7-C23	3.99	108.24	117.80	8	3
3	A	618	PX4	C7-O7-C23	3.99	108.25	117.80	9	4
3	B	312	PX4	C8-C7-C6	3.99	102.48	111.78	14	2
3	B	394	PX4	C5-N1-C4	3.99	98.49	108.98	15	2
3	C	317	PX4	O7-C23-C24	3.99	102.85	111.48	15	4
3	B	314	PX4	O7-C23-C24	3.99	102.86	111.48	12	6
3	A	605	PX4	O7-C23-O8	3.98	133.01	123.70	14	5
3	B	339	PX4	O7-C23-O8	3.98	133.00	123.70	13	3
3	B	374	PX4	C8-C7-C6	3.97	102.53	111.78	11	2
3	A	628	PX4	O7-C23-C24	3.96	102.92	111.48	10	4
3	B	379	PX4	C7-O7-C23	3.96	108.32	117.80	5	6
3	C	329	PX4	C5-N1-C4	3.96	98.58	108.98	9	3
3	B	344	PX4	O7-C23-C24	3.96	102.92	111.48	7	3
3	A	614	PX4	O5-C8-C7	3.96	119.80	108.40	12	5
3	C	364	PX4	O5-C8-C7	3.96	119.80	108.40	1	4
3	C	355	PX4	C7-O7-C23	3.95	108.33	117.80	5	5
3	C	319	PX4	O5-C8-C7	3.95	119.79	108.40	15	3
3	C	326	PX4	C8-C7-C6	3.95	102.57	111.78	12	3
3	C	313	PX4	O7-C23-C24	3.95	102.94	111.48	8	2
3	C	358	PX4	C7-O7-C23	3.95	108.35	117.80	3	8
3	B	321	PX4	C8-C7-C6	3.94	102.59	111.78	13	2
3	B	333	PX4	O5-C8-C7	3.94	119.77	108.40	1	3
3	C	315	PX4	O7-C23-C24	3.94	102.95	111.48	9	5
3	B	321	PX4	O5-C8-C7	3.94	119.76	108.40	13	4
3	C	323	PX4	C7-O7-C23	3.94	108.36	117.80	14	7
3	B	330	PX4	C5-N1-C3	3.94	98.64	108.98	4	2
3	B	328	PX4	C8-C7-C6	3.93	102.61	111.78	8	2
3	B	396	PX4	O5-C8-C7	3.93	119.73	108.40	10	5
3	A	601	PX4	C7-O7-C23	3.93	108.39	117.80	15	8
3	B	324	PX4	O7-C23-C24	3.93	102.99	111.48	12	4
3	A	634	PX4	O5-C9-C10	3.92	99.87	111.83	2	4
3	B	356	PX4	C8-C7-C6	3.92	102.64	111.78	14	3
3	A	639	PX4	O7-C23-C24	3.92	103.00	111.48	12	6
3	B	387	PX4	O7-C23-C24	3.92	103.00	111.48	5	3
3	B	369	PX4	O7-C23-C24	3.91	103.02	111.48	12	6
3	C	352	PX4	O7-C23-C24	3.91	103.02	111.48	4	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	C	360	PX4	C7-O7-C23	3.91	108.44	117.80	8	3
3	B	355	PX4	C4-N1-C3	3.90	98.72	108.98	3	2
3	B	303	PX4	C7-O7-C23	3.90	108.47	117.80	6	5
3	C	333	PX4	O7-C23-C24	3.90	103.05	111.48	8	4
3	B	327	PX4	O7-C23-C24	3.89	119.90	111.48	12	2
3	B	335	PX4	O5-C8-C7	3.89	119.60	108.40	9	2
3	C	329	PX4	C8-C7-C6	3.88	102.74	111.78	9	4
3	B	330	PX4	O7-C23-C24	3.87	103.10	111.48	5	4
3	A	648	PX4	C7-O7-C23	3.87	108.53	117.80	5	7
3	A	619	PX4	O7-C23-C24	3.87	103.11	111.48	10	4
3	B	309	PX4	C7-O7-C23	3.87	108.54	117.80	12	6
3	A	601	PX4	O7-C23-C24	3.87	103.12	111.48	12	3
3	B	372	PX4	C7-O7-C23	3.86	108.55	117.80	10	5
3	C	355	PX4	O7-C23-O8	3.87	132.74	123.70	8	4
3	B	311	PX4	O7-C23-O8	3.86	132.74	123.70	15	5
3	B	314	PX4	C5-N1-C3	3.86	98.83	108.98	10	4
3	C	336	PX4	O7-C23-C24	3.86	103.12	111.48	2	5
3	B	340	PX4	C8-C7-C6	3.86	102.79	111.78	8	4
3	B	393	PX4	O7-C23-C24	3.85	103.14	111.48	6	5
3	C	350	PX4	O5-C8-C7	3.85	119.50	108.40	1	4
3	B	400	PX4	O5-C8-C7	3.85	119.49	108.40	3	6
3	B	311	PX4	C5-N1-C4	3.85	98.87	108.98	6	1
3	C	350	PX4	C8-C7-C6	3.85	102.81	111.78	9	4
3	C	365	PX4	C7-O7-C23	3.85	108.59	117.80	15	2
3	B	346	PX4	C8-C7-C6	3.84	102.82	111.78	1	3
3	B	379	PX4	O7-C23-C24	3.85	103.16	111.48	7	5
3	A	646	PX4	C8-C7-C6	3.84	102.83	111.78	7	5
3	B	368	PX4	C7-O7-C23	3.84	108.61	117.80	11	6
3	C	319	PX4	C5-N1-C3	3.84	119.05	108.98	11	4
3	B	395	PX4	C7-O7-C23	3.83	108.62	117.80	12	8
3	B	372	PX4	C8-C7-C6	3.83	102.85	111.78	12	2
3	B	386	PX4	O5-C8-C7	3.83	119.44	108.40	4	5
3	C	322	PX4	C8-C7-C6	3.83	102.86	111.78	11	3
3	C	370	PX4	C7-O7-C23	3.82	108.65	117.80	4	7
3	B	369	PX4	C8-C7-C6	3.82	120.69	111.78	14	3
3	C	317	PX4	O5-C8-C7	3.82	119.41	108.40	4	6
3	B	334	PX4	C7-O7-C23	3.82	108.66	117.80	9	6
3	A	608	PX4	O5-C8-C7	3.81	119.38	108.40	5	2
3	C	347	PX4	C5-N1-C3	3.81	98.97	108.98	2	4
3	B	364	PX4	C5-N1-C4	3.81	98.97	108.98	11	4
3	A	615	PX4	C7-O7-C23	3.80	108.69	117.80	15	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	332	PX4	C8-C7-C6	3.80	120.65	111.78	14	1
3	B	339	PX4	C4-N1-C3	3.80	98.99	108.98	15	2
3	B	376	PX4	C7-O7-C23	3.80	108.70	117.80	2	7
3	C	351	PX4	O7-C23-C24	3.80	103.27	111.48	4	3
3	A	633	PX4	O5-C9-C10	3.79	100.28	111.83	11	1
3	B	340	PX4	O7-C23-C24	3.79	103.29	111.48	2	4
3	C	355	PX4	O7-C23-C24	3.79	103.29	111.48	1	2
3	B	355	PX4	O7-C23-C24	3.78	103.30	111.48	8	5
3	B	361	PX4	C7-O7-C23	3.78	108.75	117.80	3	4
3	A	647	PX4	O5-C9-C10	3.78	100.31	111.83	15	3
3	C	358	PX4	O5-C8-C7	3.78	119.29	108.40	14	4
3	B	327	PX4	O5-C8-C7	3.78	119.29	108.40	4	4
3	C	344	PX4	O7-C23-O8	3.78	132.54	123.70	10	1
3	B	301	PX4	C8-C7-C6	3.77	120.58	111.78	13	2
3	A	603	PX4	O7-C23-O8	3.77	132.51	123.70	2	3
3	A	622	PX4	O7-C23-C24	3.77	103.33	111.48	2	6
3	B	338	PX4	C1-C2-N1	3.76	127.90	115.82	7	2
3	A	642	PX4	C8-C7-C6	3.76	120.55	111.78	9	5
3	B	344	PX4	O7-C23-O8	3.76	132.49	123.70	7	2
3	C	341	PX4	O5-C8-C7	3.76	119.23	108.40	11	5
3	B	308	PX4	O5-C8-C7	3.76	119.23	108.40	2	3
3	C	340	PX4	O7-C23-C24	3.75	103.38	111.48	13	6
3	C	363	PX4	C7-O7-C23	3.75	108.83	117.80	6	6
3	B	393	PX4	O5-C9-O6	3.74	132.99	123.63	6	3
3	A	623	PX4	O7-C23-O8	3.74	132.44	123.70	13	3
3	B	317	PX4	O7-C23-C24	3.73	103.41	111.48	8	5
3	B	397	PX4	O7-C23-C24	3.73	103.41	111.48	14	4
3	C	305	PX4	O7-C23-C24	3.73	103.41	111.48	13	1
3	C	347	PX4	O7-C23-O8	3.73	132.42	123.70	5	3
3	C	368	PX4	C4-N1-C3	3.73	99.18	108.98	4	3
3	B	301	PX4	C7-O7-C23	3.73	108.87	117.80	3	5
3	B	307	PX4	O5-C8-C7	3.72	119.13	108.40	4	5
3	C	370	PX4	O5-C8-C7	3.72	119.13	108.40	7	4
3	B	312	PX4	C7-O7-C23	3.72	108.89	117.80	1	5
3	B	329	PX4	C8-C7-C6	3.72	103.11	111.78	13	5
3	B	332	PX4	C5-N1-C3	3.72	99.20	108.98	2	4
3	B	348	PX4	C8-C7-C6	3.72	103.12	111.78	8	4
3	A	644	PX4	C5-N1-C4	3.72	118.74	108.98	7	4
3	C	343	PX4	O5-C8-C7	3.71	119.10	108.40	15	2
3	B	339	PX4	O7-C23-C24	3.71	103.45	111.48	13	6
3	B	368	PX4	O7-C23-C24	3.71	103.45	111.48	4	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	318	PX4	C25-C24-C23	3.71	127.28	113.69	8	2
3	B	343	PX4	C8-O5-C9	3.71	103.57	117.12	14	3
3	B	353	PX4	C8-C7-C6	3.71	103.14	111.78	6	6
3	B	381	PX4	O7-C23-C24	3.71	103.46	111.48	1	2
3	B	384	PX4	C5-N1-C4	3.71	99.24	108.98	10	1
3	B	329	PX4	C7-O7-C23	3.70	108.93	117.80	10	6
3	A	624	PX4	O5-C8-C7	3.70	119.07	108.40	15	6
3	C	370	PX4	O7-C23-O8	3.70	132.36	123.70	5	3
3	B	370	PX4	O7-C23-O8	3.70	132.36	123.70	3	3
3	C	363	PX4	O5-C9-C10	3.70	100.56	111.83	7	3
3	A	627	PX4	C7-O7-C23	3.70	108.95	117.80	11	4
3	B	388	PX4	C8-C7-C6	3.70	103.17	111.78	5	2
3	C	314	PX4	C7-O7-C23	3.70	108.95	117.80	11	3
3	C	350	PX4	O5-C9-O6	3.69	132.87	123.63	15	1
3	B	342	PX4	O5-C8-C7	3.69	119.04	108.40	7	6
3	B	364	PX4	O5-C8-C7	3.68	119.00	108.40	5	8
3	C	369	PX4	C5-N1-C3	3.67	118.62	108.98	5	3
3	C	305	PX4	C7-O7-C23	3.67	126.58	117.80	6	7
3	B	341	PX4	O7-C7-C8	3.67	121.50	108.34	12	4
3	B	367	PX4	O7-C7-C6	3.67	121.49	108.34	13	2
3	A	634	PX4	C11-C10-C9	3.66	100.27	113.69	6	1
3	A	647	PX4	O5-C9-O6	3.66	132.79	123.63	15	3
3	A	609	PX4	O5-C9-O6	3.66	132.78	123.63	14	4
3	B	359	PX4	P1-O3-C1	3.66	138.68	121.26	5	1
3	B	383	PX4	O7-C23-C24	3.66	103.57	111.48	7	3
3	B	333	PX4	C4-N1-C2	3.65	95.40	109.91	5	1
3	B	362	PX4	C7-O7-C23	3.65	109.06	117.80	12	5
3	B	343	PX4	C4-N1-C3	3.65	118.55	108.98	13	2
3	A	619	PX4	O5-C8-C7	3.64	118.90	108.40	10	6
3	C	348	PX4	C7-O7-C23	3.64	109.08	117.80	8	3
3	A	623	PX4	O5-C9-C10	3.64	100.74	111.83	13	1
3	B	400	PX4	C5-N1-C4	3.64	99.42	108.98	6	3
3	A	602	PX4	O7-C23-C24	3.63	103.62	111.48	3	3
3	A	637	PX4	C7-O7-C23	3.63	109.10	117.80	14	5
3	A	646	PX4	C5-N1-C3	3.63	99.43	108.98	7	1
3	B	322	PX4	O7-C23-C24	3.64	103.62	111.48	14	3
3	C	348	PX4	O5-C8-C7	3.63	118.87	108.40	5	6
3	B	326	PX4	O5-C8-C7	3.63	118.86	108.40	12	5
3	B	364	PX4	C8-C7-C6	3.63	120.24	111.78	4	3
3	C	323	PX4	O5-C8-C7	3.63	118.85	108.40	5	4
3	B	305	PX4	O5-C9-O6	3.63	132.70	123.63	15	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	317	PX4	O5-C8-C7	3.62	118.84	108.40	12	6
3	B	336	PX4	C7-O7-C23	3.62	109.13	117.80	1	5
3	A	610	PX4	C7-O7-C23	3.62	109.13	117.80	10	8
3	B	378	PX4	O7-C23-O8	3.62	132.17	123.70	4	2
3	A	620	PX4	C7-O7-C23	3.62	109.13	117.80	14	6
3	A	632	PX4	C5-N1-C4	3.62	99.47	108.98	9	1
3	A	612	PX4	O7-C23-C24	3.62	103.66	111.48	12	3
3	A	626	PX4	O5-C8-C7	3.61	118.81	108.40	15	5
3	B	306	PX4	C7-O7-C23	3.61	126.44	117.80	1	5
3	A	647	PX4	C4-N1-C3	3.60	118.44	108.98	14	2
3	B	374	PX4	C7-O7-C23	3.60	109.17	117.80	8	5
3	A	627	PX4	O7-C23-C24	3.60	103.69	111.48	4	4
3	C	328	PX4	C4-N1-C3	3.60	99.52	108.98	13	2
3	A	607	PX4	C5-N1-C4	3.60	99.52	108.98	3	3
3	B	304	PX4	C7-O7-C23	3.60	109.18	117.80	6	5
3	C	349	PX4	O7-C23-C24	3.60	103.70	111.48	15	5
3	C	349	PX4	C7-O7-C23	3.60	109.19	117.80	7	3
3	B	310	PX4	C8-C7-C6	3.59	120.16	111.78	13	1
3	C	332	PX4	C4-N1-C3	3.59	99.54	108.98	15	2
3	B	375	PX4	O7-C23-O8	3.59	132.10	123.70	6	4
3	B	352	PX4	C5-N1-C4	3.59	99.55	108.98	5	2
3	A	637	PX4	C8-C7-C6	3.59	103.42	111.78	1	3
3	B	395	PX4	O5-C9-C10	3.59	100.90	111.83	3	1
3	C	346	PX4	C8-C7-C6	3.59	103.42	111.78	15	4
3	B	380	PX4	C8-C7-C6	3.58	120.13	111.78	12	2
3	A	637	PX4	O5-C8-C7	3.58	118.70	108.40	2	5
3	B	369	PX4	C4-N1-C3	3.58	99.58	108.98	8	2
3	B	399	PX4	C7-O7-C23	3.58	109.24	117.80	7	5
3	A	643	PX4	O5-C9-O6	3.57	132.56	123.63	1	4
3	B	334	PX4	O5-C9-C10	3.57	100.96	111.83	9	3
3	B	388	PX4	O7-C23-C24	3.57	103.76	111.48	5	4
3	C	307	PX4	C1-C2-N1	3.57	127.27	115.82	12	1
3	A	620	PX4	O5-C8-C7	3.56	118.67	108.40	1	4
3	B	315	PX4	C7-O7-C23	3.56	109.27	117.80	1	7
3	A	623	PX4	O5-C9-O6	3.56	132.54	123.63	2	4
3	B	332	PX4	C7-O7-C23	3.56	126.33	117.80	7	2
3	B	333	PX4	O7-C23-C24	3.56	103.77	111.48	1	3
3	C	320	PX4	C5-N1-C3	3.56	99.62	108.98	1	2
3	A	623	PX4	C7-O7-C23	3.56	109.28	117.80	6	4
3	C	316	PX4	C8-C7-C6	3.56	103.49	111.78	5	1
3	A	602	PX4	O5-C9-O6	3.55	132.52	123.63	9	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	375	PX4	C5-N1-C4	3.55	118.30	108.98	5	2
3	C	327	PX4	O5-C8-C7	3.55	118.63	108.40	2	5
3	C	336	PX4	C25-C24-C23	3.55	100.70	113.69	15	1
3	A	604	PX4	O5-C8-C7	3.55	118.62	108.40	15	2
3	B	304	PX4	C8-O5-C9	3.54	104.17	117.12	4	4
3	B	317	PX4	O5-C9-O6	3.54	132.49	123.63	8	4
3	A	616	PX4	O5-C9-O6	3.54	132.49	123.63	15	2
3	B	304	PX4	C1-C2-N1	3.54	127.18	115.82	5	1
3	B	394	PX4	O7-C23-O8	3.54	131.98	123.70	7	3
3	C	326	PX4	O7-C23-C24	3.54	103.82	111.48	3	5
3	C	342	PX4	O7-C23-C24	3.54	103.82	111.48	7	6
3	B	383	PX4	O7-C23-O8	3.54	131.97	123.70	5	3
3	C	340	PX4	C26-C25-C24	3.54	100.13	113.13	7	1
3	C	341	PX4	O7-C23-O8	3.54	131.97	123.70	4	2
3	A	645	PX4	C7-O7-C23	3.53	126.25	117.80	6	6
3	B	360	PX4	C7-O7-C23	3.53	126.25	117.80	1	3
3	C	322	PX4	C7-O7-C23	3.53	109.34	117.80	12	2
3	B	320	PX4	O7-C23-O8	3.53	131.95	123.70	5	3
3	A	615	PX4	C8-C7-C6	3.53	103.56	111.78	1	4
3	B	331	PX4	O5-C8-C7	3.53	118.56	108.40	15	5
3	B	365	PX4	O7-C23-O8	3.53	131.95	123.70	7	4
3	B	303	PX4	C5-N1-C3	3.52	99.72	108.98	15	3
3	B	360	PX4	O7-C23-O8	3.52	131.94	123.70	14	2
3	C	363	PX4	C5-N1-C4	3.52	118.23	108.98	13	1
3	A	605	PX4	C7-O7-C23	3.52	109.38	117.80	14	1
3	B	357	PX4	O7-C23-C24	3.52	103.87	111.48	9	4
3	C	334	PX4	O5-C8-C7	3.52	118.53	108.40	3	1
3	C	346	PX4	C7-O7-C23	3.52	109.38	117.80	3	4
3	C	369	PX4	C1-C2-N1	3.51	127.10	115.82	14	4
3	B	347	PX4	C4-N1-C3	3.51	99.75	108.98	10	5
3	C	327	PX4	C7-O7-C23	3.51	109.40	117.80	2	1
3	C	303	PX4	C8-C7-C6	3.51	103.61	111.78	11	5
3	C	312	PX4	O5-C8-C7	3.51	118.51	108.40	2	5
3	C	324	PX4	C5-N1-C3	3.51	99.76	108.98	1	4
3	A	613	PX4	O7-C23-C24	3.51	103.90	111.48	1	3
3	A	648	PX4	O7-C23-C24	3.50	103.91	111.48	15	7
3	B	302	PX4	O7-C7-C8	3.50	120.91	108.34	1	2
3	B	379	PX4	O5-C8-C7	3.50	118.49	108.40	10	5
3	C	330	PX4	O7-C23-C24	3.50	103.91	111.48	14	2
3	B	312	PX4	O5-C8-C7	3.50	118.49	108.40	15	6
3	C	357	PX4	O5-C8-C7	3.50	118.48	108.40	2	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	315	PX4	C8-C7-C6	3.50	103.63	111.78	2	4
3	B	373	PX4	C1-C2-N1	3.50	127.04	115.82	15	4
3	B	374	PX4	C1-C2-N1	3.50	127.04	115.82	6	3
3	C	325	PX4	C5-N1-C4	3.50	99.79	108.98	8	2
3	B	315	PX4	O7-C7-C8	3.49	120.87	108.34	10	2
3	B	332	PX4	C5-N1-C4	3.49	118.15	108.98	11	4
3	B	341	PX4	O5-C8-C7	3.49	118.47	108.40	10	5
3	A	608	PX4	O7-C23-C24	3.49	103.93	111.48	12	4
3	C	307	PX4	O5-C8-C7	3.49	118.46	108.40	8	1
3	B	306	PX4	O7-C23-C24	3.49	103.93	111.48	11	3
3	C	326	PX4	O7-C7-C6	3.49	120.86	108.34	3	1
3	B	356	PX4	O5-C8-C7	3.48	118.44	108.40	14	5
3	B	369	PX4	O5-C9-O6	3.48	132.34	123.63	5	4
3	B	380	PX4	C5-N1-C3	3.48	99.82	108.98	11	2
3	C	302	PX4	C7-O7-C23	3.48	109.46	117.80	7	7
3	C	328	PX4	O7-C23-C24	3.48	103.94	111.48	6	4
3	A	619	PX4	C4-N1-C3	3.48	99.83	108.98	10	3
3	A	648	PX4	C1-C2-N1	3.48	126.99	115.82	15	1
3	C	326	PX4	O5-C8-C7	3.48	118.43	108.40	9	5
3	B	327	PX4	C5-N1-C4	3.48	99.84	108.98	3	3
3	B	384	PX4	C7-O7-C23	3.48	109.47	117.80	15	5
3	B	391	PX4	O7-C23-C24	3.48	119.00	111.48	13	4
3	B	305	PX4	C4-N1-C3	3.48	118.11	108.98	6	2
3	A	602	PX4	C4-N1-C3	3.48	99.85	108.98	14	3
3	B	386	PX4	O7-C23-C24	3.47	103.97	111.48	3	5
3	C	336	PX4	O7-C23-O8	3.48	131.83	123.70	13	2
3	B	395	PX4	O5-C8-C7	3.47	118.41	108.40	13	5
3	C	336	PX4	C7-O7-C23	3.47	109.49	117.80	6	4
3	C	306	PX4	O7-C23-O8	3.47	131.81	123.70	4	2
3	B	357	PX4	C8-C7-C6	3.47	103.70	111.78	4	2
3	B	382	PX4	C7-O7-C23	3.46	109.51	117.80	10	4
3	B	398	PX4	O7-C23-O8	3.46	131.80	123.70	13	3
3	A	644	PX4	O5-C8-C7	3.46	118.37	108.40	15	3
3	B	306	PX4	C8-C7-C6	3.46	103.72	111.78	10	2
3	B	326	PX4	C8-O5-C9	3.46	104.47	117.12	2	1
3	C	303	PX4	O5-C8-C7	3.46	118.37	108.40	5	7
3	C	332	PX4	C5-N1-C3	3.46	99.89	108.98	11	3
3	C	354	PX4	C8-C7-C6	3.46	103.72	111.78	2	3
3	B	384	PX4	C8-O5-C9	3.46	104.47	117.12	10	1
3	C	321	PX4	O7-C7-C8	3.46	120.75	108.34	7	1
3	B	309	PX4	O5-C8-C7	3.46	118.36	108.40	13	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	334	PX4	O5-C8-C7	3.46	118.37	108.40	12	6
3	A	635	PX4	O7-C23-C24	3.46	104.00	111.48	2	6
3	A	648	PX4	C5-N1-C3	3.45	99.90	108.98	5	4
3	C	320	PX4	O5-C8-C7	3.46	118.36	108.40	14	3
3	C	315	PX4	O7-C23-O8	3.45	131.78	123.70	9	2
3	C	343	PX4	O7-C23-C24	3.45	104.01	111.48	1	6
3	A	644	PX4	C7-O7-C23	3.45	109.53	117.80	14	3
3	B	340	PX4	C5-N1-C3	3.45	99.91	108.98	7	1
3	B	387	PX4	C7-O7-C23	3.45	109.53	117.80	10	4
3	B	373	PX4	C8-C7-C6	3.45	119.83	111.78	3	5
3	B	365	PX4	C8-C7-C6	3.44	103.76	111.78	1	4
3	B	371	PX4	C7-O7-C23	3.44	109.56	117.80	3	6
3	B	393	PX4	C7-O7-C23	3.44	109.56	117.80	12	3
3	B	326	PX4	C8-C7-C6	3.44	103.77	111.78	3	3
3	A	634	PX4	P1-O3-C1	3.44	104.89	121.26	7	1
3	C	345	PX4	O7-C23-C24	3.44	104.05	111.48	9	6
3	B	366	PX4	C8-C7-C6	3.44	103.77	111.78	12	2
3	A	648	PX4	O5-C8-C7	3.43	118.30	108.40	10	6
3	C	324	PX4	O5-C8-C7	3.43	118.30	108.40	3	5
3	A	613	PX4	C8-C7-C6	3.43	119.79	111.78	13	4
3	C	333	PX4	O5-C8-C7	3.43	118.29	108.40	11	3
3	C	336	PX4	C8-C7-C6	3.43	103.78	111.78	6	4
3	B	348	PX4	O7-C23-C24	3.43	104.06	111.48	5	5
3	A	636	PX4	C5-N1-C2	3.43	96.29	109.91	3	1
3	C	346	PX4	O7-C23-O8	3.42	131.71	123.70	3	3
3	A	606	PX4	O7-C23-O8	3.42	131.70	123.70	4	2
3	A	619	PX4	C8-C7-C6	3.42	103.81	111.78	9	1
3	C	304	PX4	C7-O7-C23	3.42	109.61	117.80	9	4
3	A	617	PX4	C7-O7-C23	3.42	109.62	117.80	9	4
3	B	350	PX4	O7-C23-C24	3.42	104.09	111.48	9	5
3	C	338	PX4	C7-O7-C23	3.42	109.62	117.80	6	2
3	B	302	PX4	O5-C8-C7	3.41	118.23	108.40	4	2
3	A	603	PX4	C5-N1-C3	3.41	100.01	108.98	2	5
3	B	337	PX4	O5-C8-C7	3.41	118.23	108.40	11	4
3	C	353	PX4	C4-N1-C3	3.41	100.01	108.98	3	2
3	B	308	PX4	C5-N1-C3	3.41	100.03	108.98	11	3
3	A	623	PX4	O7-C23-C24	3.41	104.11	111.48	9	3
3	C	356	PX4	O5-C8-C7	3.41	118.22	108.40	11	2
3	A	633	PX4	O7-C23-C24	3.40	104.12	111.48	14	5
3	B	391	PX4	C7-O7-C23	3.40	109.65	117.80	4	6
3	B	333	PX4	C7-O7-C23	3.40	109.66	117.80	5	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	370	PX4	C4-N1-C3	3.40	117.90	108.98	6	3
3	C	353	PX4	O5-C9-O6	3.40	132.13	123.63	15	3
3	B	365	PX4	O5-C9-O6	3.39	132.12	123.63	8	4
3	C	370	PX4	C8-C7-C6	3.39	103.87	111.78	13	5
3	C	309	PX4	O7-C23-O8	3.39	131.64	123.70	1	5
3	C	343	PX4	C7-O7-C23	3.39	109.68	117.80	2	5
3	B	351	PX4	O7-C7-C6	3.39	120.50	108.34	5	5
3	B	387	PX4	O5-C8-C7	3.39	118.16	108.40	12	7
3	B	361	PX4	C8-C7-C6	3.39	103.89	111.78	10	2
3	A	638	PX4	C5-N1-C4	3.38	100.08	108.98	8	1
3	C	323	PX4	C8-O5-C9	3.38	104.75	117.12	7	3
3	C	359	PX4	C7-O7-C23	3.39	109.69	117.80	15	4
3	B	367	PX4	O5-C8-C7	3.38	118.15	108.40	8	2
3	C	351	PX4	O5-C8-C7	3.38	118.14	108.40	1	2
3	C	368	PX4	O7-C7-C6	3.38	96.23	108.34	5	1
3	B	355	PX4	C8-C7-C6	3.37	103.92	111.78	6	3
3	B	325	PX4	O5-C8-C7	3.37	118.12	108.40	2	8
3	C	315	PX4	C8-O5-C9	3.37	104.79	117.12	4	2
3	C	357	PX4	O7-C23-C24	3.37	104.18	111.48	1	5
3	B	340	PX4	O5-C8-C7	3.37	118.11	108.40	3	6
3	C	365	PX4	O5-C8-C7	3.37	118.11	108.40	11	5
3	B	320	PX4	O7-C23-C24	3.36	104.21	111.48	7	4
3	B	361	PX4	O7-C23-C24	3.36	104.21	111.48	2	4
3	C	325	PX4	O7-C23-C24	3.36	104.21	111.48	5	3
3	B	372	PX4	O7-C23-C24	3.36	104.21	111.48	7	7
3	B	398	PX4	C7-O7-C23	3.36	109.75	117.80	11	6
3	A	643	PX4	C7-O7-C23	3.36	109.76	117.80	6	2
3	B	390	PX4	O5-C8-C7	3.36	118.08	108.40	15	6
3	B	310	PX4	O7-C23-C24	3.36	104.22	111.48	11	2
3	B	324	PX4	O7-C23-O8	3.36	131.55	123.70	9	3
3	C	336	PX4	O7-C7-C8	3.36	120.39	108.34	2	1
3	B	313	PX4	C7-O7-C23	3.35	109.77	117.80	10	7
3	B	324	PX4	C7-O7-C23	3.35	109.77	117.80	1	3
3	B	359	PX4	O7-C23-O8	3.35	131.55	123.70	2	4
3	B	389	PX4	C5-N1-C4	3.35	100.17	108.98	3	1
3	B	400	PX4	C25-C24-C23	3.35	125.98	113.69	2	1
3	C	349	PX4	C8-O5-C9	3.35	104.87	117.12	15	2
3	A	630	PX4	O7-C23-C24	3.35	104.23	111.48	4	3
3	B	335	PX4	C7-O7-C23	3.35	109.78	117.80	9	4
3	B	358	PX4	C8-O5-C9	3.35	104.87	117.12	11	3
3	C	317	PX4	C7-O7-C23	3.35	109.78	117.80	6	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	C	311	PX4	C11-C10-C9	3.35	101.42	113.69	14	2
3	C	333	PX4	C4-N1-C3	3.35	100.18	108.98	14	3
3	C	303	PX4	O7-C23-O8	3.34	131.52	123.70	1	3
3	A	632	PX4	O7-C23-C24	3.34	104.26	111.48	14	3
3	B	303	PX4	C5-N1-C4	3.34	100.20	108.98	8	3
3	B	365	PX4	O7-C23-C24	3.34	104.25	111.48	5	5
3	C	304	PX4	C11-C10-C9	3.34	101.45	113.69	4	1
3	B	377	PX4	C5-N1-C3	3.34	100.21	108.98	10	2
3	A	644	PX4	O5-C9-O6	3.34	131.97	123.63	13	2
3	B	314	PX4	C7-O7-C23	3.33	109.82	117.80	11	8
3	B	363	PX4	O7-C23-C24	3.33	104.27	111.48	8	6
3	B	377	PX4	O5-C9-C10	3.33	101.67	111.83	1	2
3	B	396	PX4	O7-C23-O8	3.33	131.50	123.70	5	1
3	B	339	PX4	O5-C8-C7	3.33	118.00	108.40	15	5
3	B	343	PX4	O7-C7-C8	3.33	120.27	108.34	15	1
3	C	329	PX4	O5-C9-C10	3.33	101.70	111.83	9	3
3	A	609	PX4	O7-C23-O8	3.32	131.48	123.70	12	2
3	C	328	PX4	C5-N1-C4	3.32	117.70	108.98	1	1
3	A	606	PX4	O7-C23-C24	3.32	104.30	111.48	12	5
3	A	611	PX4	O7-C23-C24	3.32	104.30	111.48	14	5
3	C	351	PX4	C8-C7-C6	3.32	104.04	111.78	10	3
3	B	361	PX4	O5-C8-C7	3.32	117.97	108.40	1	2
3	B	346	PX4	O7-C23-C24	3.32	104.30	111.48	12	3
3	A	605	PX4	C5-N1-C4	3.32	100.27	108.98	4	1
3	C	302	PX4	O7-C23-O8	3.31	131.46	123.70	7	2
3	B	397	PX4	C7-O7-C23	3.31	109.87	117.80	13	6
3	C	366	PX4	O7-C23-O8	3.31	131.45	123.70	4	1
3	B	360	PX4	C8-C7-C6	3.31	104.06	111.78	2	5
3	B	352	PX4	C4-N1-C3	3.31	117.67	108.98	14	3
3	B	304	PX4	C11-C10-C9	3.30	101.59	113.69	12	2
3	B	349	PX4	O5-C9-O6	3.30	131.89	123.63	2	1
3	C	321	PX4	C7-O7-C23	3.30	109.89	117.80	13	5
3	B	332	PX4	O7-C23-C24	3.30	104.34	111.48	5	3
3	C	320	PX4	C8-O5-C9	3.30	105.06	117.12	15	1
3	C	362	PX4	C5-N1-C3	3.30	100.31	108.98	9	3
3	A	613	PX4	O7-C7-C6	3.30	120.17	108.34	6	1
3	A	614	PX4	O5-C9-O6	3.30	131.88	123.63	7	1
3	C	350	PX4	O7-C23-O8	3.30	131.41	123.70	3	2
3	B	335	PX4	C5-N1-C4	3.30	100.32	108.98	13	4
3	A	621	PX4	C8-C7-C6	3.29	104.11	111.78	15	2
3	B	341	PX4	C8-C7-C6	3.29	119.46	111.78	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	371	PX4	C26-C25-C24	3.29	101.03	113.13	6	1
3	C	358	PX4	O7-C23-C24	3.29	104.36	111.48	2	2
3	A	628	PX4	O5-C9-C10	3.29	101.80	111.83	13	1
3	B	395	PX4	O7-C7-C8	3.29	120.14	108.34	5	3
3	A	629	PX4	O7-C7-C8	3.29	120.14	108.34	11	2
3	A	634	PX4	O5-C8-C7	3.29	117.87	108.40	7	5
3	B	362	PX4	O7-C23-C24	3.29	104.37	111.48	8	2
3	B	370	PX4	C7-O7-C23	3.29	109.93	117.80	5	3
3	C	321	PX4	O5-C8-C7	3.28	117.86	108.40	9	2
3	A	622	PX4	C7-O7-C23	3.28	109.94	117.80	1	5
3	C	301	PX4	O7-C23-O8	3.28	131.38	123.70	12	4
3	C	354	PX4	O7-C23-C24	3.28	104.38	111.48	11	1
3	C	314	PX4	C8-O5-C9	3.28	105.13	117.12	3	4
3	C	368	PX4	O5-C9-C10	3.28	101.83	111.83	10	5
3	A	622	PX4	C5-N1-C4	3.28	100.36	108.98	11	2
3	C	308	PX4	C7-O7-C23	3.28	125.64	117.80	12	3
3	C	365	PX4	O5-C9-C10	3.28	101.84	111.83	5	1
3	B	350	PX4	C5-N1-C3	3.27	100.38	108.98	10	4
3	B	365	PX4	C7-O7-C23	3.27	109.96	117.80	12	4
3	B	356	PX4	C5-N1-C4	3.27	100.38	108.98	12	1
3	B	337	PX4	C11-C10-C9	3.27	101.72	113.69	7	1
3	B	357	PX4	C4-N1-C3	3.27	100.39	108.98	10	1
3	C	330	PX4	C7-O7-C23	3.27	109.97	117.80	13	4
3	B	303	PX4	O5-C9-O6	3.27	131.80	123.63	9	2
3	B	354	PX4	O7-C23-C24	3.27	104.42	111.48	12	2
3	A	626	PX4	O7-C23-C24	3.26	104.42	111.48	8	2
3	A	632	PX4	O7-C7-C6	3.26	120.05	108.34	8	1
3	B	313	PX4	C5-N1-C4	3.26	117.55	108.98	2	3
3	C	318	PX4	C5-N1-C4	3.26	100.41	108.98	8	2
3	B	312	PX4	C4-N1-C3	3.26	117.54	108.98	11	2
3	B	399	PX4	O5-C8-C7	3.26	117.80	108.40	8	5
3	C	330	PX4	O5-C8-C7	3.26	117.79	108.40	13	4
3	C	363	PX4	C11-C10-C9	3.26	125.64	113.69	8	1
3	B	337	PX4	O7-C23-C24	3.26	104.43	111.48	8	5
3	A	643	PX4	O5-C8-C7	3.26	117.78	108.40	10	3
3	B	366	PX4	O7-C23-C24	3.26	104.44	111.48	8	5
3	C	330	PX4	C25-C24-C23	3.25	125.62	113.69	2	1
3	B	381	PX4	C4-N1-C3	3.25	117.52	108.98	10	4
3	B	387	PX4	O5-C9-C10	3.25	101.92	111.83	12	3
3	B	330	PX4	O7-C7-C8	3.25	120.00	108.34	11	2
3	B	397	PX4	C5-N1-C4	3.25	117.51	108.98	13	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	633	PX4	O5-C9-O6	3.25	131.75	123.63	4	2
3	B	328	PX4	O7-C23-C24	3.25	104.46	111.48	7	5
3	C	332	PX4	O7-C7-C8	3.25	119.99	108.34	1	1
3	C	364	PX4	C7-O7-C23	3.24	110.03	117.80	12	3
3	A	607	PX4	C8-C7-C6	3.24	104.22	111.78	12	1
3	A	609	PX4	C8-C7-C6	3.24	104.23	111.78	15	3
3	B	311	PX4	O7-C23-C24	3.24	118.49	111.48	11	3
3	B	378	PX4	O5-C8-C7	3.24	117.74	108.40	2	5
3	A	611	PX4	O5-C8-C7	3.24	117.74	108.40	11	3
3	B	324	PX4	O5-C8-C7	3.24	117.74	108.40	11	5
3	B	326	PX4	O7-C23-C24	3.24	104.47	111.48	10	6
3	A	632	PX4	O5-C8-C7	3.24	117.73	108.40	13	3
3	A	609	PX4	O5-C8-C7	3.24	117.72	108.40	1	3
3	C	364	PX4	O7-C23-C24	3.23	104.48	111.48	10	5
3	C	341	PX4	C8-C7-C6	3.23	104.25	111.78	9	3
3	C	302	PX4	O5-C9-O6	3.23	131.71	123.63	2	4
3	A	603	PX4	C8-C7-C6	3.23	119.31	111.78	7	4
3	B	344	PX4	C4-N1-C3	3.23	100.50	108.98	1	1
3	B	344	PX4	C8-C7-C6	3.23	104.26	111.78	7	3
3	B	359	PX4	C7-O7-C23	3.23	110.07	117.80	10	4
3	C	338	PX4	C8-C7-C6	3.23	104.26	111.78	7	2
3	C	370	PX4	C5-N1-C3	3.23	100.50	108.98	2	4
3	B	323	PX4	O5-C8-C7	3.22	117.69	108.40	6	5
3	A	636	PX4	O7-C23-O8	3.22	131.24	123.70	8	3
3	B	353	PX4	C1-C2-N1	3.22	126.16	115.82	15	2
3	B	377	PX4	O7-C23-O8	3.22	131.24	123.70	14	1
3	A	620	PX4	C5-N1-C3	3.22	100.52	108.98	10	1
3	B	314	PX4	C5-N1-C4	3.22	100.52	108.98	2	1
3	A	614	PX4	O7-C23-C24	3.22	104.53	111.48	5	5
3	A	646	PX4	O5-C8-C7	3.22	117.67	108.40	11	3
3	B	306	PX4	C5-N1-C4	3.22	117.42	108.98	7	2
3	B	331	PX4	O5-C9-O6	3.22	131.67	123.63	3	2
3	A	617	PX4	O7-C23-C24	3.21	104.53	111.48	1	5
3	A	625	PX4	C7-O7-C23	3.21	110.10	117.80	15	2
3	C	361	PX4	C7-O7-C23	3.22	110.10	117.80	1	7
3	B	399	PX4	C11-C10-C9	3.21	101.92	113.69	15	1
3	B	311	PX4	C5-N1-C3	3.21	100.54	108.98	14	1
3	C	321	PX4	C8-C7-C6	3.21	119.28	111.78	14	4
3	A	639	PX4	C8-C7-C6	3.21	119.27	111.78	5	2
3	C	333	PX4	C7-O7-C23	3.21	110.11	117.80	1	6
3	C	357	PX4	O7-C23-O8	3.21	131.21	123.70	5	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	311	PX4	C8-C7-C6	3.21	119.27	111.78	9	2
3	B	323	PX4	O7-C23-C24	3.21	104.54	111.48	2	4
3	B	305	PX4	O7-C23-C24	3.21	104.54	111.48	5	5
3	B	323	PX4	C5-N1-C4	3.21	117.40	108.98	6	4
3	B	348	PX4	C7-O7-C23	3.21	110.12	117.80	5	4
3	C	347	PX4	O7-C23-C24	3.21	104.54	111.48	6	5
3	B	322	PX4	O5-C9-C10	3.20	102.06	111.83	2	2
3	B	394	PX4	O5-C9-C10	3.21	102.06	111.83	11	1
3	C	324	PX4	O7-C23-O8	3.20	131.19	123.70	8	3
3	C	351	PX4	C4-N1-C3	3.20	100.56	108.98	1	3
3	B	377	PX4	C4-N1-C3	3.20	100.57	108.98	5	3
3	C	331	PX4	C7-O7-C23	3.20	110.13	117.80	4	5
3	A	623	PX4	C8-C7-C6	3.20	119.25	111.78	14	3
3	B	345	PX4	O5-C9-O6	3.20	131.63	123.63	1	3
3	B	358	PX4	O7-C23-C24	3.20	104.56	111.48	1	6
3	C	349	PX4	C8-C7-C6	3.20	104.33	111.78	2	3
3	A	602	PX4	O7-C7-C6	3.20	96.88	108.34	1	2
3	B	356	PX4	O7-C23-C24	3.20	104.57	111.48	15	3
3	C	309	PX4	C1-C2-N1	3.19	126.08	115.82	11	1
3	B	372	PX4	O5-C8-C7	3.19	117.60	108.40	5	4
3	B	343	PX4	O5-C8-C7	3.19	117.60	108.40	14	4
3	B	385	PX4	O5-C8-C7	3.19	117.60	108.40	12	3
3	A	637	PX4	C1-C2-N1	3.19	126.06	115.82	14	1
3	B	309	PX4	O7-C23-C24	3.19	104.58	111.48	7	6
3	B	395	PX4	C8-C7-C6	3.19	104.34	111.78	15	3
3	C	341	PX4	C7-O7-C23	3.19	110.16	117.80	5	4
3	C	342	PX4	O5-C9-O6	3.19	115.65	123.63	11	2
3	C	311	PX4	C4-N1-C3	3.19	100.60	108.98	5	2
3	C	332	PX4	C5-N1-C4	3.19	100.60	108.98	14	2
3	C	314	PX4	O5-C8-C7	3.19	117.59	108.40	10	6
3	B	373	PX4	C7-O7-C23	3.19	110.17	117.80	9	3
3	C	329	PX4	C8-O5-C9	3.19	105.47	117.12	8	1
3	B	315	PX4	C5-N1-C4	3.18	100.61	108.98	1	2
3	B	336	PX4	O5-C8-C7	3.18	117.57	108.40	1	3
3	B	318	PX4	C7-O7-C23	3.18	110.19	117.80	8	5
3	B	352	PX4	O5-C8-C7	3.18	117.56	108.40	14	3
3	B	355	PX4	O5-C8-C7	3.18	117.56	108.40	15	4
3	B	384	PX4	O7-C7-C8	3.18	119.75	108.34	9	3
3	A	610	PX4	C4-N1-C3	3.18	100.63	108.98	2	1
3	A	605	PX4	O7-C23-C24	3.18	104.61	111.48	7	2
3	A	634	PX4	O5-C9-O6	3.18	131.57	123.63	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	641	PX4	O7-C23-C24	3.18	104.61	111.48	10	3
3	B	399	PX4	C5-N1-C4	3.18	117.32	108.98	7	2
3	B	314	PX4	O5-C8-C7	3.17	117.55	108.40	4	4
3	B	367	PX4	O5-C9-O6	3.17	131.57	123.63	11	4
3	B	390	PX4	O5-C9-C10	3.17	102.16	111.83	13	1
3	C	333	PX4	C5-N1-C3	3.17	117.31	108.98	14	3
3	C	333	PX4	O7-C23-O8	3.17	131.12	123.70	6	3
3	C	370	PX4	O5-C9-C10	3.17	102.16	111.83	14	3
3	B	329	PX4	C5-N1-C4	3.17	117.30	108.98	1	2
3	B	356	PX4	C1-C2-N1	3.17	126.00	115.82	9	1
3	B	396	PX4	O5-C9-C10	3.17	102.17	111.83	5	3
3	A	605	PX4	C5-N1-C3	3.17	100.65	108.98	12	3
3	A	612	PX4	C5-N1-C3	3.17	117.30	108.98	11	3
3	B	395	PX4	O7-C23-O8	3.17	131.11	123.70	4	1
3	A	607	PX4	C7-O7-C23	3.17	110.22	117.80	11	2
3	B	312	PX4	C5-N1-C4	3.17	100.66	108.98	11	2
3	C	312	PX4	P1-O3-C1	3.17	136.34	121.26	12	1
3	A	644	PX4	C4-N1-C3	3.16	117.29	108.98	15	1
3	B	346	PX4	C7-O7-C23	3.17	110.22	117.80	9	3
3	B	369	PX4	O5-C8-C7	3.16	117.52	108.40	7	5
3	C	311	PX4	O5-C8-C7	3.16	117.52	108.40	13	7
3	C	335	PX4	C7-O7-C23	3.16	110.22	117.80	12	5
3	C	313	PX4	O7-C7-C8	3.16	119.68	108.34	10	4
3	C	358	PX4	C8-C7-C6	3.16	104.42	111.78	15	4
3	A	643	PX4	C26-C25-C24	3.16	124.72	113.13	5	1
3	C	356	PX4	O7-C7-C8	3.16	119.67	108.34	8	2
3	C	361	PX4	C4-N1-C3	3.16	100.69	108.98	4	4
3	B	354	PX4	O5-C8-C7	3.15	117.49	108.40	3	2
3	A	601	PX4	O5-C8-C7	3.15	117.48	108.40	12	6
3	A	625	PX4	O5-C8-C7	3.15	99.31	108.40	6	2
3	C	355	PX4	C8-C7-C6	3.15	119.13	111.78	2	1
3	A	611	PX4	O7-C7-C8	3.15	119.64	108.34	13	4
3	A	618	PX4	C12-C11-C10	3.15	101.55	113.13	11	1
3	B	376	PX4	C8-C7-C6	3.15	104.44	111.78	1	3
3	B	391	PX4	C26-C25-C24	3.15	124.69	113.13	9	3
3	C	365	PX4	C8-C7-C6	3.15	104.44	111.78	3	3
3	A	628	PX4	O7-C23-O8	3.15	131.06	123.70	10	1
3	B	309	PX4	O5-C9-C10	3.15	102.24	111.83	1	5
3	C	365	PX4	C5-N1-C3	3.15	100.71	108.98	3	1
3	A	624	PX4	C25-C24-C23	3.14	102.17	113.69	5	1
3	B	369	PX4	O7-C23-O8	3.15	131.06	123.70	15	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	311	PX4	C12-C11-C10	3.14	101.57	113.13	8	1
3	C	316	PX4	O7-C23-C24	3.14	104.68	111.48	10	4
3	C	337	PX4	C7-O7-C23	3.14	110.27	117.80	9	5
3	B	327	PX4	O5-C9-O6	3.14	131.49	123.63	11	1
3	B	338	PX4	O7-C23-C24	3.14	104.68	111.48	1	2
3	B	354	PX4	C5-N1-C3	3.14	100.73	108.98	2	1
3	B	381	PX4	O5-C8-C7	3.14	117.45	108.40	10	4
3	A	615	PX4	C5-N1-C4	3.14	117.22	108.98	11	1
3	B	348	PX4	O7-C23-O8	3.14	131.04	123.70	6	2
3	B	399	PX4	C5-N1-C3	3.14	117.22	108.98	5	1
3	C	352	PX4	C7-O7-C23	3.14	110.28	117.80	6	2
3	A	613	PX4	C25-C24-C23	3.14	125.18	113.69	2	1
3	C	319	PX4	C8-C7-C6	3.14	104.47	111.78	7	3
3	C	308	PX4	O7-C23-C24	3.13	104.70	111.48	3	3
3	B	366	PX4	O5-C8-C7	3.13	117.43	108.40	9	3
3	C	332	PX4	O7-C23-C24	3.13	104.70	111.48	9	3
3	A	613	PX4	O7-C7-C8	3.13	119.58	108.34	3	2
3	C	362	PX4	O7-C23-O8	3.13	131.03	123.70	1	3
3	A	639	PX4	O5-C8-C7	3.13	117.42	108.40	7	4
3	A	614	PX4	C8-O5-C9	3.13	105.68	117.12	13	3
3	C	320	PX4	O7-C23-C24	3.13	104.71	111.48	2	6
3	B	352	PX4	O7-C23-C24	3.13	104.71	111.48	9	3
3	A	635	PX4	C7-O7-C23	3.13	110.31	117.80	2	5
3	B	393	PX4	C1-C2-N1	3.13	125.86	115.82	3	1
3	A	602	PX4	C7-O7-C23	3.12	110.32	117.80	7	5
3	A	613	PX4	C8-O5-C9	3.13	105.69	117.12	14	1
3	A	632	PX4	C26-C25-C24	3.12	124.61	113.13	6	1
3	B	314	PX4	O7-C23-O8	3.13	131.01	123.70	10	1
3	C	345	PX4	C5-N1-C4	3.13	100.77	108.98	11	3
3	C	357	PX4	C8-C7-C6	3.12	104.50	111.78	9	1
3	A	645	PX4	C5-N1-C4	3.12	100.77	108.98	14	3
3	C	321	PX4	C5-N1-C4	3.12	100.78	108.98	7	1
3	A	607	PX4	O5-C9-O6	3.12	131.43	123.63	4	1
3	A	609	PX4	O5-C9-C10	3.12	102.32	111.83	14	3
3	A	616	PX4	O7-C23-O8	3.12	131.00	123.70	10	3
3	C	357	PX4	C7-O7-C23	3.12	110.33	117.80	4	2
3	C	357	PX4	O5-C9-C10	3.12	102.32	111.83	4	3
3	C	362	PX4	C1-C2-N1	3.12	125.84	115.82	1	2
3	C	364	PX4	C8-C7-C6	3.12	104.51	111.78	12	2
3	A	624	PX4	O7-C23-O8	3.12	131.00	123.70	3	4
3	A	631	PX4	C4-N1-C3	3.12	117.17	108.98	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	351	PX4	C8-C7-C6	3.12	104.51	111.78	2	3
3	B	374	PX4	O7-C23-C24	3.12	104.73	111.48	15	4
3	C	345	PX4	C7-O7-C23	3.12	110.33	117.80	1	4
3	A	606	PX4	O7-C7-C8	3.12	119.53	108.34	1	3
3	A	633	PX4	O5-C8-C7	3.12	117.38	108.40	12	4
3	A	638	PX4	O7-C23-O8	3.12	130.99	123.70	13	3
3	B	306	PX4	O5-C8-C7	3.12	117.38	108.40	11	2
3	A	604	PX4	O7-C23-C24	3.11	104.74	111.48	9	1
3	B	373	PX4	O7-C23-C24	3.12	104.74	111.48	10	4
3	B	379	PX4	C8-C7-C6	3.11	104.53	111.78	4	4
3	B	398	PX4	O5-C9-O6	3.11	131.42	123.63	8	1
3	C	331	PX4	C8-C7-C6	3.11	104.53	111.78	6	3
3	B	329	PX4	O7-C23-C24	3.11	104.75	111.48	15	4
3	B	360	PX4	O5-C8-C7	3.11	117.36	108.40	8	4
3	C	331	PX4	C5-N1-C4	3.11	117.15	108.98	10	3
3	C	360	PX4	O5-C9-O6	3.11	131.41	123.63	3	2
3	B	358	PX4	O5-C8-C7	3.11	117.36	108.40	7	4
3	B	377	PX4	O5-C9-O6	3.11	131.40	123.63	6	1
3	C	340	PX4	C11-C10-C9	3.11	102.31	113.69	4	2
3	B	378	PX4	O7-C23-C24	3.11	104.76	111.48	4	4
3	A	624	PX4	C7-O7-C23	3.10	110.37	117.80	14	3
3	A	626	PX4	O7-C23-O8	3.10	130.96	123.70	4	1
3	C	318	PX4	O7-C23-O8	3.10	130.96	123.70	15	3
3	C	329	PX4	C7-O7-C23	3.10	110.37	117.80	14	7
3	B	342	PX4	C7-O7-C23	3.10	110.38	117.80	5	4
3	B	363	PX4	C5-N1-C3	3.10	100.84	108.98	7	2
3	B	380	PX4	O5-C8-C7	3.10	117.32	108.40	12	4
3	C	352	PX4	C1-C2-N1	3.10	125.76	115.82	6	1
3	B	388	PX4	C4-N1-C3	3.09	100.85	108.98	11	3
3	A	642	PX4	O7-C23-O8	3.09	130.94	123.70	13	2
3	B	399	PX4	O5-C9-O6	3.09	131.37	123.63	2	2
3	C	352	PX4	O5-C9-C10	3.09	102.40	111.83	8	2
3	B	323	PX4	C5-N1-C3	3.09	100.86	108.98	8	2
3	C	353	PX4	C5-N1-C3	3.09	117.09	108.98	4	1
3	B	336	PX4	O7-C23-C24	3.09	104.80	111.48	13	4
3	B	382	PX4	O7-C23-O8	3.09	130.93	123.70	13	2
3	B	385	PX4	O5-C9-O6	3.09	131.35	123.63	7	1
3	B	383	PX4	C8-O5-C9	3.09	105.84	117.12	7	1
3	C	339	PX4	C7-O7-C23	3.08	110.41	117.80	6	6
3	C	367	PX4	O5-C8-C7	3.08	117.29	108.40	2	5
3	A	618	PX4	C1-C2-N1	3.08	125.71	115.82	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	356	PX4	C7-O7-C23	3.08	110.42	117.80	7	3
3	A	606	PX4	O5-C9-C10	3.08	102.45	111.83	11	2
3	B	380	PX4	O5-C9-O6	3.08	131.33	123.63	14	1
3	A	607	PX4	O7-C23-C24	3.08	104.82	111.48	15	3
3	B	342	PX4	O5-C9-O6	3.08	131.33	123.63	9	1
3	B	343	PX4	O5-C9-O6	3.08	131.33	123.63	1	5
3	B	345	PX4	C8-C7-C6	3.08	104.61	111.78	5	3
3	C	313	PX4	C8-C7-C6	3.08	104.61	111.78	14	2
3	C	350	PX4	C7-O7-C23	3.08	110.43	117.80	2	4
3	C	362	PX4	C11-C10-C9	3.08	102.42	113.69	4	2
3	A	601	PX4	C1-C2-N1	3.08	125.69	115.82	10	1
3	B	345	PX4	C4-N1-C3	3.08	100.90	108.98	9	1
3	C	326	PX4	O7-C23-O8	3.07	130.89	123.70	4	2
3	C	335	PX4	O7-C23-C24	3.08	104.83	111.48	13	6
3	B	328	PX4	C7-O7-C23	3.07	110.44	117.80	6	5
3	C	361	PX4	O5-C8-C7	3.07	117.25	108.40	9	5
3	B	335	PX4	O7-C23-O8	3.07	130.89	123.70	7	2
3	B	392	PX4	O7-C23-C24	3.07	104.84	111.48	13	1
3	C	353	PX4	C8-C7-C6	3.07	104.62	111.78	15	2
3	B	357	PX4	C5-N1-C3	3.07	100.92	108.98	8	2
3	B	363	PX4	C7-O7-C23	3.07	110.46	117.80	5	4
3	C	352	PX4	O5-C9-O6	3.07	131.30	123.63	1	3
3	C	360	PX4	O5-C8-C7	3.07	117.24	108.40	6	3
3	B	319	PX4	O7-C23-C24	3.06	104.86	111.48	4	7
3	B	322	PX4	C4-N1-C3	3.06	100.93	108.98	7	1
3	B	347	PX4	O5-C9-C10	3.06	102.50	111.83	5	2
3	C	309	PX4	C7-O7-C23	3.06	110.46	117.80	2	6
3	A	610	PX4	C4-N1-C2	3.06	122.08	109.91	5	2
3	B	341	PX4	C7-O7-C23	3.06	110.47	117.80	12	3
3	B	345	PX4	O5-C9-C10	3.06	102.50	111.83	10	4
3	A	620	PX4	O7-C23-O8	3.06	130.85	123.70	8	3
3	B	301	PX4	O5-C8-C7	3.06	117.22	108.40	7	5
3	B	301	PX4	O7-C23-C24	3.06	104.86	111.48	12	3
3	B	334	PX4	O5-C9-O6	3.06	131.28	123.63	11	3
3	C	334	PX4	C5-N1-C3	3.06	100.94	108.98	15	2
3	B	307	PX4	C5-N1-C3	3.06	100.94	108.98	9	1
3	B	316	PX4	C4-N1-C3	3.06	100.94	108.98	5	3
3	B	360	PX4	C25-C24-C23	3.06	102.49	113.69	13	2
3	B	383	PX4	C7-O7-C23	3.06	110.48	117.80	2	2
3	C	323	PX4	C4-N1-C3	3.06	100.94	108.98	12	4
3	C	338	PX4	O7-C23-C24	3.06	104.86	111.48	1	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	638	PX4	C8-C7-C6	3.06	104.66	111.78	12	3
3	C	302	PX4	C4-N1-C3	3.06	100.95	108.98	10	2
3	B	310	PX4	C11-C10-C9	3.05	102.51	113.69	15	2
3	C	308	PX4	O5-C8-C7	3.05	117.20	108.40	9	2
3	B	382	PX4	O5-C8-C7	3.05	117.19	108.40	14	6
3	B	390	PX4	O7-C23-C24	3.05	104.88	111.48	1	4
3	C	367	PX4	C8-O5-C9	3.05	105.96	117.12	3	2
3	A	638	PX4	O7-C23-C24	3.05	104.88	111.48	15	4
3	B	304	PX4	O5-C8-C7	3.05	117.19	108.40	14	2
3	B	395	PX4	O7-C23-C24	3.05	104.88	111.48	5	4
3	C	368	PX4	C7-O7-C23	3.05	110.49	117.80	1	5
3	B	308	PX4	O7-C23-C24	3.05	104.88	111.48	6	4
3	C	326	PX4	C4-N1-C3	3.05	116.99	108.98	4	2
3	B	375	PX4	O7-C23-C24	3.05	104.89	111.48	11	4
3	B	349	PX4	C7-O7-C23	3.05	110.51	117.80	10	1
3	B	353	PX4	O7-C23-C24	3.05	104.89	111.48	1	2
3	C	353	PX4	O7-C23-O8	3.05	130.83	123.70	7	1
3	A	605	PX4	O5-C8-C7	3.04	117.17	108.40	10	6
3	A	648	PX4	C5-N1-C4	3.04	100.98	108.98	13	1
3	A	603	PX4	O5-C8-C7	3.04	117.17	108.40	3	4
3	A	645	PX4	C1-C2-N1	3.04	125.59	115.82	15	1
3	B	343	PX4	C26-C25-C24	3.04	124.31	113.13	5	2
3	B	394	PX4	C7-O7-C23	3.04	110.52	117.80	14	4
3	A	640	PX4	O5-C8-C7	3.04	117.16	108.40	15	3
3	B	343	PX4	O7-C23-C24	3.04	104.91	111.48	11	2
3	C	304	PX4	C8-C7-C6	3.04	104.70	111.78	3	5
3	C	364	PX4	C26-C25-C24	3.04	124.29	113.13	10	1
3	B	315	PX4	C5-N1-C3	3.04	101.00	108.98	5	1
3	C	360	PX4	C4-N1-C3	3.04	101.00	108.98	11	1
3	A	613	PX4	O7-C23-O8	3.04	130.80	123.70	3	2
3	C	322	PX4	O5-C8-C7	3.04	117.15	108.40	12	4
3	C	356	PX4	C8-O5-C9	3.04	106.02	117.12	14	1
3	A	601	PX4	C5-N1-C4	3.03	101.01	108.98	3	1
3	A	617	PX4	O5-C9-C10	3.03	102.59	111.83	2	4
3	B	382	PX4	O5-C9-C10	3.03	102.59	111.83	10	7
3	C	339	PX4	O5-C8-C7	3.03	117.14	108.40	5	5
3	C	354	PX4	P1-O3-C1	3.03	135.69	121.26	12	2
3	B	334	PX4	C5-N1-C4	3.03	116.93	108.98	8	1
3	B	340	PX4	O7-C23-O8	3.03	130.79	123.70	9	2
3	B	365	PX4	C5-N1-C3	3.03	101.02	108.98	3	1
3	C	342	PX4	C26-C25-C24	3.03	124.25	113.13	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	622	PX4	C8-C7-C6	3.02	118.84	111.78	2	4
3	B	303	PX4	C8-C7-C6	3.02	104.74	111.78	15	5
3	B	325	PX4	C1-C2-N1	3.02	125.53	115.82	11	2
3	C	312	PX4	C4-N1-C3	3.02	101.03	108.98	2	5
3	C	341	PX4	C5-N1-C4	3.02	101.03	108.98	8	3
3	B	326	PX4	O5-C9-C10	3.02	102.62	111.83	2	2
3	B	334	PX4	O7-C23-O8	3.02	130.77	123.70	14	4
3	A	629	PX4	C1-C2-N1	3.02	125.51	115.82	9	1
3	A	640	PX4	C7-O7-C23	3.02	110.57	117.80	8	1
3	B	357	PX4	O5-C9-C10	3.02	102.63	111.83	3	4
3	B	373	PX4	O5-C8-C7	3.02	117.10	108.40	10	4
3	B	335	PX4	O7-C23-C24	3.02	104.95	111.48	11	3
3	B	344	PX4	O5-C8-C7	3.01	117.09	108.40	14	8
3	A	643	PX4	O5-C9-C10	3.01	102.65	111.83	7	4
3	C	363	PX4	C8-C7-C6	3.01	104.76	111.78	5	1
3	C	306	PX4	O5-C8-C7	3.01	117.07	108.40	13	5
3	C	350	PX4	C4-N1-C3	3.01	101.08	108.98	14	2
3	A	604	PX4	C5-N1-C4	3.01	101.08	108.98	13	3
3	A	626	PX4	C27-C26-C25	3.01	129.56	114.37	7	1
3	A	647	PX4	O7-C23-C24	3.01	104.98	111.48	10	2
3	B	363	PX4	C12-C11-C10	3.01	124.17	113.13	4	1
3	B	350	PX4	C8-C7-C6	3.00	104.78	111.78	15	2
3	C	303	PX4	O7-C23-C24	3.00	104.98	111.48	6	4
3	C	320	PX4	O7-C7-C6	3.00	119.12	108.34	1	2
3	C	360	PX4	C26-C25-C24	3.00	102.09	113.13	14	1
3	C	366	PX4	C26-C25-C24	3.00	124.17	113.13	11	1
3	C	306	PX4	C4-N1-C3	3.00	116.87	108.98	2	5
3	B	377	PX4	C8-C7-C6	3.00	104.79	111.78	10	3
3	A	617	PX4	C5-N1-C3	3.00	101.10	108.98	12	2
3	B	316	PX4	C11-C10-C9	3.00	102.70	113.69	4	1
3	B	376	PX4	C26-C25-C24	3.00	102.10	113.13	2	1
3	B	360	PX4	C5-N1-C3	3.00	101.10	108.98	14	1
3	C	312	PX4	C12-C11-C10	3.00	124.14	113.13	4	2
3	B	392	PX4	C8-C7-C6	3.00	104.80	111.78	1	2
3	C	328	PX4	C1-C2-N1	3.00	125.44	115.82	15	3
3	A	634	PX4	C5-N1-C4	2.99	101.11	108.98	5	2
3	B	395	PX4	P1-O3-C1	2.99	135.51	121.26	10	1
3	A	602	PX4	O5-C9-C10	2.99	102.71	111.83	13	3
3	A	635	PX4	C8-O5-C9	2.99	106.18	117.12	5	1
3	B	350	PX4	C1-C2-N1	2.99	125.43	115.82	8	2
3	B	357	PX4	O7-C7-C8	2.99	119.08	108.34	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	C	311	PX4	O7-C23-O8	2.99	130.71	123.70	10	1
3	A	626	PX4	C7-O7-C23	2.99	110.64	117.80	4	4
3	B	330	PX4	C25-C24-C23	2.99	102.74	113.69	12	2
3	C	370	PX4	C1-C2-N1	2.99	125.41	115.82	8	1
3	B	344	PX4	C7-O7-C23	2.98	110.65	117.80	14	4
3	A	633	PX4	C12-C11-C10	2.98	102.17	113.13	12	1
3	B	306	PX4	O7-C23-O8	2.98	130.68	123.70	12	1
3	B	357	PX4	O5-C8-C7	2.98	116.99	108.40	14	5
3	C	359	PX4	C1-C2-N1	2.98	106.25	115.82	5	2
3	C	362	PX4	O5-C9-O6	2.98	131.09	123.63	8	2
3	B	391	PX4	O5-C9-O6	2.98	131.09	123.63	11	3
3	C	321	PX4	O7-C23-O8	2.98	130.68	123.70	14	2
3	B	355	PX4	C5-N1-C4	2.98	101.15	108.98	11	3
3	B	382	PX4	C4-N1-C3	2.98	101.15	108.98	5	1
3	B	325	PX4	C7-O7-C23	2.98	110.67	117.80	8	3
3	B	389	PX4	O5-C8-C7	2.98	116.98	108.40	6	3
3	C	345	PX4	O7-C23-O8	2.98	130.66	123.70	9	3
3	A	612	PX4	O5-C8-C7	2.97	116.97	108.40	13	2
3	B	335	PX4	O5-C9-C10	2.97	102.77	111.83	11	2
3	B	396	PX4	C8-C7-C6	2.97	104.86	111.78	2	2
3	B	387	PX4	O7-C23-O8	2.97	130.65	123.70	5	2
3	B	400	PX4	C5-N1-C3	2.97	116.78	108.98	12	4
3	C	324	PX4	O5-C9-C10	2.97	102.78	111.83	11	4
3	C	345	PX4	C8-C7-C6	2.97	118.71	111.78	4	4
3	A	637	PX4	O7-C23-C24	2.97	105.06	111.48	14	4
3	C	367	PX4	O5-C9-O6	2.97	131.05	123.63	4	3
3	A	622	PX4	O5-C8-C7	2.97	116.95	108.40	14	1
3	B	305	PX4	O5-C9-C10	2.97	102.79	111.83	13	3
3	B	307	PX4	O7-C23-O8	2.97	130.64	123.70	4	2
3	B	349	PX4	C1-C2-N1	2.97	125.35	115.82	14	3
3	A	627	PX4	C4-N1-C3	2.96	101.19	108.98	10	4
3	B	328	PX4	O7-C23-O8	2.96	130.63	123.70	7	2
3	B	387	PX4	C4-N1-C3	2.96	101.19	108.98	7	1
3	B	390	PX4	C5-N1-C4	2.96	101.19	108.98	9	1
3	B	398	PX4	C5-N1-C4	2.96	116.76	108.98	14	1
3	C	313	PX4	C1-C2-N1	2.96	125.33	115.82	1	3
3	B	345	PX4	C26-C25-C24	2.96	102.24	113.13	7	1
3	A	629	PX4	C4-N1-C3	2.96	101.20	108.98	7	1
3	B	337	PX4	O7-C23-O8	2.96	130.63	123.70	2	6
3	B	349	PX4	O5-C8-C7	2.96	116.93	108.40	5	3
3	C	341	PX4	O7-C23-C24	2.96	105.08	111.48	13	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	638	PX4	O5-C8-C7	2.96	116.92	108.40	4	3
3	B	309	PX4	C12-C11-C10	2.96	123.99	113.13	13	1
3	B	339	PX4	C8-C7-C6	2.96	104.89	111.78	12	1
3	C	368	PX4	O5-C8-C7	2.96	116.92	108.40	8	2
3	A	607	PX4	O7-C23-O8	2.95	130.61	123.70	15	2
3	B	315	PX4	O7-C23-C24	2.95	105.10	111.48	10	7
3	C	332	PX4	O7-C7-C6	2.95	118.92	108.34	5	2
3	A	602	PX4	C5-N1-C4	2.94	116.71	108.98	14	4
3	A	627	PX4	O5-C8-C7	2.94	116.89	108.40	8	4
3	C	304	PX4	O5-C8-C7	2.95	116.89	108.40	5	7
3	C	318	PX4	C7-O7-C23	2.95	110.75	117.80	1	3
3	A	619	PX4	C1-C2-N1	2.94	125.27	115.82	13	2
3	B	305	PX4	C8-C7-C6	2.94	104.92	111.78	6	1
3	B	337	PX4	C8-C7-C6	2.94	104.92	111.78	4	4
3	B	387	PX4	C8-C7-C6	2.94	104.92	111.78	7	3
3	C	334	PX4	C8-C7-C6	2.94	104.92	111.78	13	2
3	B	390	PX4	O5-C9-O6	2.94	130.98	123.63	8	2
3	B	392	PX4	C4-N1-C3	2.94	116.70	108.98	12	1
3	C	322	PX4	O7-C23-O8	2.94	130.58	123.70	3	6
3	C	328	PX4	C8-C7-C6	2.94	118.64	111.78	7	4
3	C	350	PX4	O7-C23-C24	2.94	105.12	111.48	7	3
3	B	345	PX4	C7-O7-C23	2.94	110.76	117.80	14	4
3	C	342	PX4	O5-C9-C10	2.94	102.87	111.83	2	1
3	B	337	PX4	C5-N1-C3	2.94	101.26	108.98	7	2
3	B	386	PX4	C7-O7-C23	2.94	110.77	117.80	2	3
3	C	344	PX4	C4-N1-C3	2.94	116.69	108.98	15	4
3	B	305	PX4	C12-C11-C10	2.94	123.91	113.13	4	1
3	C	306	PX4	C1-C2-N1	2.94	125.24	115.82	11	1
3	A	611	PX4	C12-C11-C10	2.93	102.35	113.13	5	3
3	A	616	PX4	C7-O7-C23	2.93	110.78	117.80	4	3
3	A	648	PX4	C8-C7-C6	2.93	104.95	111.78	5	4
3	B	384	PX4	O5-C8-C7	2.93	116.85	108.40	8	5
3	C	360	PX4	C11-C10-C9	2.93	102.95	113.69	14	1
3	A	635	PX4	O5-C9-O6	2.93	130.96	123.63	3	1
3	B	302	PX4	C12-C11-C10	2.93	123.90	113.13	10	1
3	B	323	PX4	C1-C2-N1	2.93	125.22	115.82	2	2
3	C	341	PX4	O5-C9-C10	2.93	102.91	111.83	2	2
3	C	351	PX4	C7-O7-C23	2.93	124.81	117.80	1	5
3	B	337	PX4	C5-N1-C4	2.93	101.29	108.98	14	3
3	C	329	PX4	O5-C8-C7	2.93	116.83	108.40	2	3
3	B	383	PX4	O3-C1-C2	2.93	123.72	109.65	14	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	C	344	PX4	C5-N1-C3	2.93	101.29	108.98	5	3
3	A	644	PX4	C5-N1-C3	2.92	101.30	108.98	10	2
3	B	361	PX4	C11-C10-C9	2.92	102.98	113.69	4	1
3	A	642	PX4	C4-N1-C3	2.92	101.30	108.98	2	2
3	A	615	PX4	O5-C8-C7	2.92	116.81	108.40	4	1
3	B	343	PX4	C7-O7-C23	2.92	110.81	117.80	9	3
3	B	375	PX4	C4-N1-C3	2.92	101.30	108.98	12	2
3	C	354	PX4	C26-C25-C24	2.92	102.39	113.13	4	1
3	B	374	PX4	O5-C8-C7	2.92	116.81	108.40	11	5
3	A	617	PX4	O5-C9-O6	2.92	130.92	123.63	13	4
3	B	397	PX4	O7-C23-O8	2.92	130.52	123.70	3	3
3	C	322	PX4	O5-C9-O6	2.92	130.93	123.63	13	4
3	B	362	PX4	O7-C7-C8	2.91	118.80	108.34	14	1
3	B	384	PX4	C4-N1-C3	2.92	101.32	108.98	5	3
3	A	627	PX4	O5-C9-O6	2.91	130.91	123.63	6	1
3	B	332	PX4	O7-C7-C8	2.91	118.80	108.34	13	1
3	A	644	PX4	C8-C7-C6	2.91	105.00	111.78	2	2
3	B	316	PX4	O7-C23-O8	2.91	130.51	123.70	5	2
3	B	315	PX4	O5-C8-C7	2.91	116.78	108.40	6	3
3	B	328	PX4	C11-C10-C9	2.91	103.03	113.69	5	1
3	B	334	PX4	C8-C7-C6	2.91	105.00	111.78	8	3
3	C	319	PX4	C1-C2-N1	2.91	125.17	115.82	4	3
3	C	353	PX4	C7-O7-C23	2.91	110.83	117.80	6	4
3	B	335	PX4	O7-C7-C6	2.91	97.91	108.34	9	1
3	B	370	PX4	C12-C11-C10	2.91	123.81	113.13	3	2
3	C	309	PX4	C5-N1-C4	2.91	101.34	108.98	3	1
3	A	626	PX4	O5-C9-C10	2.90	102.98	111.83	9	1
3	B	384	PX4	O7-C23-O8	2.90	130.49	123.70	4	2
3	B	392	PX4	C5-N1-C3	2.90	101.35	108.98	9	4
3	B	336	PX4	O5-C9-C10	2.90	102.98	111.83	9	4
3	B	310	PX4	O5-C8-C7	2.90	116.76	108.40	11	3
3	C	345	PX4	C5-N1-C3	2.90	101.36	108.98	8	3
3	C	360	PX4	O7-C7-C6	2.90	118.75	108.34	8	1
3	B	334	PX4	C5-N1-C3	2.90	101.37	108.98	11	1
3	B	331	PX4	O5-C9-C10	2.90	103.01	111.83	7	3
3	B	307	PX4	O7-C23-C24	2.89	105.22	111.48	4	3
3	C	318	PX4	O5-C9-C10	2.89	103.01	111.83	5	1
3	B	380	PX4	O7-C23-C24	2.89	105.23	111.48	7	3
3	C	321	PX4	O7-C23-C24	2.89	105.23	111.48	14	3
3	C	354	PX4	C7-O7-C23	2.89	110.88	117.80	7	3
3	A	635	PX4	C4-N1-C3	2.89	116.57	108.98	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	C	346	PX4	O7-C23-C24	2.89	105.23	111.48	4	3
3	C	358	PX4	O5-C9-O6	2.89	130.86	123.63	4	2
3	A	634	PX4	O1-P1-O3	2.89	120.66	107.57	9	1
3	A	602	PX4	C12-C11-C10	2.89	102.52	113.13	6	1
3	B	351	PX4	C5-N1-C4	2.89	101.39	108.98	8	2
3	B	363	PX4	C8-C7-C6	2.89	105.06	111.78	2	5
3	C	354	PX4	C8-O5-C9	2.88	106.58	117.12	4	1
3	B	353	PX4	O5-C9-O6	2.88	130.84	123.63	8	2
3	B	365	PX4	C1-C2-N1	2.88	125.07	115.82	13	1
3	B	396	PX4	P1-O4-C6	2.88	137.86	121.35	7	1
3	C	325	PX4	O7-C7-C6	2.88	118.69	108.34	10	3
3	B	359	PX4	O5-C9-C10	2.88	103.05	111.83	7	2
3	C	347	PX4	C8-C7-C6	2.88	105.07	111.78	9	1
3	A	636	PX4	C5-N1-C3	2.88	101.41	108.98	11	2
3	C	339	PX4	O5-C9-O6	2.88	130.83	123.63	6	1
3	A	623	PX4	O1-P1-O2	2.88	125.83	112.44	11	1
3	C	325	PX4	O5-C9-O6	2.88	130.83	123.63	5	2
3	A	614	PX4	C8-C7-C6	2.88	105.08	111.78	12	3
3	B	371	PX4	O5-C8-C7	2.88	116.69	108.40	15	2
3	C	366	PX4	C7-O7-C23	2.88	110.91	117.80	2	1
3	A	605	PX4	C8-C7-C6	2.87	105.09	111.78	9	3
3	A	618	PX4	O5-C9-O6	2.87	130.81	123.63	10	1
3	B	302	PX4	O7-C23-C24	2.87	105.27	111.48	12	4
3	C	305	PX4	O7-C7-C8	2.87	118.64	108.34	15	2
3	A	621	PX4	C1-C2-N1	2.87	125.03	115.82	5	1
3	B	345	PX4	O7-C23-O8	2.87	130.41	123.70	3	5
3	A	629	PX4	O7-C7-C6	2.87	118.63	108.34	13	1
3	A	632	PX4	C8-C7-C6	2.87	105.10	111.78	12	2
3	B	388	PX4	O7-C23-O8	2.87	130.41	123.70	14	2
3	A	622	PX4	O7-C7-C6	2.86	118.61	108.34	3	2
3	B	352	PX4	C8-C7-C6	2.86	105.11	111.78	5	5
3	B	378	PX4	O7-C7-C8	2.86	118.62	108.34	9	2
3	B	394	PX4	O7-C7-C8	2.86	118.62	108.34	14	2
3	A	636	PX4	O5-C8-C7	2.86	116.64	108.40	1	5
3	B	310	PX4	O5-C9-O6	2.86	130.79	123.63	8	1
3	B	366	PX4	O5-C9-C10	2.86	103.11	111.83	5	2
3	B	302	PX4	C8-C7-C6	2.86	105.12	111.78	11	4
3	B	313	PX4	O5-C8-C7	2.86	116.64	108.40	1	4
3	B	396	PX4	C1-C2-N1	2.86	125.00	115.82	10	2
3	A	613	PX4	C7-O7-C23	2.86	110.96	117.80	14	5
3	A	624	PX4	O7-C23-C24	2.86	105.30	111.48	11	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	331	PX4	C1-C2-N1	2.86	124.99	115.82	8	1
3	B	339	PX4	O7-C7-C8	2.86	118.59	108.34	1	2
3	B	379	PX4	C5-N1-C4	2.86	101.47	108.98	11	4
3	C	304	PX4	C5-N1-C3	2.86	101.47	108.98	2	2
3	C	306	PX4	C8-C7-C6	2.86	118.44	111.78	13	5
3	B	327	PX4	C4-N1-C3	2.85	116.47	108.98	11	1
3	C	366	PX4	O5-C9-C10	2.85	103.14	111.83	4	1
3	A	614	PX4	O7-C7-C6	2.85	118.57	108.34	12	4
3	A	632	PX4	C7-O7-C23	2.85	124.62	117.80	11	3
3	B	361	PX4	O5-C9-O6	2.85	130.76	123.63	8	2
3	A	627	PX4	O5-C9-C10	2.85	103.15	111.83	12	2
3	A	630	PX4	C7-O7-C23	2.85	110.98	117.80	14	3
3	C	311	PX4	O7-C23-C24	2.85	105.32	111.48	6	2
3	C	331	PX4	O5-C9-C10	2.85	103.16	111.83	3	3
3	A	621	PX4	C5-N1-C4	2.84	101.51	108.98	5	2
3	A	623	PX4	C3-N1-C2	2.84	98.61	109.91	9	1
3	A	637	PX4	O5-C9-O6	2.84	130.74	123.63	6	1
3	A	629	PX4	O7-C23-C24	2.84	105.33	111.48	12	2
3	A	610	PX4	O7-C23-O8	2.84	130.35	123.70	5	2
3	A	618	PX4	O5-C8-C7	2.84	116.59	108.40	6	5
3	B	338	PX4	O7-C23-O8	2.84	130.34	123.70	1	2
3	B	322	PX4	O7-C7-C8	2.84	118.53	108.34	2	4
3	A	602	PX4	C25-C24-C23	2.84	103.30	113.69	6	2
3	B	341	PX4	C8-O5-C9	2.84	106.75	117.12	11	1
3	C	348	PX4	O7-C23-O8	2.84	130.34	123.70	15	4
3	B	351	PX4	C4-N1-C3	2.83	116.42	108.98	6	2
3	A	607	PX4	O5-C8-C7	2.83	116.56	108.40	14	1
3	A	625	PX4	O7-C23-C24	2.83	105.36	111.48	8	3
3	B	332	PX4	O7-C23-O8	2.83	130.32	123.70	5	2
3	A	618	PX4	O5-C9-C10	2.83	103.21	111.83	1	1
3	A	630	PX4	C1-C2-N1	2.83	124.90	115.82	1	2
3	C	338	PX4	C5-N1-C3	2.83	101.55	108.98	14	1
3	A	634	PX4	C7-O7-C23	2.82	111.03	117.80	9	3
3	A	644	PX4	O7-C23-C24	2.82	105.37	111.48	14	2
3	A	617	PX4	O7-C7-C6	2.82	118.47	108.34	6	1
3	A	647	PX4	C25-C24-C23	2.82	124.04	113.69	13	2
3	B	326	PX4	C5-N1-C3	2.82	101.56	108.98	14	1
3	B	400	PX4	O7-C23-C24	2.82	105.37	111.48	2	5
3	C	335	PX4	C8-O5-C9	2.82	106.80	117.12	6	1
3	C	351	PX4	C8-O5-C9	2.82	106.80	117.12	9	3
3	B	323	PX4	C25-C24-C23	2.82	124.03	113.69	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	335	PX4	C8-O5-C9	2.82	106.81	117.12	14	3
3	B	362	PX4	O6-C9-C10	2.82	134.82	123.78	9	1
3	B	373	PX4	O7-C7-C8	2.82	118.46	108.34	9	4
3	B	388	PX4	C7-O7-C23	2.82	111.05	117.80	8	3
3	B	325	PX4	C8-C7-C6	2.82	105.21	111.78	2	5
3	B	338	PX4	O5-C8-C7	2.82	116.52	108.40	12	2
3	C	353	PX4	C30-C29-C28	2.82	100.12	114.37	15	1
3	C	302	PX4	C8-O5-C9	2.82	106.82	117.12	5	3
3	C	356	PX4	O7-C23-O8	2.82	130.29	123.70	13	4
3	A	643	PX4	O7-C23-O8	2.82	130.29	123.70	9	2
3	B	309	PX4	C1-C2-N1	2.82	124.86	115.82	9	3
3	B	328	PX4	C5-N1-C3	2.82	101.58	108.98	2	2
3	B	332	PX4	O5-C9-C10	2.82	103.25	111.83	7	1
3	C	349	PX4	O5-C8-C7	2.82	116.52	108.40	4	3
3	C	356	PX4	C5-N1-C4	2.82	116.37	108.98	11	3
3	B	365	PX4	C11-C10-C9	2.81	124.01	113.69	3	2
3	B	346	PX4	C26-C25-C24	2.81	102.79	113.13	2	2
3	C	369	PX4	O7-C23-O8	2.81	130.28	123.70	10	1
3	A	624	PX4	C5-N1-C4	2.81	116.36	108.98	13	3
3	C	316	PX4	C5-N1-C3	2.81	101.59	108.98	7	2
3	B	302	PX4	C5-N1-C4	2.81	116.36	108.98	8	1
3	C	329	PX4	O7-C23-C24	2.81	105.40	111.48	10	3
3	C	344	PX4	O7-C23-C24	2.81	105.40	111.48	10	5
3	B	336	PX4	O5-C9-O6	2.81	130.65	123.63	6	2
3	B	360	PX4	C4-N1-C3	2.81	116.35	108.98	3	4
3	C	360	PX4	O7-C23-O8	2.81	130.27	123.70	9	4
3	B	379	PX4	O7-C23-O8	2.81	130.27	123.70	8	1
3	B	397	PX4	C1-C2-N1	2.81	124.83	115.82	6	1
3	C	319	PX4	O7-C7-C8	2.81	118.42	108.34	10	2
3	A	613	PX4	C5-N1-C3	2.81	116.35	108.98	12	3
3	B	362	PX4	O5-C8-C7	2.81	116.49	108.40	3	4
3	C	345	PX4	O7-C7-C6	2.81	118.42	108.34	9	1
3	A	626	PX4	C5-N1-C4	2.81	116.34	108.98	8	2
3	A	633	PX4	C5-N1-C3	2.80	101.61	108.98	4	4
3	C	367	PX4	C4-N1-C3	2.81	116.34	108.98	2	1
3	C	369	PX4	C8-O5-C9	2.81	106.86	117.12	1	1
3	B	364	PX4	C26-C25-C24	2.80	123.43	113.13	13	2
3	B	366	PX4	O5-C9-O6	2.80	130.64	123.63	10	1
3	B	380	PX4	C7-O7-C23	2.80	111.08	117.80	9	2
3	B	388	PX4	C8-O5-C9	2.80	106.87	117.12	11	1
3	C	308	PX4	C26-C25-C24	2.80	123.42	113.13	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	301	PX4	O5-C9-O6	2.80	130.63	123.63	6	4
3	B	327	PX4	C8-C7-C6	2.80	105.26	111.78	9	2
3	B	329	PX4	C5-N1-C3	2.80	116.33	108.98	9	2
3	C	307	PX4	O7-C23-C24	2.80	105.42	111.48	4	5
3	A	630	PX4	O7-C23-O8	2.80	130.25	123.70	7	3
3	A	633	PX4	C1-C2-N1	2.80	124.80	115.82	2	2
3	B	343	PX4	O5-C9-C10	2.80	103.31	111.83	3	2
3	B	349	PX4	O7-C23-C24	2.80	105.43	111.48	9	7
3	B	378	PX4	C7-O7-C23	2.80	111.10	117.80	5	6
3	B	325	PX4	C5-N1-C4	2.79	101.64	108.98	7	1
3	B	338	PX4	O1-P1-O2	2.80	125.45	112.44	3	1
3	C	370	PX4	C5-N1-C4	2.80	116.32	108.98	3	4
3	B	367	PX4	O5-C9-C10	2.79	103.32	111.83	11	4
3	A	638	PX4	C7-O7-C23	2.79	124.48	117.80	3	5
3	A	639	PX4	C5-N1-C4	2.79	116.31	108.98	15	1
3	A	641	PX4	C8-C7-C6	2.79	118.29	111.78	10	3
3	A	626	PX4	C1-C2-N1	2.79	124.77	115.82	4	2
3	B	314	PX4	O7-C7-C8	2.79	118.35	108.34	14	1
3	B	338	PX4	C7-O7-C23	2.79	111.12	117.80	12	2
3	B	320	PX4	C4-N1-C3	2.79	101.65	108.98	14	2
3	B	342	PX4	C8-C7-C6	2.79	105.28	111.78	2	2
3	C	315	PX4	O5-C9-C10	2.79	103.33	111.83	9	2
3	B	382	PX4	C8-C7-C6	2.79	105.29	111.78	15	2
3	B	328	PX4	C4-N1-C3	2.78	101.66	108.98	4	1
3	C	356	PX4	O7-C23-C24	2.78	105.46	111.48	15	4
3	C	364	PX4	O5-C9-O6	2.78	130.59	123.63	11	3
3	B	324	PX4	C5-N1-C4	2.78	101.67	108.98	12	3
3	B	396	PX4	C5-N1-C3	2.78	101.67	108.98	14	1
3	B	334	PX4	C1-C2-N1	2.78	124.74	115.82	5	2
3	B	350	PX4	O5-C9-O6	2.78	130.58	123.63	15	2
3	B	370	PX4	C8-O5-C9	2.78	127.28	117.12	10	1
3	C	302	PX4	O7-C7-C8	2.78	118.31	108.34	4	1
3	C	335	PX4	C5-N1-C3	2.78	101.68	108.98	11	2
3	B	326	PX4	C5-N1-C4	2.78	116.27	108.98	15	3
3	B	345	PX4	O7-C23-C24	2.78	117.49	111.48	15	7
3	B	393	PX4	P1-O3-C1	2.78	134.48	121.26	13	2
3	C	306	PX4	O5-C9-O6	2.78	130.57	123.63	12	3
3	C	312	PX4	C8-C7-C6	2.78	105.31	111.78	9	3
3	A	631	PX4	O7-C23-C24	2.77	105.48	111.48	3	3
3	B	308	PX4	O7-C23-O8	2.77	130.19	123.70	9	3
3	A	602	PX4	C1-C2-N1	2.77	124.72	115.82	13	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	349	PX4	C8-O5-C9	2.77	106.99	117.12	12	1
3	B	355	PX4	C8-O5-C9	2.77	106.99	117.12	4	2
3	B	372	PX4	C5-N1-C3	2.77	101.69	108.98	4	2
3	B	365	PX4	O7-C7-C6	2.77	118.28	108.34	3	2
3	C	339	PX4	C1-C2-N1	2.77	124.72	115.82	1	2
3	C	325	PX4	C1-C2-N1	2.77	124.71	115.82	3	2
3	B	372	PX4	O5-C9-C10	2.77	103.39	111.83	2	4
3	B	393	PX4	O5-C8-C7	2.77	116.38	108.40	5	3
3	A	645	PX4	O7-C23-C24	2.77	105.49	111.48	14	1
3	B	346	PX4	O1-P1-O2	2.77	125.32	112.44	2	1
3	C	308	PX4	C1-C2-N1	2.77	124.70	115.82	12	2
3	C	336	PX4	C5-N1-C3	2.77	101.71	108.98	7	1
3	C	312	PX4	C1-C2-N1	2.77	124.70	115.82	2	3
3	A	628	PX4	C7-O7-C23	2.76	111.18	117.80	9	4
3	C	343	PX4	C4-N1-C2	2.77	120.90	109.91	3	1
3	B	366	PX4	O1-P1-O2	2.76	125.31	112.44	2	1
3	A	611	PX4	C5-N1-C4	2.76	116.23	108.98	11	1
3	B	376	PX4	O5-C9-O6	2.76	130.54	123.63	13	1
3	C	313	PX4	C4-N1-C3	2.76	101.72	108.98	6	1
3	C	339	PX4	O7-C23-O8	2.76	130.17	123.70	11	3
3	C	323	PX4	O5-C9-C10	2.76	103.41	111.83	11	2
3	A	618	PX4	C5-N1-C4	2.76	101.72	108.98	6	2
3	A	607	PX4	P1-O4-C6	2.76	105.54	121.35	3	1
3	A	612	PX4	C8-O5-C9	2.76	127.20	117.12	1	1
3	A	635	PX4	C8-C7-C6	2.76	105.35	111.78	10	3
3	C	302	PX4	O5-C9-C10	2.76	103.42	111.83	11	2
3	B	304	PX4	C26-C25-C24	2.76	123.26	113.13	7	2
3	C	366	PX4	O5-C9-O6	2.76	130.53	123.63	14	3
3	B	320	PX4	C5-N1-C3	2.76	101.74	108.98	6	2
3	A	625	PX4	C8-O5-C9	2.75	107.06	117.12	11	4
3	B	312	PX4	C8-O5-C9	2.75	127.18	117.12	11	1
3	B	330	PX4	C5-N1-C4	2.75	101.74	108.98	5	3
3	C	366	PX4	C8-C7-C6	2.75	118.20	111.78	12	2
3	B	303	PX4	O5-C9-C10	2.75	103.44	111.83	7	4
3	C	323	PX4	O7-C23-O8	2.75	130.14	123.70	9	2
3	C	344	PX4	O5-C8-C7	2.75	116.33	108.40	4	4
3	B	386	PX4	C4-N1-C3	2.75	101.75	108.98	11	3
3	C	342	PX4	C5-N1-C4	2.75	101.75	108.98	4	2
3	A	643	PX4	C8-O5-C9	2.75	107.08	117.12	2	2
3	B	303	PX4	C1-C2-N1	2.75	124.64	115.82	5	1
3	C	303	PX4	C7-O7-C23	2.75	111.22	117.80	4	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	625	PX4	O5-C9-C10	2.75	103.46	111.83	14	3
3	A	631	PX4	C8-C7-C6	2.75	105.38	111.78	6	6
3	B	336	PX4	O3-C1-C2	2.75	122.86	109.65	14	1
3	B	367	PX4	O7-C23-O8	2.75	130.13	123.70	7	2
3	B	388	PX4	C3-N1-C2	2.75	120.82	109.91	7	1
3	B	398	PX4	P1-O4-C6	2.75	137.09	121.35	12	1
3	C	329	PX4	O5-C9-O6	2.75	130.50	123.63	15	2
3	B	368	PX4	O5-C9-C10	2.74	103.47	111.83	15	3
3	B	394	PX4	O6-C9-C10	2.75	134.52	123.78	11	1
3	C	308	PX4	O5-C9-C10	2.75	103.46	111.83	8	2
3	C	338	PX4	O7-C7-C8	2.75	118.20	108.34	11	2
3	B	385	PX4	O7-C23-O8	2.74	130.12	123.70	3	3
3	A	620	PX4	C5-N1-C4	2.74	116.18	108.98	6	2
3	A	623	PX4	O5-C8-C7	2.74	116.30	108.40	14	4
3	B	333	PX4	C1-C2-N1	2.74	124.62	115.82	3	5
3	B	347	PX4	O7-C7-C6	2.74	118.18	108.34	1	1
3	B	301	PX4	O5-C9-C10	2.74	103.48	111.83	2	1
3	B	399	PX4	C8-C7-C6	2.74	105.39	111.78	11	2
3	C	305	PX4	C1-C2-N1	2.74	124.62	115.82	5	2
3	C	334	PX4	O7-C23-O8	2.74	130.11	123.70	11	2
3	C	336	PX4	C5-N1-C4	2.74	101.77	108.98	8	2
3	A	616	PX4	C5-N1-C4	2.74	101.78	108.98	6	4
3	A	629	PX4	O7-C23-O8	2.74	130.11	123.70	4	2
3	B	341	PX4	O7-C23-O8	2.74	130.11	123.70	8	1
3	B	350	PX4	O5-C9-C10	2.74	103.48	111.83	13	4
3	B	368	PX4	C5-N1-C4	2.74	116.17	108.98	3	2
3	C	306	PX4	C12-C11-C10	2.74	123.19	113.13	2	1
3	B	335	PX4	C8-C7-C6	2.74	105.40	111.78	3	3
3	C	330	PX4	C5-N1-C4	2.74	116.16	108.98	13	3
3	A	640	PX4	O7-C7-C8	2.73	118.15	108.34	4	3
3	A	603	PX4	C26-C25-C24	2.73	103.08	113.13	8	1
3	A	622	PX4	C25-C24-C23	2.73	123.71	113.69	14	1
3	B	330	PX4	C8-C7-C6	2.73	118.16	111.78	3	2
3	C	354	PX4	C5-N1-C4	2.74	101.79	108.98	14	2
3	B	305	PX4	O5-C8-C7	2.73	116.28	108.40	1	3
3	B	378	PX4	C5-N1-C3	2.73	101.80	108.98	1	3
3	B	394	PX4	C5-N1-C3	2.73	101.80	108.98	5	1
3	A	602	PX4	O7-C23-O8	2.73	130.09	123.70	10	3
3	C	351	PX4	O7-C23-O8	2.73	130.09	123.70	1	3
3	A	636	PX4	C8-C7-C6	2.73	118.15	111.78	1	2
3	C	334	PX4	C7-O7-C23	2.73	111.26	117.80	6	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	313	PX4	C8-O5-C9	2.73	107.15	117.12	14	1
3	B	376	PX4	O7-C23-O8	2.73	130.08	123.70	10	2
3	A	631	PX4	O7-C7-C8	2.73	118.12	108.34	5	4
3	B	318	PX4	O6-C9-C10	2.73	134.44	123.78	12	1
3	C	345	PX4	C4-N1-C3	2.73	101.81	108.98	4	3
3	A	615	PX4	C12-C11-C10	2.72	103.12	113.13	14	3
3	A	647	PX4	C5-N1-C4	2.72	101.82	108.98	14	2
3	C	362	PX4	C4-N1-C3	2.72	116.13	108.98	15	4
3	B	312	PX4	O7-C23-C24	2.72	105.59	111.48	4	3
3	B	314	PX4	O5-C9-O6	2.72	130.44	123.63	9	1
3	C	355	PX4	C25-C24-C23	2.72	103.71	113.69	14	2
3	A	630	PX4	O5-C9-C10	2.72	103.54	111.83	3	4
3	A	602	PX4	C8-C7-C6	2.72	105.44	111.78	12	1
3	A	609	PX4	O7-C23-C24	2.72	105.60	111.48	11	2
3	A	613	PX4	C5-N1-C4	2.72	116.12	108.98	10	2
3	A	646	PX4	C7-O7-C23	2.72	111.29	117.80	10	2
3	A	647	PX4	C1-C2-N1	2.72	124.55	115.82	15	1
3	B	308	PX4	O5-C9-C10	2.72	103.54	111.83	3	3
3	B	354	PX4	C4-N1-C3	2.72	116.12	108.98	4	2
3	C	315	PX4	C4-N1-C3	2.72	101.83	108.98	11	1
3	B	342	PX4	C5-N1-C4	2.72	101.83	108.98	9	2
3	C	302	PX4	C15-C14-C13	2.72	100.62	114.37	1	1
3	C	319	PX4	C7-O7-C23	2.72	111.29	117.80	13	6
3	C	324	PX4	C25-C24-C23	2.72	123.66	113.69	14	1
3	B	304	PX4	O7-C23-C24	2.72	105.61	111.48	12	4
3	B	332	PX4	O5-C8-C7	2.72	116.23	108.40	11	4
3	B	389	PX4	C8-C7-C6	2.72	118.12	111.78	10	2
3	C	318	PX4	C8-C7-C6	2.72	105.45	111.78	6	3
3	C	330	PX4	O5-C9-O6	2.72	130.42	123.63	12	1
3	C	336	PX4	O5-C8-C7	2.72	116.23	108.40	6	1
3	C	359	PX4	C5-N1-C4	2.72	101.84	108.98	3	3
3	A	601	PX4	O5-C9-C10	2.71	103.56	111.83	4	1
3	C	353	PX4	O5-C8-C7	2.71	116.22	108.40	7	1
3	A	621	PX4	O5-C9-O6	2.71	130.41	123.63	3	3
3	A	642	PX4	O5-C8-C7	2.71	116.22	108.40	13	2
3	A	646	PX4	O7-C7-C8	2.71	118.08	108.34	9	2
3	B	331	PX4	C5-N1-C4	2.71	101.85	108.98	8	3
3	B	338	PX4	C11-C10-C9	2.71	123.63	113.69	3	1
3	B	392	PX4	O5-C9-C10	2.71	103.56	111.83	14	1
3	A	638	PX4	C25-C24-C23	2.71	103.76	113.69	3	1
3	B	357	PX4	O3-C1-C2	2.71	122.70	109.65	13	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	367	PX4	C25-C24-C23	2.71	103.76	113.69	15	1
3	B	369	PX4	O5-C9-C10	2.71	103.57	111.83	13	3
3	B	386	PX4	O5-C9-C10	2.71	103.57	111.83	14	2
3	C	306	PX4	C7-O7-C23	2.71	111.31	117.80	13	2
3	A	625	PX4	C31-C30-C29	2.71	100.67	114.37	8	1
3	C	340	PX4	C8-C7-C6	2.71	118.10	111.78	14	3
3	C	369	PX4	O7-C7-C6	2.71	118.06	108.34	15	1
3	A	615	PX4	O7-C7-C8	2.71	118.06	108.34	4	2
3	A	617	PX4	O7-C23-O8	2.71	130.04	123.70	1	1
3	B	358	PX4	O7-C23-O8	2.71	130.03	123.70	1	3
3	B	397	PX4	O5-C9-C10	2.71	103.58	111.83	5	2
3	C	317	PX4	O7-C23-O8	2.71	130.03	123.70	15	3
3	A	606	PX4	C7-O7-C23	2.71	111.32	117.80	12	4
3	A	630	PX4	O3-P1-O2	2.71	119.66	108.94	3	1
3	B	304	PX4	P1-O3-C1	2.71	108.38	121.26	2	1
3	C	316	PX4	O7-C23-O8	2.71	130.03	123.70	3	2
3	A	632	PX4	O5-C9-O6	2.70	130.39	123.63	9	3
3	A	628	PX4	O6-C9-C10	2.70	134.35	123.78	13	1
3	A	629	PX4	C5-N1-C3	2.70	116.08	108.98	14	1
3	B	352	PX4	O3-C1-C2	2.70	122.66	109.65	7	1
3	C	314	PX4	C12-C11-C10	2.70	103.20	113.13	14	1
3	A	641	PX4	C18-C17-C16	2.70	100.72	114.37	11	1
3	B	357	PX4	O7-C7-C6	2.70	118.03	108.34	10	1
3	B	389	PX4	C7-O7-C23	2.70	111.33	117.80	6	3
3	C	317	PX4	C5-N1-C4	2.70	116.07	108.98	14	3
3	A	618	PX4	O7-C23-O8	2.70	130.01	123.70	15	1
3	B	398	PX4	C5-N1-C3	2.70	101.89	108.98	4	2
3	C	333	PX4	C8-C7-C6	2.70	105.49	111.78	1	4
3	C	341	PX4	C5-N1-C3	2.70	101.88	108.98	15	1
3	A	629	PX4	O5-C8-C7	2.70	116.18	108.40	7	6
3	A	617	PX4	C5-N1-C4	2.70	116.06	108.98	6	2
3	C	350	PX4	C1-C2-N1	2.70	124.48	115.82	2	2
3	C	301	PX4	C5-N1-C3	2.70	101.89	108.98	6	2
3	C	323	PX4	O5-C9-O6	2.70	130.37	123.63	9	2
3	C	337	PX4	C8-C7-C6	2.70	118.07	111.78	1	1
3	C	356	PX4	C1-C2-N1	2.70	124.47	115.82	10	2
3	C	345	PX4	O5-C9-C10	2.69	103.62	111.83	4	1
3	A	610	PX4	C8-C7-C6	2.69	105.50	111.78	6	3
3	C	318	PX4	O5-C8-C7	2.69	116.16	108.40	2	5
3	C	320	PX4	C5-N1-C4	2.69	116.05	108.98	5	4
3	C	341	PX4	C4-N1-C3	2.69	116.05	108.98	5	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	C	365	PX4	C4-N1-C3	2.69	101.90	108.98	7	3
3	B	304	PX4	O7-C7-C8	2.69	118.00	108.34	10	3
3	A	641	PX4	O7-C7-C8	2.69	118.00	108.34	13	2
3	B	318	PX4	C26-C25-C24	2.69	103.24	113.13	7	1
3	B	377	PX4	O7-C7-C8	2.69	118.00	108.34	7	4
3	B	389	PX4	C17-C16-C15	2.69	100.76	114.37	10	1
3	B	372	PX4	O7-C7-C6	2.69	118.00	108.34	7	1
3	B	399	PX4	C25-C24-C23	2.69	123.56	113.69	6	1
3	B	336	PX4	O7-C23-O8	2.69	129.99	123.70	13	2
3	B	379	PX4	O7-C7-C6	2.69	117.99	108.34	13	1
3	B	356	PX4	O5-C9-C10	2.69	103.64	111.83	13	3
3	B	392	PX4	O7-C23-O8	2.69	129.99	123.70	15	3
3	C	309	PX4	C34-C33-C32	2.69	100.78	114.37	7	1
3	C	319	PX4	O5-C9-O6	2.69	130.35	123.63	12	2
3	B	328	PX4	O7-C7-C8	2.69	117.98	108.34	4	1
3	B	370	PX4	C5-N1-C3	2.69	116.03	108.98	3	2
3	B	385	PX4	O7-C23-C24	2.69	105.67	111.48	8	4
3	C	303	PX4	C5-N1-C4	2.69	116.03	108.98	6	1
3	B	348	PX4	O5-C9-C10	2.68	103.65	111.83	9	3
3	B	378	PX4	O5-C9-O6	2.68	130.34	123.63	14	3
3	B	381	PX4	O5-C9-O6	2.68	130.34	123.63	9	2
3	B	398	PX4	C26-C25-C24	2.68	103.27	113.13	6	2
3	C	325	PX4	C25-C24-C23	2.68	103.86	113.69	8	2
3	C	328	PX4	O5-C9-O6	2.68	130.34	123.63	4	1
3	A	606	PX4	C8-C7-C6	2.68	118.04	111.78	13	4
3	A	610	PX4	C5-N1-C3	2.68	101.93	108.98	15	3
3	A	644	PX4	O7-C7-C8	2.68	117.97	108.34	7	3
3	C	369	PX4	C5-N1-C4	2.68	101.93	108.98	12	2
3	B	375	PX4	O5-C8-C7	2.68	116.12	108.40	3	4
3	C	315	PX4	C25-C24-C23	2.68	103.87	113.69	12	2
3	C	339	PX4	C12-C11-C10	2.68	103.27	113.13	7	2
3	C	361	PX4	P1-O3-C1	2.68	134.03	121.26	13	1
3	A	611	PX4	C7-O7-C23	2.68	111.38	117.80	13	4
3	A	628	PX4	O7-C7-C8	2.68	117.96	108.34	1	3
3	B	366	PX4	C5-N1-C4	2.68	101.94	108.98	5	1
3	B	379	PX4	C8-O5-C9	2.68	107.33	117.12	7	1
3	B	398	PX4	O5-C8-C7	2.68	116.12	108.40	8	3
3	C	340	PX4	O5-C9-C10	2.68	103.67	111.83	9	2
3	B	353	PX4	O7-C7-C8	2.68	117.95	108.34	11	3
3	C	330	PX4	O5-C9-C10	2.68	103.67	111.83	14	3
3	B	385	PX4	C5-N1-C4	2.68	101.94	108.98	12	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	C	347	PX4	O5-C9-O6	2.68	130.32	123.63	2	1
3	C	347	PX4	O5-C8-C7	2.68	116.11	108.40	3	2
3	C	341	PX4	O5-C9-O6	2.68	130.32	123.63	10	1
3	C	358	PX4	C5-N1-C3	2.68	101.94	108.98	2	1
3	B	350	PX4	O7-C7-C6	2.68	117.94	108.34	6	1
3	B	379	PX4	C5-N1-C3	2.68	116.00	108.98	7	2
3	A	601	PX4	C26-C25-C24	2.67	122.95	113.13	10	1
3	A	612	PX4	O7-C7-C6	2.67	117.93	108.34	4	3
3	C	314	PX4	C8-C7-C6	2.67	105.55	111.78	7	5
3	C	315	PX4	C8-C7-C6	2.67	118.02	111.78	10	2
3	C	321	PX4	C4-N1-C3	2.67	101.95	108.98	8	3
3	B	307	PX4	C7-O7-C23	2.67	111.40	117.80	9	1
3	B	322	PX4	C8-C7-C6	2.67	105.56	111.78	2	1
3	B	340	PX4	C5-N1-C4	2.67	116.00	108.98	7	2
3	A	624	PX4	C8-O5-C9	2.67	107.36	117.12	8	1
3	A	626	PX4	C5-N1-C3	2.67	101.97	108.98	3	5
3	A	632	PX4	C1-C2-N1	2.67	124.39	115.82	9	1
3	B	324	PX4	O5-C9-O6	2.67	130.30	123.63	4	1
3	B	346	PX4	C5-N1-C4	2.67	101.97	108.98	5	2
3	C	339	PX4	C8-C7-C6	2.67	105.57	111.78	8	2
3	C	344	PX4	C7-O7-C23	2.67	111.41	117.80	12	2
3	B	304	PX4	C5-N1-C3	2.67	115.98	108.98	13	2
3	A	622	PX4	C12-C11-C10	2.67	122.92	113.13	1	1
3	A	639	PX4	O5-C9-C10	2.67	103.71	111.83	15	2
3	B	329	PX4	O5-C8-C7	2.67	116.08	108.40	10	1
3	C	357	PX4	O5-C9-O6	2.67	130.30	123.63	6	4
3	B	310	PX4	C4-N1-C3	2.66	115.98	108.98	12	2
3	C	357	PX4	C5-N1-C3	2.67	101.97	108.98	12	2
3	A	602	PX4	C8-O5-C9	2.66	107.38	117.12	2	1
3	A	610	PX4	C25-C24-C23	2.66	123.45	113.69	6	2
3	B	351	PX4	C8-O5-C9	2.66	107.38	117.12	1	3
3	B	345	PX4	C1-C2-N1	2.66	124.37	115.82	11	1
3	B	346	PX4	O5-C9-C10	2.66	103.71	111.83	15	2
3	B	368	PX4	O7-C7-C8	2.66	117.90	108.34	6	1
3	C	323	PX4	C5-N1-C4	2.66	115.97	108.98	10	2
3	B	379	PX4	C4-N1-C3	2.66	101.99	108.98	7	2
3	B	395	PX4	C8-O5-C9	2.66	107.40	117.12	11	1
3	C	311	PX4	C8-C7-C6	2.66	105.58	111.78	4	1
3	B	323	PX4	C7-O7-C23	2.66	111.43	117.80	7	2
3	B	317	PX4	O7-C23-O8	2.66	129.92	123.70	3	2
3	B	303	PX4	O7-C23-O8	2.66	129.91	123.70	11	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	359	PX4	O7-C7-C6	2.66	117.87	108.34	9	1
3	C	314	PX4	O7-C23-C24	2.66	105.73	111.48	5	3
3	C	321	PX4	O5-C9-C10	2.66	103.73	111.83	12	3
3	B	316	PX4	O5-C8-C7	2.65	116.05	108.40	2	3
3	B	318	PX4	C8-C7-C6	2.65	117.97	111.78	4	4
3	B	333	PX4	O5-C9-O6	2.65	130.27	123.63	4	2
3	B	338	PX4	O5-C9-C10	2.65	103.75	111.83	2	2
3	C	324	PX4	O7-C7-C8	2.65	117.86	108.34	9	1
3	C	370	PX4	C5-N1-C2	2.65	120.46	109.91	1	1
3	A	636	PX4	C1-C2-N1	2.65	124.33	115.82	12	3
3	A	627	PX4	C5-N1-C4	2.65	102.02	108.98	5	1
3	A	639	PX4	O7-C7-C8	2.65	117.85	108.34	10	1
3	A	648	PX4	O7-C7-C6	2.65	117.85	108.34	7	2
3	B	396	PX4	C5-N1-C4	2.65	102.01	108.98	3	4
3	C	307	PX4	O7-C7-C6	2.65	98.83	108.34	9	1
3	C	312	PX4	O5-C9-C10	2.65	103.75	111.83	13	5
3	A	610	PX4	C1-C2-N1	2.65	124.32	115.82	12	3
3	A	625	PX4	C5-N1-C4	2.65	102.02	108.98	15	1
3	B	311	PX4	C7-O7-C23	2.65	111.46	117.80	11	3
3	B	342	PX4	C11-C10-C9	2.65	103.99	113.69	7	2
3	A	625	PX4	C8-C7-C6	2.65	105.61	111.78	8	1
3	C	343	PX4	C8-C7-C6	2.65	117.95	111.78	1	5
3	C	335	PX4	O8-C23-C24	2.64	134.13	123.78	15	1
3	A	606	PX4	C5-N1-C3	2.64	102.03	108.98	15	2
3	A	620	PX4	C25-C24-C23	2.64	104.01	113.69	10	1
3	B	386	PX4	C25-C24-C23	2.64	104.01	113.69	6	3
3	C	327	PX4	O1-P1-O2	2.64	124.74	112.44	8	2
3	C	327	PX4	O7-C7-C6	2.64	117.82	108.34	13	1
3	C	358	PX4	C4-N1-C3	2.64	102.03	108.98	12	3
3	C	363	PX4	O5-C9-O6	2.64	130.24	123.63	3	2
3	A	607	PX4	C5-N1-C3	2.64	115.91	108.98	14	2
3	A	619	PX4	C7-O7-C23	2.64	111.48	117.80	10	3
3	B	372	PX4	C1-C2-N1	2.64	124.30	115.82	8	2
3	B	374	PX4	C5-N1-C4	2.64	102.04	108.98	4	1
3	C	335	PX4	O5-C8-C7	2.64	116.00	108.40	8	4
3	A	636	PX4	O5-C9-O6	2.64	130.23	123.63	2	1
3	C	314	PX4	O5-C9-C10	2.64	103.79	111.83	3	1
3	C	334	PX4	C5-N1-C4	2.64	115.91	108.98	5	2
3	A	646	PX4	C1-C2-N1	2.64	124.28	115.82	6	2
3	A	603	PX4	C7-O7-C23	2.63	111.49	117.80	9	2
3	A	629	PX4	O1-P1-O2	2.63	124.70	112.44	13	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	307	PX4	C8-C7-C6	2.64	105.64	111.78	1	3
3	B	371	PX4	C8-C7-C6	2.63	105.64	111.78	5	3
3	C	338	PX4	O5-C8-C7	2.63	115.99	108.40	13	5
3	A	620	PX4	O5-C9-C10	2.63	103.81	111.83	5	2
3	C	321	PX4	O5-C9-O6	2.63	130.21	123.63	12	2
3	C	360	PX4	C5-N1-C4	2.63	115.89	108.98	3	3
3	B	369	PX4	C12-C11-C10	2.63	103.46	113.13	5	2
3	A	641	PX4	C4-N1-C3	2.63	115.89	108.98	12	1
3	C	335	PX4	C1-C2-N1	2.63	124.27	115.82	1	1
3	B	344	PX4	O5-C9-C10	2.63	103.82	111.83	3	4
3	B	357	PX4	C7-O7-C23	2.63	111.50	117.80	6	4
3	B	391	PX4	C1-C2-N1	2.63	124.26	115.82	4	1
3	B	377	PX4	O6-C9-C10	2.63	134.06	123.78	1	1
3	C	331	PX4	O7-C23-C24	2.63	105.79	111.48	9	5
3	A	630	PX4	C8-C7-C6	2.63	117.91	111.78	6	2
3	B	311	PX4	O5-C8-C7	2.63	115.97	108.40	3	3
3	B	329	PX4	C4-N1-C3	2.63	102.08	108.98	3	2
3	C	315	PX4	C11-C10-C9	2.63	123.32	113.69	8	1
3	C	317	PX4	C5-N1-C3	2.63	115.87	108.98	12	2
3	C	320	PX4	P1-O4-C6	2.63	136.40	121.35	9	1
3	C	325	PX4	O5-C9-C10	2.63	103.83	111.83	15	2
3	C	367	PX4	O7-C23-C24	2.63	105.80	111.48	3	3
3	B	308	PX4	O5-C9-O6	2.62	130.19	123.63	3	2
3	B	380	PX4	C1-C2-N1	2.62	124.25	115.82	4	1
3	B	388	PX4	O5-C9-C10	2.62	103.83	111.83	3	2
3	B	390	PX4	O7-C7-C8	2.62	117.76	108.34	5	1
3	C	327	PX4	C8-C7-C6	2.62	117.90	111.78	10	4
3	A	636	PX4	O7-C23-C24	2.62	105.81	111.48	5	3
3	B	333	PX4	C25-C24-C23	2.62	104.09	113.69	7	1
3	B	357	PX4	C1-C2-N1	2.62	124.24	115.82	4	2
3	B	335	PX4	P1-O3-C1	2.62	133.74	121.26	12	2
3	B	362	PX4	O5-C9-O6	2.62	130.19	123.63	5	2
3	C	309	PX4	O5-C9-O6	2.62	130.19	123.63	10	2
3	A	607	PX4	C5-N1-C2	2.62	120.32	109.91	3	1
3	B	373	PX4	C11-C10-C9	2.62	123.30	113.69	12	2
3	C	352	PX4	C5-N1-C4	2.62	102.09	108.98	15	2
3	B	355	PX4	C11-C10-C9	2.62	104.10	113.69	5	2
3	C	369	PX4	C26-C25-C24	2.62	122.75	113.13	12	1
3	B	386	PX4	O5-C9-O6	2.62	130.18	123.63	14	3
3	C	310	PX4	O5-C9-C10	2.62	103.85	111.83	1	2
3	B	324	PX4	C1-C2-N1	2.62	124.22	115.82	2	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	331	PX4	O7-C23-O8	2.62	129.82	123.70	9	2
3	B	347	PX4	C8-C7-C6	2.62	117.89	111.78	3	1
3	C	326	PX4	C5-N1-C4	2.62	115.85	108.98	10	4
3	C	332	PX4	O5-C8-C7	2.62	115.94	108.40	1	4
3	B	378	PX4	C1-C2-N1	2.61	107.43	115.82	14	3
3	A	627	PX4	O3-P1-O2	2.61	98.58	108.94	10	2
3	A	647	PX4	C8-C7-C6	2.61	105.70	111.78	3	2
3	B	359	PX4	O5-C8-C7	2.61	115.93	108.40	3	2
3	B	386	PX4	C5-N1-C2	2.61	120.30	109.91	11	2
3	C	308	PX4	O5-C9-O6	2.61	130.16	123.63	9	2
3	C	310	PX4	O7-C23-O8	2.61	129.81	123.70	6	4
3	C	322	PX4	O5-C9-C10	2.61	103.87	111.83	3	4
3	B	318	PX4	O5-C9-O6	2.61	117.10	123.63	12	3
3	B	361	PX4	O5-C9-C10	2.61	103.88	111.83	6	1
3	C	341	PX4	O3-C1-C2	2.61	122.21	109.65	12	1
3	C	359	PX4	C5-N1-C3	2.61	115.83	108.98	6	1
3	B	397	PX4	O5-C8-C7	2.61	115.92	108.40	15	4
3	B	397	PX4	C4-N1-C3	2.61	102.12	108.98	7	2
3	C	314	PX4	O7-C7-C8	2.61	117.70	108.34	14	3
3	C	368	PX4	C5-N1-C4	2.61	102.12	108.98	13	3
3	B	346	PX4	O7-C7-C8	2.61	117.70	108.34	4	3
3	A	647	PX4	O7-C23-O8	2.61	129.80	123.70	14	2
3	B	332	PX4	C4-N1-C3	2.61	102.13	108.98	6	4
3	B	346	PX4	C11-C10-C9	2.61	123.25	113.69	9	1
3	C	334	PX4	C1-C2-N1	2.61	124.19	115.82	10	2
3	A	601	PX4	O7-C23-O8	2.60	129.79	123.70	11	4
3	B	351	PX4	O7-C23-O8	2.61	129.80	123.70	6	3
3	A	614	PX4	O7-C23-O8	2.60	129.79	123.70	6	4
3	B	311	PX4	C4-N1-C3	2.60	102.14	108.98	15	1
3	B	320	PX4	C8-C7-C6	2.60	105.71	111.78	15	1
3	B	335	PX4	C5-N1-C3	2.60	115.82	108.98	9	1
3	B	344	PX4	O7-C7-C8	2.60	117.68	108.34	11	1
3	B	345	PX4	O7-C7-C8	2.60	117.69	108.34	7	2
3	C	328	PX4	O5-C8-C7	2.60	115.91	108.40	11	3
3	C	366	PX4	O7-C7-C6	2.60	117.69	108.34	3	1
3	B	376	PX4	C4-N1-C3	2.60	102.14	108.98	2	2
3	C	326	PX4	O1-P1-O2	2.60	124.55	112.44	14	1
3	C	327	PX4	C4-N1-C3	2.60	102.14	108.98	7	1
3	C	335	PX4	C25-C24-C23	2.60	123.23	113.69	8	1
3	C	369	PX4	C7-O7-C23	2.60	111.56	117.80	5	1
3	A	608	PX4	O5-C9-O6	2.60	130.14	123.63	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	C	351	PX4	C26-C25-C24	2.60	103.56	113.13	8	1
3	A	615	PX4	O7-C23-O8	2.60	129.78	123.70	15	1
3	A	622	PX4	C8-O5-C9	2.60	107.61	117.12	4	1
3	C	311	PX4	C5-N1-C4	2.60	102.15	108.98	9	1
3	C	344	PX4	C8-O5-C9	2.60	126.62	117.12	6	1
3	C	354	PX4	O7-C7-C6	2.60	117.67	108.34	2	1
3	B	321	PX4	C16-C15-C14	2.60	101.23	114.37	11	1
3	A	604	PX4	O7-C7-C8	2.60	117.66	108.34	6	2
3	B	313	PX4	C11-C10-C9	2.60	123.21	113.69	9	2
3	B	346	PX4	O7-C23-O8	2.60	117.63	123.70	14	1
3	C	341	PX4	C11-C10-C9	2.60	104.17	113.69	9	1
3	B	352	PX4	C1-C2-N1	2.60	124.16	115.82	6	1
3	C	341	PX4	C1-C2-N1	2.60	124.16	115.82	14	1
3	C	368	PX4	O5-C9-O6	2.60	130.13	123.63	1	2
3	B	361	PX4	C4-N1-C3	2.60	115.80	108.98	4	1
3	C	353	PX4	C11-C10-C9	2.60	104.18	113.69	1	2
3	C	355	PX4	C1-C2-N1	2.60	124.15	115.82	12	1
3	C	360	PX4	P1-O3-C1	2.60	108.91	121.26	12	1
3	C	367	PX4	C11-C10-C9	2.60	104.18	113.69	3	2
3	B	366	PX4	C12-C11-C10	2.59	103.59	113.13	7	2
3	C	346	PX4	C5-N1-C4	2.59	115.79	108.98	14	1
3	C	358	PX4	O7-C7-C6	2.59	117.65	108.34	12	2
3	B	309	PX4	C5-N1-C4	2.59	102.16	108.98	4	2
3	B	319	PX4	O5-C8-C7	2.59	115.87	108.40	5	2
3	B	350	PX4	O5-C8-C7	2.59	115.87	108.40	15	3
3	B	354	PX4	P1-O4-C6	2.59	136.21	121.35	14	1
3	B	366	PX4	C5-N1-C3	2.59	115.79	108.98	12	1
3	B	383	PX4	C1-C2-N1	2.59	124.15	115.82	1	2
3	B	320	PX4	O5-C8-C7	2.59	115.87	108.40	14	4
3	C	303	PX4	C5-N1-C3	2.59	115.78	108.98	9	5
3	C	314	PX4	C5-N1-C4	2.59	115.78	108.98	5	5
3	C	361	PX4	C12-C11-C10	2.59	103.60	113.13	14	1
3	B	306	PX4	C5-N1-C3	2.59	102.17	108.98	6	1
3	B	374	PX4	C4-N1-C3	2.59	115.78	108.98	9	1
3	B	378	PX4	C4-N1-C3	2.59	102.18	108.98	12	1
3	B	396	PX4	O6-C9-C10	2.59	133.90	123.78	6	2
3	C	308	PX4	C4-N1-C3	2.59	102.18	108.98	14	2
3	C	364	PX4	O5-C9-C10	2.59	103.94	111.83	12	1
3	B	369	PX4	C25-C24-C23	2.59	123.17	113.69	1	1
3	C	310	PX4	C13-C12-C11	2.59	101.29	114.37	7	1
3	C	344	PX4	C1-C2-N1	2.59	124.12	115.82	14	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	628	PX4	O5-C8-C7	2.58	115.85	108.40	14	2
3	A	634	PX4	C8-C7-C6	2.58	105.76	111.78	7	2
3	A	615	PX4	O5-C9-C10	2.58	103.96	111.83	4	3
3	A	620	PX4	C4-N1-C3	2.58	115.76	108.98	10	1
3	A	629	PX4	O5-C9-O6	2.58	130.09	123.63	11	2
3	B	358	PX4	C31-C30-C29	2.58	101.30	114.37	10	1
3	B	392	PX4	O7-C7-C8	2.58	117.61	108.34	8	1
3	C	332	PX4	C25-C24-C23	2.58	104.22	113.69	1	2
3	C	342	PX4	C12-C11-C10	2.58	122.62	113.13	15	1
3	A	605	PX4	O5-C9-O6	2.58	130.09	123.63	7	3
3	B	322	PX4	O5-C9-O6	2.58	130.09	123.63	2	3
3	C	326	PX4	O5-C9-C10	2.58	103.96	111.83	5	2
3	C	363	PX4	C5-N1-C3	2.58	102.19	108.98	3	3
3	C	364	PX4	C5-N1-C3	2.58	115.76	108.98	14	2
3	A	621	PX4	O7-C23-C24	2.58	105.90	111.48	7	2
3	B	376	PX4	O5-C8-C7	2.58	115.83	108.40	12	2
3	B	399	PX4	O5-C9-C10	2.58	103.97	111.83	4	2
3	C	315	PX4	C5-N1-C4	2.58	115.76	108.98	15	1
3	A	620	PX4	C26-C25-C24	2.58	103.65	113.13	6	1
3	B	327	PX4	O7-C7-C8	2.58	117.60	108.34	7	4
3	B	332	PX4	O7-C7-C6	2.58	99.09	108.34	6	1
3	B	382	PX4	C5-N1-C4	2.58	102.20	108.98	7	2
3	C	312	PX4	C5-N1-C3	2.58	102.20	108.98	1	4
3	C	307	PX4	C4-N1-C3	2.58	102.21	108.98	7	3
3	A	626	PX4	O5-C9-O6	2.57	130.07	123.63	6	1
3	B	303	PX4	O7-C23-C24	2.58	105.91	111.48	11	2
3	B	367	PX4	C5-N1-C4	2.58	115.74	108.98	6	1
3	C	347	PX4	C1-C2-N1	2.58	124.09	115.82	1	2
3	A	612	PX4	C29-C28-C27	2.57	101.36	114.37	7	1
3	B	320	PX4	C8-O5-C9	2.57	107.71	117.12	2	1
3	B	348	PX4	C5-N1-C4	2.57	115.74	108.98	12	2
3	B	400	PX4	O7-C7-C6	2.57	117.57	108.34	11	1
3	C	335	PX4	C26-C25-C24	2.57	103.67	113.13	15	2
3	A	612	PX4	O7-C23-O8	2.57	129.72	123.70	7	1
3	C	314	PX4	C4-N1-C3	2.57	102.22	108.98	12	2
3	B	321	PX4	O7-C7-C6	2.57	117.56	108.34	2	2
3	B	377	PX4	O1-P1-O4	2.57	119.22	107.57	7	1
3	C	323	PX4	C8-C7-C6	2.57	105.79	111.78	12	1
3	B	386	PX4	C5-N1-C4	2.57	115.72	108.98	13	4
3	B	393	PX4	C4-N1-C3	2.57	102.23	108.98	10	4
3	C	307	PX4	O7-C7-C8	2.57	117.56	108.34	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	C	364	PX4	C1-C2-N1	2.57	124.07	115.82	13	4
3	A	606	PX4	O5-C9-O6	2.57	130.05	123.63	11	2
3	B	353	PX4	O5-C8-C7	2.57	115.79	108.40	9	2
3	C	330	PX4	C8-C7-C6	2.56	117.76	111.78	6	3
3	C	337	PX4	C5-N1-C4	2.56	102.24	108.98	6	1
3	A	619	PX4	C32-C31-C30	2.56	127.33	114.37	6	1
3	B	366	PX4	O7-C23-O8	2.56	129.70	123.70	7	3
3	B	305	PX4	C5-N1-C3	2.56	102.25	108.98	7	2
3	B	339	PX4	O5-C9-C10	2.56	104.03	111.83	8	2
3	B	357	PX4	C31-C30-C29	2.56	101.42	114.37	8	1
3	B	393	PX4	C8-C7-C6	2.56	105.81	111.78	9	2
3	B	374	PX4	C5-N1-C3	2.56	102.25	108.98	12	2
3	C	348	PX4	O7-C7-C8	2.56	117.52	108.34	6	3
3	B	326	PX4	C11-C10-C9	2.56	104.32	113.69	9	2
3	C	354	PX4	C11-C10-C9	2.56	123.07	113.69	6	1
3	B	340	PX4	C7-O7-C23	2.56	111.68	117.80	1	3
3	B	370	PX4	O5-C8-C7	2.56	115.77	108.40	14	6
3	B	400	PX4	C26-C25-C24	2.56	122.52	113.13	3	1
3	B	323	PX4	O5-C9-O6	2.55	130.02	123.63	10	1
3	B	389	PX4	O7-C23-C24	2.55	105.95	111.48	15	1
3	B	391	PX4	O5-C8-C7	2.55	115.76	108.40	1	2
3	C	333	PX4	C1-C2-N1	2.55	124.02	115.82	8	1
3	A	616	PX4	C12-C11-C10	2.55	103.75	113.13	15	2
3	A	621	PX4	C4-N1-C3	2.55	102.27	108.98	6	2
3	B	346	PX4	O5-C9-O6	2.55	130.01	123.63	14	2
3	C	309	PX4	C5-N1-C3	2.55	102.27	108.98	4	2
3	C	346	PX4	P1-O3-C1	2.55	133.40	121.26	1	1
3	B	323	PX4	P1-O3-C1	2.55	133.39	121.26	10	1
3	B	331	PX4	C7-O7-C23	2.55	111.70	117.80	5	4
3	B	354	PX4	C1-C2-N1	2.55	124.00	115.82	6	1
3	B	358	PX4	C5-N1-C2	2.55	99.78	109.91	3	1
3	B	371	PX4	C25-C24-C23	2.55	104.36	113.69	2	1
3	B	380	PX4	C8-O5-C9	2.55	107.80	117.12	12	1
3	C	331	PX4	O5-C9-O6	2.55	130.00	123.63	1	2
3	A	620	PX4	O5-C9-O6	2.55	130.00	123.63	11	2
3	C	303	PX4	O7-C7-C8	2.55	117.48	108.34	3	1
3	C	328	PX4	C7-O7-C23	2.55	111.70	117.80	5	2
3	A	631	PX4	C12-C11-C10	2.54	103.78	113.13	15	2
3	B	306	PX4	O8-C23-C24	2.54	133.73	123.78	11	1
3	C	303	PX4	C1-C2-N1	2.55	123.99	115.82	13	4
3	C	314	PX4	O7-C7-C6	2.54	117.47	108.34	1	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	373	PX4	C5-N1-C3	2.54	115.66	108.98	15	2
3	B	394	PX4	C12-C11-C10	2.54	103.79	113.13	4	1
3	C	330	PX4	C11-C10-C9	2.54	104.38	113.69	14	1
3	B	338	PX4	C26-C25-C24	2.54	122.45	113.13	3	1
3	B	364	PX4	C7-O7-C23	2.54	111.72	117.80	3	3
3	B	371	PX4	C1-C2-N1	2.54	123.97	115.82	10	2
3	B	384	PX4	C11-C10-C9	2.54	104.39	113.69	2	1
3	B	390	PX4	C8-C7-C6	2.54	117.70	111.78	1	2
3	C	309	PX4	O7-C7-C8	2.54	117.45	108.34	6	3
3	C	310	PX4	O5-C9-O6	2.54	129.98	123.63	3	2
3	B	325	PX4	O7-C23-O8	2.54	117.78	123.70	2	2
3	B	399	PX4	C4-N1-C3	2.54	102.32	108.98	6	3
3	C	302	PX4	O7-C7-C6	2.54	117.44	108.34	9	1
3	A	612	PX4	O5-C9-O6	2.53	129.96	123.63	6	2
3	B	313	PX4	O7-C23-O8	2.53	129.63	123.70	11	1
3	B	327	PX4	P1-O3-C1	2.53	133.32	121.26	1	1
3	B	386	PX4	C8-C7-C6	2.53	105.88	111.78	10	2
3	B	388	PX4	C12-C11-C10	2.53	122.44	113.13	3	1
3	A	638	PX4	C5-N1-C2	2.53	119.97	109.91	9	1
3	B	310	PX4	C1-C2-N1	2.53	123.95	115.82	5	2
3	B	375	PX4	C7-O7-C23	2.53	111.74	117.80	7	3
3	B	386	PX4	C12-C11-C10	2.53	122.43	113.13	5	1
3	B	394	PX4	C1-C2-N1	2.53	123.95	115.82	2	2
3	C	337	PX4	C5-N1-C3	2.53	115.62	108.98	9	2
3	A	602	PX4	O7-C7-C8	2.53	117.42	108.34	1	3
3	B	305	PX4	C25-C24-C23	2.53	122.97	113.69	9	3
3	B	350	PX4	C5-N1-C4	2.53	102.33	108.98	2	2
3	C	305	PX4	C8-C7-C6	2.53	117.68	111.78	15	1
3	A	615	PX4	C3-N1-C2	2.53	119.95	109.91	5	3
3	A	619	PX4	C5-N1-C4	2.53	102.34	108.98	9	2
3	B	315	PX4	O7-C23-O8	2.53	129.61	123.70	15	2
3	B	341	PX4	O5-C9-C10	2.53	104.13	111.83	9	2
3	B	394	PX4	O5-C9-O6	2.53	129.95	123.63	15	2
3	A	639	PX4	C7-O7-C23	2.52	111.75	117.80	5	3
3	B	308	PX4	O7-C7-C6	2.52	117.40	108.34	3	3
3	B	357	PX4	O7-C23-O8	2.52	129.61	123.70	11	1
3	C	313	PX4	O5-C9-C10	2.52	104.14	111.83	7	1
3	A	626	PX4	O7-C7-C6	2.52	99.30	108.34	6	2
3	A	628	PX4	C8-C7-C6	2.52	117.67	111.78	13	2
3	B	396	PX4	O7-C7-C8	2.52	117.39	108.34	4	1
3	C	329	PX4	O7-C23-O8	2.52	129.60	123.70	8	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	330	PX4	C26-C25-C24	2.52	122.39	113.13	8	1
3	C	349	PX4	C5-N1-C3	2.52	102.35	108.98	4	2
3	A	634	PX4	C8-O5-C9	2.52	107.91	117.12	11	1
3	A	645	PX4	C8-C7-C6	2.52	105.91	111.78	2	2
3	C	342	PX4	O5-C8-C7	2.52	115.66	108.40	1	5
3	B	312	PX4	O5-C9-C10	2.52	104.16	111.83	13	3
3	B	356	PX4	C11-C10-C9	2.52	122.92	113.69	13	1
3	B	362	PX4	C5-N1-C4	2.52	115.59	108.98	9	1
3	C	361	PX4	O5-C9-C10	2.52	104.15	111.83	15	1
3	B	377	PX4	O5-C8-C7	2.52	115.66	108.40	14	3
3	B	393	PX4	C25-C24-C23	2.52	104.47	113.69	1	1
3	C	337	PX4	O5-C9-O6	2.52	129.93	123.63	3	3
3	B	394	PX4	P1-O3-C1	2.52	133.24	121.26	9	1
3	C	319	PX4	C12-C11-C10	2.52	122.38	113.13	5	1
3	C	347	PX4	C7-O7-C23	2.52	123.82	117.80	5	3
3	A	601	PX4	C4-N1-C3	2.52	102.37	108.98	1	1
3	C	351	PX4	O7-C7-C6	2.52	117.37	108.34	11	2
3	C	359	PX4	C26-C25-C24	2.52	103.88	113.13	5	1
3	A	609	PX4	C12-C11-C10	2.52	103.88	113.13	9	1
3	B	375	PX4	O5-C9-C10	2.52	104.16	111.83	7	1
3	B	312	PX4	C11-C10-C9	2.51	104.48	113.69	4	1
3	B	370	PX4	C8-C7-C6	2.51	105.92	111.78	2	1
3	A	633	PX4	O7-C7-C6	2.51	117.36	108.34	1	2
3	B	310	PX4	C26-C25-C24	2.51	122.36	113.13	7	1
3	C	355	PX4	C5-N1-C3	2.51	102.38	108.98	11	1
3	A	614	PX4	O1-P1-O3	2.51	118.94	107.57	2	1
3	A	648	PX4	O7-C7-C8	2.51	117.35	108.34	15	4
3	B	363	PX4	O7-C23-O8	2.51	129.57	123.70	4	1
3	B	382	PX4	C5-N1-C3	2.51	102.38	108.98	5	1
3	B	349	PX4	C4-N1-C3	2.51	102.39	108.98	10	1
3	B	370	PX4	O5-C9-C10	2.51	104.18	111.83	11	3
3	B	387	PX4	O5-C9-O6	2.51	129.90	123.63	12	2
3	B	393	PX4	O7-C7-C8	2.51	117.34	108.34	9	1
3	C	350	PX4	C5-N1-C3	2.51	102.38	108.98	15	1
3	B	370	PX4	C1-C2-N1	2.51	123.87	115.82	12	2
3	C	303	PX4	C25-C24-C23	2.51	104.51	113.69	8	2
3	C	307	PX4	C11-C10-C9	2.51	104.51	113.69	2	2
3	A	641	PX4	C5-N1-C3	2.51	115.56	108.98	15	2
3	B	306	PX4	O7-C7-C8	2.51	117.33	108.34	9	2
3	B	366	PX4	C26-C25-C24	2.51	122.33	113.13	12	2
3	B	385	PX4	C5-N1-C3	2.50	102.40	108.98	10	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	624	PX4	O5-C9-C10	2.50	104.20	111.83	15	2
3	C	360	PX4	C5-N1-C2	2.50	119.86	109.91	1	1
3	B	375	PX4	C26-C25-C24	2.50	122.32	113.13	3	1
3	B	385	PX4	C29-C28-C27	2.50	101.72	114.37	12	1
3	C	332	PX4	O5-C9-C10	2.50	104.20	111.83	4	1
3	C	348	PX4	C5-N1-C4	2.50	115.55	108.98	7	2
3	A	614	PX4	O3-C1-C2	2.50	97.61	109.65	3	2
3	A	612	PX4	C5-N1-C4	2.50	102.41	108.98	5	1
3	A	623	PX4	P1-O3-C1	2.50	109.36	121.26	10	1
3	B	308	PX4	C7-O7-C23	2.50	111.81	117.80	8	2
3	C	306	PX4	C8-O5-C9	2.50	107.98	117.12	3	1
3	A	636	PX4	C5-N1-C4	2.50	102.41	108.98	1	1
3	C	346	PX4	O7-C7-C8	2.50	117.31	108.34	10	2
3	B	345	PX4	C5-N1-C4	2.50	115.54	108.98	11	1
3	A	610	PX4	O5-C8-C7	2.50	115.59	108.40	12	3
3	A	626	PX4	C8-O5-C9	2.50	126.24	117.12	14	1
3	A	635	PX4	O5-C8-C7	2.49	115.59	108.40	8	1
3	B	325	PX4	C5-N1-C3	2.49	102.42	108.98	3	1
3	B	333	PX4	O1-P1-O2	2.49	124.05	112.44	9	1
3	B	382	PX4	O3-C1-C2	2.49	121.65	109.65	9	1
3	B	368	PX4	C5-N1-C3	2.49	115.53	108.98	9	2
3	C	334	PX4	O7-C7-C8	2.49	117.29	108.34	8	2
3	C	352	PX4	O7-C7-C8	2.49	117.29	108.34	13	2
3	A	632	PX4	C5-N1-C3	2.49	102.43	108.98	14	3
3	A	646	PX4	O7-C23-O8	2.49	129.53	123.70	2	1
3	B	301	PX4	C4-N1-C3	2.49	115.52	108.98	10	1
3	B	345	PX4	O5-C8-C7	2.49	115.58	108.40	2	3
3	B	381	PX4	C5-N1-C3	2.49	102.43	108.98	3	1
3	C	308	PX4	C11-C10-C9	2.49	104.57	113.69	2	1
3	C	348	PX4	C26-C25-C24	2.49	103.97	113.13	10	1
3	C	361	PX4	O7-C7-C8	2.49	117.28	108.34	15	1
3	A	607	PX4	C34-C33-C32	2.49	126.95	114.37	7	1
3	B	380	PX4	C25-C24-C23	2.49	122.81	113.69	11	1
3	C	339	PX4	C5-N1-C3	2.49	102.44	108.98	15	2
3	B	319	PX4	C7-O7-C23	2.49	123.75	117.80	11	1
3	B	343	PX4	C1-C2-N1	2.49	123.81	115.82	8	1
3	C	364	PX4	P1-O4-C6	2.49	135.60	121.35	7	1
3	A	628	PX4	C12-C11-C10	2.48	104.00	113.13	3	3
3	B	348	PX4	C4-N1-C3	2.48	102.45	108.98	12	3
3	B	351	PX4	C26-C25-C24	2.48	122.25	113.13	1	1
3	C	347	PX4	O5-C9-C10	2.48	104.26	111.83	2	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	630	PX4	O5-C9-O6	2.48	129.84	123.63	11	4
3	A	614	PX4	P1-O3-C1	2.48	133.07	121.26	2	1
3	B	350	PX4	O1-P1-O2	2.48	123.99	112.44	6	1
3	B	386	PX4	P1-O4-C6	2.48	135.57	121.35	3	1
3	B	329	PX4	P1-O3-C1	2.48	133.06	121.26	6	1
3	C	354	PX4	C25-C24-C23	2.48	104.61	113.69	9	1
3	A	640	PX4	O5-C9-O6	2.48	129.83	123.63	11	3
3	A	620	PX4	O7-C23-C24	2.48	106.12	111.48	3	2
3	A	608	PX4	C5-N1-C4	2.48	115.48	108.98	3	2
3	B	322	PX4	C5-N1-C3	2.48	102.47	108.98	15	1
3	B	341	PX4	C5-N1-C4	2.48	102.47	108.98	12	2
3	B	347	PX4	C14-C13-C12	2.48	101.85	114.37	15	2
3	B	348	PX4	O5-C9-O6	2.48	129.82	123.63	8	1
3	B	309	PX4	O5-C9-O6	2.47	129.82	123.63	2	3
3	B	383	PX4	C4-N1-C3	2.47	115.47	108.98	9	2
3	B	393	PX4	O7-C7-C6	2.47	117.22	108.34	1	1
3	C	356	PX4	C12-C11-C10	2.48	104.03	113.13	13	1
3	B	332	PX4	C11-C10-C9	2.47	122.76	113.69	8	2
3	B	400	PX4	C1-C2-N1	2.47	123.76	115.82	15	2
3	C	317	PX4	C8-C7-C6	2.47	117.55	111.78	4	3
3	A	625	PX4	O5-C9-O6	2.47	129.81	123.63	1	1
3	C	309	PX4	O8-C23-C24	2.47	114.12	123.78	1	1
3	C	309	PX4	O7-C7-C6	2.47	117.21	108.34	13	1
3	A	603	PX4	O7-C7-C8	2.47	117.20	108.34	6	4
3	A	613	PX4	C11-C10-C9	2.47	122.74	113.69	7	1
3	A	615	PX4	O7-C7-C6	2.47	117.20	108.34	11	2
3	C	367	PX4	O5-C9-C10	2.47	104.31	111.83	4	2
3	C	366	PX4	O5-C8-C7	2.47	115.51	108.40	4	1
3	B	306	PX4	O5-C9-O6	2.47	129.80	123.63	3	1
3	C	342	PX4	C5-N1-C3	2.47	102.50	108.98	2	2
3	A	645	PX4	O5-C9-O6	2.46	129.79	123.63	11	2
3	B	304	PX4	O5-C9-O6	2.46	129.79	123.63	3	1
3	B	322	PX4	C26-C25-C24	2.46	104.07	113.13	13	1
3	B	328	PX4	O5-C9-O6	2.47	129.79	123.63	12	2
3	C	316	PX4	O7-C7-C8	2.47	117.19	108.34	5	2
3	C	354	PX4	C4-N1-C3	2.47	102.50	108.98	10	2
3	B	318	PX4	O7-C23-C24	2.46	106.15	111.48	6	1
3	B	357	PX4	C8-O5-C9	2.46	108.11	117.12	13	1
3	C	366	PX4	C11-C10-C9	2.46	122.72	113.69	10	2
3	B	319	PX4	P1-O3-C1	2.46	132.98	121.26	6	1
3	A	627	PX4	C8-C7-C6	2.46	106.05	111.78	15	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	367	PX4	C1-C2-N1	2.46	123.72	115.82	4	1
3	B	381	PX4	C8-O5-C9	2.46	108.13	117.12	3	2
3	B	383	PX4	C5-N1-C3	2.46	115.44	108.98	2	2
3	B	390	PX4	O6-C9-C10	2.46	133.41	123.78	13	1
3	C	311	PX4	O7-C7-C6	2.46	117.17	108.34	3	2
3	A	629	PX4	C4-N1-C2	2.46	119.69	109.91	7	1
3	A	627	PX4	P1-O3-C1	2.46	109.55	121.26	2	1
3	C	338	PX4	O7-C23-O8	2.46	129.45	123.70	4	2
3	C	365	PX4	C5-N1-C4	2.46	102.52	108.98	1	4
3	B	311	PX4	C1-C2-N1	2.46	123.71	115.82	15	3
3	B	380	PX4	C4-N1-C3	2.46	102.52	108.98	11	1
3	A	627	PX4	O1-P1-O2	2.45	123.86	112.44	10	1
3	A	639	PX4	O7-C7-C6	2.45	117.15	108.34	3	2
3	A	648	PX4	C25-C24-C23	2.46	104.70	113.69	5	2
3	B	312	PX4	C1-C2-N1	2.46	123.70	115.82	12	1
3	B	315	PX4	C4-N1-C2	2.46	119.67	109.91	8	1
3	C	308	PX4	C5-N1-C3	2.46	102.52	108.98	5	2
3	C	323	PX4	C1-C2-N1	2.46	123.70	115.82	1	1
3	B	327	PX4	O5-C9-C10	2.45	104.35	111.83	10	2
3	B	367	PX4	C4-N1-C3	2.45	115.42	108.98	10	1
3	B	376	PX4	C34-C33-C32	2.45	101.97	114.37	4	1
3	B	385	PX4	O7-C7-C8	2.45	117.14	108.34	12	2
3	C	340	PX4	O5-C8-C7	2.45	115.47	108.40	6	1
3	B	347	PX4	O5-C9-O6	2.45	129.76	123.63	5	1
3	B	357	PX4	P1-O3-C1	2.45	109.58	121.26	15	2
3	C	338	PX4	O5-C9-O6	2.45	129.76	123.63	4	1
3	C	342	PX4	C19-C18-C17	2.45	101.97	114.37	11	1
3	A	605	PX4	O3-C1-C2	2.45	97.85	109.65	2	1
3	B	349	PX4	C8-C7-C6	2.45	117.50	111.78	15	1
3	B	353	PX4	C4-N1-C3	2.45	115.41	108.98	5	2
3	C	310	PX4	O7-C23-C24	2.45	116.78	111.48	11	1
3	C	314	PX4	C25-C24-C23	2.45	122.67	113.69	15	1
3	C	315	PX4	O1-P1-O2	2.45	123.84	112.44	2	1
3	A	610	PX4	O5-C9-O6	2.45	129.75	123.63	12	4
3	B	359	PX4	O7-C7-C8	2.45	117.13	108.34	2	1
3	A	634	PX4	O7-C7-C8	2.45	117.12	108.34	7	2
3	A	640	PX4	O1-P1-O3	2.45	118.66	107.57	4	1
3	B	311	PX4	C13-C12-C11	2.45	126.73	114.37	12	1
3	B	329	PX4	C26-C25-C24	2.45	104.14	113.13	12	1
3	A	639	PX4	C31-C30-C29	2.45	102.01	114.37	10	1
3	B	305	PX4	C1-C2-N1	2.45	123.67	115.82	11	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	351	PX4	O5-C9-O6	2.44	129.74	123.63	15	1
3	B	380	PX4	C11-C10-C9	2.44	104.74	113.69	12	2
3	A	604	PX4	O7-C23-O8	2.44	129.42	123.70	4	1
3	B	357	PX4	C5-N1-C4	2.44	102.56	108.98	12	1
3	C	312	PX4	C5-N1-C4	2.44	115.39	108.98	7	2
3	A	634	PX4	C4-N1-C3	2.44	102.56	108.98	7	2
3	A	639	PX4	O5-C9-O6	2.44	129.73	123.63	15	1
3	B	316	PX4	O7-C23-C24	2.44	106.20	111.48	6	1
3	B	364	PX4	C5-N1-C3	2.44	102.56	108.98	8	2
3	C	312	PX4	C25-C24-C23	2.44	104.75	113.69	3	1
3	B	381	PX4	P1-O4-C6	2.44	135.33	121.35	10	1
3	C	314	PX4	O5-C9-O6	2.44	129.73	123.63	8	2
3	B	308	PX4	O8-C23-C24	2.44	133.32	123.78	4	1
3	C	330	PX4	C5-N1-C3	2.44	102.56	108.98	13	1
3	C	359	PX4	C13-C12-C11	2.44	102.03	114.37	4	1
3	A	615	PX4	O7-C23-C24	2.44	106.21	111.48	9	1
3	B	346	PX4	C4-N1-C3	2.44	102.57	108.98	13	1
3	A	611	PX4	O1-P1-O2	2.44	123.78	112.44	8	1
3	A	636	PX4	O5-C9-C10	2.44	104.40	111.83	2	3
3	B	348	PX4	O7-C7-C6	2.44	117.09	108.34	2	2
3	B	384	PX4	C1-C2-N1	2.44	123.65	115.82	10	2
3	C	358	PX4	O7-C23-O8	2.44	129.40	123.70	9	2
3	A	642	PX4	C1-C2-N1	2.43	123.64	115.82	12	2
3	B	304	PX4	C25-C24-C23	2.44	104.77	113.69	1	3
3	B	338	PX4	C8-C7-C6	2.44	117.46	111.78	11	1
3	B	363	PX4	O7-C7-C8	2.44	117.08	108.34	4	1
3	C	327	PX4	O7-C23-C24	2.44	106.21	111.48	2	2
3	A	630	PX4	O7-C7-C8	2.43	117.07	108.34	10	1
3	A	644	PX4	C3-N1-C2	2.43	119.58	109.91	1	2
3	B	332	PX4	C26-C25-C24	2.43	104.18	113.13	10	1
3	C	321	PX4	O6-C9-C10	2.43	114.26	123.78	11	1
3	C	324	PX4	C15-C14-C13	2.43	102.06	114.37	2	1
3	C	370	PX4	C11-C10-C9	2.43	104.77	113.69	2	2
3	C	353	PX4	O7-C23-C24	2.43	106.22	111.48	2	3
3	C	358	PX4	O5-C9-C10	2.43	104.42	111.83	10	1
3	A	601	PX4	C5-N1-C3	2.43	102.59	108.98	8	2
3	A	605	PX4	C25-C24-C23	2.43	104.79	113.69	12	2
3	A	614	PX4	C25-C24-C23	2.43	104.78	113.69	9	1
3	B	333	PX4	C11-C10-C9	2.43	104.79	113.69	14	2
3	B	400	PX4	O7-C7-C8	2.43	99.63	108.34	8	1
3	A	616	PX4	C25-C24-C23	2.43	122.59	113.69	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	317	PX4	C8-O5-C9	2.43	108.25	117.12	10	2
3	B	345	PX4	C12-C11-C10	2.43	104.21	113.13	14	1
3	C	302	PX4	O5-C8-C7	2.43	115.39	108.40	3	3
3	C	334	PX4	C31-C30-C29	2.43	102.10	114.37	14	1
3	A	602	PX4	C3-N1-C2	2.42	119.55	109.91	6	1
3	A	635	PX4	P1-O4-C6	2.43	107.45	121.35	15	1
3	C	370	PX4	O7-C7-C8	2.43	117.05	108.34	8	1
3	A	601	PX4	O5-C9-O6	2.42	129.69	123.63	11	2
3	B	322	PX4	O7-C23-O8	2.42	129.37	123.70	14	2
3	C	320	PX4	O7-C23-O8	2.42	129.37	123.70	8	2
3	C	330	PX4	O7-C7-C8	2.42	117.04	108.34	10	1
3	C	333	PX4	O7-C7-C6	2.42	117.04	108.34	13	1
3	C	368	PX4	C25-C24-C23	2.43	122.58	113.69	14	2
3	C	368	PX4	O8-C23-C24	2.42	133.27	123.78	8	1
3	A	633	PX4	C11-C10-C9	2.42	104.81	113.69	12	1
3	A	647	PX4	C5-N1-C3	2.42	102.61	108.98	8	1
3	B	354	PX4	O7-C7-C6	2.42	99.65	108.34	14	2
3	C	314	PX4	C3-N1-C2	2.42	100.28	109.91	15	1
3	C	366	PX4	O7-C23-C24	2.42	106.24	111.48	4	7
3	C	368	PX4	C12-C11-C10	2.42	104.22	113.13	4	1
3	B	310	PX4	C25-C24-C23	2.42	122.56	113.69	15	1
3	B	359	PX4	C5-N1-C4	2.42	115.33	108.98	6	3
3	C	306	PX4	O7-C7-C6	2.42	117.03	108.34	5	1
3	A	612	PX4	C4-N1-C3	2.42	115.33	108.98	3	1
3	C	308	PX4	C25-C24-C23	2.42	104.82	113.69	15	1
3	B	357	PX4	O5-C9-O6	2.42	129.68	123.63	13	2
3	B	363	PX4	O3-P1-O2	2.42	118.53	108.94	6	1
3	C	337	PX4	C5-N1-C2	2.42	119.53	109.91	8	1
3	C	345	PX4	O5-C9-O6	2.42	129.68	123.63	6	1
3	C	347	PX4	O7-C7-C8	2.42	117.02	108.34	10	2
3	B	337	PX4	C12-C11-C10	2.42	104.25	113.13	8	2
3	B	384	PX4	O3-P1-O2	2.42	99.36	108.94	7	1
3	C	312	PX4	O5-C9-O6	2.42	129.67	123.63	8	2
3	C	336	PX4	O5-C9-C10	2.41	104.47	111.83	3	1
3	C	367	PX4	O7-C23-O8	2.42	129.35	123.70	10	1
3	B	315	PX4	C4-N1-C3	2.41	115.31	108.98	1	2
3	B	325	PX4	P1-O3-C1	2.41	109.77	121.26	8	1
3	C	311	PX4	C7-O7-C23	2.41	112.02	117.80	3	1
3	A	640	PX4	C8-C7-C6	2.41	117.41	111.78	8	1
3	A	643	PX4	O4-P1-O2	2.41	118.49	108.94	15	1
3	B	319	PX4	O5-C9-O6	2.41	129.66	123.63	12	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	325	PX4	O7-C23-C24	2.41	106.27	111.48	6	3
3	C	317	PX4	O5-C9-C10	2.41	104.48	111.83	15	2
3	C	348	PX4	C8-C7-C6	2.41	117.41	111.78	3	3
3	B	349	PX4	C25-C24-C23	2.41	104.86	113.69	9	1
3	A	605	PX4	C26-C25-C24	2.41	121.97	113.13	7	1
3	B	383	PX4	C11-C10-C9	2.41	104.87	113.69	7	2
3	A	625	PX4	C25-C24-C23	2.41	122.52	113.69	2	1
3	C	304	PX4	O7-C7-C8	2.41	116.98	108.34	13	2
3	C	368	PX4	C8-O5-C9	2.41	108.31	117.12	2	2
3	B	360	PX4	O5-C9-C10	2.41	104.50	111.83	10	2
3	C	343	PX4	O7-C23-O8	2.41	129.33	123.70	1	1
3	B	371	PX4	C12-C11-C10	2.41	121.97	113.13	2	1
3	B	315	PX4	O5-C9-O6	2.41	129.64	123.63	4	1
3	C	310	PX4	C12-C11-C10	2.40	121.96	113.13	11	1
3	A	624	PX4	C14-C13-C12	2.40	102.22	114.37	10	1
3	A	647	PX4	C12-C11-C10	2.40	104.30	113.13	14	2
3	C	329	PX4	C29-C28-C27	2.40	102.21	114.37	12	1
3	C	359	PX4	C4-N1-C2	2.40	119.46	109.91	8	1
3	C	362	PX4	C5-N1-C4	2.40	115.29	108.98	10	3
3	C	302	PX4	O7-C23-C24	2.40	106.28	111.48	6	2
3	C	309	PX4	O6-C9-C10	2.40	114.39	123.78	5	1
3	C	330	PX4	C1-C2-N1	2.40	123.53	115.82	2	2
3	C	343	PX4	O1-P1-O2	2.40	123.62	112.44	12	3
3	C	346	PX4	C1-C2-N1	2.40	123.53	115.82	3	2
3	C	363	PX4	C4-N1-C3	2.40	102.67	108.98	1	2
3	B	301	PX4	O7-C23-O8	2.40	129.32	123.70	10	3
3	B	304	PX4	C12-C11-C10	2.40	104.31	113.13	2	2
3	B	358	PX4	C8-C7-C6	2.40	106.19	111.78	12	2
3	B	390	PX4	C1-C2-N1	2.40	123.53	115.82	2	1
3	A	644	PX4	O7-C23-O8	2.40	129.31	123.70	15	2
3	B	336	PX4	C1-C2-N1	2.40	123.52	115.82	7	1
3	B	339	PX4	C5-N1-C3	2.40	115.27	108.98	13	1
3	B	364	PX4	C4-N1-C3	2.40	102.68	108.98	4	1
3	B	374	PX4	C26-C25-C24	2.40	104.32	113.13	1	1
3	C	342	PX4	O7-C23-O8	2.40	129.31	123.70	10	1
3	C	344	PX4	O5-C9-O6	2.40	129.63	123.63	9	1
3	B	370	PX4	O7-C7-C6	2.40	116.94	108.34	12	1
3	C	331	PX4	C5-N1-C3	2.40	102.68	108.98	13	2
3	B	310	PX4	O5-C9-C10	2.39	104.53	111.83	7	1
3	B	384	PX4	C5-N1-C3	2.39	102.69	108.98	4	1
3	B	394	PX4	C31-C30-C29	2.39	102.26	114.37	3	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	C	344	PX4	C5-N1-C4	2.39	115.27	108.98	3	2
3	C	308	PX4	C8-C7-C6	2.39	117.37	111.78	1	2
3	C	355	PX4	C4-N1-C3	2.39	102.69	108.98	7	5
3	C	361	PX4	C8-C7-C6	2.39	117.37	111.78	3	3
3	A	605	PX4	C12-C11-C10	2.39	104.33	113.13	14	1
3	A	632	PX4	C12-C11-C10	2.39	104.33	113.13	8	2
3	B	315	PX4	O5-C9-C10	2.39	104.54	111.83	15	1
3	B	384	PX4	O3-C1-C2	2.39	121.16	109.65	8	1
3	C	326	PX4	O7-C7-C8	2.39	116.92	108.34	9	1
3	C	341	PX4	C4-N1-C2	2.39	119.42	109.91	13	1
3	A	620	PX4	O7-C7-C8	2.39	116.92	108.34	8	1
3	C	350	PX4	P1-O3-C1	2.39	132.64	121.26	2	1
3	B	340	PX4	O5-C9-O6	2.39	129.60	123.63	11	1
3	B	353	PX4	O1-P1-O2	2.39	123.56	112.44	13	1
3	B	360	PX4	O7-C7-C8	2.39	116.92	108.34	8	1
3	B	306	PX4	O5-C9-C10	2.39	104.55	111.83	3	3
3	B	381	PX4	P1-O3-C1	2.39	132.63	121.26	13	1
3	B	363	PX4	O5-C9-O6	2.39	129.60	123.63	13	2
3	B	395	PX4	C26-C25-C24	2.39	121.90	113.13	3	1
3	C	360	PX4	C5-N1-C3	2.39	102.70	108.98	6	5
3	C	364	PX4	C25-C24-C23	2.39	122.45	113.69	4	1
3	C	343	PX4	C12-C11-C10	2.39	121.90	113.13	8	2
3	C	365	PX4	O1-P1-O4	2.39	118.39	107.57	12	1
3	A	619	PX4	C25-C24-C23	2.39	104.95	113.69	6	1
3	A	644	PX4	C26-C25-C24	2.39	104.36	113.13	2	1
3	B	315	PX4	C1-C2-N1	2.39	123.48	115.82	1	3
3	B	343	PX4	C5-N1-C4	2.39	102.71	108.98	2	2
3	B	354	PX4	C7-O7-C23	2.39	123.51	117.80	15	3
3	B	390	PX4	C7-O7-C23	2.39	112.08	117.80	11	2
3	B	386	PX4	O7-C23-O8	2.39	129.28	123.70	7	1
3	C	325	PX4	C8-C7-C6	2.38	106.23	111.78	6	3
3	C	360	PX4	O5-C9-C10	2.38	104.57	111.83	11	2
3	A	609	PX4	C5-N1-C3	2.38	115.23	108.98	10	3
3	A	620	PX4	C5-N1-C2	2.38	119.38	109.91	7	2
3	A	616	PX4	O5-C8-C7	2.38	115.26	108.40	6	4
3	A	625	PX4	O7-C23-O8	2.38	129.27	123.70	11	1
3	A	633	PX4	C8-O5-C9	2.38	125.83	117.12	4	1
3	B	312	PX4	O1-P1-O4	2.38	118.36	107.57	4	1
3	C	364	PX4	C20-C19-C18	2.38	102.33	114.37	11	1
3	A	637	PX4	O7-C23-O8	2.38	129.27	123.70	14	1
3	B	320	PX4	P1-O3-C1	2.38	132.59	121.26	7	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	610	PX4	C11-C10-C9	2.38	122.41	113.69	7	1
3	B	338	PX4	O5-C9-O6	2.38	129.58	123.63	11	3
3	B	355	PX4	O7-C23-O8	2.38	129.27	123.70	15	2
3	C	309	PX4	O7-C23-C24	2.38	106.33	111.48	11	1
3	C	313	PX4	O7-C7-C6	2.38	116.88	108.34	4	1
3	C	346	PX4	C8-O5-C9	2.38	108.42	117.12	2	2
3	B	303	PX4	O1-P1-O3	2.38	118.34	107.57	14	1
3	A	607	PX4	C1-C2-N1	2.38	123.45	115.82	1	2
3	A	641	PX4	C5-N1-C4	2.38	115.22	108.98	2	1
3	B	343	PX4	O7-C23-O8	2.38	129.26	123.70	11	2
3	B	350	PX4	O7-C23-O8	2.38	129.26	123.70	10	3
3	B	359	PX4	C8-O5-C9	2.38	108.43	117.12	4	3
3	B	354	PX4	C8-C7-C6	2.38	106.25	111.78	6	2
3	B	354	PX4	C8-O5-C9	2.38	125.80	117.12	6	2
3	B	392	PX4	O5-C9-O6	2.38	129.57	123.63	11	3
3	C	321	PX4	O3-C1-C2	2.38	98.22	109.65	7	1
3	C	328	PX4	P1-O3-C1	2.37	109.96	121.26	8	1
3	C	339	PX4	C33-C32-C31	2.38	102.36	114.37	3	2
3	C	343	PX4	O7-C7-C8	2.38	116.87	108.34	9	2
3	C	307	PX4	O5-C9-C10	2.37	104.59	111.83	11	1
3	C	354	PX4	C12-C11-C10	2.38	104.40	113.13	14	1
3	A	601	PX4	C25-C24-C23	2.37	105.00	113.69	8	3
3	A	612	PX4	O5-C9-C10	2.37	104.60	111.83	4	3
3	A	638	PX4	O5-C9-O6	2.37	129.56	123.63	3	1
3	B	313	PX4	C5-N1-C3	2.37	102.74	108.98	8	2
3	A	635	PX4	O1-P1-O2	2.37	123.48	112.44	3	1
3	A	639	PX4	O8-C23-C24	2.37	133.06	123.78	12	1
3	A	640	PX4	C28-C27-C26	2.37	102.38	114.37	8	1
3	B	326	PX4	O7-C7-C8	2.37	116.85	108.34	3	2
3	B	368	PX4	C8-C7-C6	2.37	106.25	111.78	4	2
3	B	393	PX4	C5-N1-C3	2.37	115.21	108.98	2	3
3	A	645	PX4	C12-C11-C10	2.37	121.83	113.13	3	2
3	B	301	PX4	C5-N1-C4	2.37	102.75	108.98	7	1
3	B	318	PX4	C20-C19-C18	2.37	102.39	114.37	1	1
3	C	306	PX4	C5-N1-C4	2.37	102.75	108.98	2	3
3	C	324	PX4	C4-N1-C3	2.37	102.75	108.98	13	3
3	A	604	PX4	C16-C15-C14	2.37	102.40	114.37	1	1
3	B	318	PX4	O5-C8-C7	2.37	115.22	108.40	8	2
3	B	333	PX4	O5-C9-C10	2.37	104.61	111.83	3	2
3	B	371	PX4	C5-N1-C4	2.37	102.75	108.98	7	2
3	C	314	PX4	O7-C23-O8	2.37	129.24	123.70	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	C	345	PX4	O5-C8-C7	2.37	115.22	108.40	13	4
3	A	626	PX4	C8-C7-C6	2.37	117.31	111.78	4	1
3	B	350	PX4	C15-C14-C13	2.37	102.40	114.37	11	1
3	B	377	PX4	C5-N1-C4	2.37	102.76	108.98	1	1
3	B	380	PX4	O5-C9-C10	2.37	104.62	111.83	3	3
3	C	331	PX4	O1-P1-O2	2.37	123.46	112.44	14	1
3	C	365	PX4	O6-C9-C10	2.37	133.04	123.78	5	1
3	B	366	PX4	C4-N1-C2	2.37	100.51	109.91	11	1
3	C	351	PX4	O1-P1-O2	2.37	123.45	112.44	13	1
3	C	367	PX4	C7-O7-C23	2.37	112.14	117.80	7	4
3	B	342	PX4	C26-C25-C24	2.36	104.44	113.13	1	1
3	A	603	PX4	O7-C7-C6	2.36	116.82	108.34	15	1
3	A	641	PX4	C8-O5-C9	2.36	108.48	117.12	3	1
3	B	302	PX4	O5-C9-C10	2.36	104.63	111.83	4	1
3	B	306	PX4	C13-C12-C11	2.36	102.42	114.37	1	2
3	B	354	PX4	O7-C7-C8	2.36	116.82	108.34	5	2
3	B	392	PX4	C12-C11-C10	2.36	121.81	113.13	3	2
3	B	363	PX4	C8-O5-C9	2.36	108.48	117.12	13	3
3	B	302	PX4	C25-C24-C23	2.36	122.35	113.69	4	1
3	B	316	PX4	O7-C7-C8	2.36	116.82	108.34	4	2
3	B	385	PX4	C4-N1-C3	2.36	102.77	108.98	6	2
3	B	395	PX4	C5-N1-C3	2.36	102.77	108.98	8	3
3	C	338	PX4	C1-C2-N1	2.36	123.41	115.82	8	2
3	B	318	PX4	C11-C10-C9	2.36	105.04	113.69	14	1
3	B	345	PX4	C8-O5-C9	2.36	125.75	117.12	15	2
3	C	303	PX4	O5-C9-O6	2.36	129.53	123.63	10	2
3	C	362	PX4	O5-C9-C10	2.36	104.64	111.83	8	1
3	B	367	PX4	C5-N1-C3	2.36	102.78	108.98	7	4
3	C	336	PX4	C4-N1-C3	2.36	115.17	108.98	7	1
3	C	361	PX4	O7-C23-C24	2.36	106.38	111.48	15	1
3	B	314	PX4	O1-P1-O4	2.36	118.26	107.57	15	2
3	B	314	PX4	C26-C25-C24	2.36	121.79	113.13	15	1
3	B	375	PX4	C5-N1-C3	2.36	102.78	108.98	12	1
3	B	397	PX4	O5-C9-O6	2.36	129.53	123.63	5	2
3	A	631	PX4	O5-C8-C7	2.36	115.19	108.40	14	4
3	B	337	PX4	C26-C25-C24	2.36	121.79	113.13	15	1
3	B	393	PX4	O7-C23-O8	2.36	129.22	123.70	13	3
3	B	320	PX4	C14-C13-C12	2.35	102.46	114.37	6	1
3	B	335	PX4	C1-C2-N1	2.36	123.38	115.82	5	2
3	B	356	PX4	O5-C9-O6	2.36	129.52	123.63	15	1
3	C	333	PX4	C26-C25-C24	2.35	121.78	113.13	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	301	PX4	C5-N1-C3	2.35	102.79	108.98	14	2
3	B	328	PX4	C5-N1-C4	2.35	102.79	108.98	1	2
3	B	336	PX4	C5-N1-C3	2.35	102.79	108.98	4	2
3	A	619	PX4	O5-C9-O6	2.35	129.51	123.63	13	2
3	B	385	PX4	C26-C25-C24	2.35	104.48	113.13	2	1
3	B	352	PX4	O1-P1-O2	2.35	123.39	112.44	5	3
3	B	368	PX4	C31-C30-C29	2.35	102.49	114.37	1	1
3	C	325	PX4	C11-C10-C9	2.35	105.08	113.69	4	1
3	C	342	PX4	P1-O3-C1	2.35	132.45	121.26	12	2
3	C	361	PX4	O5-C9-O6	2.35	129.51	123.63	15	2
3	B	342	PX4	O7-C23-O8	2.35	129.20	123.70	5	2
3	B	342	PX4	C4-N1-C3	2.35	102.80	108.98	4	4
3	B	388	PX4	O6-C9-C10	2.35	114.59	123.78	14	1
3	B	397	PX4	C8-C7-C6	2.35	106.31	111.78	2	2
3	C	339	PX4	O7-C23-C24	2.35	106.40	111.48	11	4
3	C	364	PX4	C4-N1-C3	2.35	102.80	108.98	14	2
3	A	645	PX4	C25-C24-C23	2.35	122.30	113.69	15	1
3	B	360	PX4	O5-C9-O6	2.35	129.50	123.63	8	3
3	C	345	PX4	C12-C11-C10	2.35	104.50	113.13	6	2
3	C	303	PX4	C12-C11-C10	2.35	104.50	113.13	10	1
3	C	304	PX4	O5-C9-C10	2.35	104.68	111.83	2	2
3	C	335	PX4	O5-C9-C10	2.35	104.68	111.83	15	2
3	C	346	PX4	C3-N1-C2	2.35	100.58	109.91	8	1
3	C	347	PX4	C4-N1-C3	2.35	115.14	108.98	2	2
3	B	317	PX4	C25-C24-C23	2.35	105.10	113.69	13	1
3	B	326	PX4	C27-C26-C25	2.35	102.51	114.37	3	1
3	B	331	PX4	C25-C24-C23	2.35	122.29	113.69	5	2
3	B	363	PX4	C4-N1-C3	2.35	102.81	108.98	6	1
3	B	390	PX4	C5-N1-C3	2.35	102.81	108.98	11	1
3	C	340	PX4	O7-C7-C8	2.35	116.76	108.34	6	2
3	A	603	PX4	C5-N1-C4	2.34	115.13	108.98	2	2
3	B	334	PX4	O7-C7-C8	2.34	116.76	108.34	6	1
3	A	605	PX4	C15-C14-C13	2.34	102.53	114.37	2	1
3	A	609	PX4	C4-N1-C3	2.34	115.13	108.98	9	3
3	A	609	PX4	C5-N1-C4	2.34	102.82	108.98	10	2
3	B	318	PX4	C1-C2-N1	2.34	123.34	115.82	4	1
3	C	327	PX4	C5-N1-C3	2.34	102.82	108.98	4	1
3	A	630	PX4	C11-C10-C9	2.34	122.27	113.69	2	1
3	B	337	PX4	C5-N1-C2	2.34	100.61	109.91	8	1
3	B	380	PX4	O6-C9-C10	2.34	132.94	123.78	3	3
3	C	362	PX4	C8-O5-C9	2.34	108.56	117.12	13	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	631	PX4	C5-N1-C4	2.34	115.12	108.98	6	2
3	A	633	PX4	C5-N1-C4	2.34	102.83	108.98	9	1
3	B	336	PX4	C8-C7-C6	2.34	117.24	111.78	4	2
3	B	365	PX4	O5-C9-C10	2.34	104.70	111.83	5	1
3	C	334	PX4	O3-C1-C2	2.34	120.91	109.65	15	1
3	A	622	PX4	C19-C18-C17	2.33	102.57	114.37	7	1
3	B	313	PX4	O5-C9-O6	2.33	129.47	123.63	6	2
3	B	334	PX4	O6-C9-C10	2.33	132.91	123.78	9	1
3	B	347	PX4	O7-C23-O8	2.33	129.16	123.70	10	1
3	C	322	PX4	C5-N1-C4	2.33	102.84	108.98	15	3
3	C	354	PX4	O7-C23-O8	2.33	129.16	123.70	13	1
3	B	396	PX4	C11-C10-C9	2.33	122.25	113.69	11	1
3	A	626	PX4	C26-C25-C24	2.33	104.56	113.13	10	1
3	B	308	PX4	C25-C24-C23	2.33	105.15	113.69	10	1
3	B	310	PX4	P1-O4-C6	2.33	134.71	121.35	8	2
3	B	344	PX4	C11-C10-C9	2.33	105.15	113.69	11	1
3	B	370	PX4	O3-C1-C2	2.33	120.87	109.65	8	1
3	B	375	PX4	C11-C10-C9	2.33	122.24	113.69	14	1
3	C	305	PX4	O7-C23-O8	2.33	129.16	123.70	6	1
3	C	322	PX4	O7-C7-C6	2.33	116.71	108.34	3	1
3	B	323	PX4	C8-O5-C9	2.33	108.60	117.12	2	1
3	B	381	PX4	C8-C7-C6	2.33	106.35	111.78	3	2
3	C	320	PX4	C1-C2-N1	2.33	123.30	115.82	12	2
3	B	381	PX4	O5-C9-C10	2.33	104.73	111.83	3	1
3	C	335	PX4	C4-N1-C3	2.33	102.86	108.98	12	1
3	C	335	PX4	C5-N1-C2	2.33	119.17	109.91	14	1
3	C	338	PX4	C28-C27-C26	2.33	102.59	114.37	2	1
3	B	307	PX4	P1-O3-C1	2.33	132.34	121.26	6	1
3	C	310	PX4	C30-C29-C28	2.33	102.60	114.37	11	1
3	A	611	PX4	C5-N1-C3	2.33	115.09	108.98	12	1
3	A	616	PX4	C8-O5-C9	2.33	108.62	117.12	14	1
3	A	629	PX4	C25-C24-C23	2.33	105.17	113.69	10	1
3	B	338	PX4	O3-C1-C2	2.33	120.84	109.65	3	1
3	B	345	PX4	C33-C32-C31	2.33	126.13	114.37	9	1
3	B	399	PX4	C1-C2-N1	2.33	123.29	115.82	15	1
3	C	367	PX4	O3-P1-O2	2.33	99.72	108.94	6	1
3	B	372	PX4	O7-C23-O8	2.32	129.14	123.70	14	1
3	B	374	PX4	O7-C23-O8	2.32	129.14	123.70	8	2
3	B	377	PX4	C34-C33-C32	2.32	126.12	114.37	6	1
3	B	378	PX4	C8-O5-C9	2.33	108.62	117.12	11	2
3	B	387	PX4	C5-N1-C4	2.32	102.87	108.98	10	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	C	357	PX4	C1-C2-N1	2.32	123.28	115.82	11	2
3	C	362	PX4	C4-N1-C2	2.33	119.15	109.91	6	1
3	A	641	PX4	O7-C23-O8	2.32	129.14	123.70	1	2
3	B	304	PX4	C5-N1-C4	2.32	115.08	108.98	4	1
3	B	306	PX4	O7-C7-C6	2.32	116.68	108.34	11	1
3	B	328	PX4	O3-C1-C2	2.32	120.83	109.65	14	3
3	B	336	PX4	O1-P1-O2	2.32	123.25	112.44	10	1
3	C	318	PX4	C12-C11-C10	2.32	104.59	113.13	12	1
3	C	338	PX4	O5-C9-C10	2.32	104.75	111.83	4	3
3	B	390	PX4	C4-N1-C3	2.32	115.07	108.98	11	2
3	C	327	PX4	O7-C23-O8	2.32	129.13	123.70	3	3
3	A	635	PX4	O1-P1-O4	2.32	118.08	107.57	15	1
3	A	648	PX4	O7-C23-O8	2.32	129.13	123.70	12	1
3	B	319	PX4	O7-C23-O8	2.32	129.13	123.70	14	2
3	B	321	PX4	C25-C24-C23	2.32	122.19	113.69	5	1
3	B	400	PX4	C8-C7-C6	2.32	117.20	111.78	8	2
3	C	330	PX4	O8-C23-C24	2.32	132.86	123.78	14	1
3	C	333	PX4	C11-C10-C9	2.32	105.19	113.69	15	1
3	C	365	PX4	C12-C11-C10	2.32	104.60	113.13	3	2
3	B	352	PX4	O5-C9-C10	2.32	104.76	111.83	6	1
3	B	354	PX4	O5-C9-C10	2.32	104.76	111.83	10	2
3	B	358	PX4	C1-C2-N1	2.32	123.27	115.82	14	1
3	C	302	PX4	C11-C10-C9	2.32	122.19	113.69	5	1
3	A	615	PX4	O5-C9-O6	2.32	129.42	123.63	3	1
3	A	633	PX4	C26-C25-C24	2.32	121.64	113.13	15	1
3	A	640	PX4	C5-N1-C4	2.32	115.06	108.98	13	1
3	B	308	PX4	C3-N1-C2	2.32	100.70	109.91	6	1
3	B	388	PX4	C11-C10-C9	2.32	105.20	113.69	3	1
3	C	305	PX4	O5-C9-C10	2.32	104.77	111.83	3	4
3	C	310	PX4	C1-C2-N1	2.32	123.26	115.82	13	1
3	C	354	PX4	C27-C26-C25	2.32	102.65	114.37	3	1
3	A	637	PX4	C5-N1-C2	2.32	100.70	109.91	9	2
3	C	314	PX4	C5-N1-C3	2.32	115.06	108.98	9	1
3	B	325	PX4	O5-C9-O6	2.32	129.42	123.63	13	1
3	A	631	PX4	O7-C23-O8	2.31	129.12	123.70	8	1
3	A	641	PX4	C30-C29-C28	2.31	102.67	114.37	5	1
3	C	318	PX4	C5-N1-C2	2.31	119.11	109.91	8	1
3	B	310	PX4	O7-C7-C6	2.31	100.04	108.34	8	1
3	C	343	PX4	C4-N1-C3	2.31	115.05	108.98	14	1
3	C	344	PX4	O5-C9-C10	2.31	104.78	111.83	11	4
3	A	608	PX4	C4-N1-C3	2.31	102.90	108.98	4	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	617	PX4	C8-C7-C6	2.31	117.17	111.78	8	1
3	A	642	PX4	C5-N1-C4	2.31	115.05	108.98	11	2
3	A	643	PX4	C5-N1-C3	2.31	115.05	108.98	1	4
3	B	322	PX4	O7-C7-C6	2.31	116.64	108.34	6	2
3	B	312	PX4	O3-P1-O2	2.31	118.09	108.94	5	1
3	B	354	PX4	P1-O3-C1	2.31	132.26	121.26	1	1
3	B	375	PX4	C8-C7-C6	2.31	106.39	111.78	2	2
3	A	635	PX4	C33-C32-C31	2.31	102.70	114.37	1	1
3	B	330	PX4	C4-N1-C3	2.31	115.04	108.98	4	1
3	B	346	PX4	C15-C14-C13	2.31	102.70	114.37	13	1
3	B	387	PX4	C5-N1-C3	2.31	115.04	108.98	7	1
3	B	397	PX4	O1-P1-O2	2.31	123.19	112.44	11	1
3	C	322	PX4	C17-C16-C15	2.31	102.70	114.37	6	1
3	C	329	PX4	P1-O3-C1	2.31	110.27	121.26	11	1
3	C	364	PX4	C8-O5-C9	2.31	108.68	117.12	3	1
3	A	615	PX4	C5-N1-C2	2.31	119.08	109.91	8	1
3	B	349	PX4	C11-C10-C9	2.31	105.24	113.69	12	1
3	C	366	PX4	C4-N1-C3	2.31	102.91	108.98	8	1
3	B	353	PX4	C11-C10-C9	2.31	105.24	113.69	5	1
3	C	305	PX4	C4-N1-C3	2.31	102.92	108.98	7	2
3	C	348	PX4	O5-C9-C10	2.31	104.80	111.83	11	2
3	A	624	PX4	O1-P1-O4	2.31	118.02	107.57	14	1
3	A	615	PX4	C25-C24-C23	2.30	105.25	113.69	3	1
3	A	616	PX4	C5-N1-C3	2.31	102.92	108.98	13	2
3	B	326	PX4	O7-C23-O8	2.31	118.32	123.70	3	1
3	B	334	PX4	O3-C1-C2	2.31	120.74	109.65	7	1
3	B	363	PX4	C5-N1-C4	2.31	102.92	108.98	3	1
3	B	391	PX4	O7-C7-C6	2.31	116.61	108.34	15	1
3	C	364	PX4	C5-N1-C4	2.31	115.03	108.98	5	2
3	B	366	PX4	C4-N1-C3	2.30	115.03	108.98	5	3
3	A	630	PX4	C4-N1-C3	2.30	102.93	108.98	7	1
3	B	377	PX4	C25-C24-C23	2.30	105.26	113.69	12	1
3	B	385	PX4	C8-C7-C6	2.30	117.15	111.78	13	1
3	A	630	PX4	C25-C24-C23	2.30	105.26	113.69	11	1
3	A	644	PX4	C1-C2-N1	2.30	123.21	115.82	4	2
3	B	369	PX4	O1-P1-O2	2.30	123.15	112.44	7	1
3	C	325	PX4	C4-N1-C2	2.30	119.06	109.91	8	1
3	C	347	PX4	O7-C7-C6	2.30	116.60	108.34	9	1
3	C	356	PX4	O5-C9-C10	2.30	104.82	111.83	6	1
3	C	368	PX4	C8-C7-C6	2.30	117.15	111.78	5	2
3	A	636	PX4	O7-C7-C6	2.30	100.09	108.34	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	305	PX4	C5-N1-C4	2.30	102.94	108.98	8	2
3	B	327	PX4	O7-C23-O8	2.30	129.08	123.70	15	2
3	B	388	PX4	O7-C7-C8	2.30	116.59	108.34	9	1
3	C	302	PX4	C26-C25-C24	2.30	104.68	113.13	10	1
3	C	318	PX4	C4-N1-C3	2.30	102.94	108.98	14	1
3	C	333	PX4	O7-C7-C8	2.30	116.59	108.34	6	2
3	C	336	PX4	O5-C9-O6	2.30	129.38	123.63	7	3
3	A	608	PX4	O5-C9-C10	2.30	104.83	111.83	3	1
3	A	627	PX4	C1-C2-N1	2.30	123.19	115.82	14	1
3	A	640	PX4	C11-C10-C9	2.30	105.28	113.69	12	2
3	A	645	PX4	C8-O5-C9	2.30	108.72	117.12	9	1
3	B	308	PX4	C4-N1-C3	2.30	102.94	108.98	5	1
3	B	335	PX4	O5-C9-O6	2.30	129.37	123.63	11	2
3	C	337	PX4	O3-C1-C2	2.30	98.59	109.65	7	1
3	C	350	PX4	O5-C9-C10	2.30	104.83	111.83	14	2
3	B	309	PX4	C34-C33-C32	2.30	102.76	114.37	3	1
3	B	329	PX4	C8-O5-C9	2.30	108.73	117.12	12	1
3	B	379	PX4	C11-C10-C9	2.30	122.10	113.69	7	2
3	C	311	PX4	C25-C24-C23	2.29	105.28	113.69	2	1
3	C	315	PX4	O3-C1-C2	2.30	120.69	109.65	12	1
3	C	348	PX4	C8-O5-C9	2.30	108.72	117.12	8	1
3	A	607	PX4	C4-N1-C2	2.29	119.02	109.91	14	2
3	A	620	PX4	C34-C33-C32	2.29	102.78	114.37	3	1
3	A	622	PX4	O5-C9-C10	2.29	104.85	111.83	7	1
3	A	642	PX4	O8-C23-C24	2.29	132.75	123.78	12	1
3	B	301	PX4	C4-N1-C2	2.29	100.79	109.91	13	1
3	B	391	PX4	O7-C7-C8	2.29	116.57	108.34	8	1
3	C	323	PX4	C11-C10-C9	2.29	105.29	113.69	12	1
3	B	355	PX4	P1-O3-C1	2.29	132.17	121.26	15	1
3	B	311	PX4	C8-O5-C9	2.29	108.75	117.12	15	3
3	B	323	PX4	C12-C11-C10	2.29	104.71	113.13	8	1
3	B	329	PX4	C25-C24-C23	2.29	122.09	113.69	2	1
3	B	357	PX4	C11-C10-C9	2.29	122.09	113.69	14	2
3	B	370	PX4	O7-C7-C8	2.29	116.57	108.34	11	1
3	A	620	PX4	O7-C7-C6	2.29	100.13	108.34	15	1
3	B	330	PX4	O5-C8-C7	2.29	115.00	108.40	12	3
3	A	618	PX4	C5-N1-C3	2.29	114.99	108.98	13	3
3	B	336	PX4	P1-O4-C6	2.29	134.47	121.35	3	1
3	B	338	PX4	C16-C15-C14	2.29	102.79	114.37	2	1
3	A	642	PX4	O3-C1-C2	2.29	120.66	109.65	7	2
3	B	314	PX4	C12-C11-C10	2.29	121.53	113.13	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	320	PX4	C5-N1-C4	2.29	102.97	108.98	15	1
3	B	351	PX4	C5-N1-C3	2.29	102.96	108.98	6	1
3	B	351	PX4	P1-O4-C6	2.29	108.23	121.35	8	1
3	C	307	PX4	O5-C9-O6	2.29	129.35	123.63	5	1
3	C	318	PX4	C5-N1-C3	2.29	114.99	108.98	6	2
3	C	315	PX4	C1-C2-N1	2.29	123.17	115.82	14	2
3	C	334	PX4	O7-C7-C6	2.29	100.13	108.34	8	1
3	B	320	PX4	C1-C2-N1	2.29	123.16	115.82	8	2
3	B	350	PX4	C8-O5-C9	2.29	108.76	117.12	4	1
3	C	352	PX4	O5-C8-C7	2.29	114.99	108.40	10	2
3	A	615	PX4	P1-O3-C1	2.29	132.14	121.26	3	1
3	A	633	PX4	O7-C23-O8	2.29	129.05	123.70	3	2
3	B	335	PX4	C5-N1-C2	2.29	119.00	109.91	13	1
3	B	364	PX4	C25-C24-C23	2.29	122.07	113.69	7	1
3	B	392	PX4	O1-P1-O4	2.29	117.93	107.57	1	1
3	A	612	PX4	C8-C7-C6	2.28	117.11	111.78	12	2
3	B	356	PX4	C5-N1-C3	2.28	102.97	108.98	10	1
3	B	368	PX4	O5-C9-O6	2.29	129.34	123.63	13	3
3	B	372	PX4	C4-N1-C3	2.28	102.97	108.98	14	1
3	C	319	PX4	O1-P1-O2	2.28	123.07	112.44	11	1
3	C	361	PX4	C26-C25-C24	2.28	121.52	113.13	1	2
3	B	340	PX4	O7-C7-C6	2.28	116.53	108.34	8	1
3	B	341	PX4	C25-C24-C23	2.28	122.06	113.69	15	1
3	B	376	PX4	O7-C7-C8	2.28	116.53	108.34	1	1
3	B	399	PX4	C26-C25-C24	2.28	104.74	113.13	14	2
3	A	612	PX4	C25-C24-C23	2.28	105.33	113.69	2	3
3	A	615	PX4	C1-C2-N1	2.28	123.14	115.82	9	1
3	A	640	PX4	C12-C11-C10	2.28	104.74	113.13	9	1
3	B	319	PX4	C8-C7-C6	2.28	106.47	111.78	6	5
3	B	350	PX4	C4-N1-C3	2.28	102.98	108.98	9	1
3	B	389	PX4	P1-O3-C1	2.28	132.12	121.26	12	1
3	C	340	PX4	O7-C7-C6	2.28	116.53	108.34	5	2
3	C	349	PX4	O5-C9-C10	2.28	104.88	111.83	10	2
3	A	621	PX4	O3-C1-C2	2.28	120.61	109.65	9	1
3	C	328	PX4	O7-C23-O8	2.28	129.03	123.70	5	3
3	C	355	PX4	O5-C9-O6	2.28	129.33	123.63	5	1
3	B	308	PX4	C26-C25-C24	2.28	104.75	113.13	7	2
3	C	355	PX4	O7-C7-C8	2.28	116.52	108.34	5	1
3	A	623	PX4	C1-C2-N1	2.28	123.13	115.82	13	2
3	A	634	PX4	O6-C9-C10	2.28	132.69	123.78	2	1
3	B	302	PX4	C1-C2-N1	2.28	123.13	115.82	8	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	C	304	PX4	O7-C23-C24	2.28	106.55	111.48	12	1
3	B	324	PX4	O7-C7-C8	2.28	116.51	108.34	7	1
3	B	369	PX4	C5-N1-C3	2.28	103.00	108.98	7	1
3	B	395	PX4	C5-N1-C4	2.28	103.00	108.98	3	3
3	B	400	PX4	O5-C9-O6	2.28	129.32	123.63	12	1
3	C	345	PX4	C18-C17-C16	2.28	102.86	114.37	3	1
3	C	362	PX4	O1-P1-O2	2.28	123.03	112.44	3	1
3	B	378	PX4	C8-C7-C6	2.27	117.08	111.78	15	4
3	B	394	PX4	O4-P1-O2	2.27	99.93	108.94	2	1
3	C	311	PX4	O5-C9-C10	2.27	104.90	111.83	13	2
3	C	366	PX4	C5-N1-C3	2.28	103.00	108.98	2	1
3	B	320	PX4	O7-C7-C8	2.27	116.50	108.34	14	1
3	B	326	PX4	C3-N1-C2	2.27	118.95	109.91	1	1
3	C	324	PX4	O5-C9-O6	2.27	129.31	123.63	8	3
3	C	336	PX4	C26-C25-C24	2.27	104.77	113.13	9	1
3	A	627	PX4	O3-C1-C2	2.27	120.58	109.65	1	1
3	A	621	PX4	C12-C11-C10	2.27	121.47	113.13	7	1
3	A	630	PX4	C5-N1-C4	2.27	114.94	108.98	4	1
3	B	395	PX4	C4-N1-C3	2.27	114.94	108.98	14	3
3	C	321	PX4	C4-N1-C2	2.27	118.94	109.91	5	1
3	C	335	PX4	C8-C7-C6	2.27	106.49	111.78	11	3
3	B	335	PX4	O1-P1-O3	2.27	117.86	107.57	11	1
3	C	318	PX4	C4-N1-C2	2.27	100.88	109.91	13	1
3	C	325	PX4	C5-N1-C3	2.27	103.01	108.98	9	1
3	B	303	PX4	C5-N1-C2	2.27	118.93	109.91	15	1
3	B	308	PX4	C8-C7-C6	2.27	106.50	111.78	15	2
3	B	313	PX4	C25-C24-C23	2.27	105.38	113.69	11	1
3	C	359	PX4	O7-C23-O8	2.27	129.01	123.70	13	4
3	A	607	PX4	C26-C25-C24	2.27	121.46	113.13	2	1
3	B	304	PX4	O5-C9-C10	2.27	104.92	111.83	4	2
3	B	318	PX4	O1-P1-O2	2.27	123.00	112.44	6	1
3	B	335	PX4	C4-N1-C3	2.27	103.02	108.98	9	2
3	C	315	PX4	C36-C35-C34	2.27	128.67	113.36	7	1
3	A	601	PX4	C8-C7-C6	2.27	106.50	111.78	4	1
3	B	389	PX4	O1-P1-O2	2.27	122.99	112.44	7	2
3	A	640	PX4	C16-C15-C14	2.27	102.92	114.37	4	1
3	A	645	PX4	O1-P1-O3	2.26	117.83	107.57	12	1
3	B	307	PX4	O5-C9-C10	2.26	104.93	111.83	5	2
3	B	333	PX4	C12-C11-C10	2.26	121.45	113.13	4	1
3	B	334	PX4	C8-O5-C9	2.26	125.39	117.12	9	1
3	C	337	PX4	O1-P1-O2	2.27	122.98	112.44	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	340	PX4	O5-C9-C10	2.26	104.93	111.83	13	1
3	B	351	PX4	C31-C30-C29	2.26	102.93	114.37	8	1
3	B	358	PX4	C11-C10-C9	2.26	105.40	113.69	9	1
3	B	390	PX4	O1-P1-O2	2.26	122.97	112.44	1	1
3	B	397	PX4	O6-C9-C10	2.26	132.63	123.78	1	1
3	B	397	PX4	C26-C25-C24	2.26	121.44	113.13	10	1
3	C	332	PX4	O5-C9-O6	2.26	129.29	123.63	3	1
3	C	335	PX4	P1-O4-C6	2.26	134.32	121.35	4	1
3	C	338	PX4	C15-C14-C13	2.26	102.93	114.37	15	1
3	B	346	PX4	O1-P1-O3	2.26	117.81	107.57	14	1
3	B	353	PX4	O7-C7-C6	2.26	116.45	108.34	8	2
3	B	373	PX4	O1-P1-O3	2.26	117.81	107.57	10	1
3	B	384	PX4	C30-C29-C28	2.26	102.94	114.37	14	1
3	C	352	PX4	O3-C1-C2	2.26	120.53	109.65	13	2
3	B	360	PX4	C26-C25-C24	2.26	104.82	113.13	8	1
3	A	615	PX4	C5-N1-C3	2.26	114.91	108.98	6	1
3	B	338	PX4	O7-C7-C6	2.26	116.45	108.34	12	3
3	B	340	PX4	C11-C10-C9	2.26	105.41	113.69	1	1
3	C	314	PX4	C11-C10-C9	2.26	121.98	113.69	7	2
3	A	636	PX4	C25-C24-C23	2.26	105.42	113.69	3	1
3	C	326	PX4	C32-C31-C30	2.26	125.79	114.37	6	1
3	B	372	PX4	C32-C31-C30	2.26	102.96	114.37	10	1
3	B	393	PX4	C30-C29-C28	2.26	102.96	114.37	8	1
3	B	325	PX4	C11-C10-C9	2.26	121.96	113.69	2	1
3	B	338	PX4	C5-N1-C3	2.26	103.05	108.98	11	2
3	C	339	PX4	O5-C9-C10	2.26	104.96	111.83	2	1
3	A	611	PX4	C1-C2-N1	2.25	123.06	115.82	15	1
3	A	605	PX4	O5-C9-C10	2.25	104.97	111.83	13	1
3	A	629	PX4	C11-C10-C9	2.25	105.44	113.69	15	1
3	A	637	PX4	O7-C7-C8	2.25	116.43	108.34	1	1
3	A	610	PX4	O5-C9-C10	2.25	104.97	111.83	7	1
3	A	634	PX4	O8-C23-C24	2.25	132.59	123.78	11	1
3	A	645	PX4	O7-C7-C6	2.25	116.42	108.34	4	1
3	A	648	PX4	C14-C13-C12	2.25	102.98	114.37	4	1
3	B	303	PX4	O1-P1-O2	2.25	122.93	112.44	12	1
3	C	325	PX4	O7-C23-O8	2.25	128.97	123.70	7	2
3	C	355	PX4	O5-C8-C7	2.25	114.89	108.40	14	2
3	B	372	PX4	C3-N1-C2	2.25	118.86	109.91	11	1
3	C	316	PX4	O7-C7-C6	2.25	116.42	108.34	1	1
3	C	340	PX4	C8-O5-C9	2.25	125.35	117.12	13	1
3	A	636	PX4	C34-C33-C32	2.25	103.00	114.37	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	302	PX4	C5-N1-C3	2.25	103.06	108.98	4	1
3	B	346	PX4	C1-C2-N1	2.25	123.04	115.82	7	1
3	B	353	PX4	O8-C23-C24	2.25	132.58	123.78	2	1
3	C	338	PX4	C25-C24-C23	2.25	121.94	113.69	2	1
3	A	634	PX4	C1-C2-N1	2.25	123.04	115.82	2	1
3	B	314	PX4	C8-C7-C6	2.25	117.03	111.78	6	2
3	B	340	PX4	O1-P1-O2	2.25	122.91	112.44	4	2
3	B	369	PX4	O7-C7-C8	2.25	116.41	108.34	11	2
3	A	639	PX4	C26-C25-C24	2.25	121.38	113.13	15	1
3	A	646	PX4	C16-C15-C14	2.25	103.01	114.37	1	1
3	B	356	PX4	C4-N1-C3	2.25	103.07	108.98	11	2
3	B	397	PX4	C11-C10-C9	2.25	105.46	113.69	3	1
3	C	316	PX4	O5-C9-C10	2.25	104.98	111.83	4	1
3	C	360	PX4	O7-C7-C8	2.25	116.41	108.34	14	2
3	A	606	PX4	C26-C25-C24	2.25	121.38	113.13	6	1
3	A	619	PX4	C5-N1-C3	2.25	114.87	108.98	10	1
3	A	602	PX4	C5-N1-C3	2.24	114.87	108.98	14	3
3	A	610	PX4	C5-N1-C4	2.24	103.08	108.98	5	3
3	A	625	PX4	O3-P1-O2	2.24	100.04	108.94	2	1
3	B	320	PX4	C26-C25-C24	2.24	104.88	113.13	6	1
3	B	360	PX4	C12-C11-C10	2.25	104.88	113.13	5	1
3	B	387	PX4	O4-P1-O2	2.25	117.83	108.94	8	3
3	C	320	PX4	C31-C30-C29	2.24	103.02	114.37	8	1
3	C	363	PX4	O5-C8-C7	2.25	114.87	108.40	7	2
3	A	627	PX4	C5-N1-C3	2.24	103.08	108.98	4	2
3	A	630	PX4	C8-O5-C9	2.24	125.32	117.12	14	2
3	A	646	PX4	O7-C7-C6	2.24	100.29	108.34	13	1
3	B	334	PX4	C27-C26-C25	2.24	125.71	114.37	13	1
3	B	369	PX4	C19-C18-C17	2.24	103.03	114.37	14	1
3	B	374	PX4	O5-C9-C10	2.24	105.00	111.83	13	5
3	B	381	PX4	O1-P1-O4	2.24	117.73	107.57	1	1
3	C	306	PX4	C11-C10-C9	2.24	105.47	113.69	5	1
3	A	621	PX4	C29-C28-C27	2.24	103.04	114.37	3	1
3	A	624	PX4	C12-C11-C10	2.24	104.89	113.13	8	1
3	B	301	PX4	C1-C2-N1	2.24	123.02	115.82	2	1
3	B	361	PX4	O7-C7-C6	2.24	116.39	108.34	14	2
3	C	310	PX4	C11-C10-C9	2.24	105.48	113.69	7	1
3	B	386	PX4	P1-O3-C1	2.24	131.93	121.26	2	1
3	B	317	PX4	O5-C9-C10	2.24	105.01	111.83	8	2
3	B	400	PX4	C20-C19-C18	2.24	103.04	114.37	1	1
3	A	606	PX4	C4-N1-C3	2.24	114.85	108.98	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	629	PX4	C8-C7-C6	2.24	106.57	111.78	3	1
3	A	648	PX4	C8-O5-C9	2.24	108.94	117.12	1	1
3	B	312	PX4	O7-C7-C8	2.24	116.37	108.34	2	1
3	C	307	PX4	C26-C25-C24	2.24	104.90	113.13	13	1
3	B	374	PX4	O7-C7-C6	2.24	116.37	108.34	6	1
3	C	330	PX4	C5-N1-C2	2.24	118.81	109.91	9	1
3	B	327	PX4	C26-C25-C24	2.24	104.91	113.13	4	1
3	B	322	PX4	C1-C2-N1	2.24	123.00	115.82	9	2
3	C	301	PX4	O5-C9-O6	2.24	129.22	123.63	1	1
3	C	331	PX4	O7-C23-O8	2.24	118.48	123.70	11	2
3	C	361	PX4	C5-N1-C3	2.24	114.85	108.98	11	3
3	A	621	PX4	C5-N1-C3	2.23	103.11	108.98	9	1
3	B	342	PX4	C5-N1-C3	2.23	114.84	108.98	10	1
3	B	390	PX4	O7-C7-C6	2.23	100.33	108.34	1	1
3	B	392	PX4	C5-N1-C4	2.23	103.11	108.98	3	2
3	B	396	PX4	O1-P1-O2	2.23	122.83	112.44	14	1
3	C	309	PX4	C26-C25-C24	2.23	121.34	113.13	9	1
3	C	329	PX4	C5-N1-C3	2.23	103.11	108.98	4	1
3	C	326	PX4	C1-C2-N1	2.23	122.99	115.82	13	1
3	C	362	PX4	O7-C23-C24	2.23	106.65	111.48	6	3
3	A	630	PX4	C12-C11-C10	2.23	121.33	113.13	7	1
3	A	643	PX4	C1-C2-N1	2.23	122.99	115.82	6	1
3	A	603	PX4	C30-C29-C28	2.23	103.09	114.37	7	1
3	A	610	PX4	C33-C32-C31	2.23	125.65	114.37	11	1
3	A	617	PX4	C12-C11-C10	2.23	104.93	113.13	10	1
3	B	343	PX4	C4-N1-C2	2.23	118.78	109.91	5	1
3	B	376	PX4	C5-N1-C3	2.23	114.84	108.98	12	1
3	C	321	PX4	C26-C25-C24	2.23	121.32	113.13	8	1
3	C	323	PX4	C27-C26-C25	2.23	103.10	114.37	2	1
3	C	354	PX4	O3-C1-C2	2.23	120.38	109.65	2	2
3	C	363	PX4	O3-P1-O2	2.23	100.09	108.94	10	1
3	C	370	PX4	C4-N1-C3	2.23	114.84	108.98	14	1
3	A	622	PX4	C4-N1-C3	2.23	114.83	108.98	1	2
3	A	624	PX4	C8-C7-C6	2.23	106.59	111.78	1	2
3	A	632	PX4	C25-C24-C23	2.23	105.53	113.69	6	1
3	A	623	PX4	C31-C30-C29	2.23	103.11	114.37	1	1
3	B	316	PX4	O5-C9-C10	2.23	105.04	111.83	10	1
3	B	388	PX4	O5-C9-O6	2.23	129.20	123.63	2	1
3	B	394	PX4	C3-N1-C2	2.23	118.77	109.91	8	1
3	C	339	PX4	C5-N1-C4	2.23	103.12	108.98	15	1
3	C	345	PX4	C8-O5-C9	2.23	108.97	117.12	12	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	C	368	PX4	O7-C7-C8	2.23	116.34	108.34	10	1
3	C	370	PX4	C16-C15-C14	2.23	103.10	114.37	10	2
3	A	643	PX4	C25-C24-C23	2.23	105.53	113.69	8	1
3	B	371	PX4	C4-N1-C3	2.23	103.12	108.98	5	2
3	B	371	PX4	C28-C27-C26	2.23	103.11	114.37	11	2
3	B	365	PX4	O5-C8-C7	2.23	114.81	108.40	5	3
3	B	400	PX4	O5-C9-C10	2.23	105.04	111.83	14	1
3	C	365	PX4	O5-C9-O6	2.23	129.20	123.63	13	2
3	A	618	PX4	O7-C7-C6	2.23	116.33	108.34	9	3
3	B	314	PX4	O5-C9-C10	2.22	105.05	111.83	15	1
3	B	352	PX4	O7-C23-O8	2.23	128.91	123.70	6	1
3	C	303	PX4	C4-N1-C3	2.23	103.13	108.98	7	2
3	C	310	PX4	C8-C7-C6	2.23	116.97	111.78	2	2
3	A	616	PX4	C26-C25-C24	2.22	121.30	113.13	4	1
3	B	395	PX4	C1-C2-N1	2.22	122.96	115.82	10	2
3	C	323	PX4	O1-P1-O3	2.22	117.65	107.57	3	1
3	A	627	PX4	C25-C24-C23	2.22	105.55	113.69	7	1
3	A	629	PX4	O5-C9-C10	2.22	105.06	111.83	10	3
3	B	327	PX4	C1-C2-N1	2.22	122.95	115.82	12	1
3	B	345	PX4	C11-C10-C9	2.22	105.55	113.69	9	1
3	C	327	PX4	O7-C7-C8	2.22	116.32	108.34	6	1
3	C	333	PX4	O5-C9-C10	2.22	105.05	111.83	1	1
3	A	644	PX4	O3-C1-C2	2.22	120.34	109.65	12	1
3	B	303	PX4	O7-C7-C6	2.22	116.31	108.34	11	1
3	B	329	PX4	O5-C9-C10	2.22	105.06	111.83	14	2
3	B	334	PX4	C25-C24-C23	2.22	121.83	113.69	10	1
3	C	304	PX4	C26-C25-C24	2.22	121.29	113.13	12	1
3	B	370	PX4	O5-C9-O6	2.22	129.18	123.63	10	2
3	B	375	PX4	C1-C2-N1	2.22	122.95	115.82	10	1
3	B	362	PX4	C3-N1-C2	2.22	101.08	109.91	1	1
3	C	314	PX4	O3-C1-C2	2.22	120.33	109.65	8	1
3	B	365	PX4	O3-P1-O2	2.22	100.14	108.94	15	1
3	C	314	PX4	P1-O3-C1	2.22	131.83	121.26	11	1
3	C	366	PX4	C33-C32-C31	2.22	125.59	114.37	12	1
3	B	308	PX4	O7-C7-C8	2.22	116.30	108.34	5	2
3	B	314	PX4	P1-O3-C1	2.22	131.82	121.26	4	1
3	B	355	PX4	C1-C2-N1	2.22	122.94	115.82	1	1
3	C	317	PX4	O7-C7-C8	2.22	116.30	108.34	12	2
3	B	340	PX4	C25-C24-C23	2.22	121.82	113.69	9	2
3	B	399	PX4	O7-C23-O8	2.22	128.89	123.70	11	1
3	B	364	PX4	O5-C9-O6	2.22	129.17	123.63	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	383	PX4	C8-C7-C6	2.22	116.95	111.78	10	1
3	C	356	PX4	C4-N1-C3	2.22	103.15	108.98	3	1
3	A	606	PX4	O7-C7-C6	2.21	116.29	108.34	2	1
3	A	631	PX4	O5-C9-C10	2.21	105.08	111.83	15	1
3	A	635	PX4	O7-C7-C6	2.21	116.29	108.34	3	2
3	B	322	PX4	C13-C12-C11	2.21	103.17	114.37	9	1
3	B	384	PX4	O5-C9-C10	2.22	105.08	111.83	9	1
3	C	313	PX4	C5-N1-C4	2.21	103.16	108.98	4	1
3	C	331	PX4	O3-C1-C2	2.22	120.31	109.65	2	1
3	B	325	PX4	C26-C25-C24	2.21	104.99	113.13	7	2
3	B	352	PX4	C8-O5-C9	2.21	109.03	117.12	3	2
3	B	379	PX4	O5-C9-C10	2.21	105.09	111.83	15	1
3	C	344	PX4	C28-C27-C26	2.21	103.18	114.37	6	1
3	C	360	PX4	C8-O5-C9	2.21	109.03	117.12	11	1
3	B	384	PX4	C8-C7-C6	2.21	106.63	111.78	2	1
3	B	391	PX4	O7-C23-O8	2.21	128.88	123.70	11	1
3	C	363	PX4	O7-C23-O8	2.21	128.88	123.70	2	2
3	A	622	PX4	C1-C2-N1	2.21	122.92	115.82	7	1
3	A	642	PX4	O7-C7-C6	2.21	116.28	108.34	3	1
3	B	303	PX4	O5-C8-C7	2.21	114.77	108.40	13	4
3	B	349	PX4	O7-C7-C6	2.21	116.28	108.34	5	2
3	B	359	PX4	O7-C23-C24	2.21	106.70	111.48	12	2
3	B	365	PX4	C3-N1-C2	2.21	118.70	109.91	2	2
3	B	400	PX4	O4-P1-O2	2.21	100.17	108.94	1	1
3	C	301	PX4	O5-C9-C10	2.21	105.09	111.83	5	2
3	C	304	PX4	O3-C1-C2	2.21	120.29	109.65	3	1
3	C	309	PX4	O5-C9-C10	2.21	105.09	111.83	13	1
3	C	311	PX4	C13-C12-C11	2.21	103.19	114.37	2	2
3	C	318	PX4	C26-C25-C24	2.21	105.00	113.13	10	2
3	C	321	PX4	C1-C2-N1	2.21	122.92	115.82	13	1
3	C	338	PX4	P1-O3-C1	2.21	131.79	121.26	3	2
3	A	633	PX4	C30-C29-C28	2.21	103.20	114.37	13	1
3	B	316	PX4	C1-C2-N1	2.21	122.92	115.82	10	1
3	A	645	PX4	O5-C9-C10	2.21	105.10	111.83	11	2
3	B	316	PX4	C8-O5-C9	2.21	109.04	117.12	6	1
3	B	340	PX4	P1-O4-C6	2.21	108.70	121.35	9	1
3	B	345	PX4	O1-P1-O2	2.21	122.71	112.44	9	1
3	C	350	PX4	C15-C14-C13	2.21	125.53	114.37	15	1
3	C	359	PX4	O5-C8-C7	2.21	114.76	108.40	15	1
3	C	368	PX4	C26-C25-C24	2.21	121.24	113.13	8	1
3	B	305	PX4	C4-N1-C2	2.21	118.67	109.91	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	342	PX4	O8-C23-C24	2.21	132.41	123.78	4	1
3	B	348	PX4	C1-C2-N1	2.21	122.90	115.82	1	1
3	B	381	PX4	C12-C11-C10	2.21	121.23	113.13	1	1
3	B	369	PX4	C8-O5-C9	2.20	109.06	117.12	15	1
3	C	307	PX4	C5-N1-C3	2.20	103.19	108.98	7	1
3	C	310	PX4	C5-N1-C4	2.21	103.18	108.98	5	1
3	C	319	PX4	C5-N1-C2	2.21	118.68	109.91	10	1
3	C	334	PX4	C8-O5-C9	2.20	109.06	117.12	10	1
3	C	343	PX4	O5-C9-C10	2.20	105.11	111.83	11	1
3	C	352	PX4	C8-O5-C9	2.21	109.06	117.12	6	1
3	C	357	PX4	P1-O3-C1	2.20	131.75	121.26	13	1
3	C	359	PX4	O5-C9-O6	2.21	129.14	123.63	1	2
3	B	305	PX4	O7-C7-C6	2.20	100.44	108.34	14	1
3	B	341	PX4	C12-C11-C10	2.20	121.22	113.13	12	2
3	B	309	PX4	O7-C7-C6	2.20	100.44	108.34	7	1
3	B	357	PX4	O1-P1-O2	2.20	122.69	112.44	6	1
3	B	384	PX4	O1-P1-O2	2.20	122.69	112.44	8	2
3	B	386	PX4	C32-C31-C30	2.20	125.50	114.37	9	1
3	C	301	PX4	O3-C1-C2	2.20	120.25	109.65	2	2
3	C	342	PX4	O3-P1-O2	2.20	100.20	108.94	10	1
3	A	644	PX4	O4-P1-O2	2.20	117.66	108.94	12	1
3	A	646	PX4	C5-N1-C4	2.20	114.76	108.98	13	2
3	B	325	PX4	O7-C7-C8	2.20	116.24	108.34	6	1
3	B	350	PX4	P1-O3-C1	2.20	131.74	121.26	11	1
3	B	387	PX4	O7-C7-C6	2.20	116.24	108.34	8	1
3	C	304	PX4	P1-O4-C6	2.20	133.97	121.35	2	1
3	A	611	PX4	O7-C23-O8	2.20	128.85	123.70	4	1
3	B	330	PX4	C1-C2-N1	2.20	122.89	115.82	15	1
3	C	309	PX4	P1-O3-C1	2.20	110.78	121.26	10	1
3	C	325	PX4	O1-P1-O2	2.20	122.68	112.44	12	1
3	B	303	PX4	C8-O5-C9	2.20	109.08	117.12	14	2
3	C	322	PX4	C5-N1-C2	2.20	118.65	109.91	5	1
3	B	313	PX4	C31-C30-C29	2.20	103.26	114.37	12	1
3	B	320	PX4	C11-C10-C9	2.20	105.64	113.69	2	2
3	B	359	PX4	O1-P1-O3	2.20	117.53	107.57	3	1
3	C	316	PX4	C1-C2-N1	2.20	122.88	115.82	12	1
3	C	351	PX4	C11-C10-C9	2.20	105.64	113.69	11	1
3	C	370	PX4	P1-O4-C6	2.20	133.96	121.35	11	1
3	C	328	PX4	O5-C9-C10	2.20	105.13	111.83	15	1
3	C	346	PX4	C34-C33-C32	2.20	103.26	114.37	1	1
3	C	365	PX4	C31-C30-C29	2.20	103.25	114.37	14	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	643	PX4	C8-C7-C6	2.20	116.91	111.78	12	1
3	C	320	PX4	C8-C7-C6	2.20	106.66	111.78	15	2
3	C	335	PX4	C5-N1-C4	2.20	103.20	108.98	1	2
3	C	369	PX4	O5-C9-O6	2.20	129.13	123.63	3	1
3	B	318	PX4	C27-C26-C25	2.20	103.26	114.37	7	1
3	A	620	PX4	P1-O3-C1	2.20	131.71	121.26	3	1
3	B	310	PX4	O7-C7-C8	2.20	116.22	108.34	9	1
3	B	380	PX4	O7-C23-O8	2.20	128.84	123.70	12	2
3	B	351	PX4	O5-C8-C7	2.20	114.72	108.40	15	3
3	A	608	PX4	C15-C14-C13	2.19	125.46	114.37	7	1
3	A	624	PX4	C16-C15-C14	2.19	103.28	114.37	15	1
3	A	642	PX4	P1-O3-C1	2.19	131.71	121.26	13	1
3	B	352	PX4	C25-C24-C23	2.19	121.74	113.69	10	1
3	B	386	PX4	O7-C7-C8	2.19	116.21	108.34	11	2
3	B	393	PX4	C8-O5-C9	2.19	109.10	117.12	6	1
3	A	601	PX4	C12-C11-C10	2.19	105.07	113.13	6	1
3	A	629	PX4	C26-C25-C24	2.19	105.07	113.13	13	1
3	B	308	PX4	C16-C15-C14	2.19	103.28	114.37	2	1
3	B	330	PX4	O7-C23-O8	2.19	128.83	123.70	8	2
3	C	318	PX4	O7-C23-C24	2.19	106.74	111.48	9	1
3	C	348	PX4	C25-C24-C23	2.19	105.66	113.69	11	2
3	C	353	PX4	O5-C9-C10	2.19	105.15	111.83	6	2
3	B	311	PX4	O5-C9-O6	2.19	129.11	123.63	6	1
3	B	312	PX4	O7-C23-O8	2.19	128.83	123.70	11	2
3	B	319	PX4	C5-N1-C4	2.19	103.22	108.98	14	1
3	C	311	PX4	O5-C9-O6	2.19	129.11	123.63	5	1
3	A	636	PX4	C8-O5-C9	2.19	109.11	117.12	11	1
3	B	319	PX4	O7-C7-C6	2.19	116.20	108.34	1	1
3	B	354	PX4	O5-C9-O6	2.19	129.11	123.63	5	3
3	C	314	PX4	P1-O4-C6	2.19	108.79	121.35	10	1
3	B	354	PX4	O8-C23-C24	2.19	132.35	123.78	10	1
3	B	373	PX4	C25-C24-C23	2.19	121.72	113.69	5	1
3	C	356	PX4	O5-C9-O6	2.19	129.11	123.63	5	1
3	C	359	PX4	C8-O5-C9	2.19	109.11	117.12	2	2
3	B	362	PX4	O7-C7-C6	2.19	116.19	108.34	11	1
3	C	325	PX4	C5-N1-C2	2.19	118.60	109.91	14	1
3	A	637	PX4	O5-C9-C10	2.18	105.17	111.83	6	1
3	B	348	PX4	O3-P1-O2	2.19	100.27	108.94	6	1
3	B	354	PX4	O7-C23-O8	2.19	128.81	123.70	6	4
3	B	379	PX4	O7-C7-C8	2.19	116.18	108.34	7	1
3	B	391	PX4	C19-C18-C17	2.19	125.41	114.37	2	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	C	317	PX4	C25-C24-C23	2.19	121.70	113.69	5	2
3	C	337	PX4	C1-C2-N1	2.19	122.84	115.82	14	1
3	C	366	PX4	C8-O5-C9	2.19	109.13	117.12	9	1
3	A	644	PX4	C25-C24-C23	2.18	105.69	113.69	3	1
3	A	611	PX4	C19-C18-C17	2.18	103.33	114.37	8	1
3	A	630	PX4	C28-C27-C26	2.18	103.33	114.37	13	1
3	A	640	PX4	C31-C30-C29	2.18	103.33	114.37	3	1
3	B	393	PX4	O1-P1-O4	2.18	117.47	107.57	7	1
3	B	381	PX4	O7-C23-O8	2.18	128.81	123.70	5	2
3	B	382	PX4	C28-C27-C26	2.18	103.33	114.37	1	1
3	C	331	PX4	C8-O5-C9	2.18	109.13	117.12	13	1
3	A	644	PX4	O8-C23-C24	2.18	132.32	123.78	14	1
3	A	604	PX4	C4-N1-C3	2.18	103.24	108.98	13	2
3	B	306	PX4	C4-N1-C3	2.18	114.71	108.98	5	2
3	B	324	PX4	O5-C9-C10	2.18	105.18	111.83	10	1
3	C	330	PX4	P1-O3-C1	2.18	131.65	121.26	9	1
3	B	354	PX4	C13-C12-C11	2.18	103.34	114.37	6	1
3	B	372	PX4	C5-N1-C4	2.18	103.25	108.98	11	1
3	B	399	PX4	O7-C23-C24	2.18	106.76	111.48	14	2
3	C	351	PX4	C27-C26-C25	2.18	103.34	114.37	4	2
3	C	361	PX4	C17-C16-C15	2.18	103.34	114.37	14	1
3	B	309	PX4	P1-O4-C6	2.18	133.85	121.35	8	1
3	A	609	PX4	C1-C2-N1	2.18	122.82	115.82	2	1
3	A	621	PX4	C25-C24-C23	2.18	105.71	113.69	2	1
3	B	374	PX4	O5-C9-O6	2.18	129.08	123.63	2	3
3	C	340	PX4	O7-C23-O8	2.18	128.80	123.70	10	1
3	C	354	PX4	O5-C9-O6	2.18	129.08	123.63	14	3
3	A	621	PX4	O5-C9-C10	2.18	105.19	111.83	11	2
3	B	358	PX4	C25-C24-C23	2.18	105.71	113.69	14	1
3	B	382	PX4	O7-C23-C24	2.18	106.77	111.48	9	1
3	B	388	PX4	C5-N1-C4	2.18	103.25	108.98	5	3
3	B	384	PX4	C16-C15-C14	2.18	103.36	114.37	1	1
3	C	324	PX4	C8-O5-C9	2.18	109.16	117.12	7	1
3	C	328	PX4	C5-N1-C3	2.18	103.25	108.98	2	1
3	C	349	PX4	C25-C24-C23	2.18	121.68	113.69	3	1
3	C	358	PX4	C26-C25-C24	2.18	121.13	113.13	10	1
3	A	610	PX4	O7-C7-C6	2.18	116.15	108.34	15	1
3	A	624	PX4	O5-C9-O6	2.18	129.07	123.63	12	1
3	B	376	PX4	O1-P1-O2	2.18	122.57	112.44	5	2
3	C	301	PX4	C8-O5-C9	2.18	125.07	117.12	8	2
3	C	349	PX4	C20-C19-C18	2.18	103.36	114.37	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	C	304	PX4	C4-N1-C2	2.18	118.56	109.91	14	1
3	A	648	PX4	C26-C25-C24	2.17	121.11	113.13	9	1
3	B	373	PX4	O3-C1-C2	2.17	120.11	109.65	13	1
3	C	307	PX4	C5-N1-C4	2.17	103.27	108.98	11	2
3	C	337	PX4	O5-C9-C10	2.17	105.21	111.83	5	1
3	B	355	PX4	O1-P1-O2	2.17	122.55	112.44	7	1
3	B	359	PX4	C12-C11-C10	2.17	105.14	113.13	9	1
3	B	395	PX4	O5-C9-O6	2.17	129.06	123.63	6	3
3	A	648	PX4	O5-C9-O6	2.17	129.06	123.63	11	2
3	B	307	PX4	C30-C29-C28	2.17	103.39	114.37	10	1
3	C	312	PX4	C11-C10-C9	2.17	121.65	113.69	12	1
3	C	337	PX4	C4-N1-C3	2.17	103.27	108.98	9	2
3	C	341	PX4	O6-C9-C10	2.17	132.28	123.78	9	1
3	B	326	PX4	O3-P1-O2	2.17	117.54	108.94	6	1
3	C	350	PX4	C4-N1-C2	2.17	118.54	109.91	15	1
3	B	384	PX4	C12-C11-C10	2.17	105.16	113.13	14	1
3	C	322	PX4	C8-O5-C9	2.17	109.19	117.12	1	1
3	C	322	PX4	O3-C1-C2	2.17	120.08	109.65	15	1
3	C	332	PX4	C7-O7-C23	2.17	112.60	117.80	8	1
3	C	342	PX4	C8-C7-C6	2.17	106.72	111.78	8	1
3	A	608	PX4	C1-C2-N1	2.17	122.78	115.82	4	1
3	A	624	PX4	P1-O3-C1	2.17	110.94	121.26	7	1
3	B	316	PX4	P1-O4-C6	2.17	108.92	121.35	7	2
3	B	378	PX4	O5-C9-C10	2.17	105.23	111.83	5	1
3	B	381	PX4	O7-C7-C8	2.17	100.57	108.34	7	1
3	C	302	PX4	C33-C32-C31	2.17	103.41	114.37	10	1
3	A	641	PX4	C31-C30-C29	2.17	103.42	114.37	9	1
3	B	311	PX4	O3-C1-C2	2.16	120.06	109.65	11	1
3	B	316	PX4	O5-C9-O6	2.17	129.04	123.63	10	1
3	C	316	PX4	P1-O4-C6	2.16	108.95	121.35	6	1
3	C	316	PX4	C4-N1-C3	2.17	103.29	108.98	7	1
3	C	331	PX4	C4-N1-C3	2.17	114.67	108.98	14	1
3	C	363	PX4	C1-C2-N1	2.17	122.77	115.82	4	2
3	A	643	PX4	C4-N1-C3	2.16	114.66	108.98	14	1
3	B	318	PX4	C4-N1-C3	2.16	103.29	108.98	1	1
3	C	340	PX4	O3-C1-C2	2.16	120.07	109.65	2	1
3	C	370	PX4	C8-O5-C9	2.17	109.20	117.12	6	1
3	B	319	PX4	C11-C10-C9	2.16	105.77	113.69	1	1
3	B	308	PX4	C4-N1-C2	2.16	101.32	109.91	15	1
3	B	328	PX4	P1-O3-C1	2.16	131.55	121.26	7	1
3	B	372	PX4	O7-C7-C8	2.16	116.10	108.34	15	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	C	302	PX4	C19-C18-C17	2.16	125.30	114.37	8	1
3	C	362	PX4	C8-C7-C6	2.16	106.74	111.78	4	1
3	C	307	PX4	O7-C23-O8	2.16	128.76	123.70	11	3
3	C	316	PX4	O3-P1-O2	2.16	117.50	108.94	8	2
3	B	393	PX4	C5-N1-C4	2.16	103.30	108.98	11	1
3	B	398	PX4	C4-N1-C3	2.16	114.65	108.98	13	1
3	C	319	PX4	O7-C23-O8	2.16	128.76	123.70	14	1
3	C	326	PX4	C11-C10-C9	2.16	105.78	113.69	1	2
3	C	331	PX4	C11-C10-C9	2.16	105.78	113.69	6	3
3	A	606	PX4	C25-C24-C23	2.16	105.78	113.69	3	2
3	A	628	PX4	C5-N1-C3	2.16	103.30	108.98	13	2
3	B	339	PX4	C26-C25-C24	2.16	121.06	113.13	6	2
3	A	624	PX4	O1-P1-O2	2.16	122.48	112.44	11	1
3	B	309	PX4	O7-C23-O8	2.16	128.75	123.70	3	2
3	B	330	PX4	O1-P1-O2	2.16	122.48	112.44	15	1
3	B	323	PX4	C11-C10-C9	2.16	105.79	113.69	15	1
3	B	339	PX4	C1-C2-N1	2.16	122.74	115.82	11	1
3	B	345	PX4	C29-C28-C27	2.16	103.47	114.37	8	1
3	B	373	PX4	P1-O3-C1	2.16	131.53	121.26	12	1
3	B	383	PX4	P1-O3-C1	2.16	110.99	121.26	7	2
3	B	398	PX4	C19-C18-C17	2.16	103.46	114.37	14	1
3	A	641	PX4	O5-C8-C7	2.15	114.61	108.40	9	1
3	A	647	PX4	O7-C7-C8	2.16	100.61	108.34	13	1
3	B	353	PX4	C18-C17-C16	2.16	103.47	114.37	2	1
3	B	353	PX4	C32-C31-C30	2.16	103.47	114.37	10	1
3	B	357	PX4	C25-C24-C23	2.16	121.59	113.69	12	1
3	C	355	PX4	O3-C1-C2	2.16	120.03	109.65	14	1
3	B	317	PX4	C8-C7-C6	2.15	106.76	111.78	1	1
3	B	317	PX4	O7-C7-C8	2.15	116.07	108.34	6	2
3	B	319	PX4	C5-N1-C3	2.15	103.32	108.98	2	2
3	B	363	PX4	C4-N1-C2	2.15	101.35	109.91	8	2
3	B	399	PX4	C27-C26-C25	2.16	103.47	114.37	13	1
3	C	353	PX4	C25-C24-C23	2.16	105.80	113.69	2	1
3	C	364	PX4	O7-C7-C8	2.16	116.08	108.34	8	1
3	B	382	PX4	C1-C2-N1	2.15	122.73	115.82	1	1
3	C	322	PX4	C1-C2-N1	2.15	122.74	115.82	10	1
3	A	601	PX4	O7-C7-C6	2.15	100.62	108.34	3	1
3	A	634	PX4	C5-N1-C3	2.15	103.32	108.98	13	1
3	A	637	PX4	C5-N1-C3	2.15	114.63	108.98	12	1
3	B	313	PX4	C8-C7-C6	2.15	116.80	111.78	15	1
3	B	391	PX4	C28-C27-C26	2.15	103.49	114.37	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	C	317	PX4	O5-C9-O6	2.15	129.01	123.63	11	1
3	A	608	PX4	C33-C32-C31	2.15	103.50	114.37	10	1
3	C	323	PX4	O1-P1-O4	2.15	117.31	107.57	12	1
3	C	326	PX4	C5-N1-C2	2.15	118.46	109.91	5	1
3	B	346	PX4	C5-N1-C2	2.15	118.45	109.91	4	1
3	B	396	PX4	O1-P1-O4	2.15	117.31	107.57	2	1
3	C	359	PX4	C25-C24-C23	2.15	105.82	113.69	9	2
3	A	629	PX4	C12-C11-C10	2.15	121.02	113.13	2	1
3	C	343	PX4	O5-C9-O6	2.15	129.00	123.63	10	2
3	B	341	PX4	C4-N1-C3	2.15	103.34	108.98	8	1
3	B	363	PX4	C18-C17-C16	2.15	103.52	114.37	4	1
3	B	382	PX4	C11-C10-C9	2.15	105.83	113.69	3	2
3	B	302	PX4	C4-N1-C3	2.15	114.61	108.98	2	3
3	B	342	PX4	O5-C9-C10	2.15	105.29	111.83	9	2
3	C	369	PX4	C32-C31-C30	2.15	125.22	114.37	7	1
3	B	302	PX4	C8-O5-C9	2.15	109.28	117.12	11	1
3	A	606	PX4	C5-N1-C4	2.14	103.34	108.98	5	1
3	B	321	PX4	C13-C12-C11	2.14	103.53	114.37	5	1
3	C	301	PX4	O7-C7-C8	2.14	116.04	108.34	9	2
3	C	340	PX4	C1-C2-N1	2.14	122.71	115.82	11	1
3	B	313	PX4	O5-C9-C10	2.14	105.30	111.83	1	1
3	B	316	PX4	O7-C7-C6	2.14	116.03	108.34	6	1
3	B	322	PX4	C5-N1-C4	2.14	103.35	108.98	8	2
3	B	332	PX4	C8-O5-C9	2.14	109.29	117.12	1	1
3	B	359	PX4	C4-N1-C3	2.14	114.60	108.98	1	1
3	B	359	PX4	C4-N1-C2	2.14	118.43	109.91	2	1
3	C	310	PX4	C27-C26-C25	2.14	103.53	114.37	9	1
3	C	343	PX4	C33-C32-C31	2.14	125.20	114.37	10	1
3	B	362	PX4	C8-O5-C9	2.14	109.29	117.12	8	1
3	C	324	PX4	C26-C25-C24	2.14	105.25	113.13	1	1
3	C	325	PX4	O4-P1-O2	2.14	100.45	108.94	15	1
3	C	332	PX4	O6-C9-C10	2.14	132.16	123.78	12	1
3	A	635	PX4	C1-C2-N1	2.14	122.69	115.82	4	1
3	A	646	PX4	O3-P1-O2	2.14	100.45	108.94	15	2
3	B	331	PX4	O7-C7-C8	2.14	116.02	108.34	9	1
3	C	360	PX4	O6-C9-C10	2.14	132.15	123.78	6	1
3	C	365	PX4	C8-O5-C9	2.14	124.94	117.12	13	1
3	B	313	PX4	C27-C26-C25	2.14	103.56	114.37	8	1
3	B	316	PX4	C4-N1-C2	2.14	101.41	109.91	14	1
3	B	319	PX4	O5-C9-C10	2.14	105.31	111.83	13	2
3	B	392	PX4	O7-C7-C6	2.14	116.02	108.34	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	400	PX4	C19-C18-C17	2.14	103.55	114.37	10	1
3	A	604	PX4	C8-C7-C6	2.14	106.80	111.78	10	1
3	A	640	PX4	C26-C25-C24	2.14	105.27	113.13	2	1
3	A	617	PX4	P1-O4-C6	2.14	133.59	121.35	12	1
3	A	623	PX4	O3-C1-C2	2.14	119.93	109.65	15	1
3	A	639	PX4	C5-N1-C3	2.14	103.36	108.98	14	1
3	A	641	PX4	O5-C9-C10	2.14	105.32	111.83	1	1
3	B	315	PX4	C14-C13-C12	2.14	103.57	114.37	6	1
3	B	319	PX4	C25-C24-C23	2.14	105.86	113.69	4	1
3	B	321	PX4	O7-C23-C24	2.14	106.86	111.48	3	2
3	A	648	PX4	C5-N1-C2	2.14	101.42	109.91	3	1
3	B	325	PX4	O5-C9-C10	2.14	105.32	111.83	7	1
3	B	378	PX4	C26-C25-C24	2.14	120.98	113.13	7	1
3	C	370	PX4	C18-C17-C16	2.14	125.17	114.37	10	1
3	A	634	PX4	C12-C11-C10	2.13	120.97	113.13	12	1
3	B	309	PX4	P1-O3-C1	2.13	131.41	121.26	1	1
3	B	319	PX4	C4-N1-C3	2.13	103.38	108.98	1	1
3	B	320	PX4	C22-C21-C20	2.13	127.76	113.36	6	1
3	B	325	PX4	O8-C23-C24	2.13	132.12	123.78	2	1
3	B	331	PX4	C3-N1-C2	2.13	118.39	109.91	8	1
3	B	338	PX4	C15-C14-C13	2.13	103.59	114.37	6	1
3	B	362	PX4	C33-C32-C31	2.13	103.58	114.37	6	1
3	B	370	PX4	C5-N1-C4	2.13	103.38	108.98	15	1
3	B	376	PX4	C27-C26-C25	2.13	103.59	114.37	11	1
3	A	647	PX4	C8-O5-C9	2.13	109.33	117.12	1	1
3	B	356	PX4	C18-C17-C16	2.13	103.59	114.37	2	1
3	B	370	PX4	C11-C10-C9	2.13	121.50	113.69	9	1
3	B	393	PX4	O5-C9-C10	2.13	105.33	111.83	11	2
3	C	310	PX4	C8-O5-C9	2.13	109.33	117.12	15	1
3	C	351	PX4	C3-N1-C2	2.13	101.44	109.91	13	2
3	C	356	PX4	O1-P1-O2	2.13	122.36	112.44	2	2
3	A	617	PX4	O7-C7-C8	2.13	115.98	108.34	11	1
3	A	607	PX4	C8-O5-C9	2.13	109.34	117.12	15	1
3	A	623	PX4	C8-O5-C9	2.13	109.34	117.12	4	1
3	A	648	PX4	O3-P1-O2	2.13	100.50	108.94	3	1
3	B	331	PX4	C26-C25-C24	2.13	120.95	113.13	13	1
3	B	357	PX4	C12-C11-C10	2.13	120.95	113.13	6	1
3	C	349	PX4	C1-C2-N1	2.13	122.66	115.82	3	1
3	A	634	PX4	O7-C23-O8	2.13	128.68	123.70	9	2
3	B	306	PX4	C5-N1-C2	2.13	118.37	109.91	10	1
3	B	318	PX4	C12-C11-C10	2.13	105.31	113.13	10	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	378	PX4	C25-C24-C23	2.13	105.90	113.69	14	1
3	C	326	PX4	C27-C26-C25	2.13	103.61	114.37	15	1
3	C	330	PX4	O7-C23-O8	2.13	128.68	123.70	12	2
3	B	368	PX4	C4-N1-C3	2.13	114.56	108.98	7	2
3	B	369	PX4	C4-N1-C2	2.13	118.36	109.91	14	1
3	C	336	PX4	C8-O5-C9	2.13	124.89	117.12	15	2
3	C	341	PX4	C25-C24-C23	2.13	105.90	113.69	4	1
3	B	331	PX4	C4-N1-C3	2.12	103.40	108.98	13	1
3	B	340	PX4	C34-C33-C32	2.12	103.63	114.37	1	1
3	C	339	PX4	C11-C10-C9	2.12	105.91	113.69	8	1
3	C	340	PX4	O5-C9-O6	2.13	128.94	123.63	9	1
3	A	618	PX4	O1-P1-O2	2.12	122.32	112.44	11	2
3	A	621	PX4	O7-C23-O8	2.12	128.67	123.70	1	3
3	A	627	PX4	C31-C30-C29	2.12	103.64	114.37	3	1
3	A	631	PX4	O1-P1-O2	2.12	122.32	112.44	14	2
3	B	317	PX4	C5-N1-C3	2.12	103.40	108.98	4	1
3	B	342	PX4	C3-N1-C2	2.12	101.47	109.91	10	1
3	B	360	PX4	C11-C10-C9	2.12	105.91	113.69	4	1
3	B	377	PX4	C1-C2-N1	2.12	122.64	115.82	13	2
3	B	386	PX4	O8-C23-C24	2.12	132.09	123.78	11	1
3	B	367	PX4	C4-N1-C2	2.12	101.47	109.91	15	1
3	B	393	PX4	C26-C25-C24	2.12	120.93	113.13	3	1
3	C	304	PX4	O1-P1-O2	2.12	122.32	112.44	3	1
3	C	356	PX4	C26-C25-C24	2.12	120.93	113.13	12	1
3	B	331	PX4	O1-P1-O4	2.12	117.18	107.57	14	1
3	B	327	PX4	O3-P1-O2	2.12	117.34	108.94	4	1
3	B	346	PX4	C5-N1-C3	2.12	103.41	108.98	10	1
3	B	355	PX4	O8-C23-C24	2.12	132.08	123.78	8	1
3	B	363	PX4	O5-C9-C10	2.12	105.37	111.83	4	1
3	B	399	PX4	O1-P1-O2	2.12	122.31	112.44	8	1
3	C	327	PX4	C28-C27-C26	2.12	103.64	114.37	5	1
3	C	331	PX4	C14-C13-C12	2.12	103.65	114.37	14	1
3	C	333	PX4	C5-N1-C4	2.12	103.40	108.98	12	1
3	C	350	PX4	C19-C18-C17	2.12	103.64	114.37	10	2
3	A	619	PX4	C11-C10-C9	2.12	121.46	113.69	1	1
3	A	620	PX4	C17-C16-C15	2.12	125.08	114.37	12	1
3	B	314	PX4	O8-C23-C24	2.12	132.07	123.78	12	1
3	B	315	PX4	C16-C15-C14	2.12	103.66	114.37	5	1
3	B	317	PX4	C4-N1-C3	2.12	114.54	108.98	2	1
3	B	332	PX4	C12-C11-C10	2.12	105.34	113.13	7	1
3	C	304	PX4	C25-C24-C23	2.12	105.93	113.69	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	C	359	PX4	O7-C7-C6	2.12	100.74	108.34	2	1
3	A	609	PX4	O7-C7-C8	2.12	115.94	108.34	9	2
3	A	640	PX4	C20-C19-C18	2.12	103.67	114.37	14	1
3	A	641	PX4	P1-O4-C6	2.12	133.48	121.35	8	1
3	B	357	PX4	C30-C29-C28	2.12	103.66	114.37	5	1
3	B	366	PX4	O7-C7-C6	2.12	115.94	108.34	3	2
3	C	327	PX4	C5-N1-C4	2.12	103.41	108.98	12	1
3	C	332	PX4	C1-C2-N1	2.12	122.62	115.82	12	2
3	A	623	PX4	O7-C7-C6	2.12	115.94	108.34	15	2
3	A	648	PX4	O5-C9-C10	2.12	105.38	111.83	10	2
3	B	340	PX4	C18-C17-C16	2.12	103.67	114.37	14	1
3	B	341	PX4	C1-C2-N1	2.12	122.62	115.82	2	2
3	B	346	PX4	O7-C7-C6	2.12	115.94	108.34	3	2
3	B	354	PX4	C4-N1-C2	2.12	101.50	109.91	15	1
3	B	360	PX4	C13-C12-C11	2.12	103.67	114.37	9	1
3	B	393	PX4	C33-C32-C31	2.12	103.66	114.37	5	1
3	B	400	PX4	C4-N1-C3	2.12	103.42	108.98	14	1
3	C	317	PX4	C4-N1-C2	2.12	101.49	109.91	12	1
3	C	319	PX4	C5-N1-C4	2.12	114.54	108.98	12	1
3	C	329	PX4	C12-C11-C10	2.12	120.90	113.13	13	1
3	C	342	PX4	C4-N1-C3	2.12	114.54	108.98	15	2
3	C	349	PX4	O5-C9-O6	2.12	128.92	123.63	10	1
3	A	608	PX4	C5-N1-C3	2.11	103.42	108.98	5	1
3	A	617	PX4	P1-O3-C1	2.11	111.19	121.26	6	1
3	B	309	PX4	C8-C7-C6	2.11	116.72	111.78	5	1
3	B	313	PX4	O4-P1-O2	2.12	100.55	108.94	7	1
3	B	382	PX4	O5-C9-O6	2.12	128.92	123.63	8	2
3	B	383	PX4	C15-C14-C13	2.11	103.68	114.37	3	1
3	B	397	PX4	C8-O5-C9	2.11	109.39	117.12	10	1
3	C	322	PX4	C5-N1-C3	2.11	114.53	108.98	1	1
3	C	351	PX4	O5-C9-C10	2.12	105.39	111.83	11	1
3	A	642	PX4	O7-C7-C8	2.11	115.92	108.34	11	1
3	B	307	PX4	O1-P1-O2	2.11	122.27	112.44	4	1
3	B	351	PX4	C25-C24-C23	2.11	105.95	113.69	14	1
3	B	323	PX4	C26-C25-C24	2.11	105.37	113.13	5	1
3	B	329	PX4	C12-C11-C10	2.11	105.37	113.13	2	1
3	B	335	PX4	C3-N1-C2	2.11	118.30	109.91	6	1
3	B	381	PX4	C26-C25-C24	2.11	105.36	113.13	10	1
3	B	400	PX4	C5-N1-C2	2.11	118.31	109.91	6	1
3	C	342	PX4	C25-C24-C23	2.11	105.95	113.69	9	1
3	B	366	PX4	P1-O3-C1	2.11	111.22	121.26	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	379	PX4	O5-C9-O6	2.11	128.90	123.63	3	2
3	B	394	PX4	C11-C10-C9	2.11	105.97	113.69	14	1
3	C	304	PX4	O7-C23-O8	2.11	128.64	123.70	11	1
3	C	325	PX4	P1-O4-C6	2.11	109.25	121.35	10	1
3	C	345	PX4	C26-C25-C24	2.11	105.37	113.13	7	1
3	A	644	PX4	O5-C9-C10	2.11	105.40	111.83	13	2
3	A	614	PX4	C5-N1-C4	2.11	103.44	108.98	13	1
3	A	621	PX4	O5-C8-C7	2.11	114.47	108.40	1	1
3	B	307	PX4	C11-C10-C9	2.11	105.97	113.69	6	1
3	B	324	PX4	C8-O5-C9	2.11	124.82	117.12	5	1
3	B	349	PX4	O1-P1-O4	2.11	98.01	107.57	2	1
3	A	614	PX4	C5-N1-C3	2.11	103.44	108.98	10	1
3	B	368	PX4	P1-O4-C6	2.11	109.28	121.35	8	1
3	B	373	PX4	C5-N1-C4	2.11	103.44	108.98	8	3
3	B	398	PX4	C11-C10-C9	2.11	105.98	113.69	8	1
3	B	398	PX4	O5-C9-C10	2.11	105.41	111.83	10	1
3	C	331	PX4	C17-C16-C15	2.11	103.72	114.37	13	1
3	C	362	PX4	O7-C7-C8	2.11	115.90	108.34	11	1
3	C	367	PX4	C1-C2-N1	2.11	122.58	115.82	8	1
3	B	313	PX4	C26-C25-C24	2.11	105.39	113.13	8	1
3	B	317	PX4	O4-P1-O2	2.11	100.59	108.94	8	1
3	B	330	PX4	O8-C23-C24	2.11	132.02	123.78	5	1
3	A	607	PX4	C11-C10-C9	2.10	121.41	113.69	10	1
3	B	378	PX4	C12-C11-C10	2.10	120.86	113.13	10	1
3	B	390	PX4	O7-C23-O8	2.11	128.63	123.70	4	1
3	B	391	PX4	C8-C7-C6	2.10	116.69	111.78	3	1
3	B	374	PX4	C28-C27-C26	2.10	103.73	114.37	1	1
3	C	304	PX4	C19-C18-C17	2.10	103.73	114.37	13	1
3	C	317	PX4	P1-O4-C6	2.10	133.41	121.35	13	1
3	C	334	PX4	O5-C9-C10	2.10	105.42	111.83	12	1
3	A	633	PX4	O3-P1-O2	2.10	100.60	108.94	10	2
3	A	632	PX4	C11-C10-C9	2.10	121.40	113.69	9	1
3	A	647	PX4	O8-C23-C24	2.10	132.01	123.78	5	2
3	C	302	PX4	C34-C33-C32	2.10	103.74	114.37	9	1
3	C	339	PX4	C30-C29-C28	2.10	103.74	114.37	6	1
3	A	614	PX4	C26-C25-C24	2.10	120.85	113.13	7	2
3	A	614	PX4	O3-P1-O2	2.10	100.61	108.94	9	1
3	B	383	PX4	O7-C7-C6	2.10	100.81	108.34	7	1
3	C	301	PX4	C7-O7-C23	2.10	112.77	117.80	5	1
3	C	352	PX4	C5-N1-C3	2.10	103.45	108.98	2	2
3	C	362	PX4	C33-C32-C31	2.10	103.74	114.37	10	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	C	367	PX4	C13-C12-C11	2.10	103.74	114.37	6	1
3	B	347	PX4	C5-N1-C4	2.10	103.46	108.98	12	1
3	A	640	PX4	O5-C9-C10	2.10	105.43	111.83	10	1
3	B	366	PX4	O7-C7-C8	2.10	115.88	108.34	8	1
3	C	304	PX4	C1-C2-N1	2.10	122.56	115.82	3	1
3	B	315	PX4	O3-C1-C2	2.10	119.75	109.65	2	1
3	A	608	PX4	O7-C23-O8	2.10	128.61	123.70	13	1
3	A	616	PX4	C8-C7-C6	2.10	106.90	111.78	3	1
3	A	626	PX4	O1-P1-O2	2.10	122.20	112.44	3	1
3	C	335	PX4	O1-P1-O2	2.10	122.21	112.44	3	1
3	C	346	PX4	O5-C9-O6	2.10	128.88	123.63	11	1
3	C	351	PX4	C5-N1-C4	2.10	103.46	108.98	14	1
3	A	611	PX4	C8-C7-C6	2.10	116.67	111.78	11	3
3	B	311	PX4	O5-C9-C10	2.10	105.44	111.83	6	1
3	B	353	PX4	O5-C9-C10	2.10	105.44	111.83	8	1
3	B	377	PX4	C4-N1-C2	2.10	118.24	109.91	6	1
3	B	395	PX4	C3-N1-C2	2.10	101.58	109.91	2	1
3	C	313	PX4	C25-C24-C23	2.10	121.37	113.69	4	1
3	C	317	PX4	O4-P1-O2	2.10	117.24	108.94	7	1
3	C	318	PX4	C20-C19-C18	2.10	103.77	114.37	1	1
3	B	356	PX4	C25-C24-C23	2.10	121.37	113.69	7	2
3	C	359	PX4	O1-P1-O2	2.10	122.20	112.44	2	1
3	A	633	PX4	O6-C9-C10	2.09	131.97	123.78	11	1
3	A	642	PX4	C17-C16-C15	2.09	124.95	114.37	8	1
3	B	312	PX4	O1-P1-O3	2.09	117.06	107.57	11	1
3	B	338	PX4	P1-O3-C1	2.09	131.23	121.26	9	1
3	B	375	PX4	C28-C27-C26	2.09	103.79	114.37	6	1
3	B	376	PX4	O5-C9-C10	2.09	105.45	111.83	4	1
3	B	384	PX4	O7-C7-C6	2.09	100.83	108.34	6	1
3	B	389	PX4	C29-C28-C27	2.09	103.78	114.37	1	1
3	C	309	PX4	C25-C24-C23	2.09	106.02	113.69	7	1
3	C	329	PX4	O3-P1-O2	2.09	117.24	108.94	9	1
3	B	397	PX4	C5-N1-C3	2.09	114.47	108.98	7	1
3	C	338	PX4	C34-C33-C32	2.09	103.78	114.37	1	1
3	A	608	PX4	C29-C28-C27	2.09	103.80	114.37	8	1
3	A	608	PX4	C4-N1-C2	2.09	118.22	109.91	15	1
3	B	313	PX4	O7-C23-C24	2.09	106.96	111.48	1	1
3	B	317	PX4	O1-P1-O2	2.09	122.17	112.44	2	1
3	B	321	PX4	P1-O4-C6	2.09	133.33	121.35	15	1
3	B	328	PX4	C1-C2-N1	2.09	122.53	115.82	8	1
3	A	627	PX4	C4-N1-C2	2.09	118.21	109.91	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	647	PX4	O3-C1-C2	2.09	99.60	109.65	5	1
3	B	316	PX4	O1-P1-O2	2.09	122.16	112.44	13	1
3	C	301	PX4	C11-C10-C9	2.09	106.03	113.69	8	1
3	C	303	PX4	C26-C25-C24	2.09	105.45	113.13	15	1
3	C	342	PX4	C5-N1-C2	2.09	118.22	109.91	5	1
3	C	347	PX4	C5-N1-C2	2.09	101.61	109.91	10	1
3	C	360	PX4	C19-C18-C17	2.09	103.80	114.37	5	1
3	B	339	PX4	C5-N1-C4	2.09	114.46	108.98	2	1
3	B	301	PX4	C8-O5-C9	2.09	109.49	117.12	7	1
3	B	318	PX4	C30-C29-C28	2.09	103.82	114.37	13	1
3	B	396	PX4	C12-C11-C10	2.09	105.46	113.13	13	1
3	C	307	PX4	O1-P1-O2	2.09	122.15	112.44	4	1
3	C	310	PX4	P1-O3-C1	2.09	131.20	121.26	9	1
3	C	352	PX4	P1-O4-C6	2.09	109.39	121.35	9	1
3	C	302	PX4	O3-C1-C2	2.09	119.69	109.65	12	1
3	A	623	PX4	C4-N1-C3	2.08	114.45	108.98	9	1
3	A	624	PX4	O3-C1-C2	2.08	119.67	109.65	14	1
3	B	302	PX4	O3-C1-C2	2.08	119.68	109.65	1	1
3	B	307	PX4	C26-C25-C24	2.08	120.78	113.13	14	1
3	B	340	PX4	C26-C25-C24	2.08	120.78	113.13	11	1
3	C	313	PX4	C13-C12-C11	2.09	103.83	114.37	1	1
3	B	386	PX4	C1-C2-N1	2.08	122.51	115.82	1	1
3	B	389	PX4	C11-C10-C9	2.09	121.33	113.69	5	1
3	C	302	PX4	P1-O4-C6	2.08	133.29	121.35	2	1
3	C	304	PX4	P1-O3-C1	2.08	111.34	121.26	15	1
3	C	308	PX4	C5-N1-C2	2.08	118.20	109.91	14	1
3	A	643	PX4	O8-C23-C24	2.08	131.93	123.78	12	1
3	B	358	PX4	C27-C26-C25	2.08	103.84	114.37	11	1
3	C	342	PX4	O6-C9-C10	2.08	131.93	123.78	11	1
3	B	312	PX4	C12-C11-C10	2.08	105.48	113.13	2	1
3	C	359	PX4	O5-C9-C10	2.08	105.49	111.83	14	1
3	A	633	PX4	C14-C13-C12	2.08	103.85	114.37	3	1
3	B	375	PX4	C12-C11-C10	2.08	105.48	113.13	11	1
3	B	396	PX4	C4-N1-C3	2.08	103.51	108.98	9	1
3	C	301	PX4	C8-C7-C6	2.08	116.64	111.78	6	1
3	C	323	PX4	C16-C15-C14	2.08	103.85	114.37	8	1
3	B	348	PX4	O3-C1-C2	2.08	119.66	109.65	13	1
3	A	604	PX4	C34-C33-C32	2.08	124.87	114.37	13	1
3	B	360	PX4	C5-N1-C4	2.08	103.51	108.98	4	1
3	C	330	PX4	C8-O5-C9	2.08	109.52	117.12	5	1
3	C	349	PX4	C26-C25-C24	2.08	120.77	113.13	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	C	357	PX4	C8-O5-C9	2.08	109.52	117.12	13	1
3	B	337	PX4	O3-C1-C2	2.08	119.64	109.65	3	1
3	C	367	PX4	C5-N1-C4	2.08	114.44	108.98	3	1
3	B	368	PX4	C32-C31-C30	2.08	103.87	114.37	13	1
3	C	307	PX4	C27-C26-C25	2.08	103.87	114.37	8	1
3	A	621	PX4	O7-C7-C6	2.08	115.79	108.34	2	1
3	B	311	PX4	P1-O3-C1	2.07	131.14	121.26	2	1
3	B	314	PX4	C29-C28-C27	2.07	103.88	114.37	8	1
3	B	352	PX4	O4-P1-O2	2.08	100.71	108.94	13	1
3	B	359	PX4	C8-C7-C6	2.08	116.62	111.78	1	1
3	B	369	PX4	C5-N1-C4	2.07	103.53	108.98	14	1
3	B	389	PX4	O5-C9-C10	2.08	118.16	111.83	3	2
3	C	303	PX4	C30-C29-C28	2.08	103.88	114.37	14	1
3	C	312	PX4	O3-C1-C2	2.08	119.64	109.65	14	1
3	C	368	PX4	C1-C2-N1	2.08	122.49	115.82	8	1
3	C	331	PX4	O7-C7-C6	2.07	115.79	108.34	5	1
3	C	339	PX4	C28-C27-C26	2.08	103.88	114.37	4	1
3	C	305	PX4	C5-N1-C4	2.07	103.53	108.98	15	1
3	C	318	PX4	C25-C24-C23	2.07	106.10	113.69	5	1
3	C	338	PX4	O7-C7-C6	2.07	100.91	108.34	7	1
3	C	342	PX4	C28-C27-C26	2.07	124.85	114.37	14	1
3	B	325	PX4	C25-C24-C23	2.07	106.10	113.69	5	1
3	B	337	PX4	O7-C7-C6	2.07	115.78	108.34	13	2
3	C	357	PX4	O3-C1-C2	2.07	119.62	109.65	7	1
3	C	357	PX4	C3-N1-C2	2.07	118.15	109.91	11	1
3	A	610	PX4	C32-C31-C30	2.07	103.90	114.37	4	1
3	A	613	PX4	C12-C11-C10	2.07	120.74	113.13	8	2
3	A	626	PX4	C4-N1-C3	2.07	114.41	108.98	2	1
3	A	643	PX4	O7-C7-C6	2.07	115.77	108.34	13	1
3	B	322	PX4	O5-C8-C7	2.07	114.37	108.40	11	1
3	B	329	PX4	C11-C10-C9	2.07	106.11	113.69	10	1
3	B	341	PX4	O1-P1-O2	2.07	122.08	112.44	7	1
3	C	304	PX4	C3-N1-C2	2.07	118.14	109.91	2	1
3	C	336	PX4	C1-C2-N1	2.07	122.47	115.82	2	1
3	C	332	PX4	C11-C10-C9	2.07	106.11	113.69	14	1
3	A	648	PX4	O4-P1-O2	2.07	100.73	108.94	8	1
3	B	301	PX4	P1-O3-C1	2.07	131.11	121.26	12	2
3	B	320	PX4	O1-P1-O3	2.07	116.94	107.57	11	1
3	B	392	PX4	C8-O5-C9	2.07	109.56	117.12	5	1
3	C	363	PX4	C29-C28-C27	2.07	103.91	114.37	12	1
3	B	384	PX4	O5-C9-O6	2.07	128.80	123.63	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	615	PX4	C26-C25-C24	2.07	105.54	113.13	4	1
3	B	307	PX4	C25-C24-C23	2.07	121.27	113.69	6	1
3	A	619	PX4	C8-O5-C9	2.06	109.57	117.12	2	1
3	B	311	PX4	O8-C23-C24	2.07	115.70	123.78	15	1
3	B	317	PX4	C34-C33-C32	2.07	103.93	114.37	4	1
3	B	385	PX4	C4-N1-C2	2.07	118.12	109.91	14	1
3	B	346	PX4	P1-O3-C1	2.06	111.44	121.26	12	1
3	B	351	PX4	C5-N1-C2	2.06	101.70	109.91	13	1
3	C	313	PX4	C26-C25-C24	2.06	105.54	113.13	6	1
3	C	352	PX4	C4-N1-C3	2.06	114.40	108.98	5	1
3	B	367	PX4	C8-C7-C6	2.06	106.97	111.78	5	1
3	B	380	PX4	C33-C32-C31	2.06	103.94	114.37	14	1
3	B	385	PX4	C1-C2-N1	2.06	122.44	115.82	15	1
3	B	396	PX4	O5-C9-O6	2.06	118.47	123.63	6	1
3	C	332	PX4	C8-O5-C9	2.06	109.58	117.12	7	1
3	C	335	PX4	O7-C7-C6	2.06	115.75	108.34	13	1
3	B	322	PX4	C8-O5-C9	2.06	109.58	117.12	10	1
3	C	337	PX4	C11-C10-C9	2.06	121.25	113.69	6	1
3	A	606	PX4	C16-C15-C14	2.06	103.95	114.37	5	1
3	A	632	PX4	C4-N1-C3	2.06	103.56	108.98	14	1
3	B	307	PX4	C34-C33-C32	2.06	103.95	114.37	14	1
3	B	327	PX4	C11-C10-C9	2.06	106.14	113.69	2	1
3	B	391	PX4	C4-N1-C3	2.06	103.56	108.98	13	1
3	B	395	PX4	C14-C13-C12	2.06	124.79	114.37	5	1
3	C	301	PX4	C12-C11-C10	2.06	120.70	113.13	5	1
3	C	316	PX4	C8-O5-C9	2.06	124.65	117.12	8	1
3	C	317	PX4	C27-C26-C25	2.06	103.95	114.37	8	1
3	C	344	PX4	C11-C10-C9	2.06	106.14	113.69	8	1
3	B	358	PX4	O7-C7-C8	2.06	115.74	108.34	6	1
3	B	386	PX4	C27-C26-C25	2.06	103.95	114.37	2	1
3	C	309	PX4	C8-C7-C6	2.06	116.59	111.78	8	1
3	B	312	PX4	O5-C9-O6	2.06	128.78	123.63	1	1
3	B	368	PX4	C1-C2-N1	2.06	122.43	115.82	15	1
3	B	374	PX4	O1-P1-O2	2.06	122.02	112.44	3	1
3	A	615	PX4	C4-N1-C3	2.06	114.38	108.98	1	2
3	B	321	PX4	C26-C25-C24	2.06	120.69	113.13	10	1
3	B	358	PX4	O7-C7-C6	2.06	115.73	108.34	2	1
3	C	370	PX4	O7-C7-C6	2.06	115.73	108.34	6	1
3	A	610	PX4	C34-C33-C32	2.05	103.98	114.37	8	1
3	A	632	PX4	C31-C30-C29	2.06	103.98	114.37	11	1
3	A	633	PX4	O1-P1-O3	2.06	116.89	107.57	10	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	646	PX4	C26-C25-C24	2.06	120.68	113.13	15	1
3	C	311	PX4	C8-O5-C9	2.06	109.60	117.12	15	1
3	C	329	PX4	C26-C25-C24	2.06	105.57	113.13	9	1
3	A	645	PX4	O7-C23-O8	2.06	128.51	123.70	8	2
3	B	305	PX4	P1-O3-C1	2.06	131.05	121.26	5	2
3	B	333	PX4	C26-C25-C24	2.05	105.58	113.13	13	1
3	B	344	PX4	O5-C9-O6	2.06	128.77	123.63	1	1
3	B	380	PX4	C20-C19-C18	2.06	103.97	114.37	8	1
3	C	353	PX4	C20-C19-C18	2.06	103.97	114.37	9	1
3	A	605	PX4	C8-O5-C9	2.05	109.61	117.12	9	1
3	A	613	PX4	O1-P1-O3	2.05	116.88	107.57	14	1
3	B	390	PX4	C16-C15-C14	2.05	103.98	114.37	13	1
3	B	400	PX4	C8-O5-C9	2.05	109.61	117.12	8	1
3	C	323	PX4	C18-C17-C16	2.05	103.98	114.37	10	1
3	C	341	PX4	O7-C7-C6	2.05	100.97	108.34	13	1
3	C	344	PX4	C25-C24-C23	2.06	106.16	113.69	12	1
3	C	355	PX4	C26-C25-C24	2.05	105.58	113.13	13	1
3	A	643	PX4	C12-C11-C10	2.05	105.58	113.13	4	1
3	B	319	PX4	C22-C21-C20	2.05	127.23	113.36	4	1
3	B	339	PX4	C8-O5-C9	2.05	109.61	117.12	6	1
3	B	400	PX4	P1-O3-C1	2.05	131.03	121.26	2	1
3	C	353	PX4	C5-N1-C4	2.05	103.58	108.98	3	1
3	A	618	PX4	C4-N1-C3	2.05	114.37	108.98	2	1
3	B	330	PX4	O5-C9-O6	2.05	128.76	123.63	13	2
3	B	308	PX4	C17-C16-C15	2.05	124.73	114.37	12	2
3	B	318	PX4	C5-N1-C2	2.05	118.06	109.91	7	1
3	C	311	PX4	C5-N1-C3	2.05	103.58	108.98	1	1
3	C	315	PX4	O1-P1-O4	2.05	116.87	107.57	8	1
3	A	604	PX4	C8-O5-C9	2.05	109.62	117.12	8	1
3	B	352	PX4	O1-P1-O4	2.05	116.86	107.57	3	1
3	B	358	PX4	C4-N1-C3	2.05	103.59	108.98	9	1
3	C	313	PX4	O7-C23-O8	2.05	128.50	123.70	12	2
3	C	346	PX4	C25-C24-C23	2.05	121.21	113.69	2	1
3	C	368	PX4	O7-C23-O8	2.05	128.50	123.70	4	1
3	A	634	PX4	C25-C24-C23	2.05	121.20	113.69	6	3
3	A	639	PX4	O3-C1-C2	2.05	119.51	109.65	7	1
3	B	330	PX4	O5-C9-C10	2.05	105.58	111.83	6	1
3	B	309	PX4	C26-C25-C24	2.05	105.60	113.13	14	1
3	B	359	PX4	C1-C2-N1	2.05	122.40	115.82	4	1
3	B	376	PX4	C16-C15-C14	2.05	104.01	114.37	14	1
3	B	393	PX4	C31-C30-C29	2.05	104.01	114.37	10	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	C	301	PX4	C26-C25-C24	2.05	105.60	113.13	9	1
3	C	346	PX4	C5-N1-C3	2.05	103.59	108.98	5	1
3	C	366	PX4	C18-C17-C16	2.05	104.01	114.37	1	1
3	A	620	PX4	C8-C7-C6	2.05	116.56	111.78	9	1
3	A	641	PX4	C25-C24-C23	2.05	106.19	113.69	14	1
3	C	337	PX4	P1-O4-C6	2.05	133.09	121.35	2	1
3	C	366	PX4	C12-C11-C10	2.05	105.60	113.13	10	1
3	C	367	PX4	O7-C7-C8	2.05	115.69	108.34	14	1
3	B	302	PX4	C15-C14-C13	2.05	104.02	114.37	3	1
3	B	318	PX4	O7-C23-O8	2.05	128.49	123.70	12	1
3	B	318	PX4	C5-N1-C4	2.05	103.60	108.98	15	1
3	B	351	PX4	P1-O3-C1	2.05	131.01	121.26	7	1
3	B	353	PX4	C26-C25-C24	2.05	120.65	113.13	13	1
3	B	383	PX4	O5-C9-O6	2.05	128.75	123.63	1	1
3	C	311	PX4	O1-P1-O2	2.05	121.97	112.44	11	1
3	C	314	PX4	C19-C18-C17	2.05	104.02	114.37	6	1
3	C	323	PX4	C25-C24-C23	2.05	106.19	113.69	15	1
3	C	349	PX4	C5-N1-C4	2.05	103.60	108.98	14	1
3	A	619	PX4	O7-C7-C6	2.05	115.68	108.34	4	1
3	A	632	PX4	C30-C29-C28	2.05	104.03	114.37	15	2
3	A	635	PX4	C28-C27-C26	2.05	104.03	114.37	12	1
3	A	648	PX4	C12-C11-C10	2.05	105.61	113.13	4	1
3	A	612	PX4	O1-P1-O2	2.04	121.95	112.44	2	1
3	A	619	PX4	C27-C26-C25	2.04	104.03	114.37	13	1
3	B	313	PX4	C4-N1-C3	2.05	103.60	108.98	2	1
3	B	313	PX4	O7-C7-C6	2.05	101.01	108.34	3	2
3	C	310	PX4	C17-C16-C15	2.05	104.03	114.37	12	1
3	C	321	PX4	P1-O3-C1	2.04	111.53	121.26	4	1
3	C	367	PX4	C20-C19-C18	2.05	104.03	114.37	1	1
3	B	302	PX4	C26-C25-C24	2.04	105.62	113.13	14	1
3	B	341	PX4	C11-C10-C9	2.04	106.20	113.69	14	1
3	B	356	PX4	C17-C16-C15	2.04	104.03	114.37	10	1
3	B	343	PX4	C17-C16-C15	2.04	104.04	114.37	9	1
3	B	345	PX4	C32-C31-C30	2.04	104.04	114.37	15	1
3	A	641	PX4	O5-C9-O6	2.04	118.52	123.63	15	1
3	A	648	PX4	O1-P1-O4	2.04	116.82	107.57	11	1
3	A	615	PX4	O1-P1-O2	2.04	121.94	112.44	5	1
3	A	617	PX4	C11-C10-C9	2.04	106.22	113.69	4	1
3	A	646	PX4	C17-C16-C15	2.04	104.05	114.37	1	1
3	B	396	PX4	O3-C1-C2	2.04	119.47	109.65	3	1
3	B	399	PX4	C5-N1-C2	2.04	118.02	109.91	12	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	C	324	PX4	C8-C7-C6	2.04	107.03	111.78	14	1
3	C	339	PX4	C26-C25-C24	2.04	120.63	113.13	9	1
3	C	301	PX4	O4-P1-O2	2.04	100.85	108.94	14	1
3	C	348	PX4	C12-C11-C10	2.04	105.63	113.13	11	1
3	C	349	PX4	O1-P1-O2	2.04	121.94	112.44	10	1
3	C	316	PX4	C4-N1-C2	2.04	118.02	109.91	15	1
3	C	365	PX4	O7-C7-C8	2.04	115.67	108.34	8	1
3	A	602	PX4	O6-C9-C10	2.04	115.81	123.78	9	1
3	A	607	PX4	O7-C7-C8	2.04	115.66	108.34	12	1
3	A	624	PX4	O7-C7-C6	2.04	115.66	108.34	7	1
3	A	642	PX4	C25-C24-C23	2.04	106.22	113.69	7	1
3	A	645	PX4	C5-N1-C3	2.04	103.62	108.98	11	1
3	B	317	PX4	P1-O3-C1	2.04	111.55	121.26	2	1
3	A	616	PX4	O5-C9-C10	2.04	105.62	111.83	15	1
3	A	636	PX4	O7-C7-C8	2.04	115.65	108.34	15	1
3	A	644	PX4	C19-C18-C17	2.04	104.07	114.37	13	1
3	B	317	PX4	C7-O7-C23	2.04	112.92	117.80	9	2
3	B	367	PX4	C11-C10-C9	2.04	106.22	113.69	5	1
3	B	382	PX4	C27-C26-C25	2.04	104.06	114.37	11	1
3	C	308	PX4	O7-C7-C8	2.04	115.66	108.34	2	3
3	C	312	PX4	O1-P1-O2	2.04	121.93	112.44	14	1
3	B	311	PX4	C30-C29-C28	2.04	104.07	114.37	6	1
3	B	337	PX4	O5-C9-C10	2.04	105.62	111.83	6	2
3	B	341	PX4	C3-N1-C2	2.04	101.81	109.91	14	1
3	C	330	PX4	C31-C30-C29	2.04	104.06	114.37	14	1
3	C	361	PX4	C5-N1-C4	2.04	114.33	108.98	13	1
3	B	376	PX4	C5-N1-C4	2.04	103.62	108.98	7	1
3	B	399	PX4	C4-N1-C2	2.04	101.81	109.91	15	1
3	A	623	PX4	C4-N1-C2	2.04	101.81	109.91	4	1
3	B	308	PX4	C5-N1-C4	2.04	103.63	108.98	5	1
3	B	364	PX4	C12-C11-C10	2.04	120.61	113.13	11	1
3	B	367	PX4	C12-C11-C10	2.04	105.64	113.13	9	1
3	C	317	PX4	C15-C14-C13	2.04	104.07	114.37	15	1
3	C	328	PX4	C12-C11-C10	2.04	105.64	113.13	11	2
3	A	609	PX4	C34-C33-C32	2.03	104.09	114.37	14	1
3	A	634	PX4	C26-C25-C24	2.03	105.65	113.13	14	1
3	B	337	PX4	P1-O4-C6	2.03	133.01	121.35	11	1
3	B	373	PX4	O4-P1-O2	2.03	100.87	108.94	10	1
3	A	632	PX4	O7-C23-O8	2.03	128.46	123.70	10	1
3	A	611	PX4	C11-C10-C9	2.03	106.25	113.69	8	1
3	A	614	PX4	C1-C2-N1	2.03	122.35	115.82	15	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	305	PX4	O4-P1-O2	2.03	116.99	108.94	5	1
3	B	327	PX4	O3-C1-C2	2.03	99.87	109.65	12	1
3	B	340	PX4	O7-C7-C8	2.03	115.64	108.34	15	1
3	B	392	PX4	O1-P1-O2	2.03	121.91	112.44	8	1
3	B	397	PX4	O7-C7-C6	2.03	115.64	108.34	8	1
3	C	327	PX4	C8-O5-C9	2.03	109.69	117.12	10	1
3	B	371	PX4	O3-P1-O2	2.03	116.99	108.94	2	1
3	C	322	PX4	C34-C33-C32	2.03	104.10	114.37	4	1
3	C	345	PX4	C5-N1-C2	2.03	117.99	109.91	8	1
3	A	639	PX4	O7-C23-O8	2.03	128.45	123.70	6	1
3	B	324	PX4	O6-C9-C10	2.03	131.72	123.78	10	1
3	C	310	PX4	C5-N1-C3	2.03	103.64	108.98	7	1
3	C	327	PX4	C25-C24-C23	2.03	106.25	113.69	4	1
3	A	602	PX4	C27-C26-C25	2.03	104.12	114.37	6	1
3	A	615	PX4	C27-C26-C25	2.03	104.11	114.37	14	1
3	A	611	PX4	C17-C16-C15	2.03	104.12	114.37	10	1
3	A	632	PX4	O7-C7-C8	2.03	101.07	108.34	7	1
3	B	353	PX4	C3-N1-C2	2.03	117.97	109.91	12	1
3	B	358	PX4	C5-N1-C3	2.03	114.31	108.98	14	1
3	C	337	PX4	O4-P1-O2	2.03	100.89	108.94	5	1
3	C	323	PX4	C26-C25-C24	2.03	105.68	113.13	7	1
3	C	341	PX4	C8-O5-C9	2.03	109.70	117.12	9	1
3	C	350	PX4	O1-P1-O2	2.03	121.88	112.44	3	1
3	B	305	PX4	C8-O5-C9	2.03	124.53	117.12	5	1
3	A	609	PX4	C8-O5-C9	2.03	109.71	117.12	14	1
3	A	627	PX4	C18-C17-C16	2.03	104.12	114.37	9	1
3	B	348	PX4	C4-N1-C2	2.03	101.85	109.91	2	1
3	B	349	PX4	P1-O3-C1	2.03	111.61	121.26	13	1
3	A	614	PX4	C27-C26-C25	2.03	104.13	114.37	10	1
3	A	626	PX4	C18-C17-C16	2.03	104.13	114.37	6	1
3	B	313	PX4	C1-C2-N1	2.03	122.33	115.82	2	1
3	B	319	PX4	C8-O5-C9	2.03	109.71	117.12	5	1
3	B	355	PX4	O5-C9-O6	2.03	128.70	123.63	6	1
3	B	364	PX4	C3-N1-C2	2.03	101.85	109.91	3	2
3	C	366	PX4	C31-C30-C29	2.03	104.12	114.37	8	1
3	A	646	PX4	C12-C11-C10	2.02	120.57	113.13	4	1
3	B	307	PX4	C5-N1-C4	2.02	103.66	108.98	7	2
3	A	619	PX4	O7-C23-O8	2.02	118.97	123.70	15	1
3	A	620	PX4	C1-C2-N1	2.02	122.32	115.82	9	1
3	B	316	PX4	O3-C1-C2	2.02	99.91	109.65	12	1
3	B	321	PX4	C29-C28-C27	2.02	104.13	114.37	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	370	PX4	O4-P1-O2	2.03	116.96	108.94	13	1
3	B	393	PX4	O1-P1-O2	2.02	121.86	112.44	14	1
3	A	623	PX4	C5-N1-C3	2.02	103.66	108.98	6	1
3	C	349	PX4	O7-C7-C8	2.02	115.61	108.34	2	1
3	C	358	PX4	P1-O4-C6	2.02	132.95	121.35	7	1
3	B	364	PX4	O7-C23-O8	2.02	128.44	123.70	11	1
3	C	369	PX4	O5-C9-C10	2.02	105.67	111.83	13	1
3	A	605	PX4	C13-C12-C11	2.02	104.15	114.37	7	1
3	A	608	PX4	C5-N1-C2	2.02	117.95	109.91	5	1
3	A	627	PX4	C26-C25-C24	2.02	105.70	113.13	3	1
3	A	639	PX4	C11-C10-C9	2.02	106.29	113.69	13	1
3	A	646	PX4	P1-O3-C1	2.02	111.64	121.26	4	1
3	B	326	PX4	C25-C24-C23	2.02	106.29	113.69	3	1
3	B	332	PX4	O6-C9-C10	2.02	131.69	123.78	10	1
3	B	347	PX4	C1-C2-N1	2.02	122.31	115.82	11	1
3	B	354	PX4	O1-P1-O2	2.02	121.85	112.44	5	1
3	B	372	PX4	C12-C11-C10	2.02	120.56	113.13	8	1
3	B	368	PX4	O5-C8-C7	2.02	114.22	108.40	7	1
3	C	318	PX4	C1-C2-N1	2.02	122.31	115.82	2	1
3	C	335	PX4	O7-C23-O8	2.02	128.43	123.70	12	1
3	C	340	PX4	C5-N1-C4	2.02	103.67	108.98	4	1
3	C	323	PX4	P1-O3-C1	2.02	111.64	121.26	4	1
3	C	327	PX4	O6-C9-C10	2.02	131.69	123.78	8	1
3	C	342	PX4	C32-C31-C30	2.02	124.58	114.37	6	1
3	C	367	PX4	O1-P1-O2	2.02	121.85	112.44	1	1
3	A	626	PX4	C12-C11-C10	2.02	120.55	113.13	9	1
3	A	636	PX4	C4-N1-C3	2.02	103.67	108.98	14	1
3	A	640	PX4	P1-O3-C1	2.02	130.87	121.26	7	1
3	B	329	PX4	O7-C7-C8	2.02	115.59	108.34	10	1
3	B	398	PX4	O1-P1-O3	2.02	116.72	107.57	12	1
3	C	325	PX4	C13-C12-C11	2.02	104.16	114.37	2	1
3	C	346	PX4	O3-P1-O2	2.02	116.94	108.94	12	1
3	C	363	PX4	O8-C23-C24	2.02	131.68	123.78	7	1
3	B	309	PX4	O7-C7-C8	2.02	115.58	108.34	11	1
3	A	602	PX4	C11-C10-C9	2.02	121.08	113.69	14	1
3	A	616	PX4	O8-C23-C24	2.02	115.89	123.78	10	1
3	A	631	PX4	O5-C9-O6	2.02	128.67	123.63	12	1
3	A	633	PX4	O7-C7-C8	2.02	115.58	108.34	2	2
3	A	623	PX4	C20-C19-C18	2.02	104.18	114.37	12	1
3	A	624	PX4	C4-N1-C3	2.02	103.68	108.98	15	1
3	B	308	PX4	C11-C10-C9	2.02	106.31	113.69	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	310	PX4	C5-N1-C2	2.02	101.90	109.91	8	1
3	B	334	PX4	C4-N1-C3	2.02	103.68	108.98	5	1
3	B	340	PX4	C4-N1-C3	2.02	103.68	108.98	13	1
3	B	346	PX4	C30-C29-C28	2.02	104.17	114.37	5	1
3	B	353	PX4	C19-C18-C17	2.02	104.17	114.37	2	1
3	B	399	PX4	C8-O5-C9	2.02	124.49	117.12	1	1
3	C	316	PX4	C5-N1-C2	2.02	117.93	109.91	7	1
3	C	317	PX4	O1-P1-O2	2.02	121.83	112.44	8	1
3	A	647	PX4	C15-C14-C13	2.02	104.18	114.37	11	1
3	B	306	PX4	O1-P1-O2	2.02	121.82	112.44	9	1
3	B	349	PX4	O6-C9-C10	2.02	131.66	123.78	15	1
3	C	341	PX4	O1-P1-O2	2.02	121.82	112.44	12	1
3	C	343	PX4	C30-C29-C28	2.02	124.56	114.37	10	1
3	B	317	PX4	C5-N1-C4	2.01	103.69	108.98	8	2
3	B	326	PX4	O5-C9-O6	2.01	128.66	123.63	13	1
3	B	346	PX4	O5-C8-C7	2.01	114.20	108.40	1	1
3	B	365	PX4	C31-C30-C29	2.01	104.19	114.37	14	1
3	B	367	PX4	C7-O7-C23	2.01	112.98	117.80	4	1
3	B	375	PX4	C36-C35-C34	2.01	126.96	113.36	3	1
3	C	308	PX4	C20-C19-C18	2.01	104.19	114.37	14	1
3	C	321	PX4	C5-N1-C3	2.01	103.69	108.98	1	1
3	C	327	PX4	O5-C9-C10	2.01	105.69	111.83	14	1
3	B	375	PX4	O7-C7-C8	2.01	115.56	108.34	2	1
3	B	390	PX4	O8-C23-C24	2.01	131.65	123.78	7	1
3	C	341	PX4	C5-N1-C2	2.01	117.91	109.91	15	1
3	B	341	PX4	O8-C23-C24	2.01	131.65	123.78	1	1
3	A	603	PX4	C8-O5-C9	2.01	109.77	117.12	6	1
3	A	622	PX4	C15-C14-C13	2.01	104.21	114.37	14	1
3	A	637	PX4	C26-C25-C24	2.01	105.74	113.13	7	1
3	B	340	PX4	C20-C19-C18	2.01	124.53	114.37	10	1
3	B	371	PX4	C5-N1-C3	2.01	103.69	108.98	12	1
3	B	391	PX4	O5-C9-C10	2.01	105.70	111.83	10	1
3	C	342	PX4	C1-C2-N1	2.01	122.28	115.82	7	1
3	B	335	PX4	O7-C7-C8	2.01	115.55	108.34	15	1
3	B	361	PX4	C15-C14-C13	2.01	104.21	114.37	11	1
3	B	371	PX4	O7-C23-O8	2.01	119.01	123.70	12	1
3	B	380	PX4	C5-N1-C4	2.01	103.70	108.98	7	1
3	B	392	PX4	C5-N1-C2	2.01	117.90	109.91	9	1
3	B	396	PX4	C27-C26-C25	2.01	124.53	114.37	4	1
3	C	365	PX4	C33-C32-C31	2.01	104.20	114.37	6	1
3	B	324	PX4	C4-N1-C3	2.01	114.25	108.98	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	328	PX4	C25-C24-C23	2.01	106.33	113.69	6	1
3	C	311	PX4	P1-O3-C1	2.01	130.82	121.26	10	1
3	C	327	PX4	O8-C23-C24	2.01	131.64	123.78	10	1
3	C	342	PX4	O7-C7-C6	2.01	115.55	108.34	4	1
3	C	359	PX4	C5-N1-C2	2.01	101.92	109.91	11	1
3	B	304	PX4	O7-C23-O8	2.01	128.40	123.70	12	1
3	B	305	PX4	C28-C27-C26	2.01	104.22	114.37	4	1
3	B	307	PX4	O6-C9-C10	2.01	131.63	123.78	12	1
3	B	391	PX4	C5-N1-C4	2.01	103.70	108.98	4	1
3	C	329	PX4	C11-C10-C9	2.01	106.34	113.69	5	1
3	C	330	PX4	O7-C7-C6	2.01	101.14	108.34	15	1
3	C	356	PX4	O6-C9-C10	2.01	131.63	123.78	7	1
3	A	605	PX4	C4-N1-C3	2.01	103.71	108.98	4	1
3	A	617	PX4	O6-C9-C10	2.00	115.94	123.78	7	1
3	A	635	PX4	O5-C9-C10	2.01	105.72	111.83	12	1
3	B	339	PX4	C12-C11-C10	2.01	105.76	113.13	6	1
3	B	341	PX4	C5-N1-C3	2.01	103.71	108.98	5	1
3	B	348	PX4	C25-C24-C23	2.01	106.35	113.69	2	1
3	C	308	PX4	O7-C23-O8	2.01	128.40	123.70	2	1
3	B	376	PX4	C8-O5-C9	2.00	109.79	117.12	14	1
3	B	385	PX4	O3-C1-C2	2.01	119.30	109.65	12	1
3	B	389	PX4	O7-C7-C6	2.01	101.15	108.34	6	1
3	C	354	PX4	C1-C2-N1	2.01	122.26	115.82	11	1
3	A	622	PX4	C33-C32-C31	2.00	124.50	114.37	12	1
3	B	309	PX4	C4-N1-C3	2.00	103.72	108.98	4	1
3	B	310	PX4	C5-N1-C3	2.00	114.24	108.98	10	1
3	B	339	PX4	C11-C10-C9	2.00	121.04	113.69	6	1
3	B	355	PX4	C15-C14-C13	2.00	104.24	114.37	9	1
3	C	330	PX4	O1-P1-O2	2.00	121.76	112.44	5	1
3	C	354	PX4	O1-P1-O2	2.00	121.77	112.44	13	1
3	C	312	PX4	C8-O5-C9	2.00	124.44	117.12	2	1
3	A	620	PX4	C27-C26-C25	2.00	104.25	114.37	14	1
3	A	642	PX4	O4-P1-O2	2.00	116.87	108.94	13	1
3	C	303	PX4	C34-C33-C32	2.00	104.25	114.37	13	1
3	B	377	PX4	C8-O5-C9	2.00	109.81	117.12	1	1
3	C	307	PX4	C25-C24-C23	2.00	106.36	113.69	9	1
3	C	307	PX4	P1-O3-C1	2.00	130.79	121.26	14	1
3	C	316	PX4	C30-C29-C28	2.00	104.25	114.37	11	1
3	C	317	PX4	C12-C11-C10	2.00	105.77	113.13	6	1
3	C	321	PX4	O7-C7-C6	2.00	115.53	108.34	2	1
3	C	327	PX4	C12-C11-C10	2.00	105.77	113.13	14	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	623	PX4	C18-C17-C16	2.00	104.26	114.37	5	1
3	B	348	PX4	C32-C31-C30	2.00	104.26	114.37	10	1
3	B	382	PX4	O7-C7-C8	2.00	115.52	108.34	3	1
3	C	321	PX4	C12-C11-C10	2.00	105.78	113.13	15	1
3	C	347	PX4	C8-O5-C9	2.00	109.81	117.12	15	1

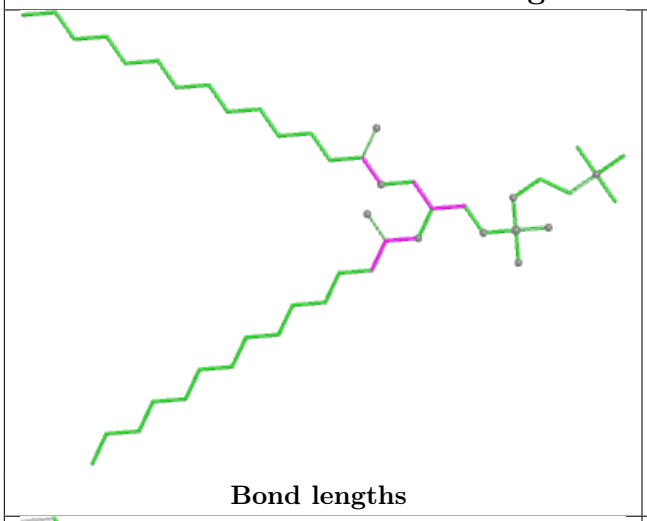
There are no chirality outliers.

There are no torsion outliers.

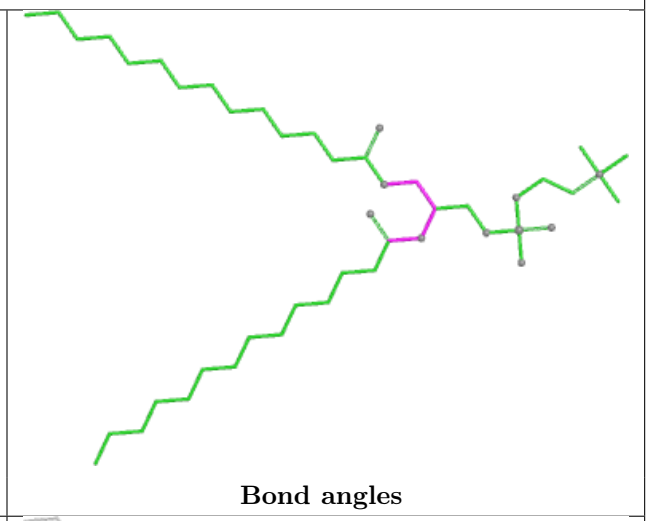
There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

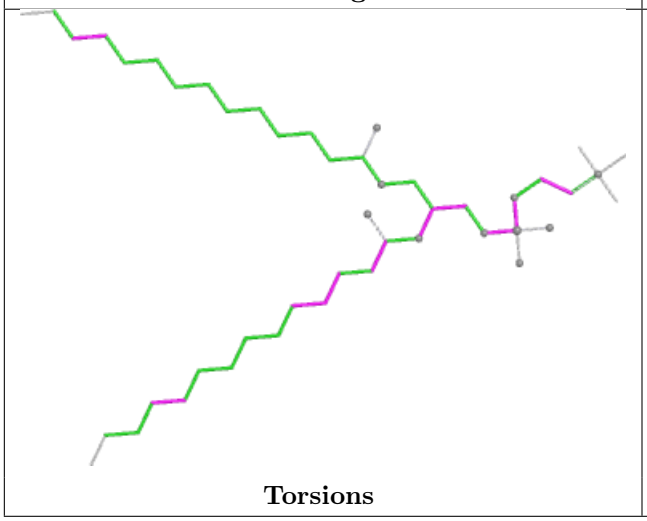
Ligand PX4 C 350



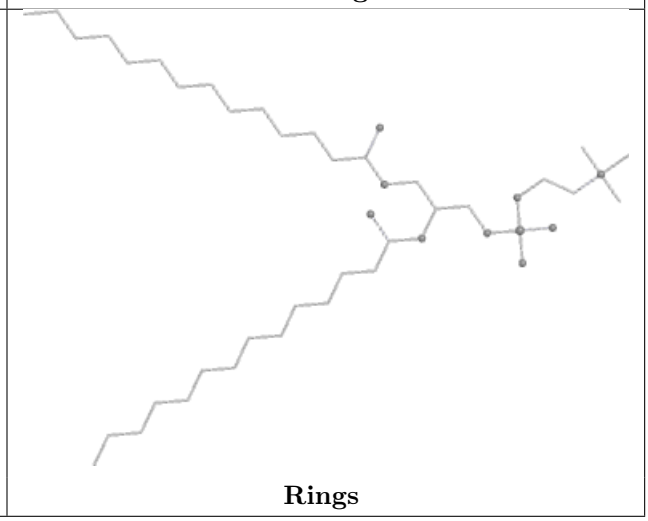
Bond lengths



Bond angles

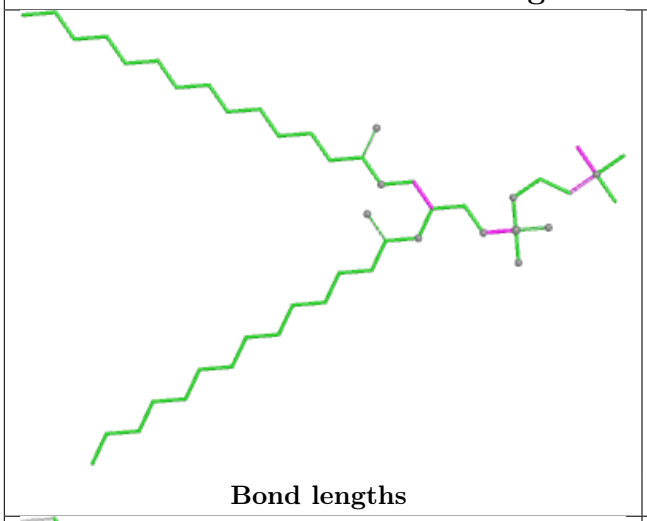


Torsions

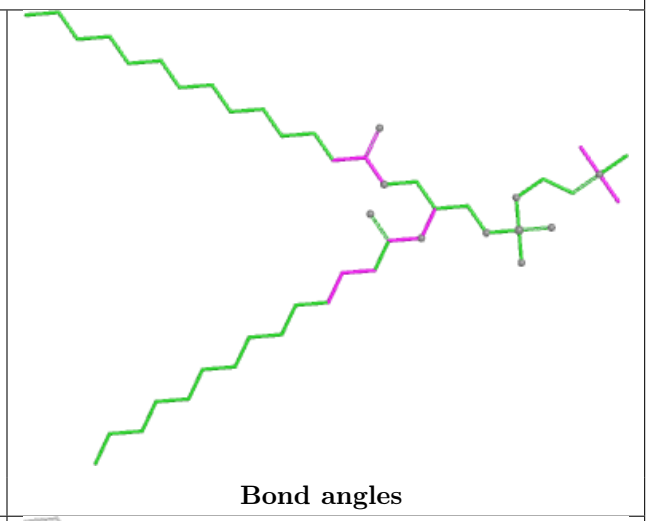


Rings

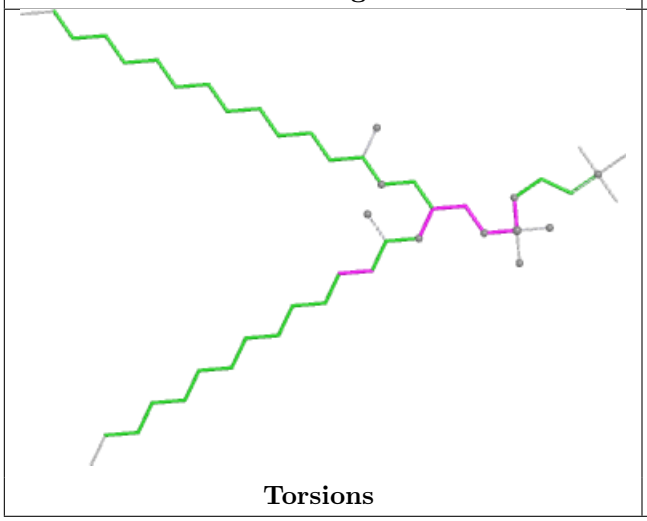
Ligand PX4 C 324



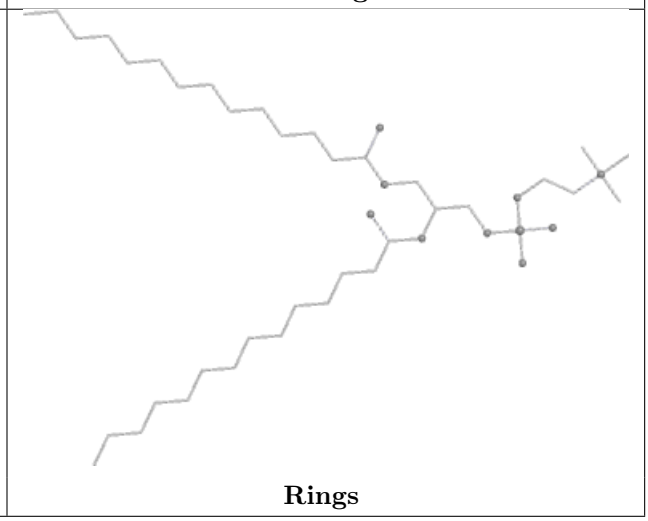
Bond lengths



Bond angles

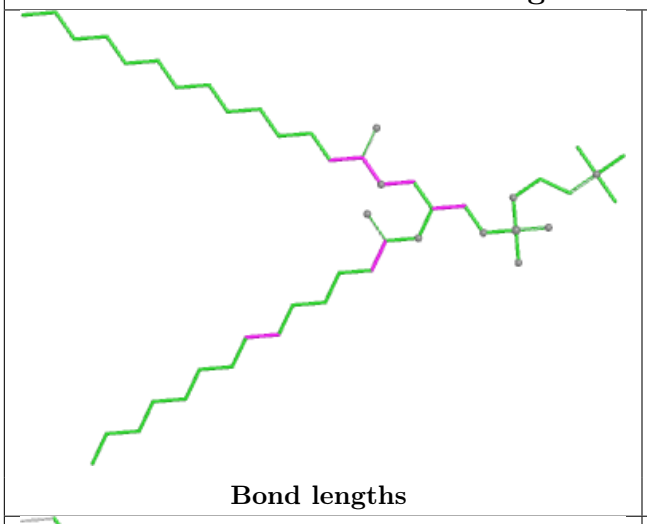


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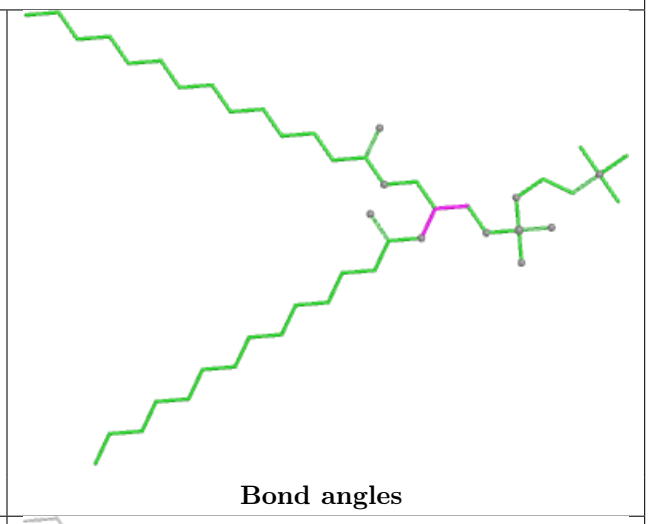


Rings

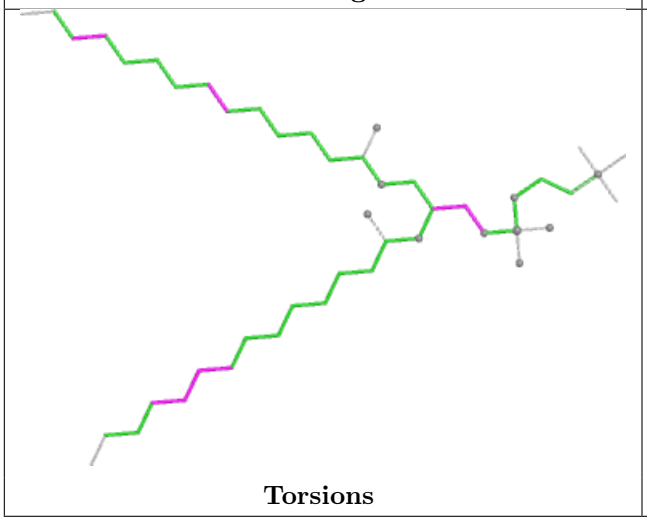
Ligand PX4 C 316



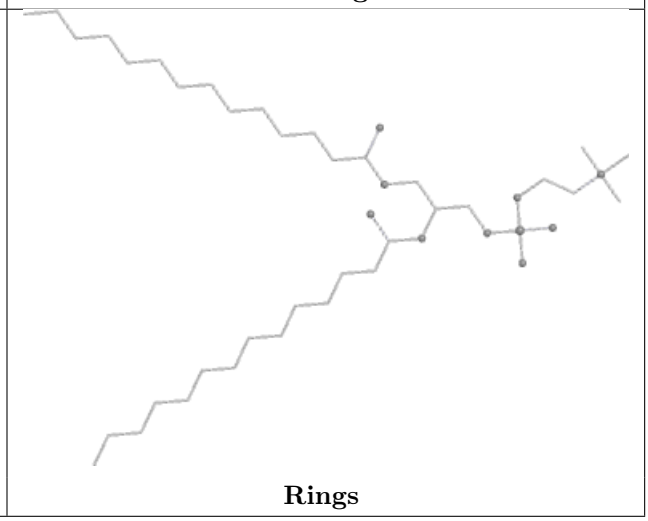
Bond lengths



Bond angles

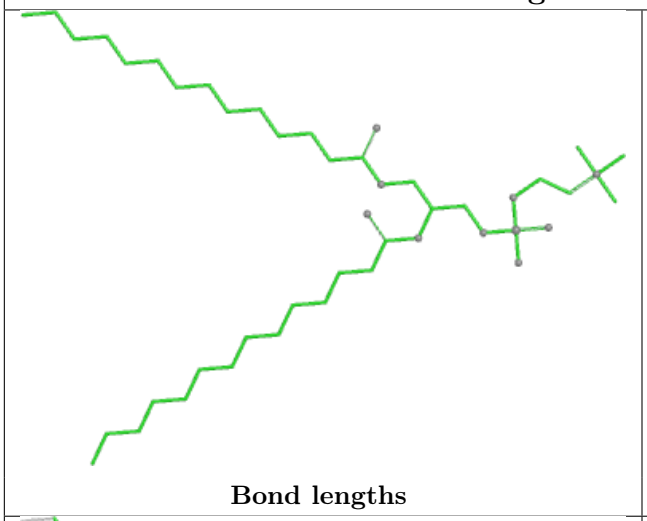


Torsions

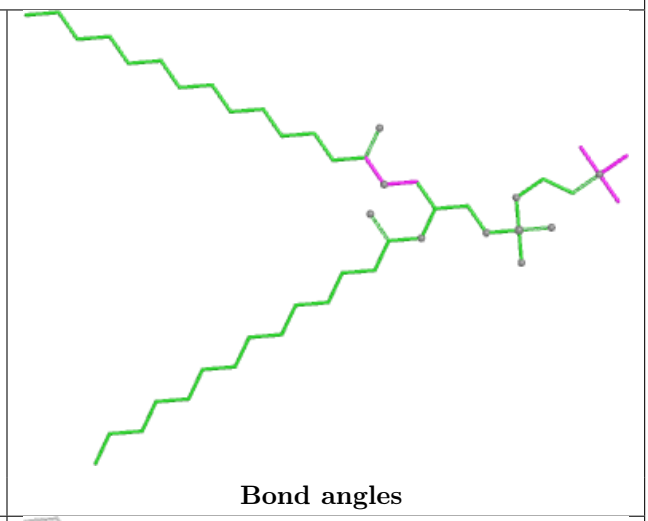


Rings

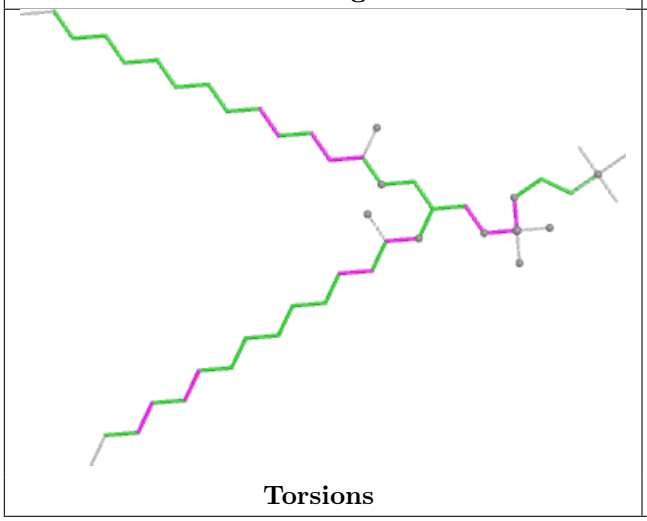
Ligand PX4 B 332



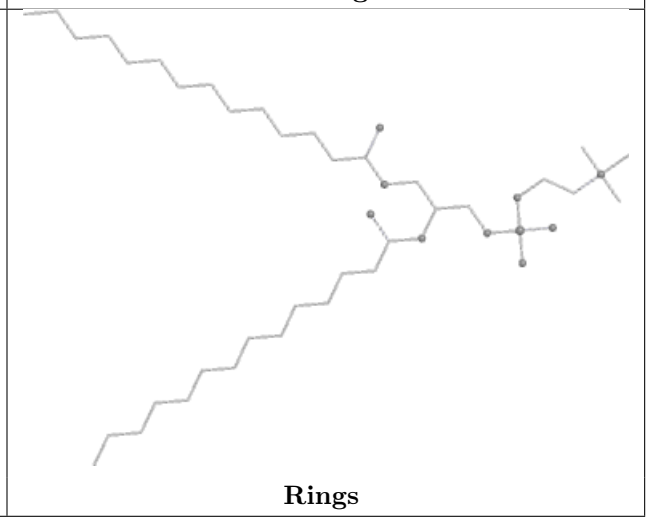
Bond lengths



Bond angles

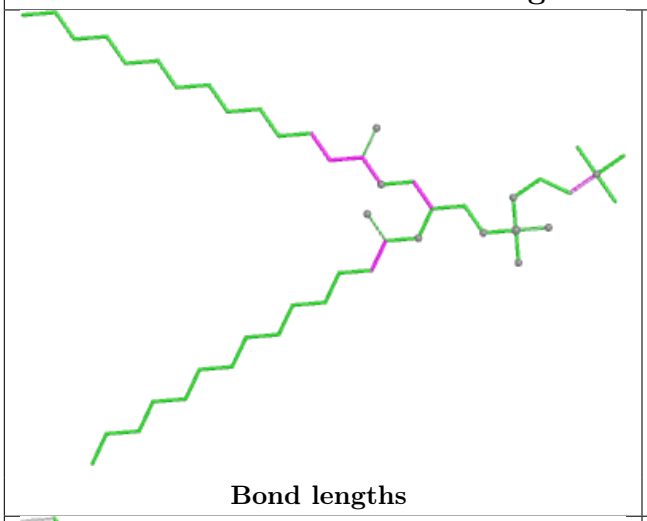


Torsions

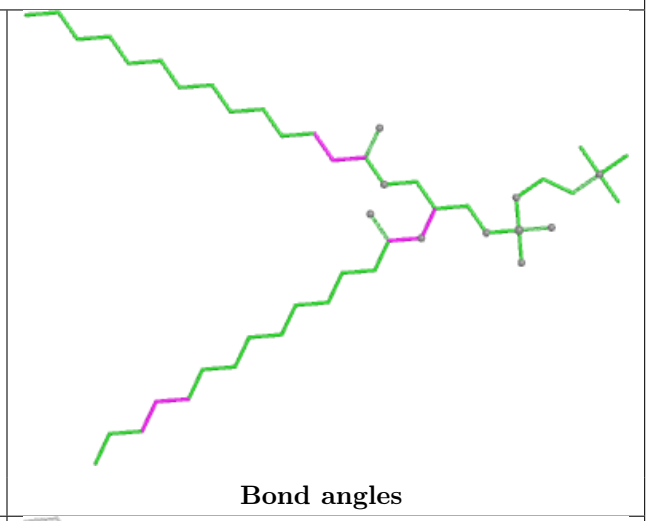


Rings

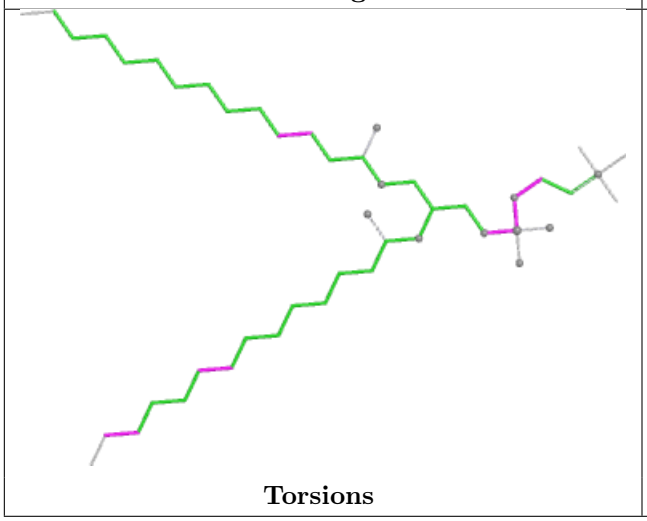
Ligand PX4 B 340



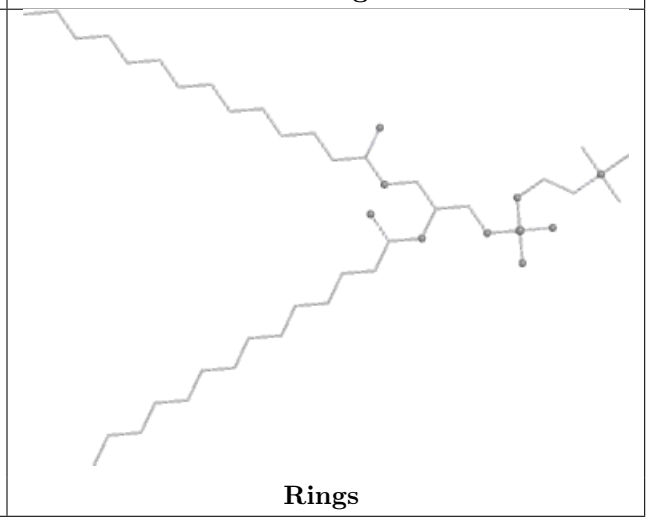
Bond lengths



Bond angles

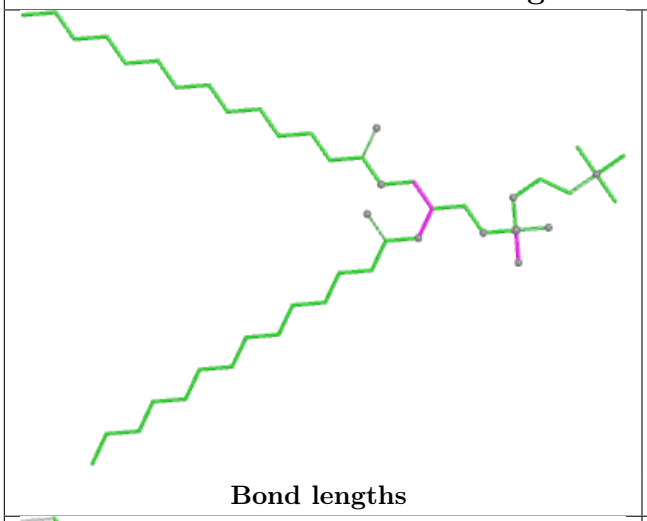


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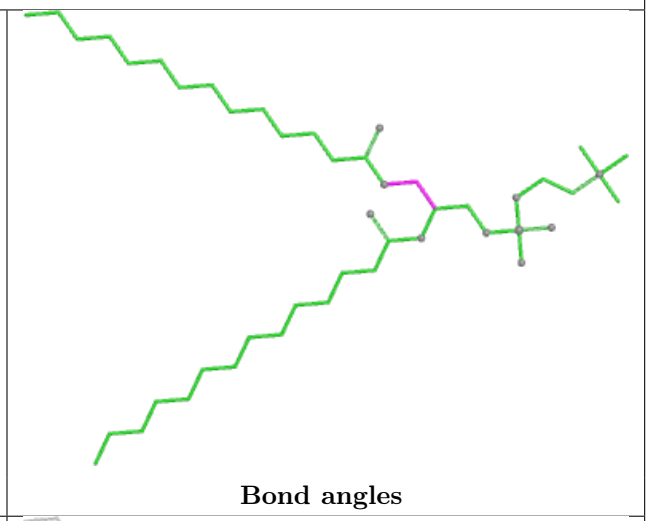


Rings

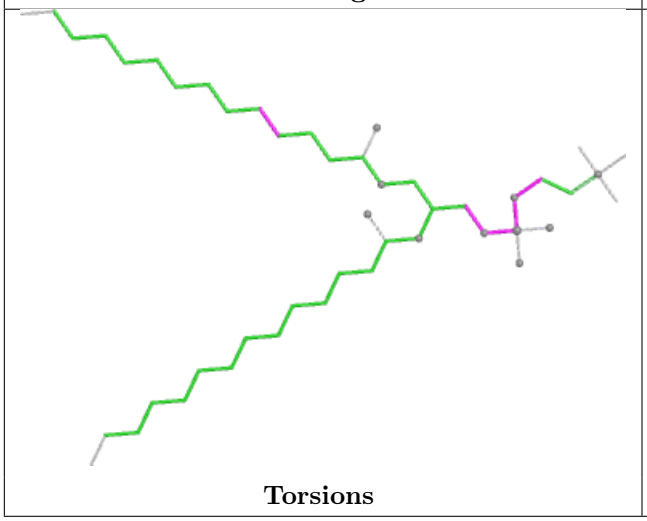
Ligand PX4 A 620



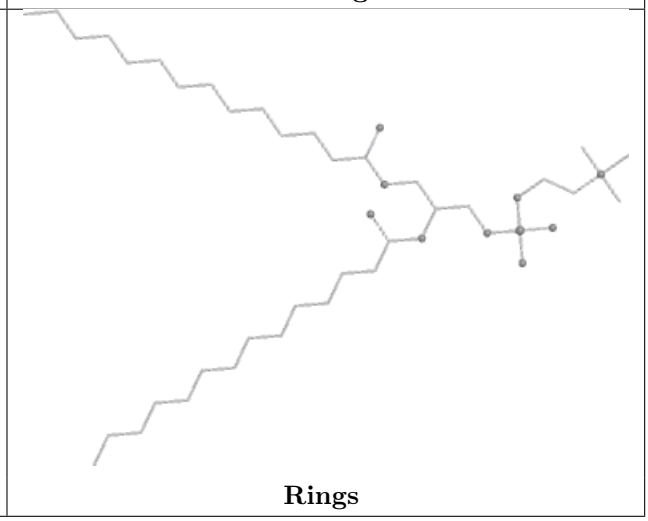
Bond lengths



Bond angles

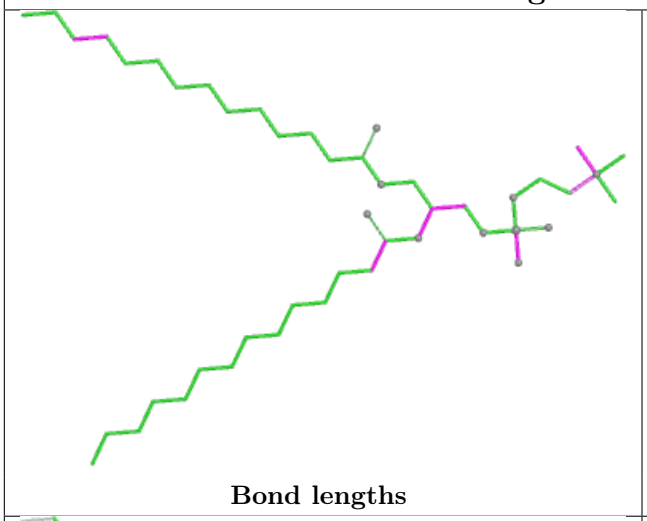


Torsions

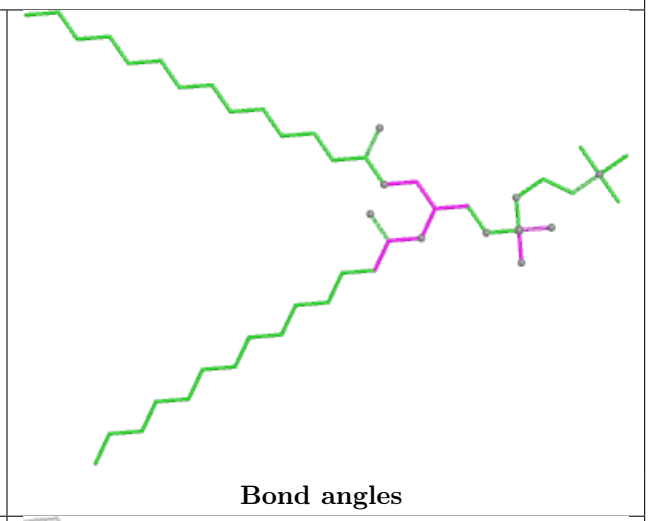


Rings

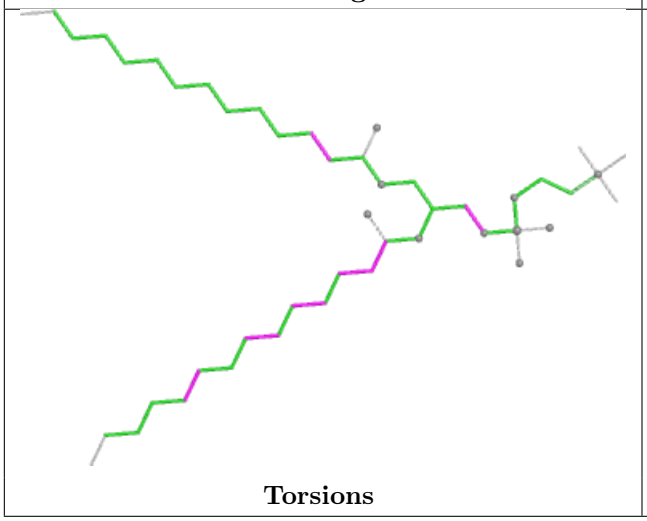
Ligand PX4 B 390



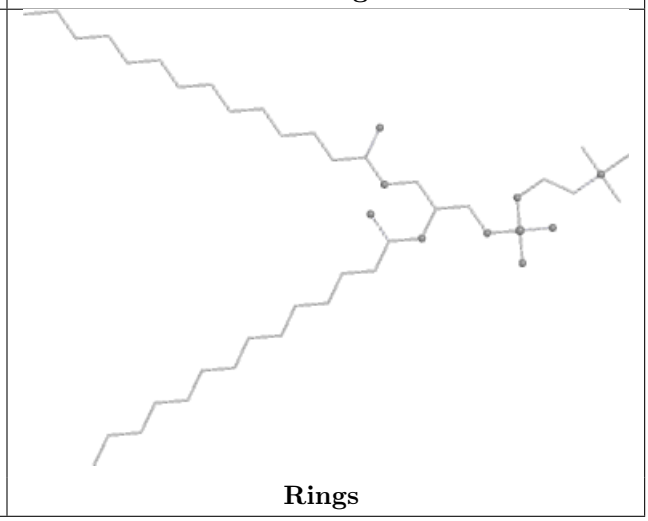
Bond lengths



Bond angles

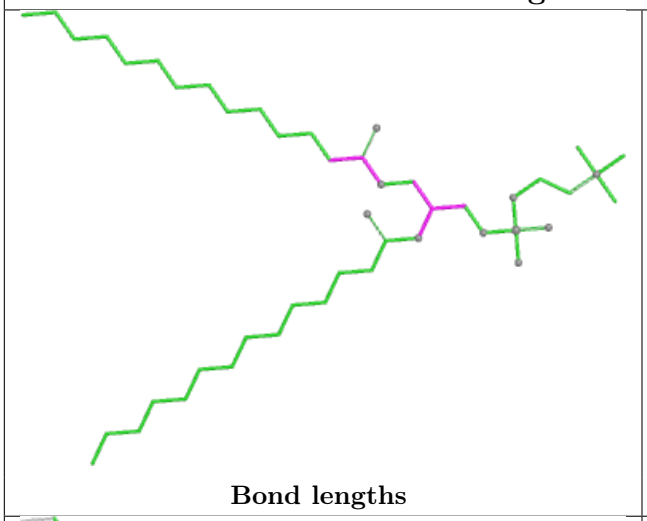


Torsions

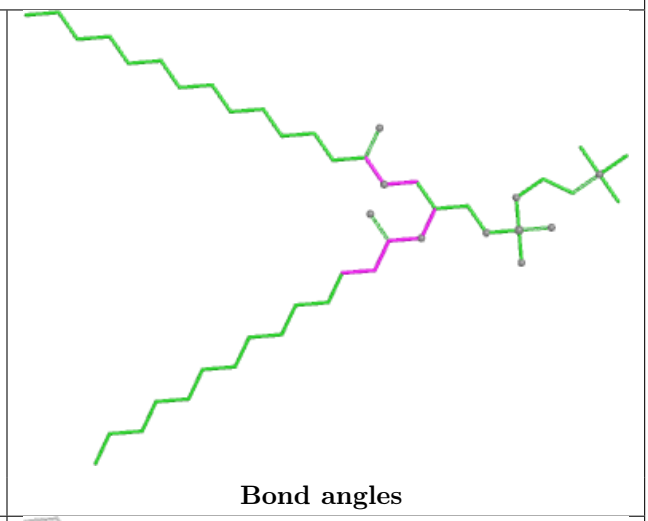


Rings

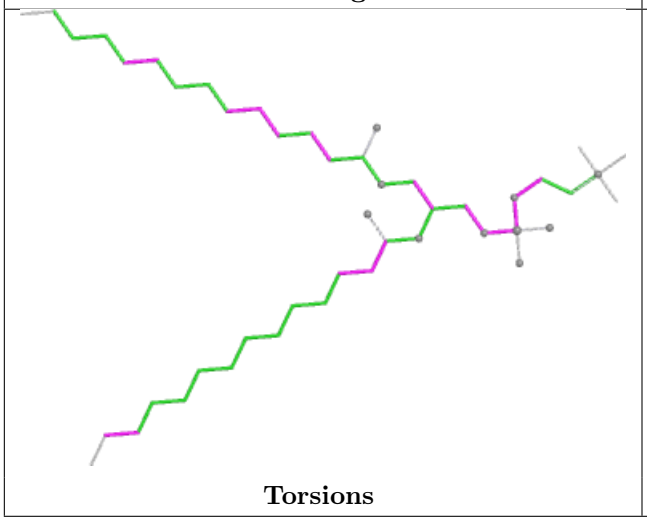
Ligand PX4 B 304



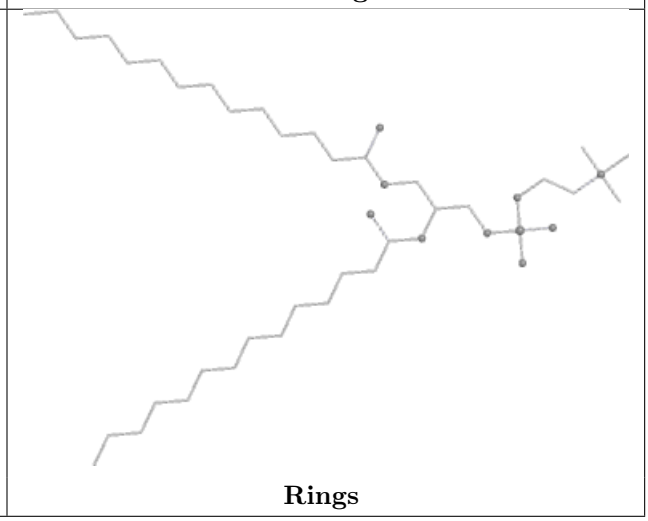
Bond lengths



Bond angles

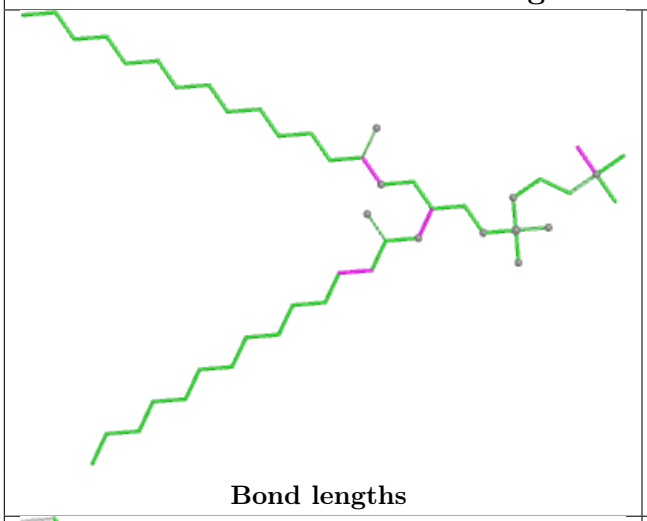


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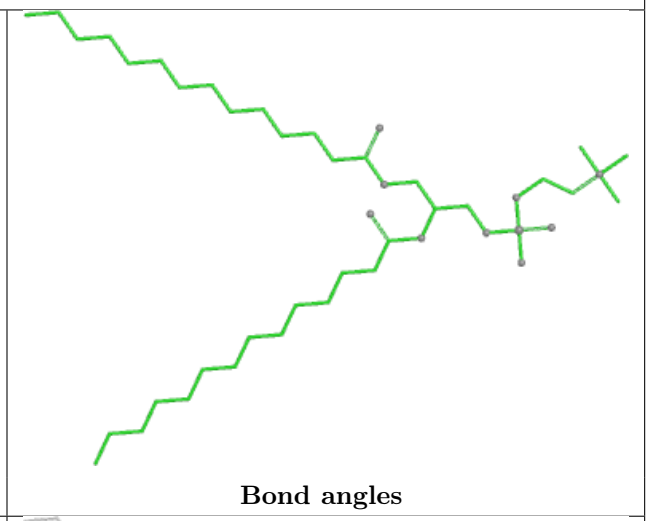


Rings

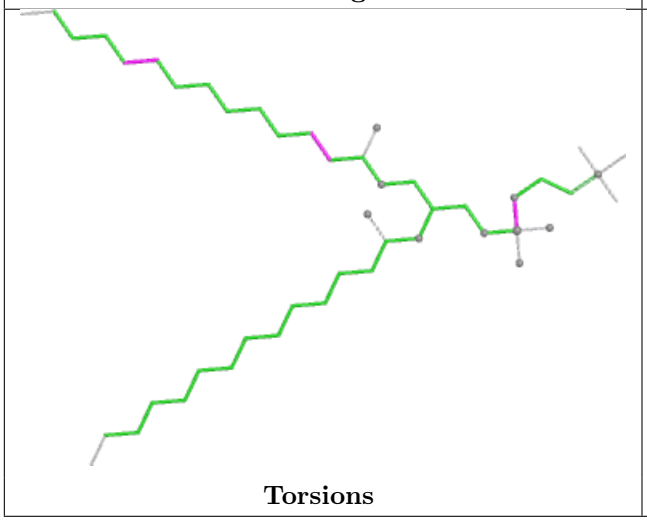
Ligand PX4 C 354



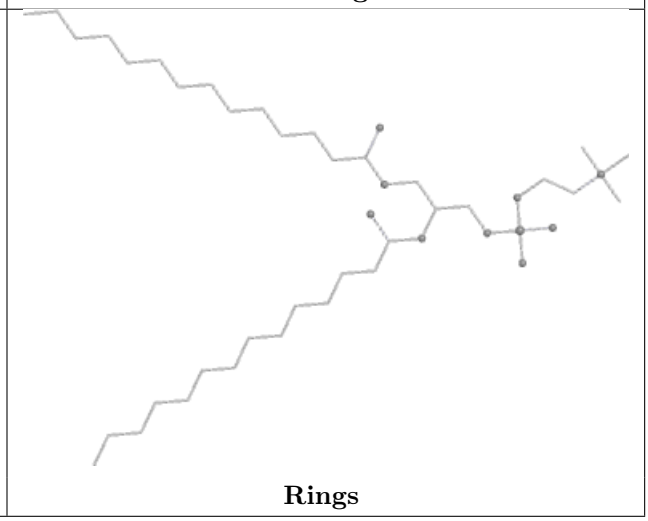
Bond lengths



Bond angles

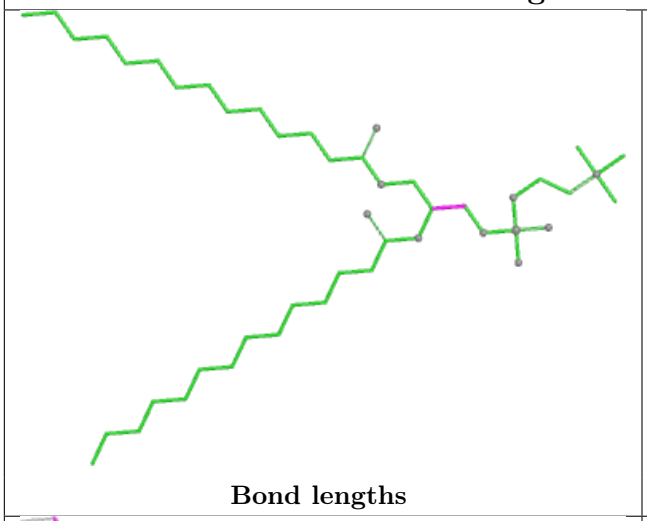


Torsions

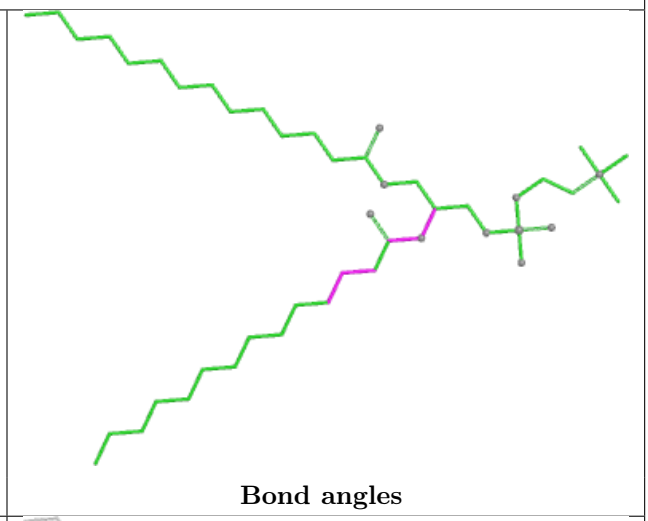


Rings

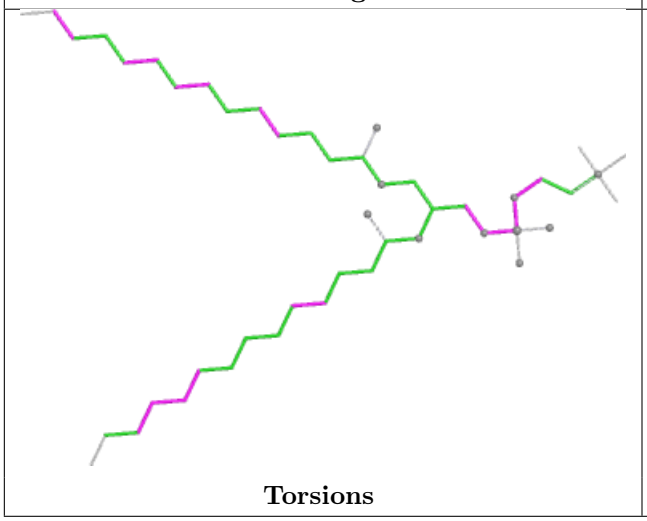
Ligand PX4 C 361



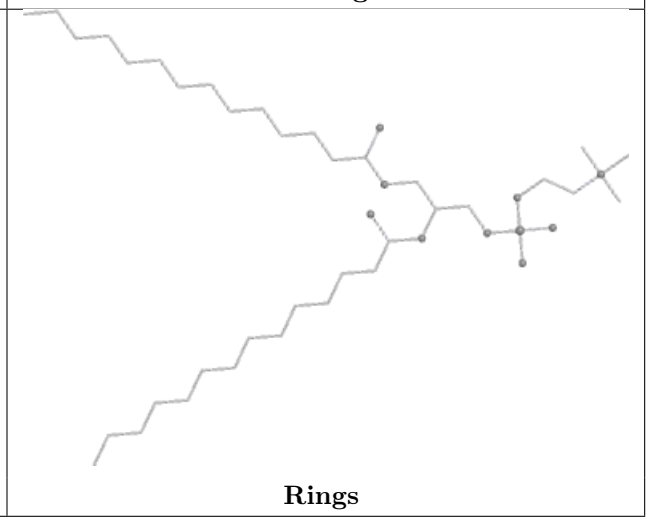
Bond lengths



Bond angles

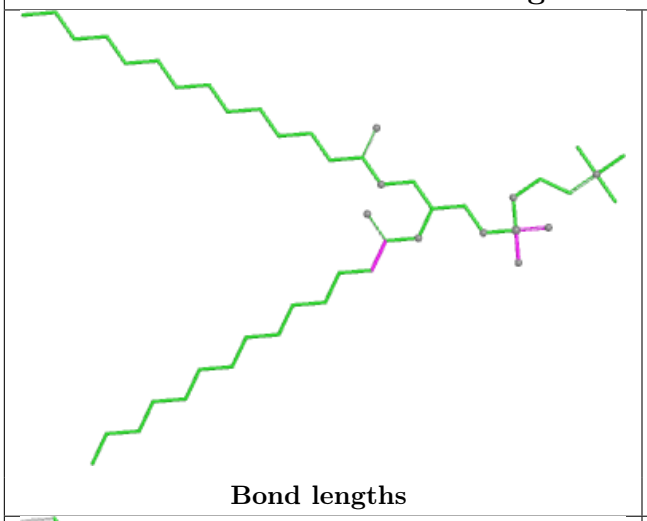


Torsions

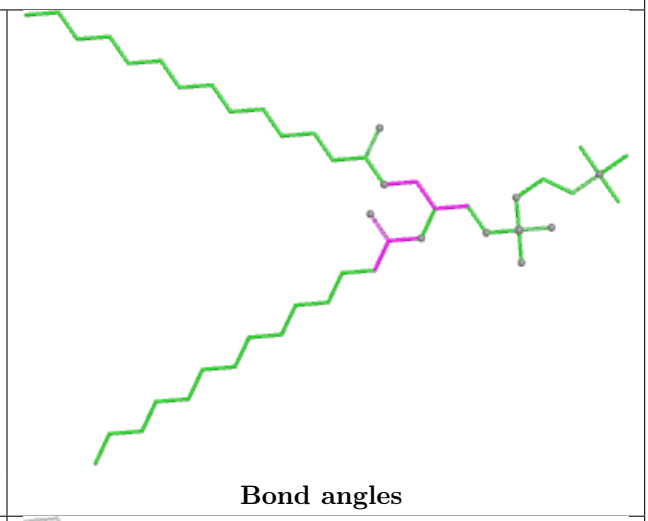


Rings

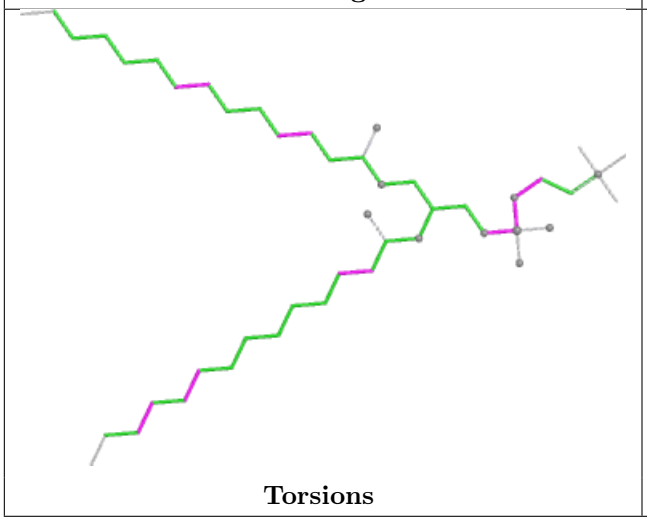
Ligand PX4 C 337



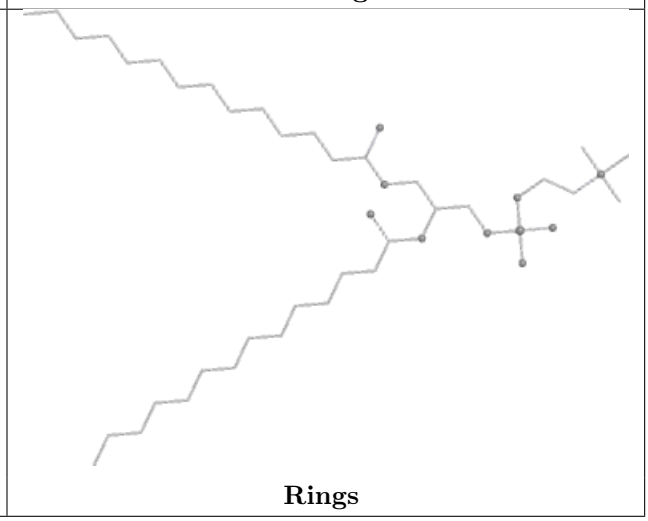
Bond lengths



Bond angles

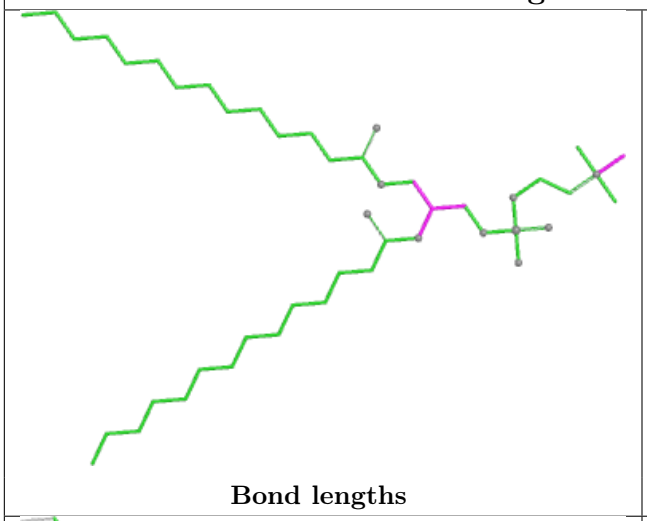


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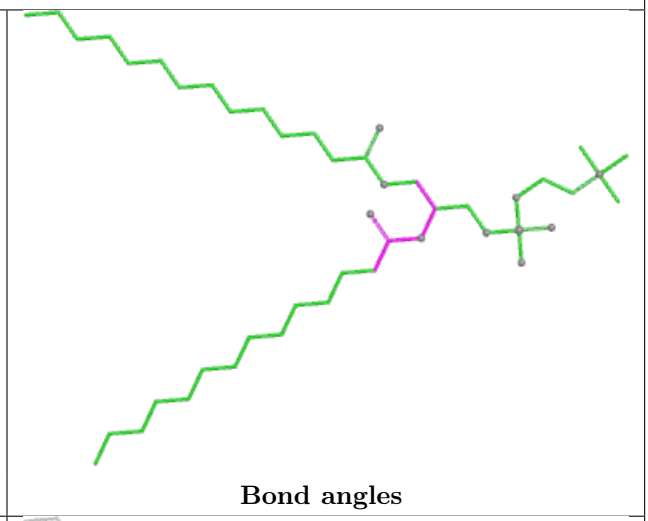


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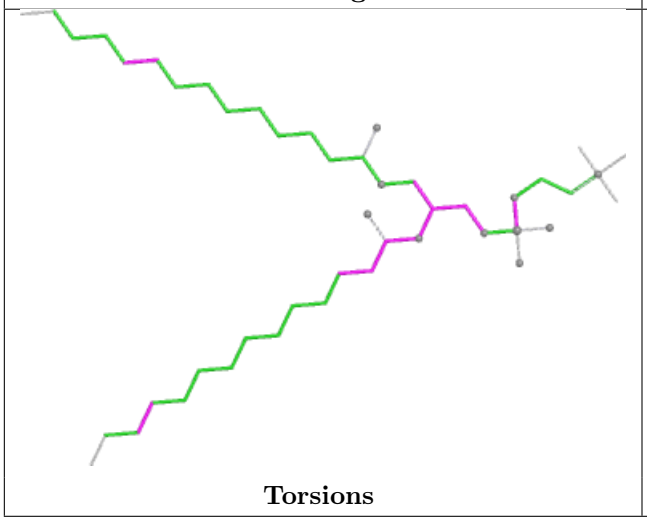
Ligand PX4 C 309



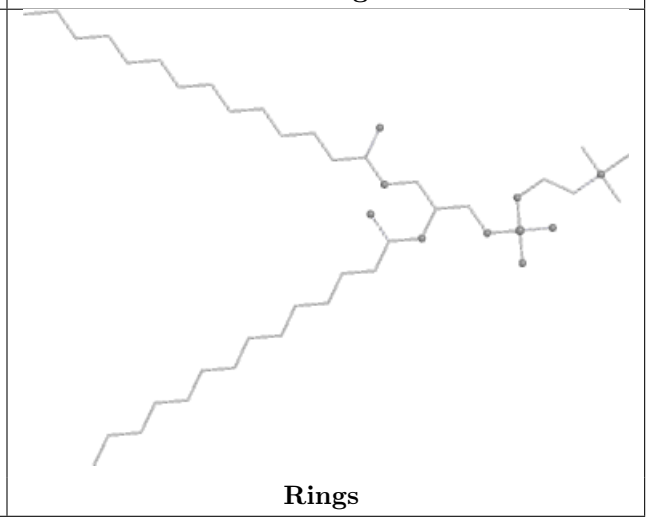
Bond lengths



Bond angles

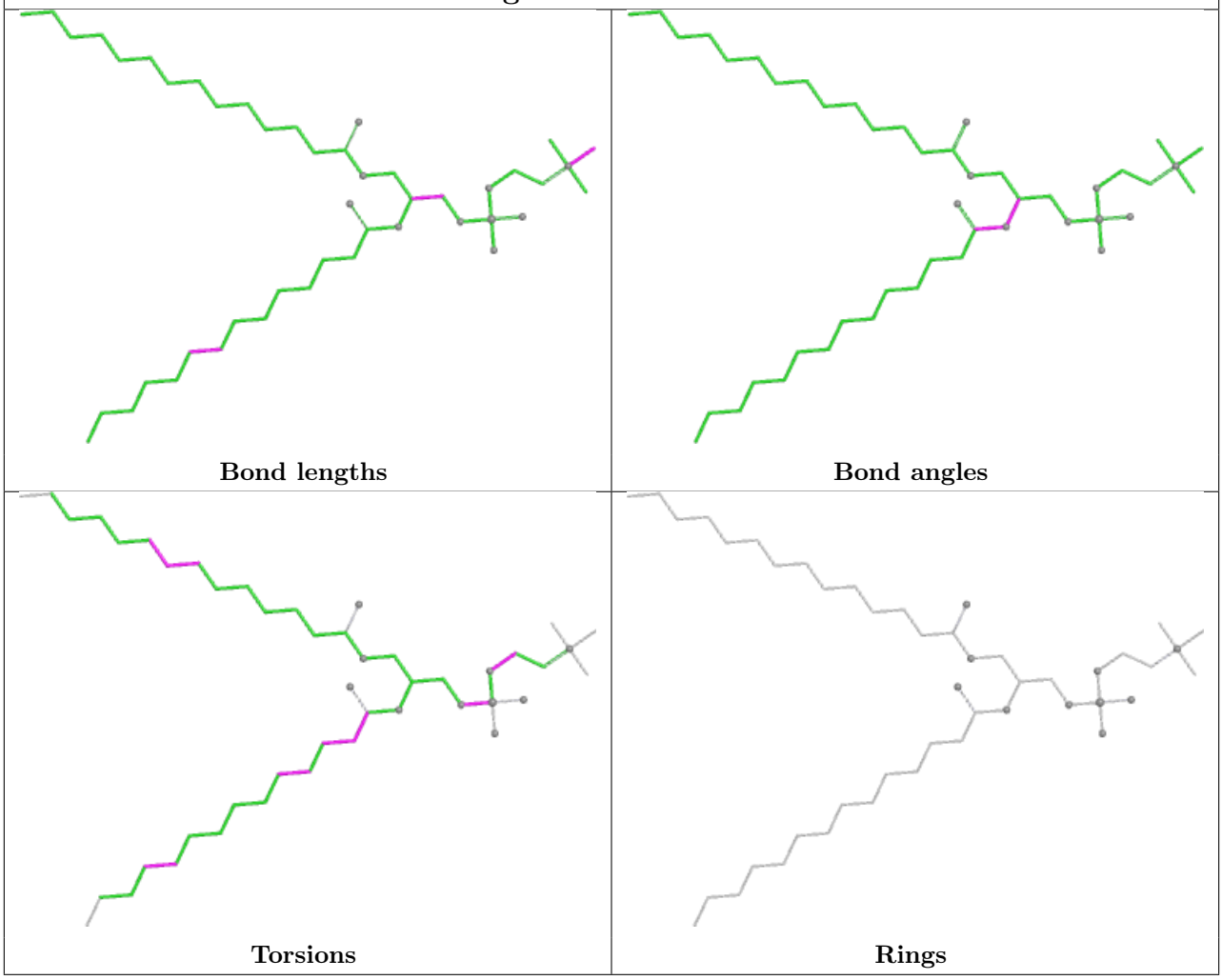


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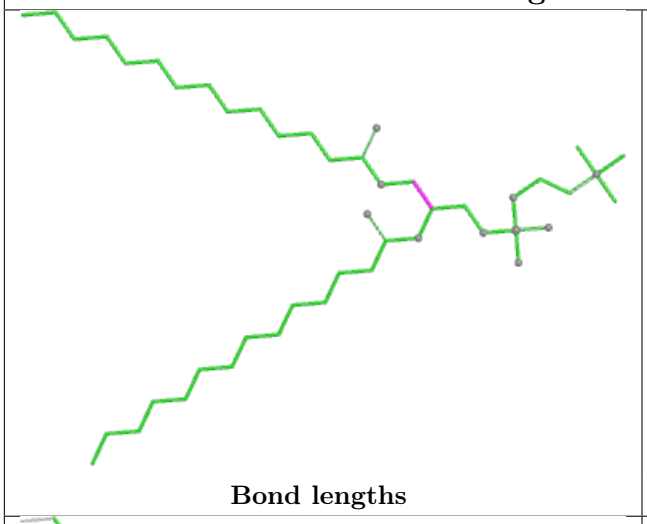


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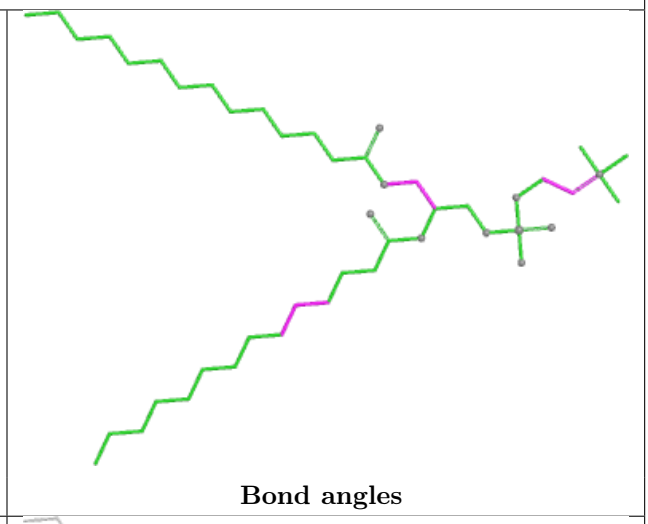
Ligand PX4 B 321



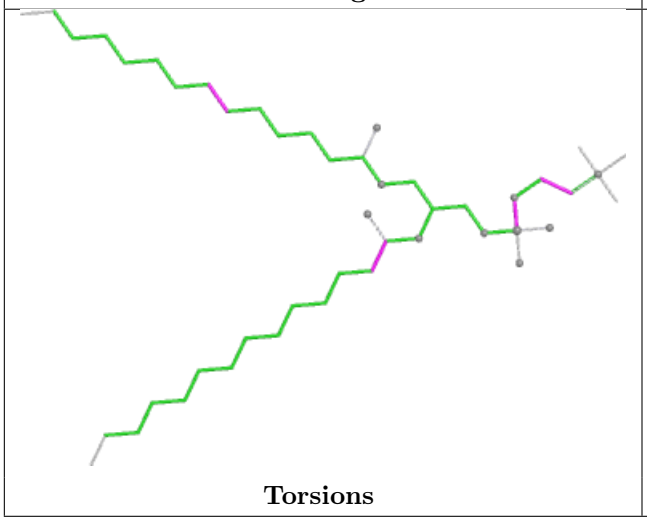
Ligand PX4 B 382



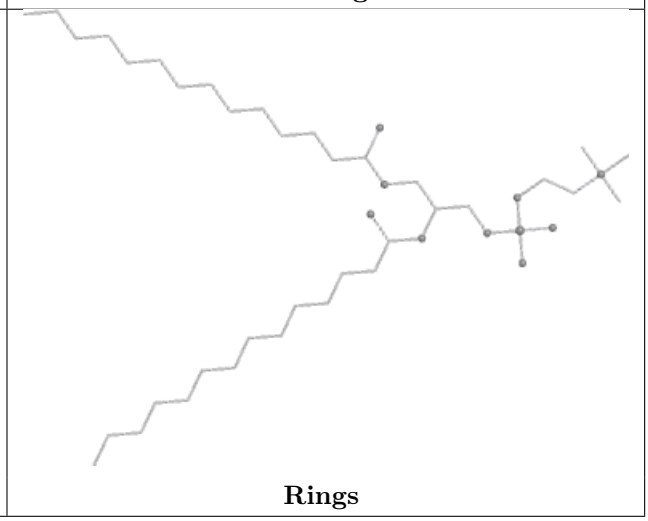
Bond lengths



Bond angles

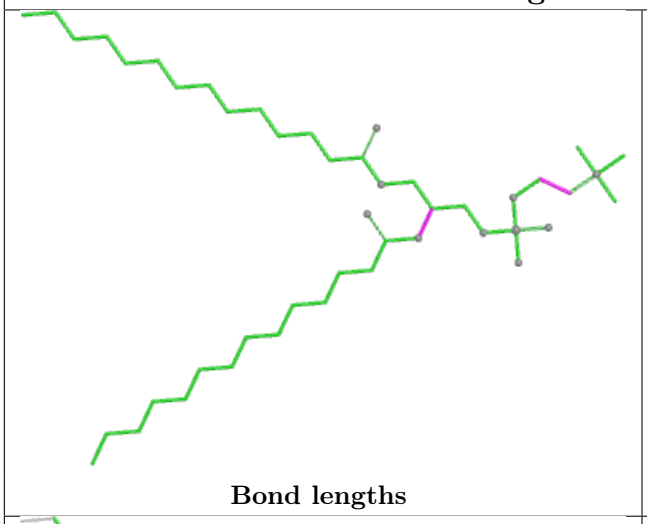


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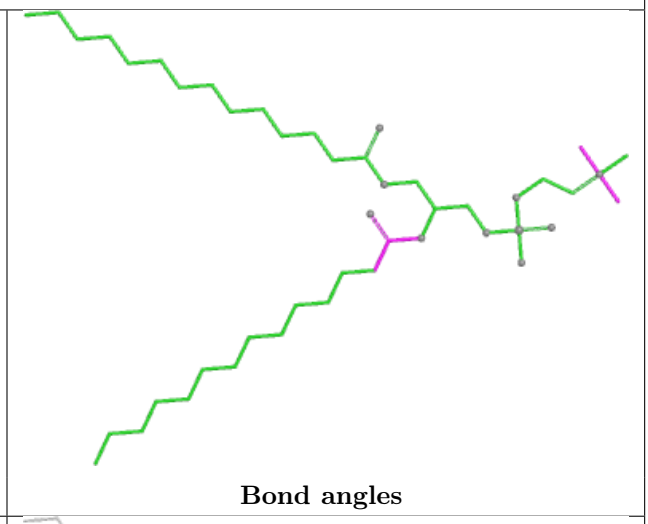


Rings

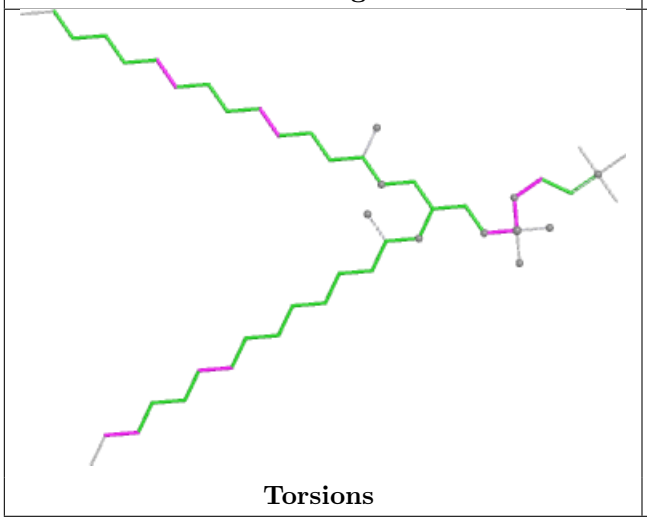
Ligand PX4 C 303



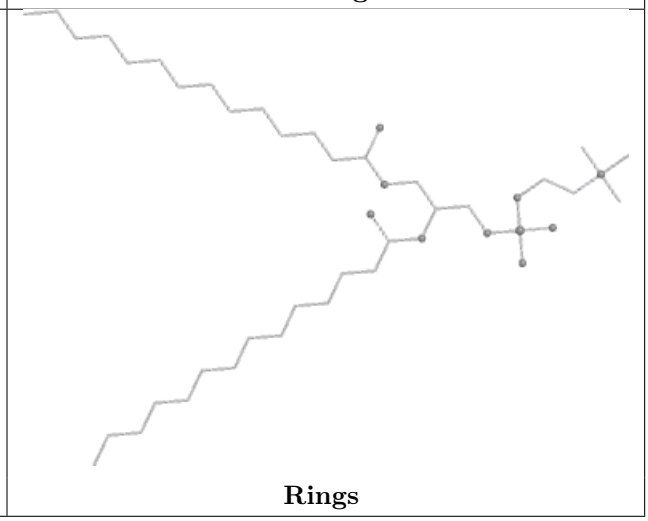
Bond lengths



Bond angles

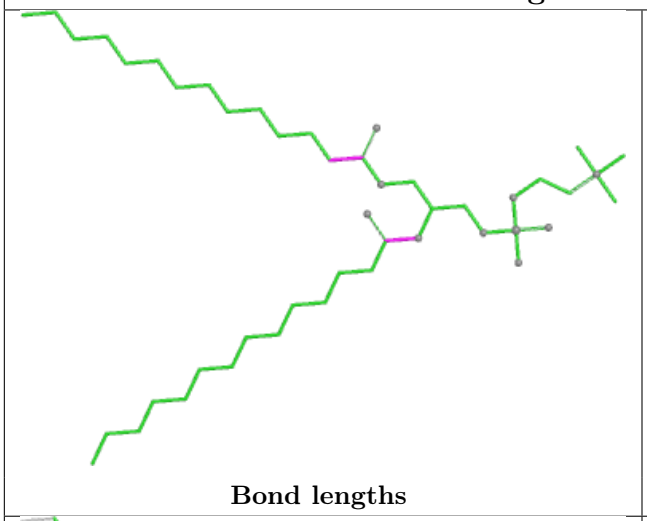


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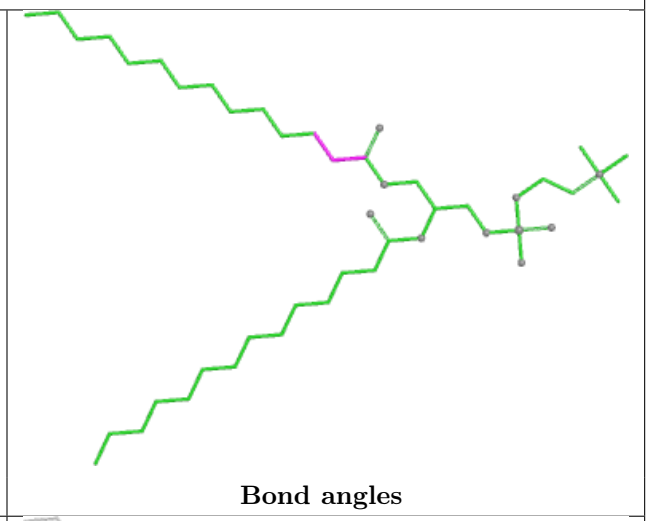


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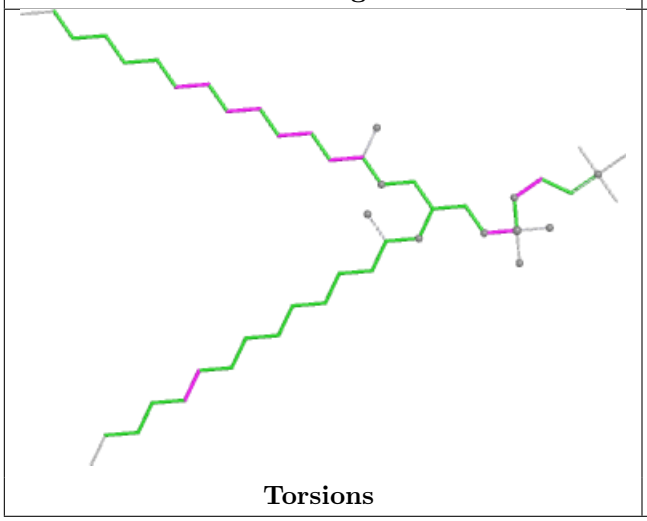
Ligand PX4 C 353



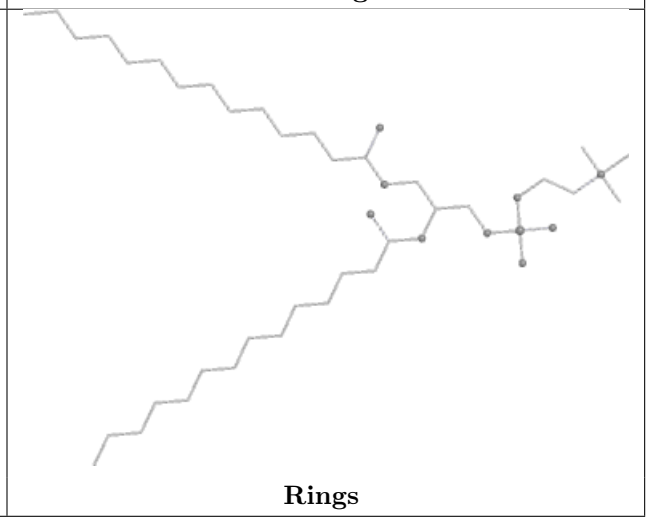
Bond lengths



Bond angles

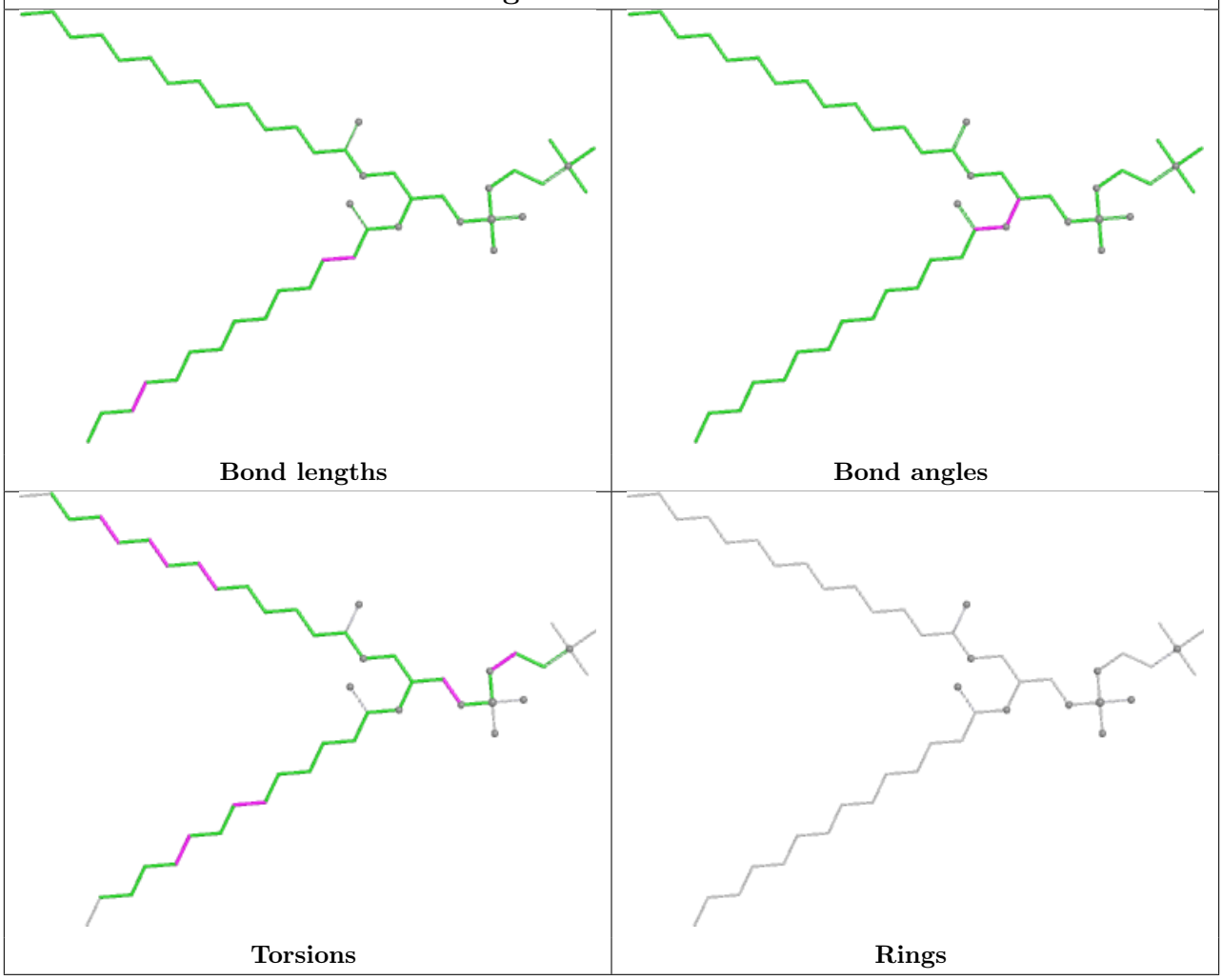


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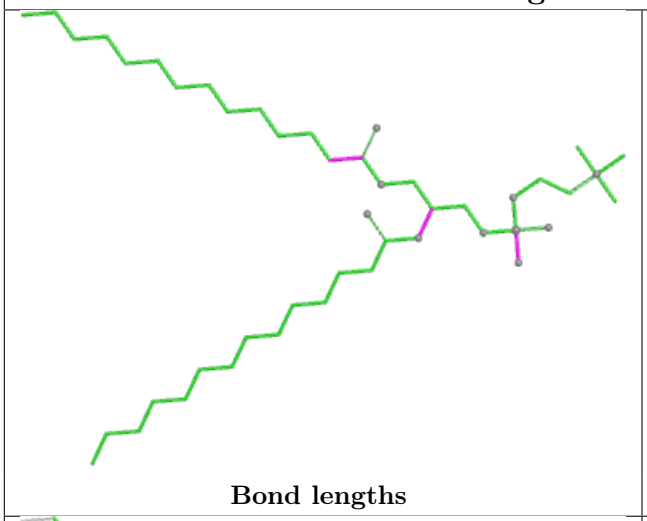


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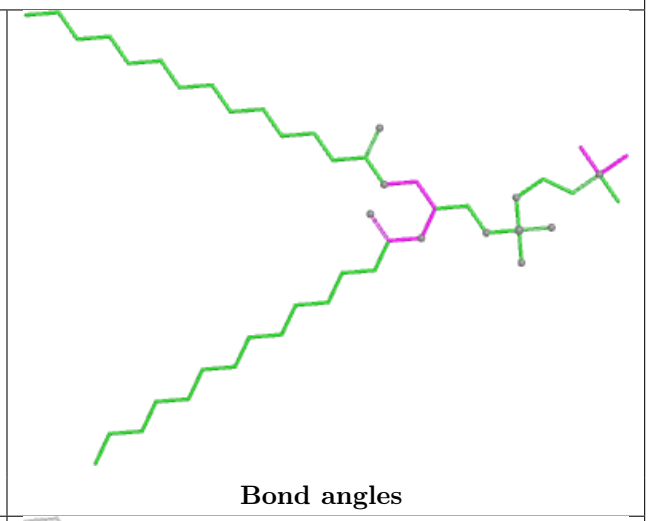
Ligand PX4 B 379



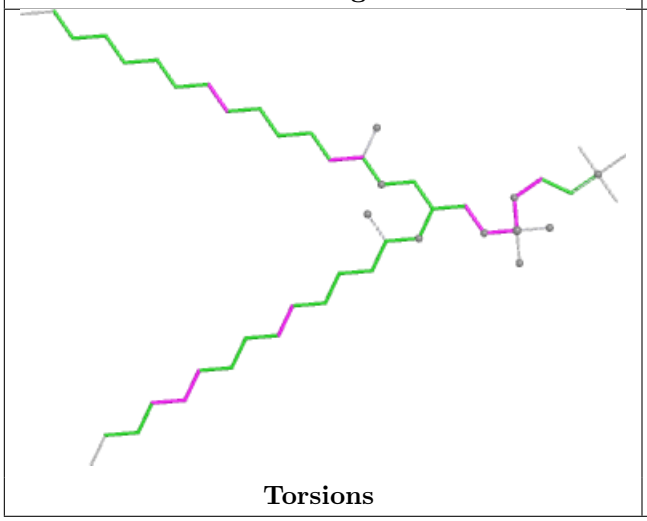
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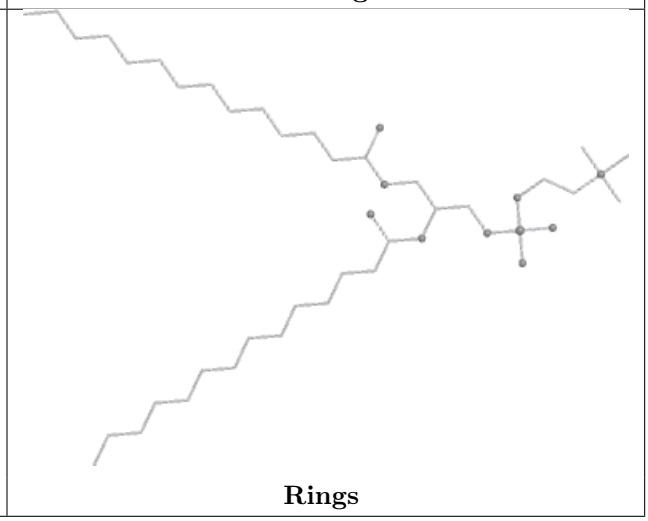
Bond lengths



Bond angles

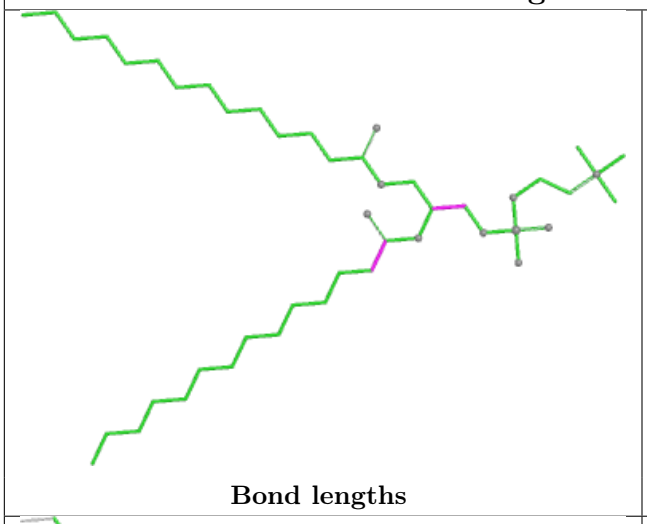


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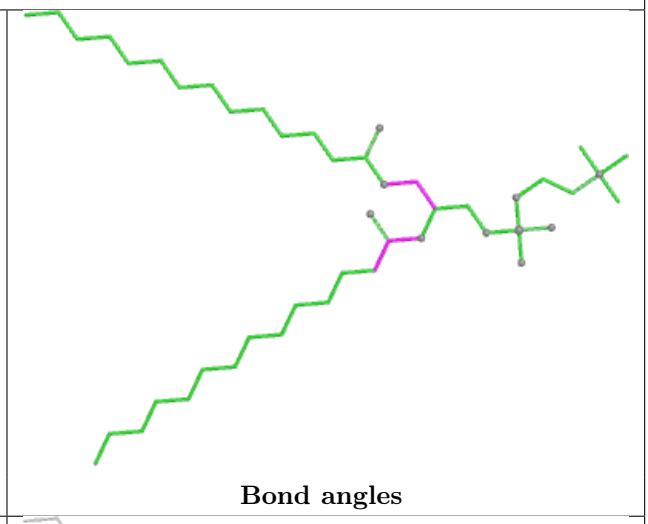


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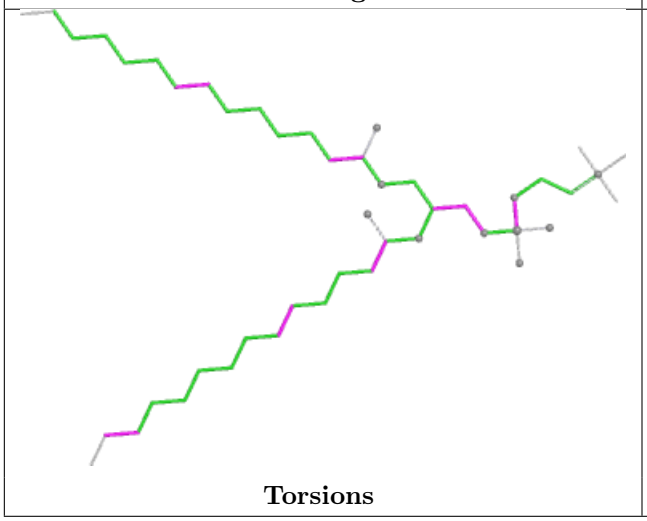
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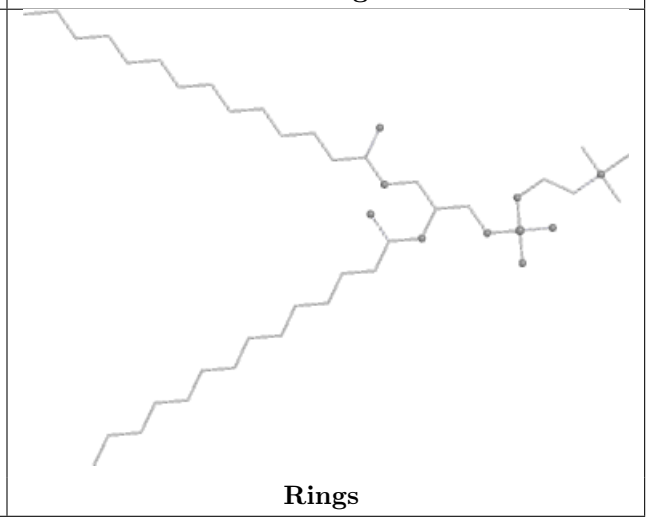
Bond lengths



Bond angles

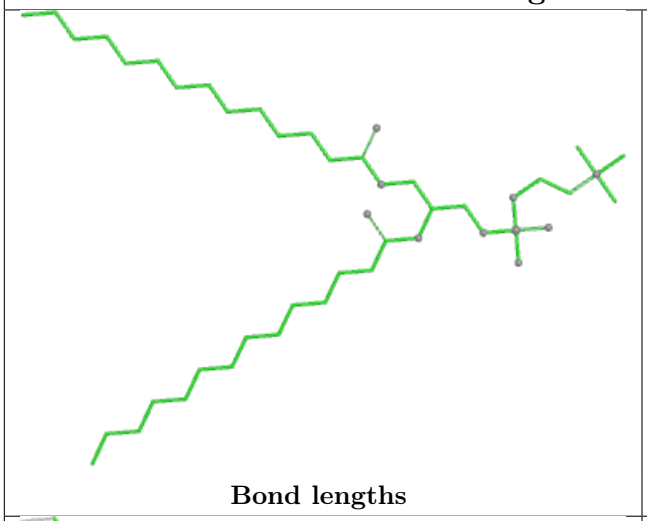


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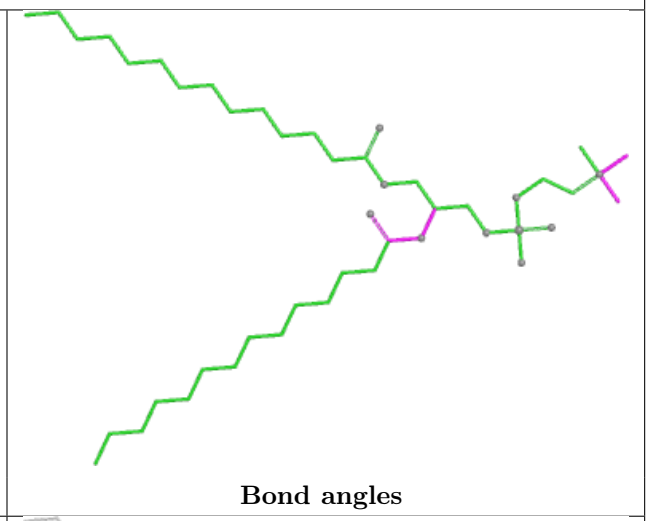


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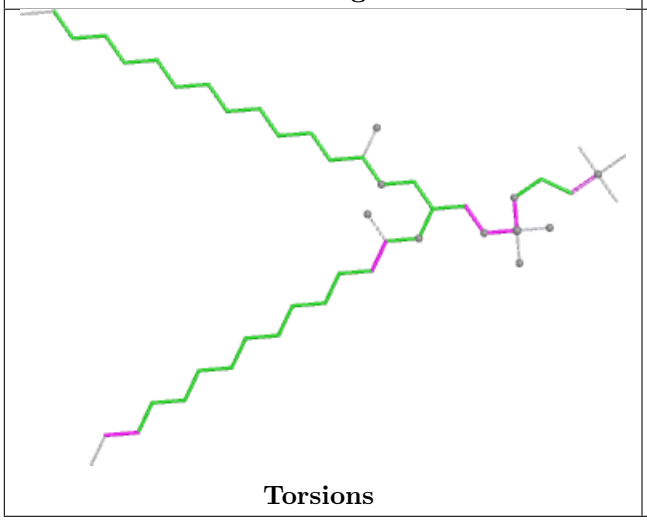
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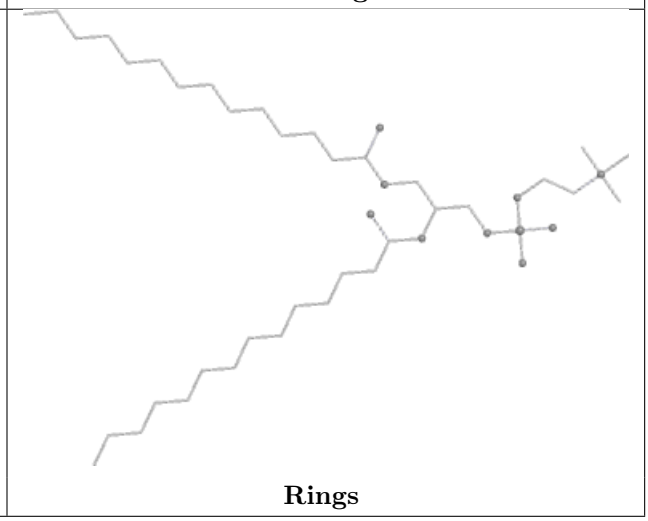
Bond lengths



Bond angles

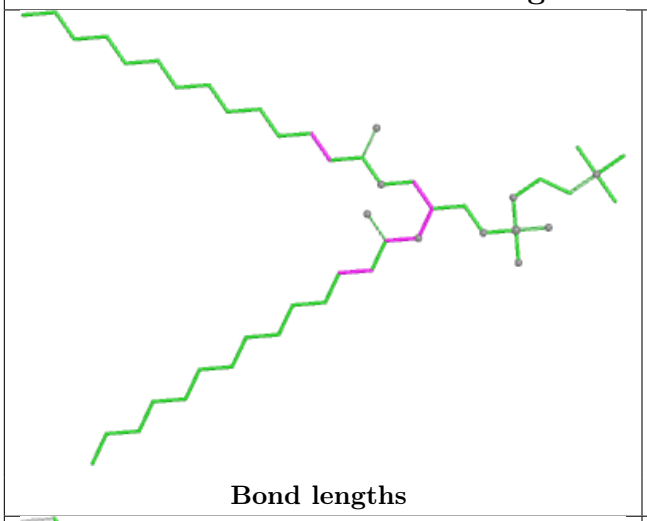


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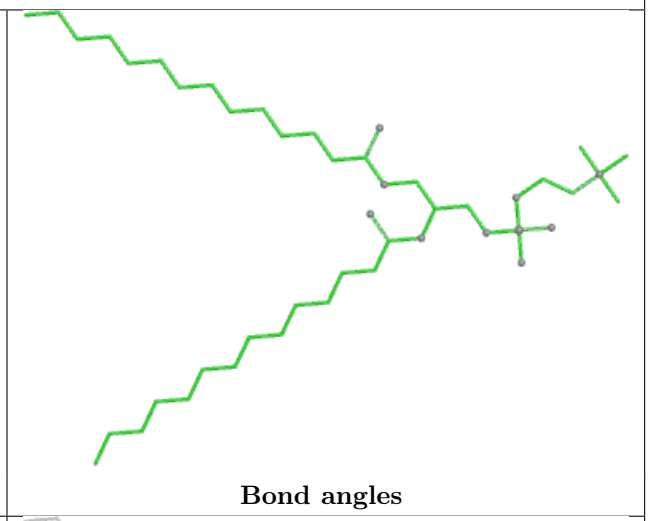


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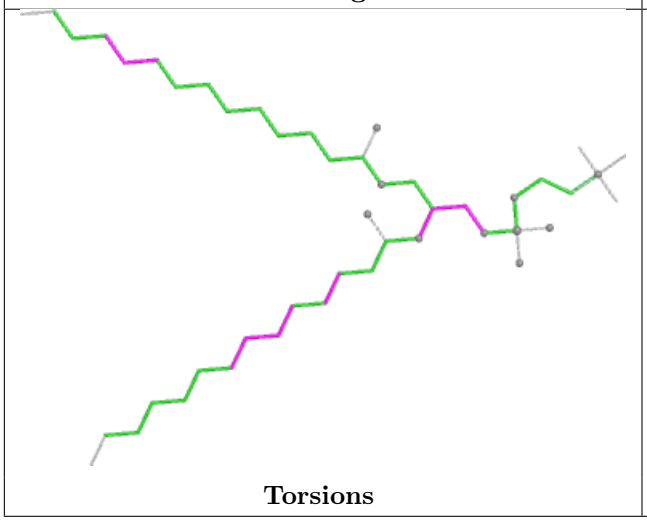
Ligand PX4 C 356



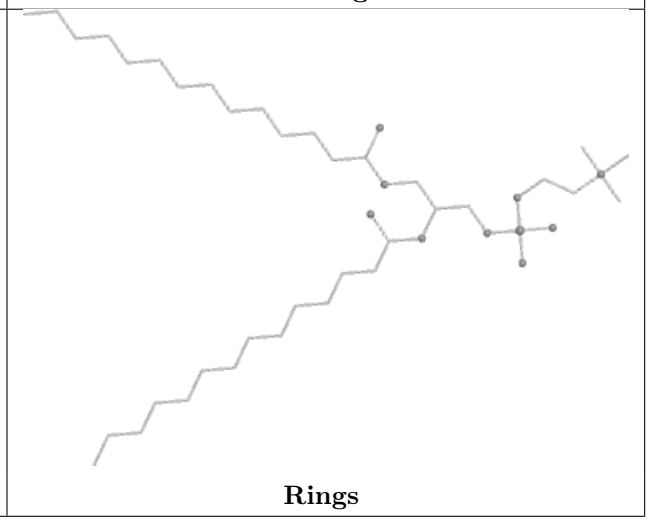
Bond lengths



Bond angles

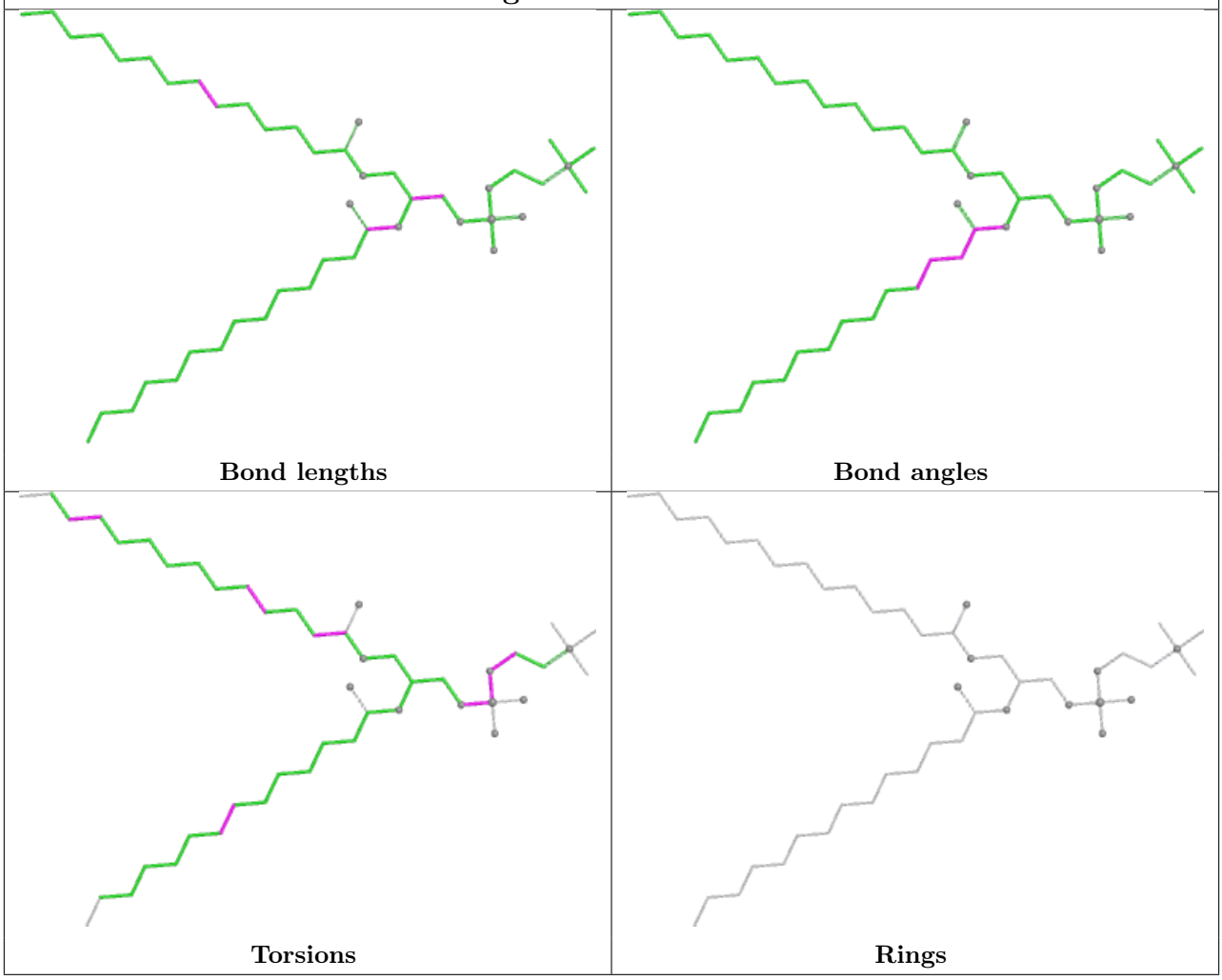


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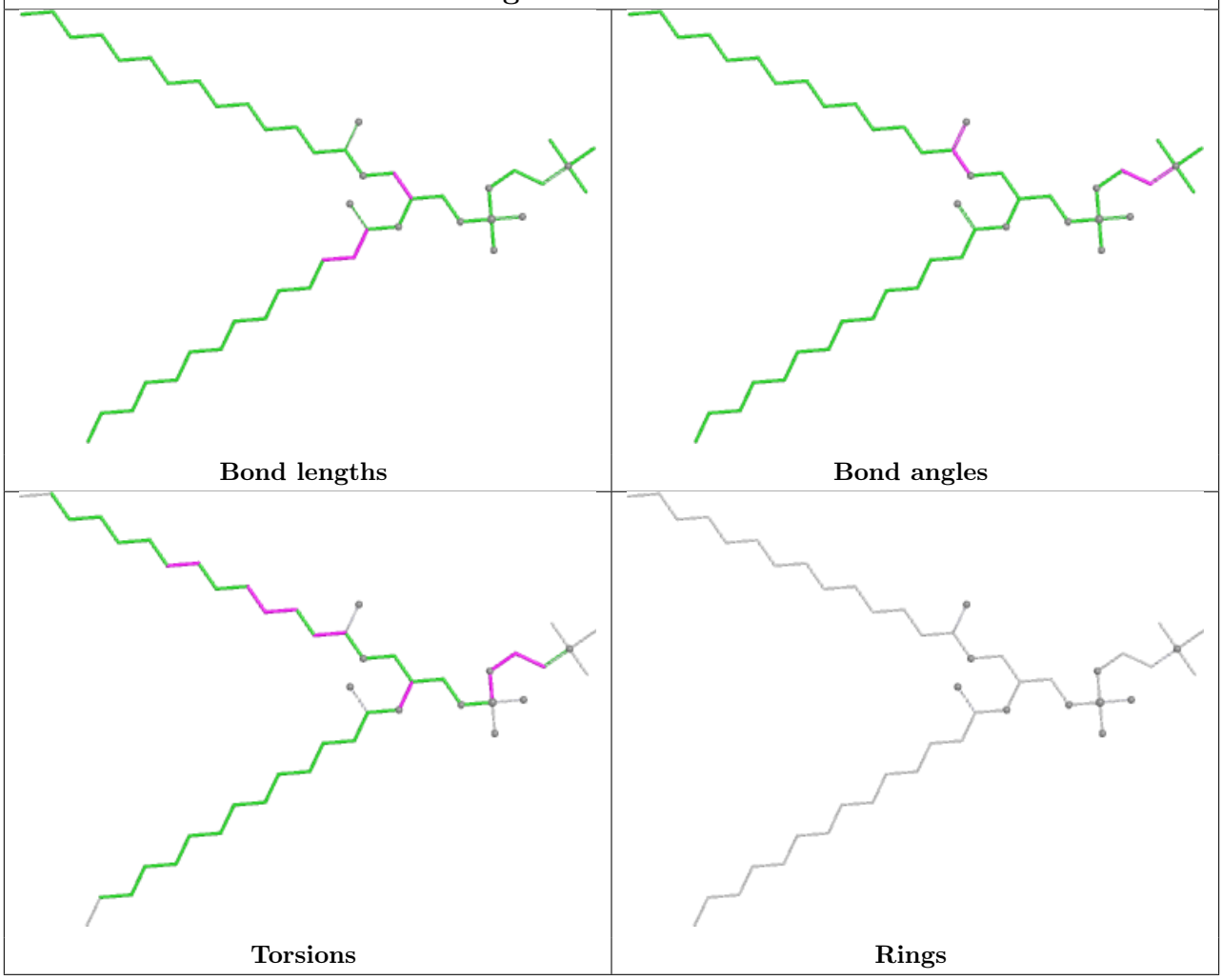


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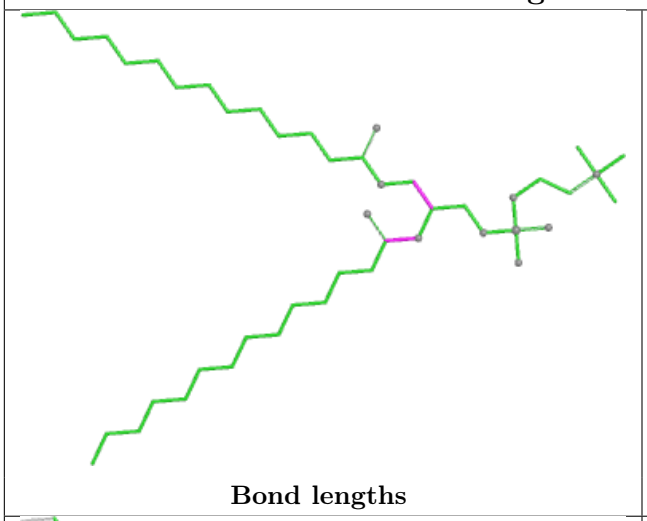
Ligand PX4 B 398



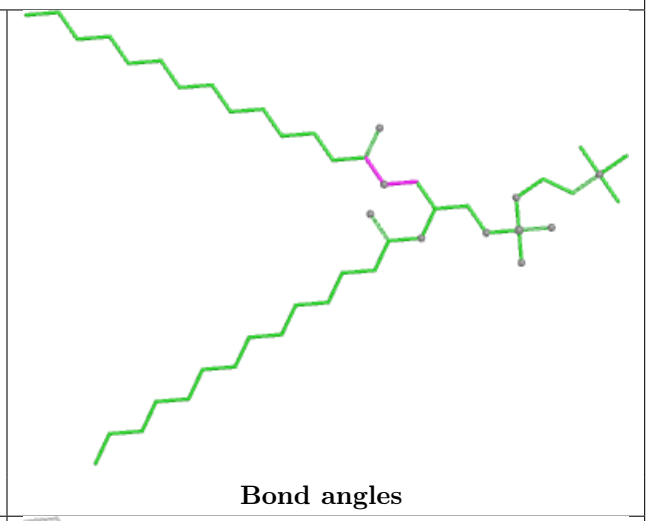
Ligand PX4 B 383



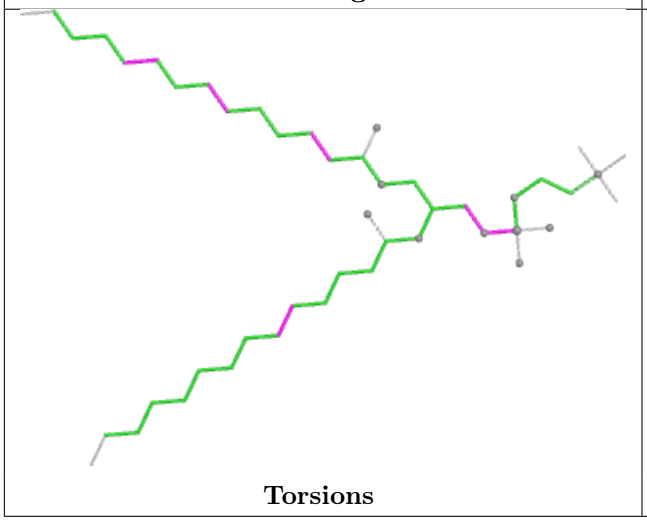
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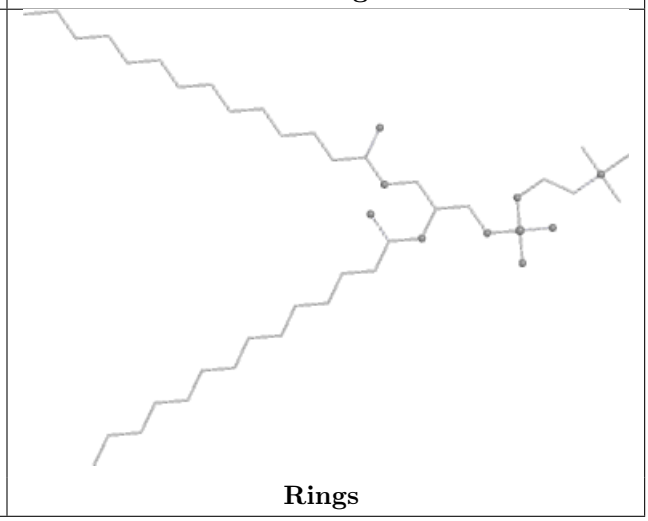
Bond lengths



Bond angles

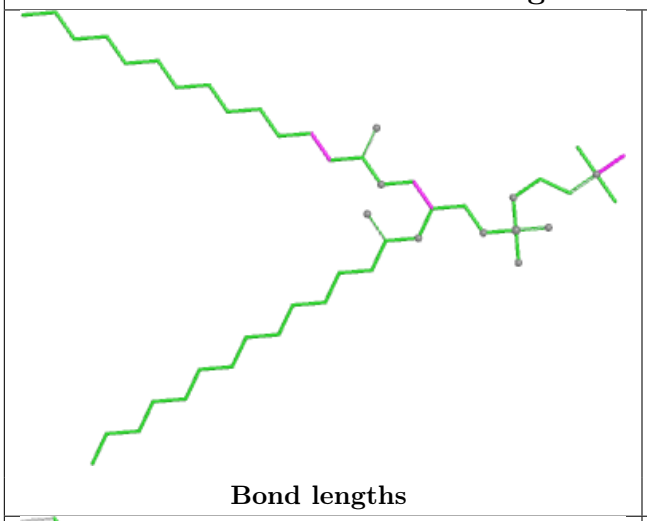


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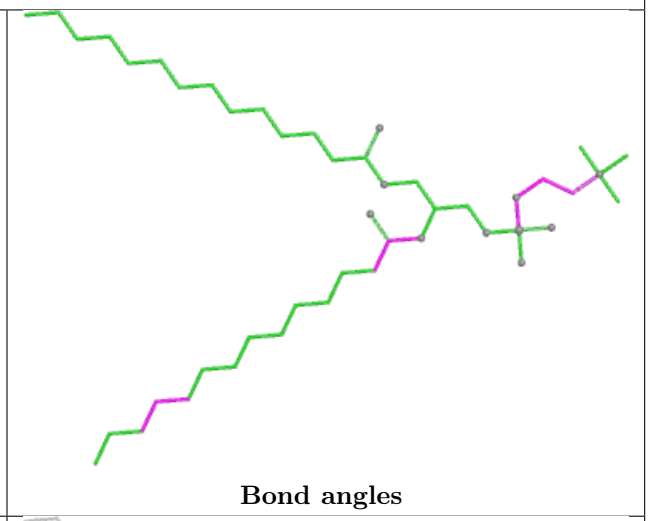


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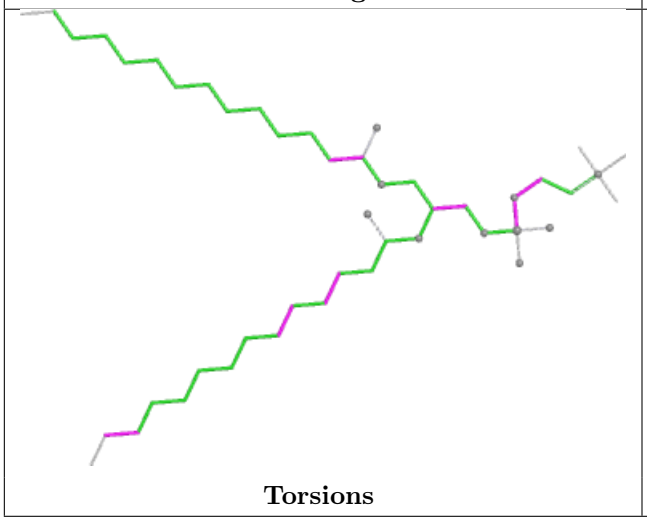
Ligand PX4 C 346



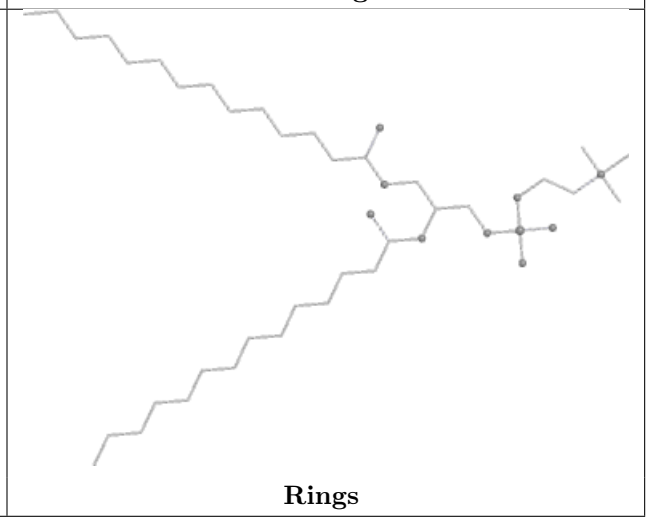
Bond lengths



Bond angles

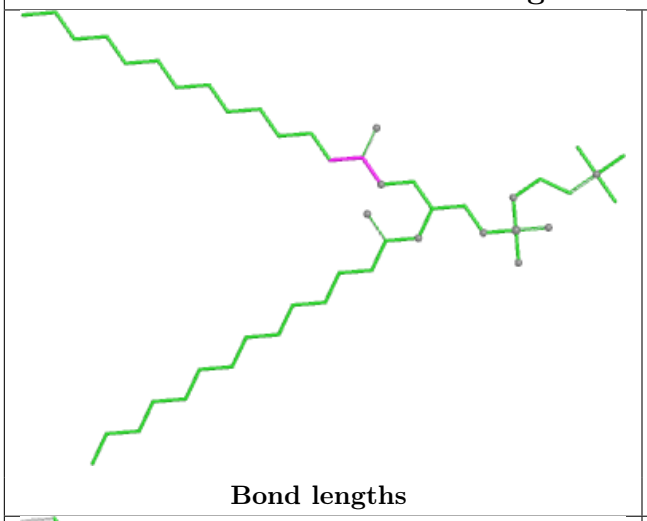


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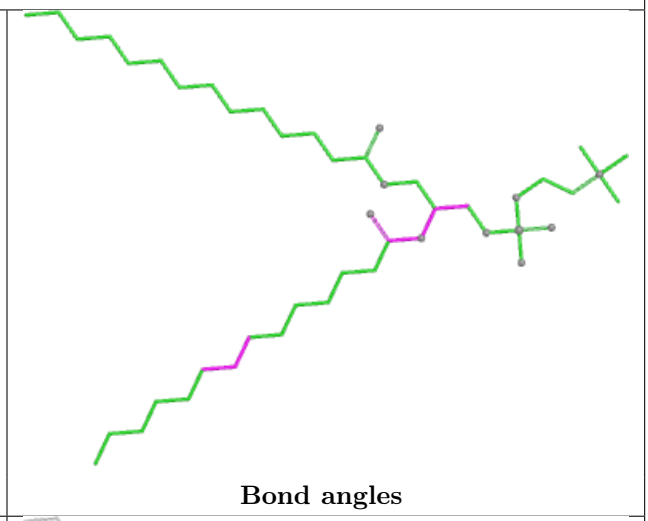


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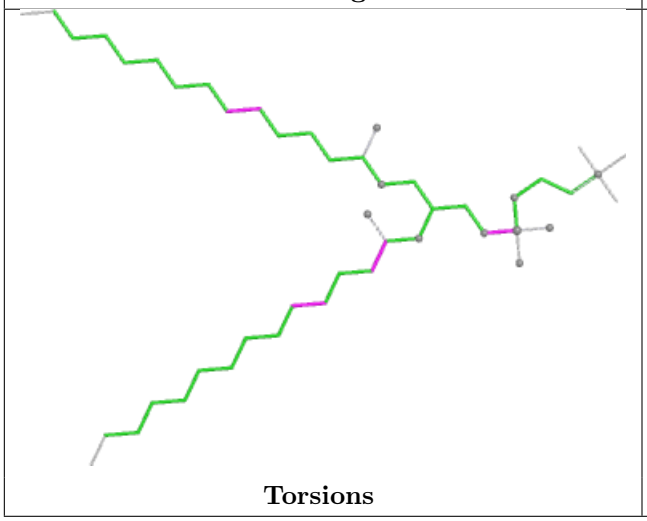
Ligand PX4 A 623



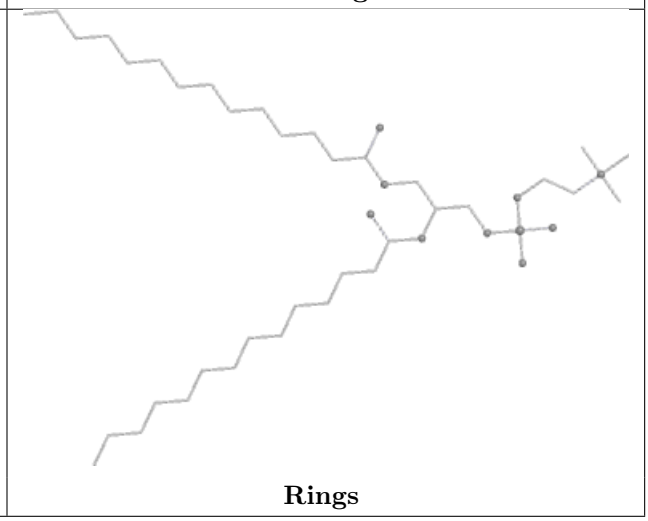
Bond lengths



Bond angles

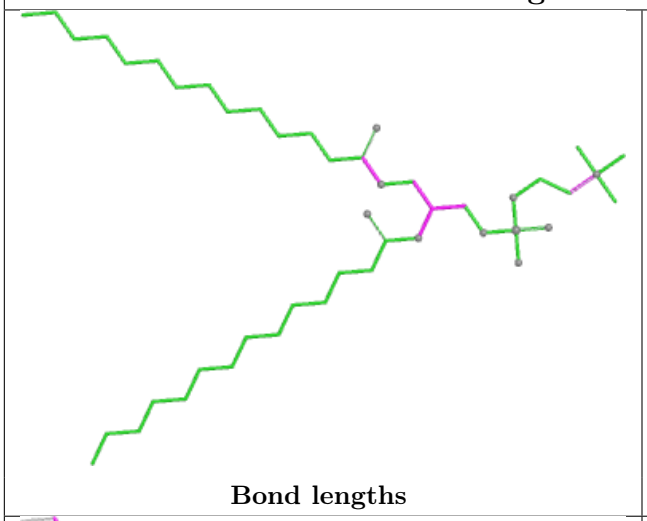


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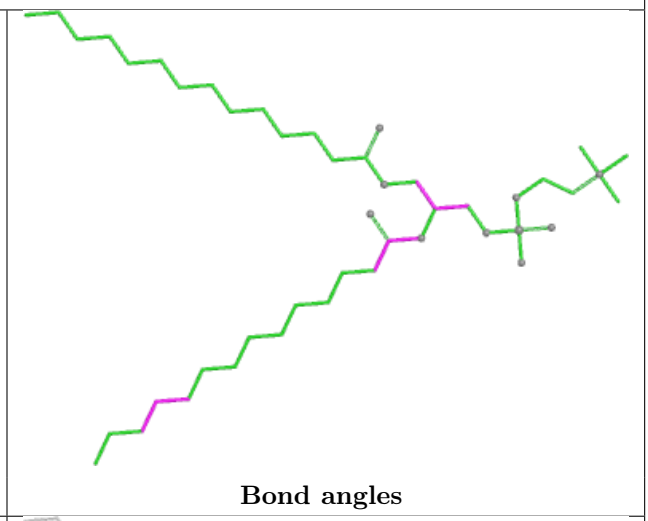


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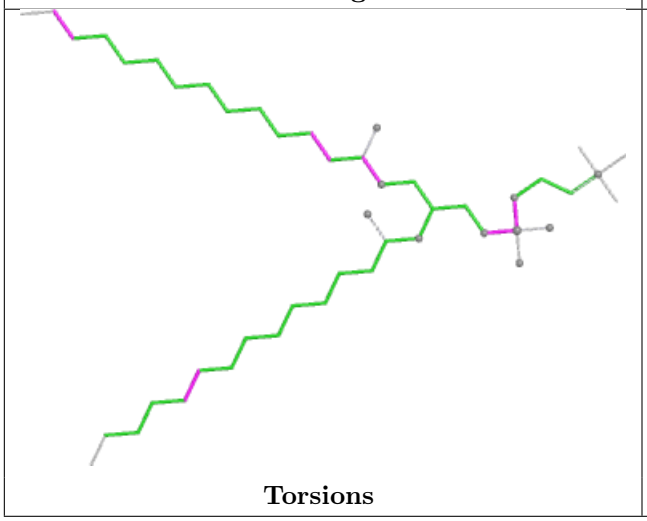
Ligand PX4 C 338



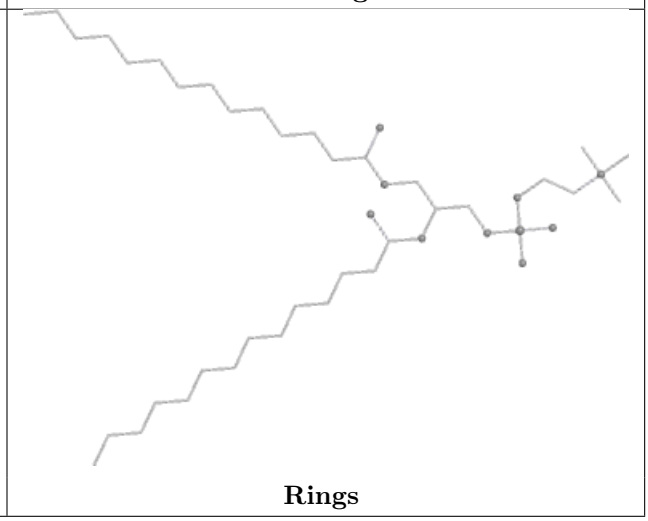
Bond lengths



Bond angles

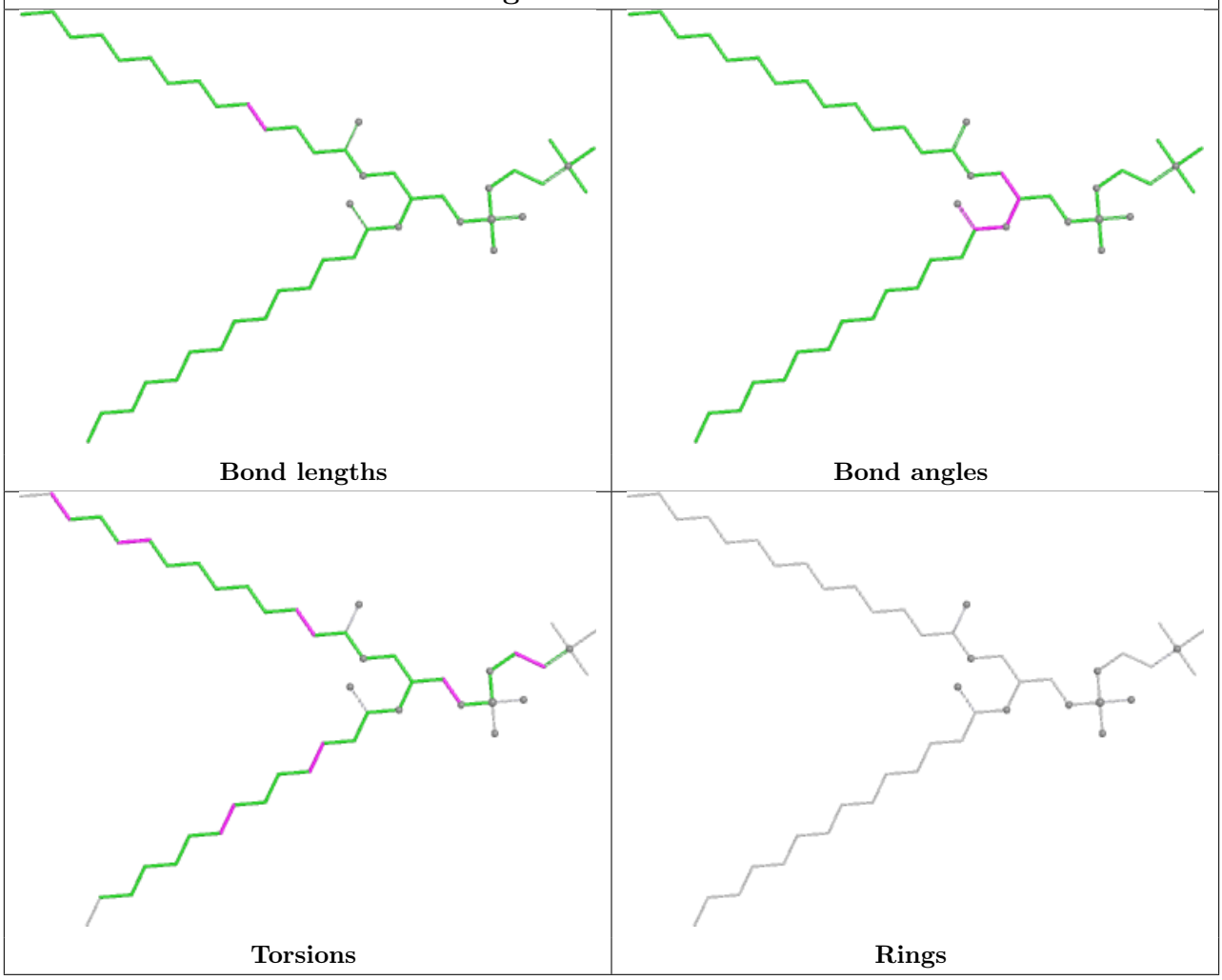


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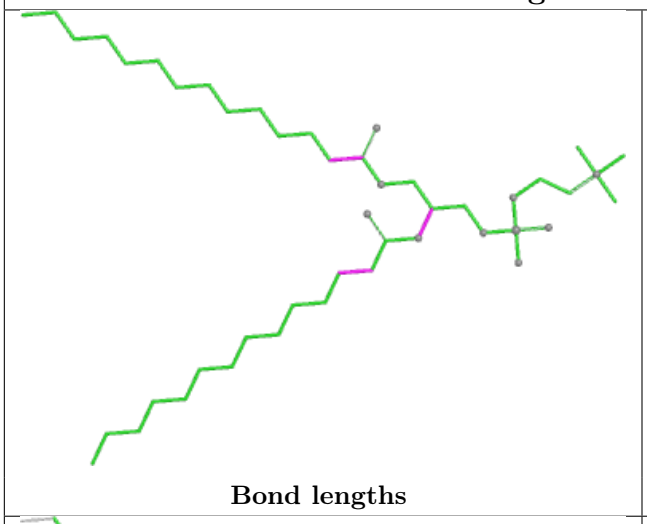


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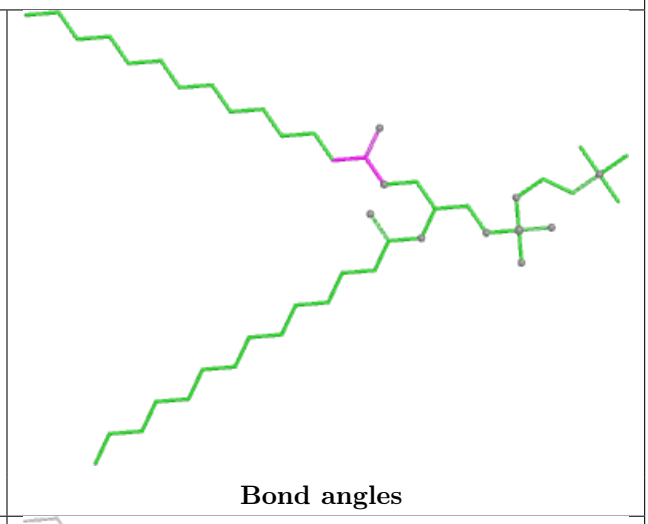
Ligand PX4 B 339



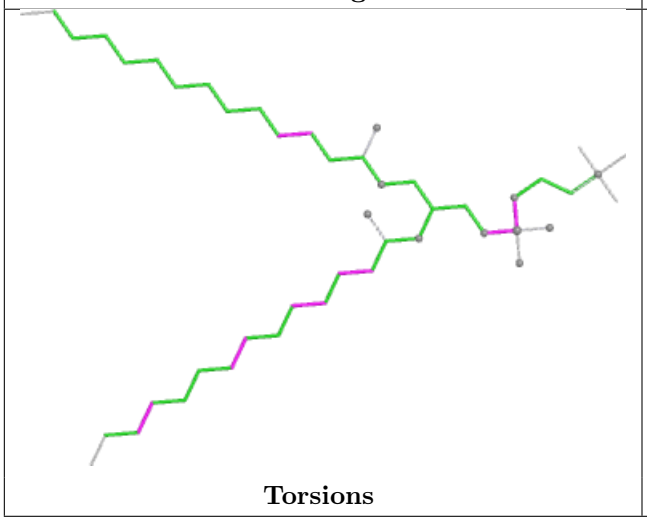
Ligand PX4 B 345



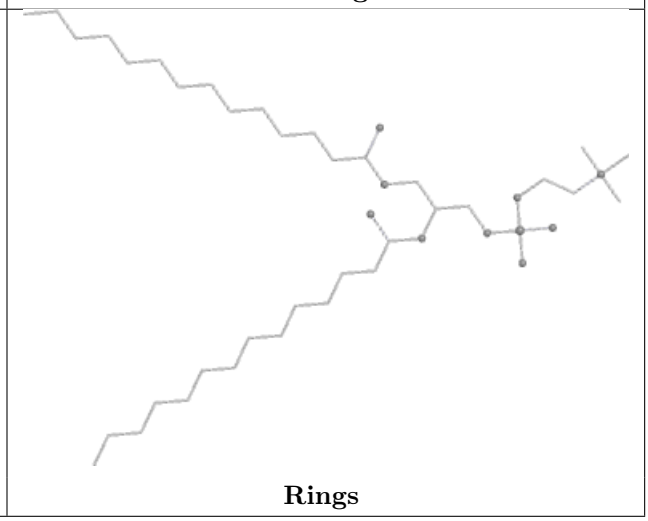
Bond lengths



Bond angles

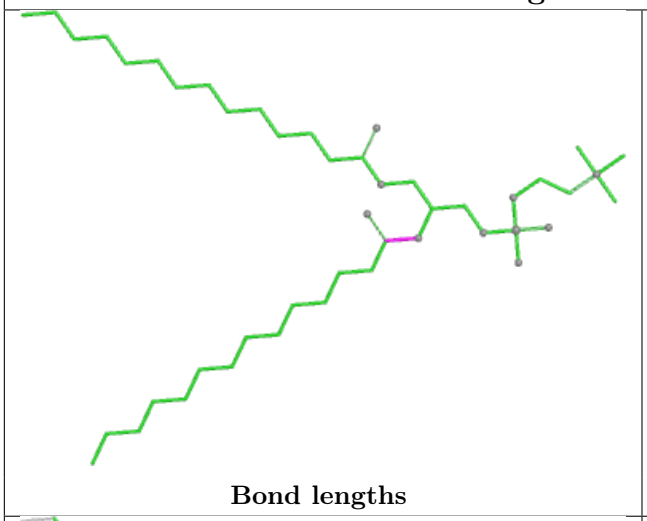


Torsions

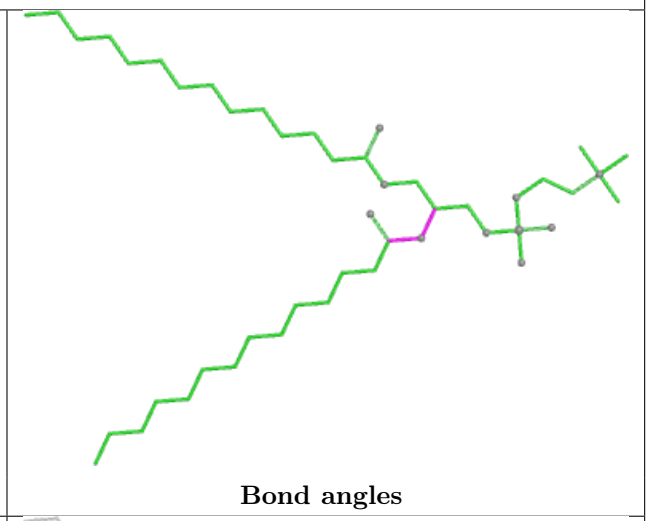


Rings

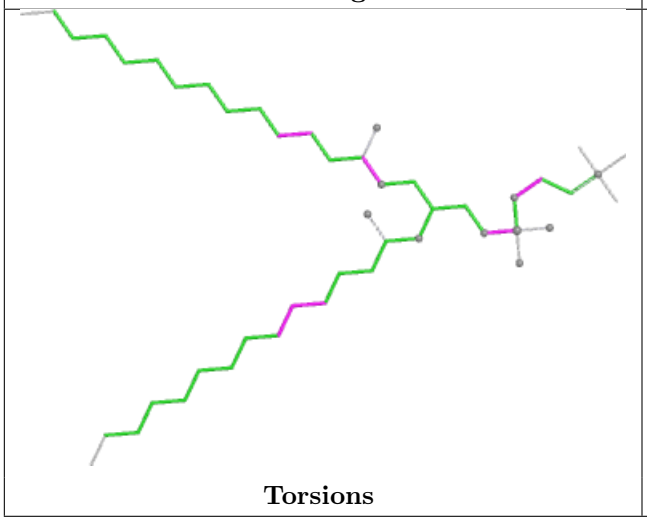
Ligand PX4 C 358



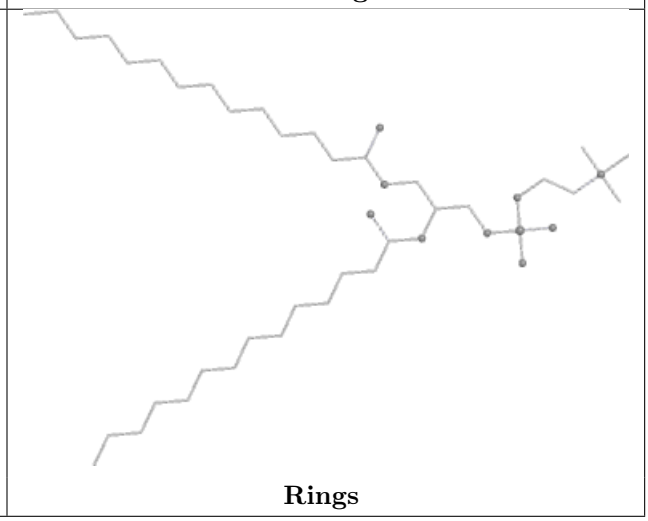
Bond lengths



Bond angles

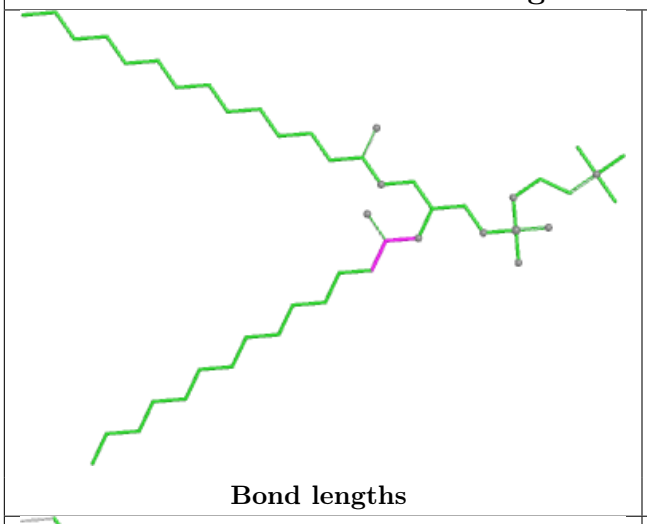


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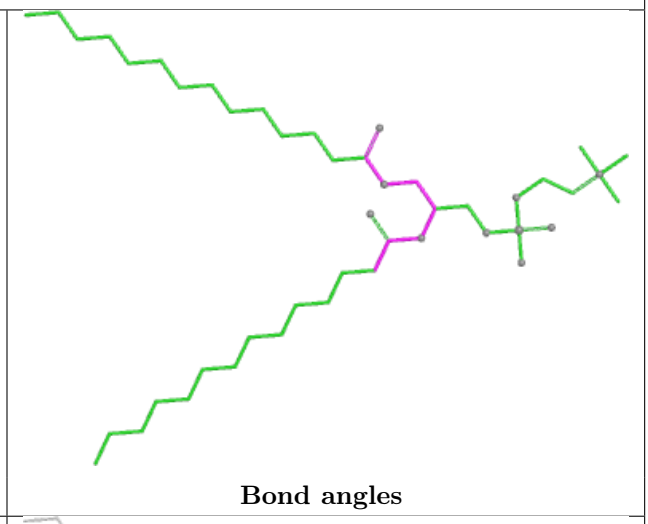


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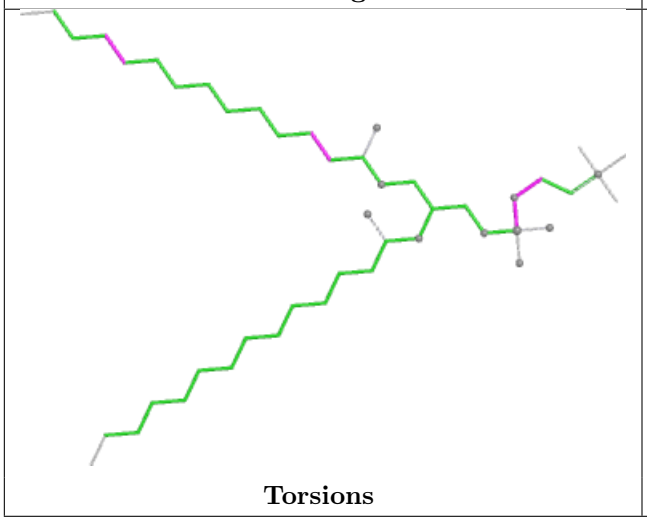
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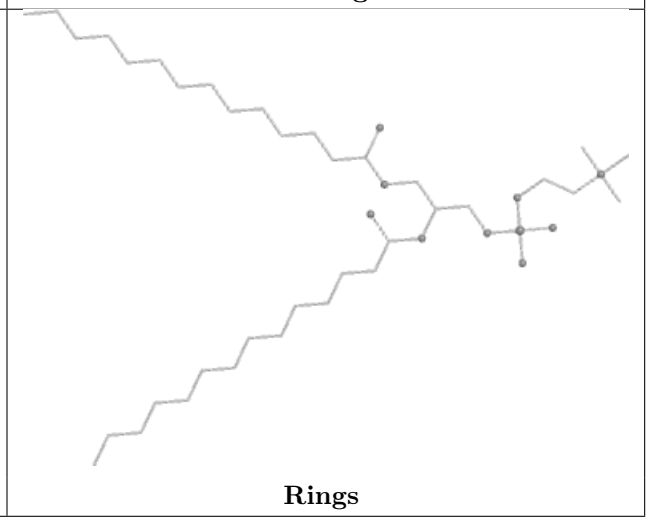
Bond lengths



Bond angles

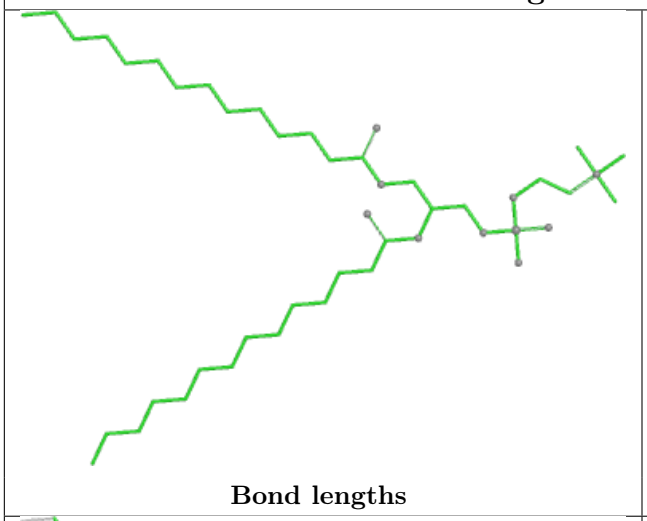


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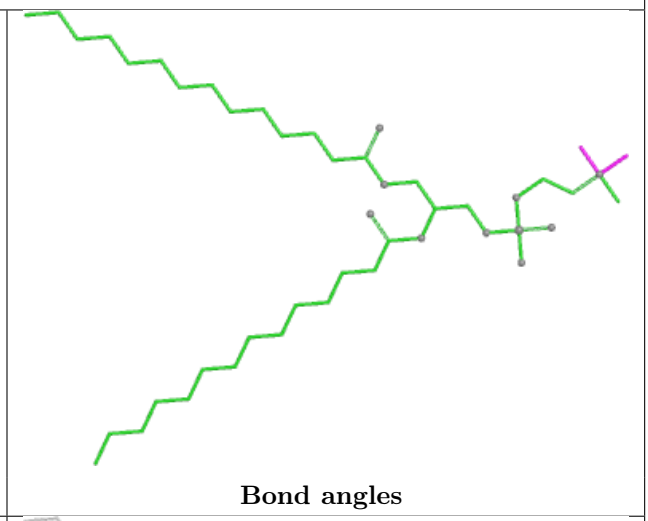


Rings

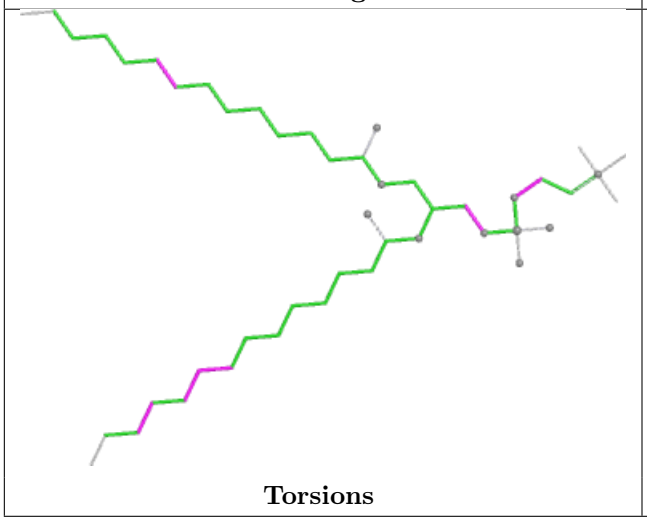
Ligand PX4 A 601



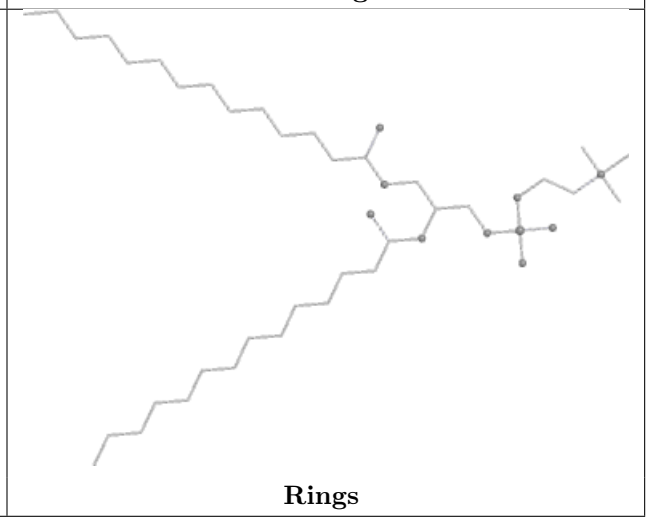
Bond lengths



Bond angles

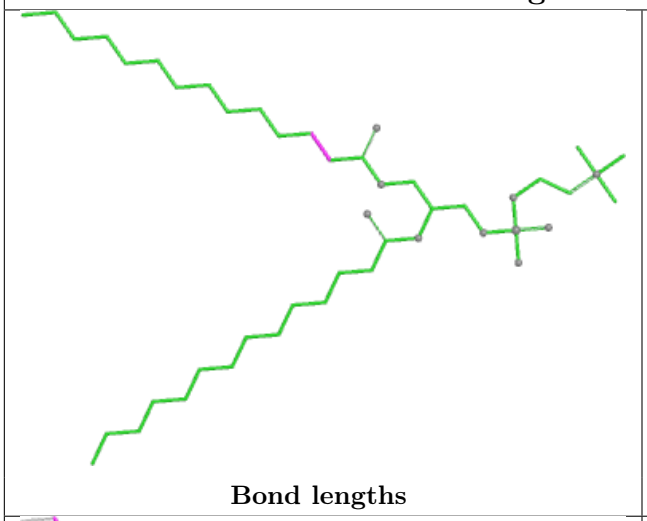


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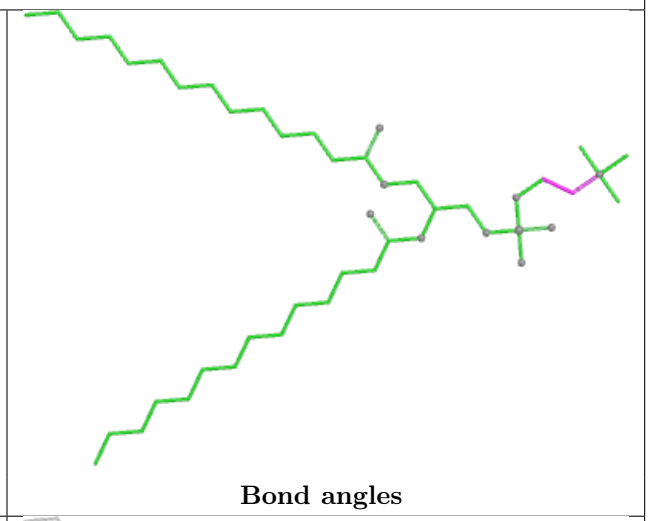


Rings

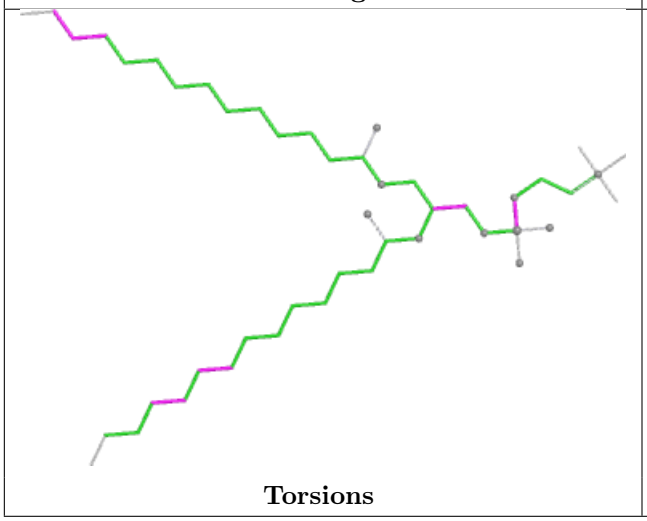
Ligand PX4 B 349



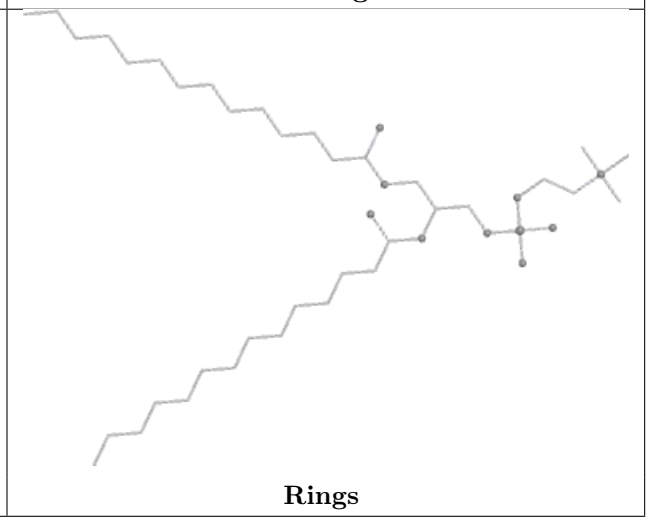
Bond lengths



Bond angles

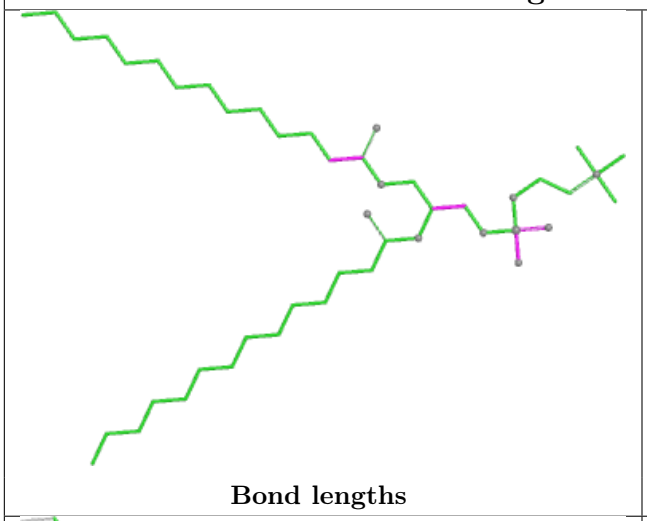


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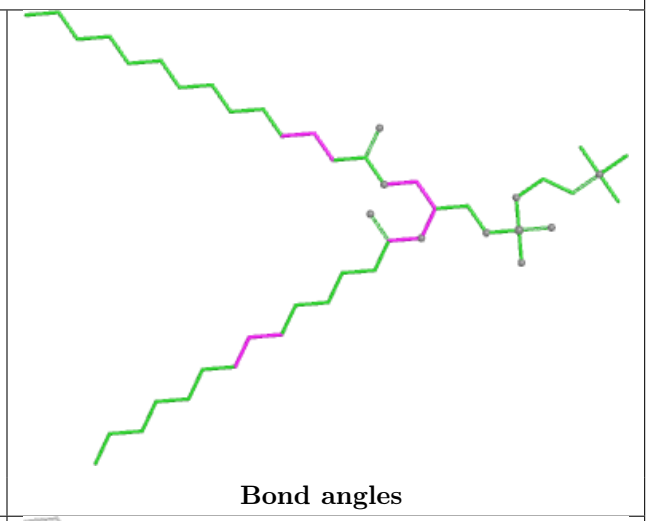


Rings

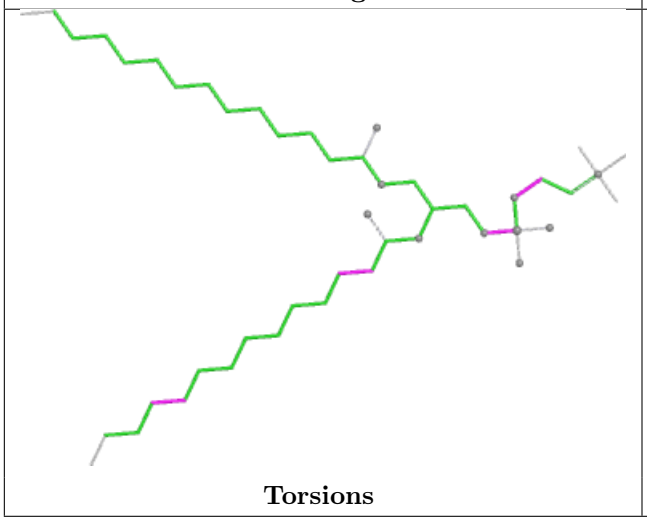
Ligand PX4 A 632



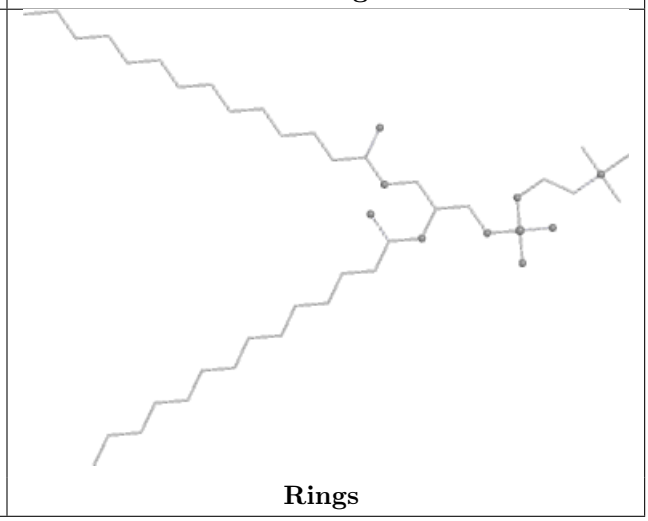
Bond lengths



Bond angles

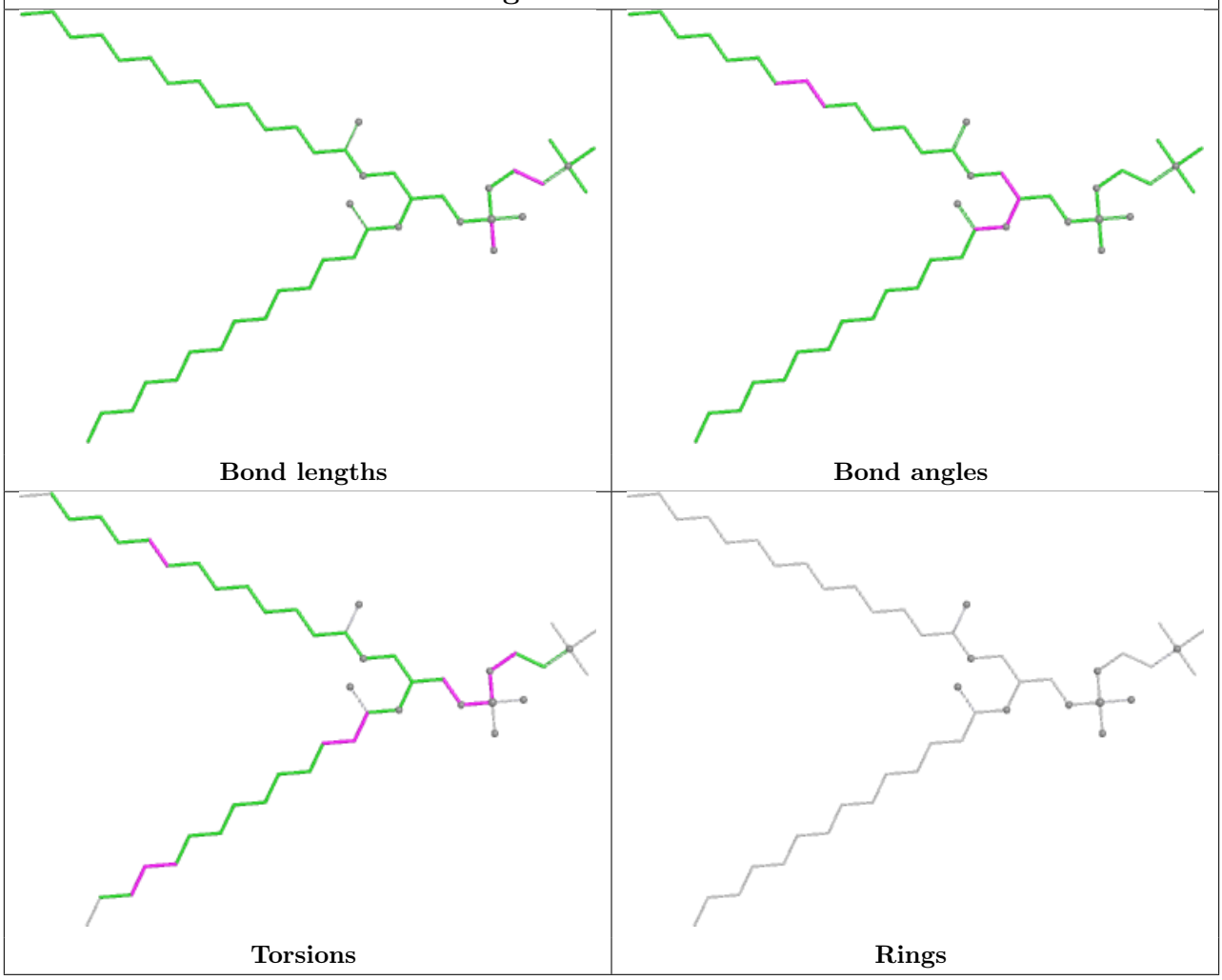


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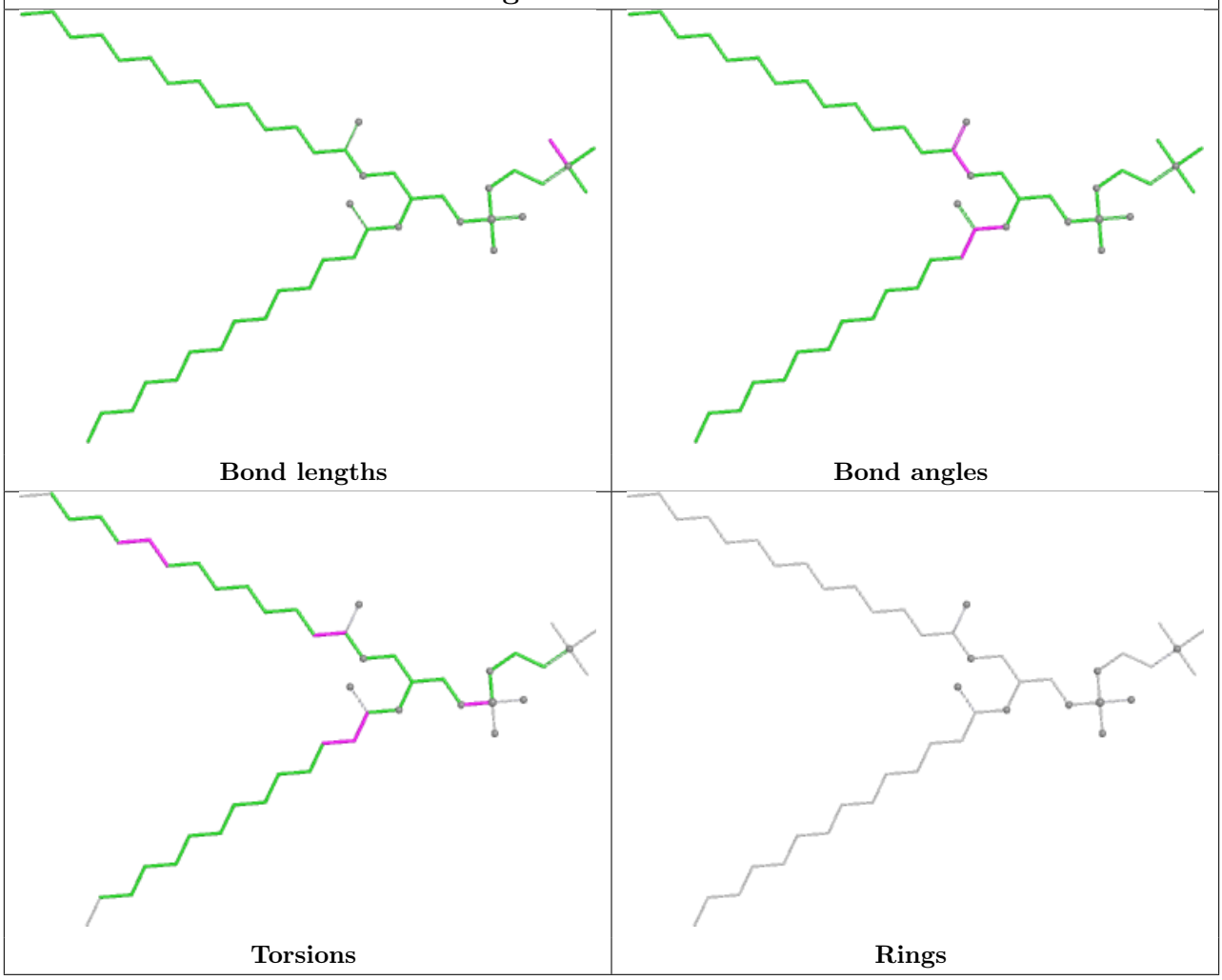


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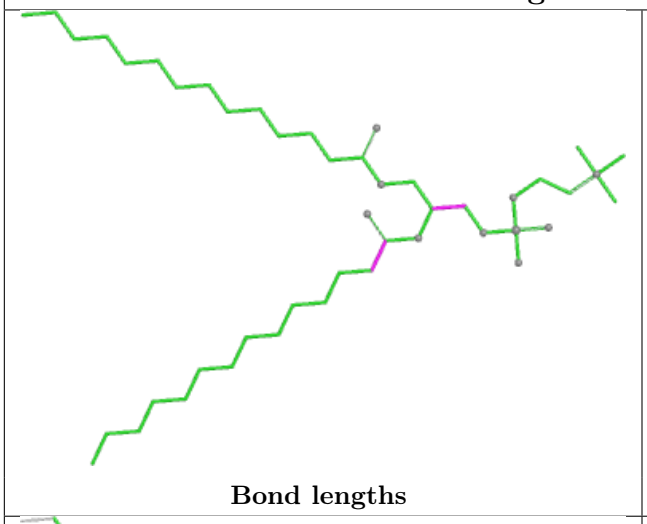
Ligand PX4 B 384



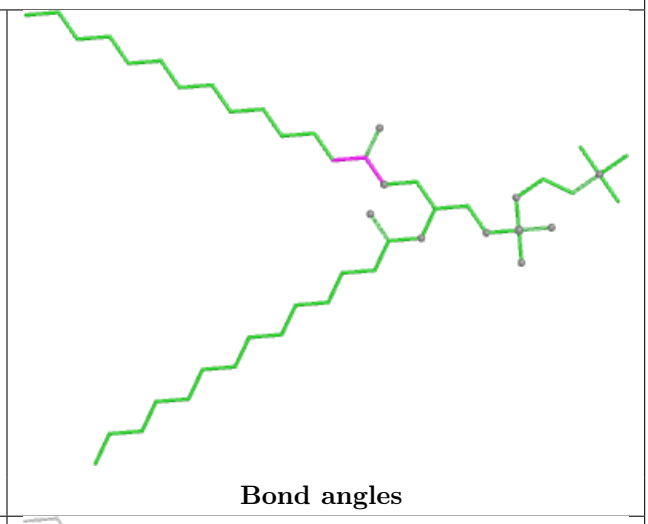
Ligand PX4 C 331



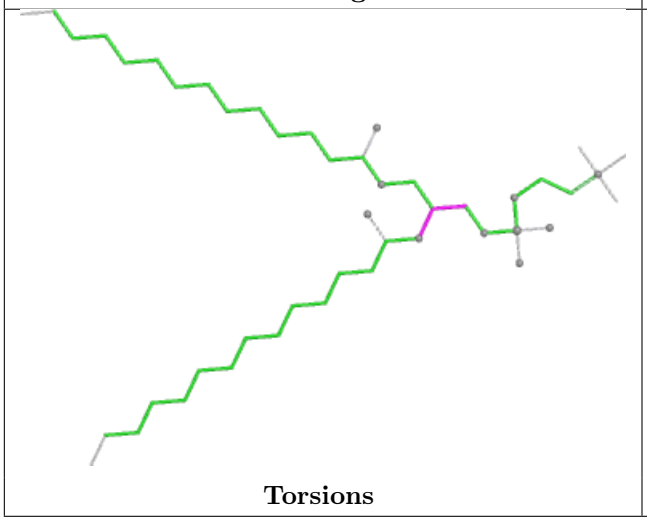
Ligand PX4 C 325



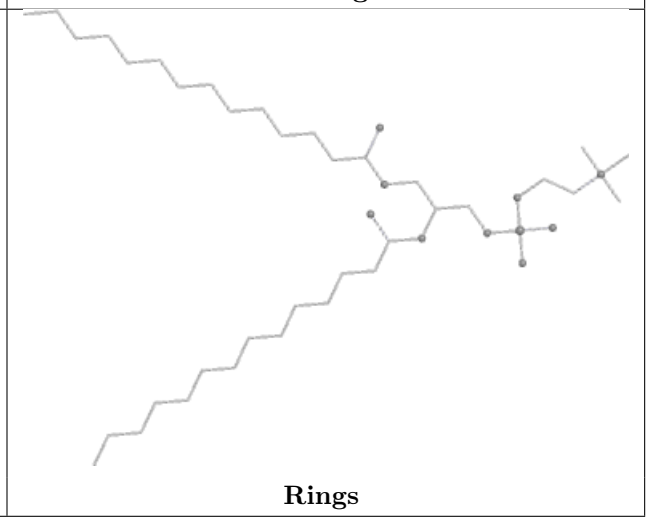
Bond lengths



Bond angles

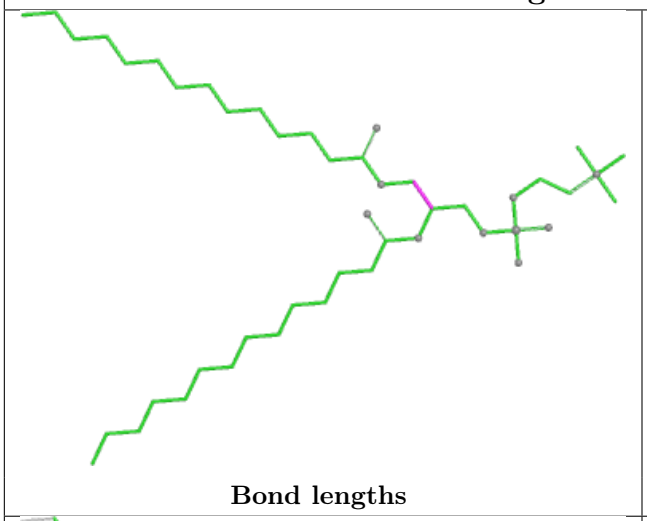


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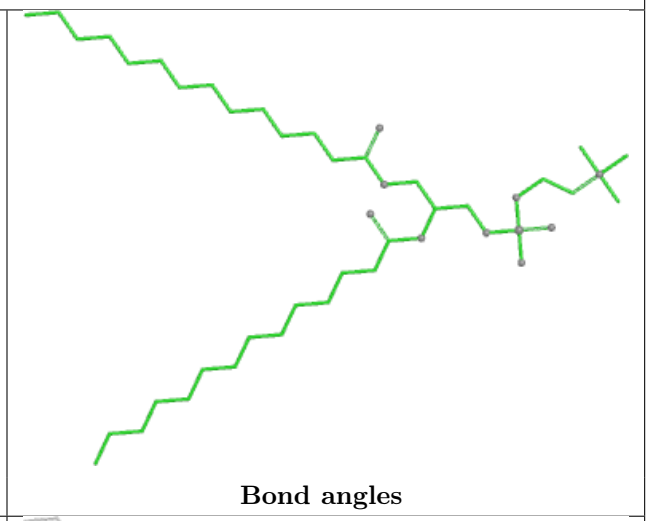


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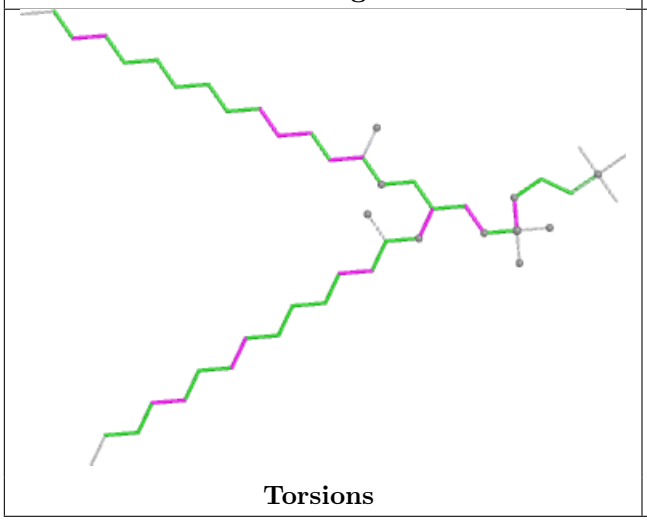
Ligand PX4 B 334



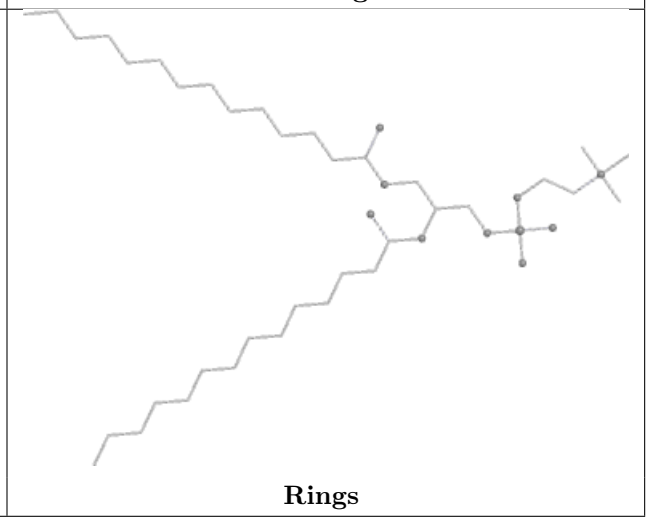
Bond lengths



Bond angles

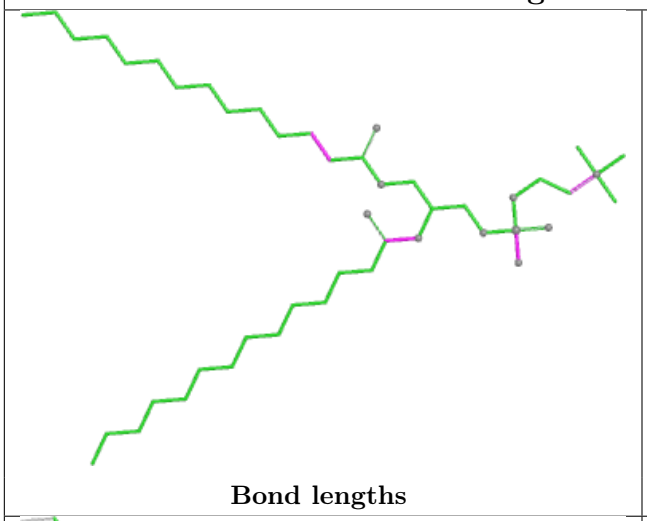


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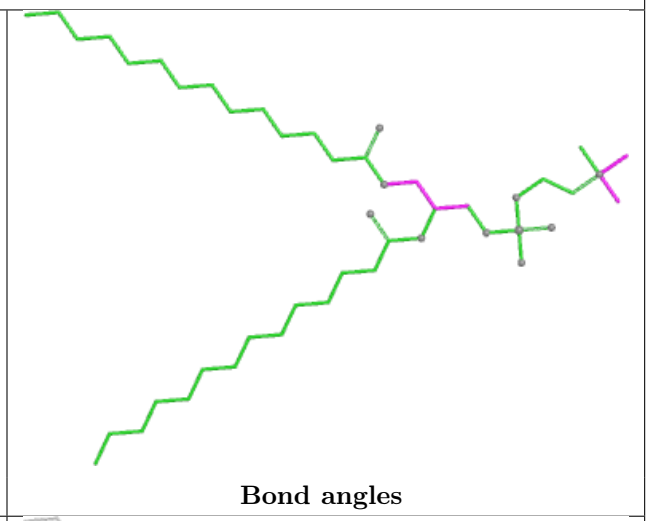


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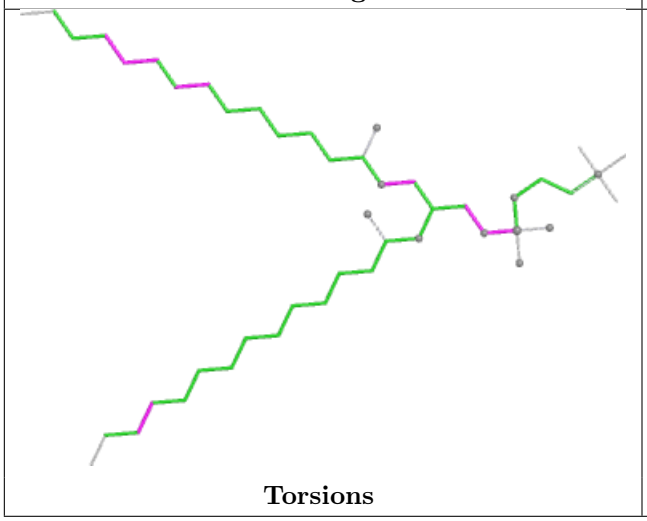
Ligand PX4 A 636



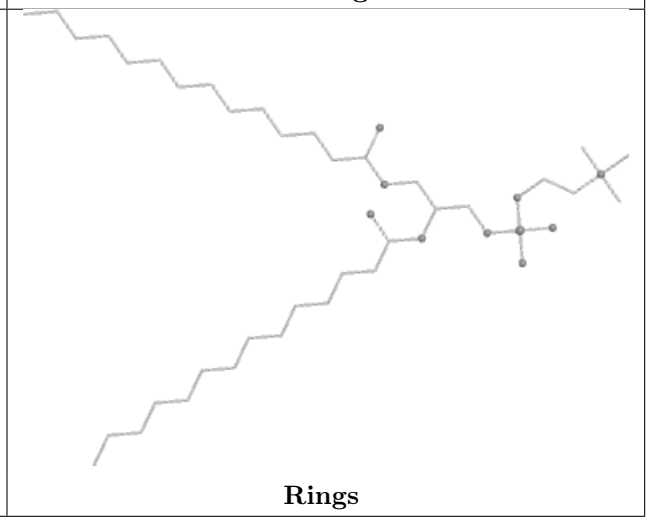
Bond lengths



Bond angles

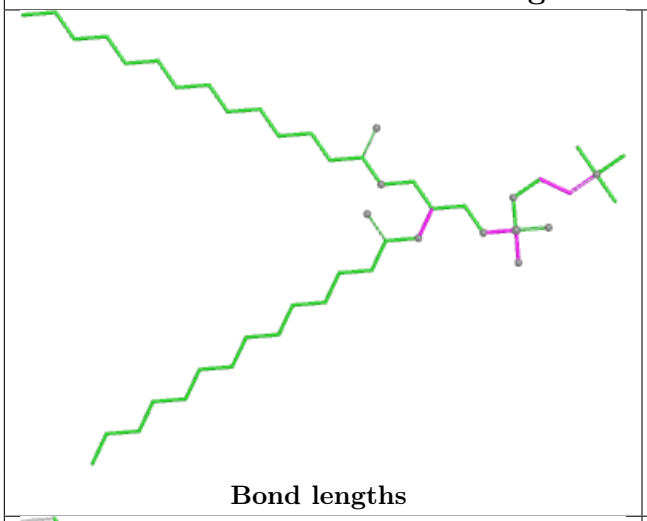


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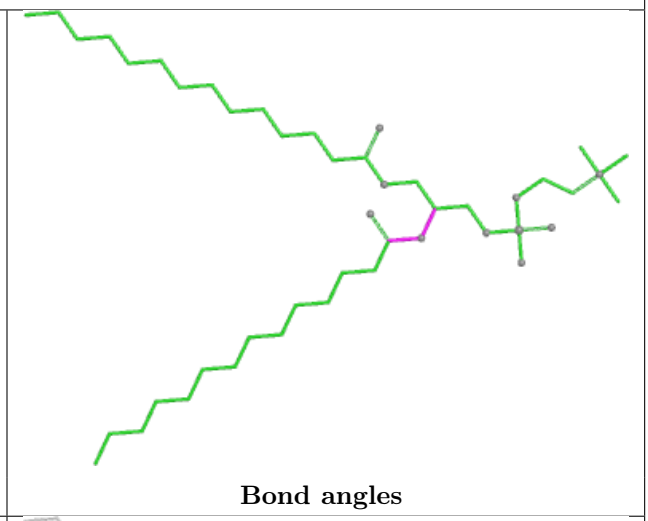


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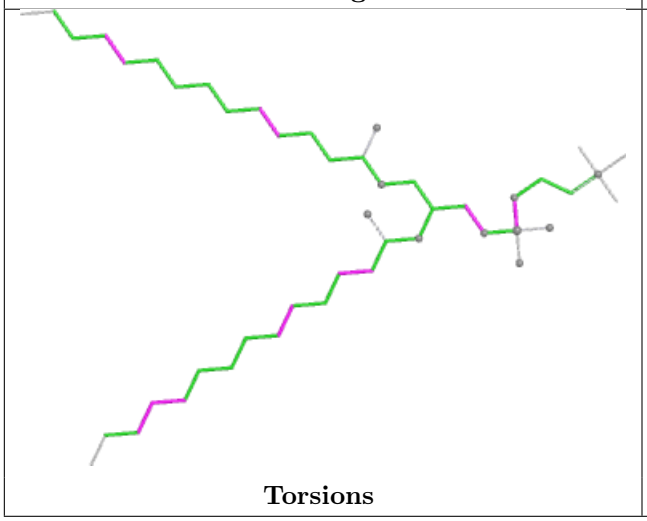
Ligand PX4 B 372



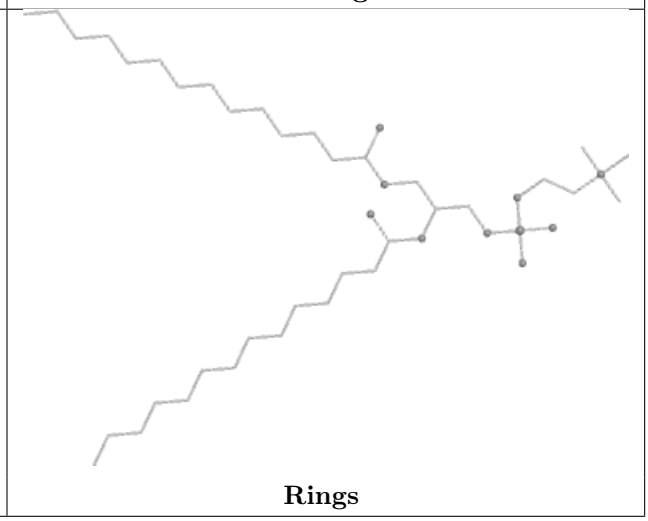
Bond lengths



Bond angles

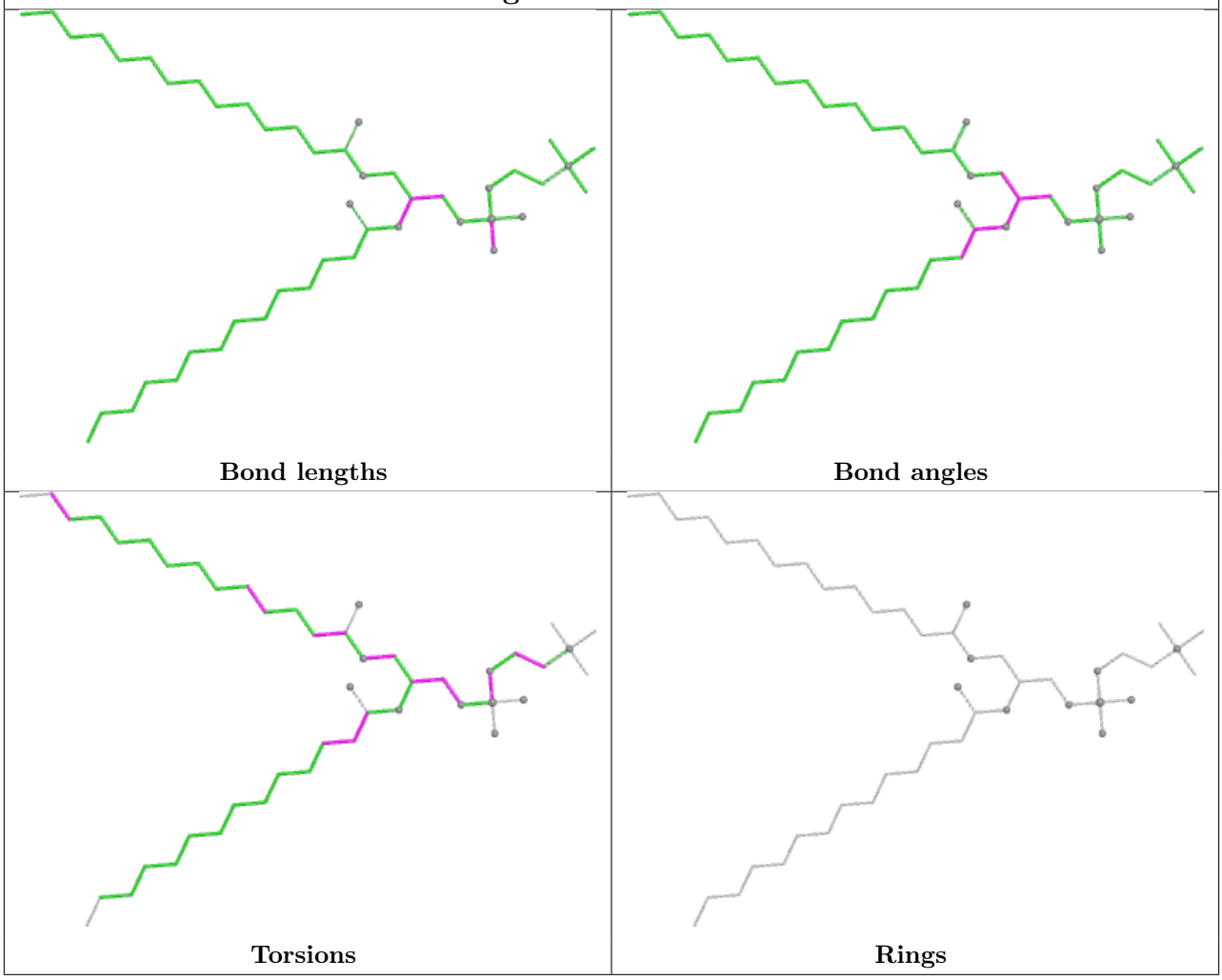


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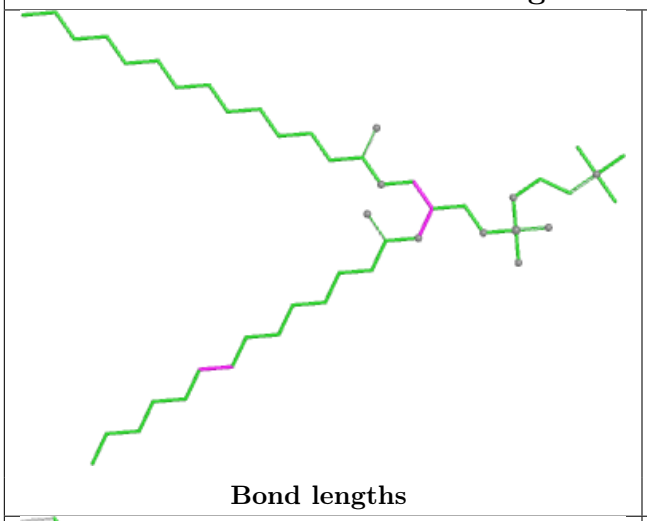


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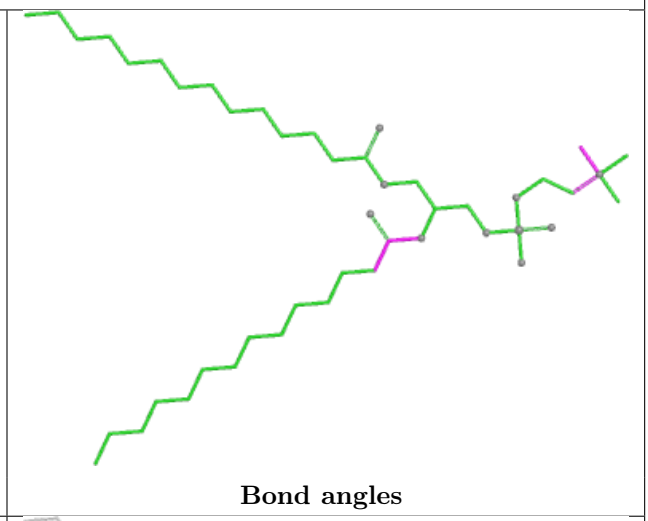
Ligand PX4 B 360



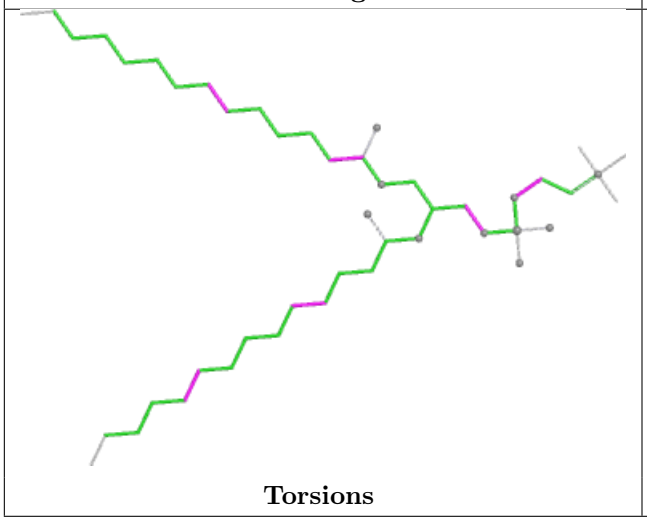
Ligand PX4 B 326



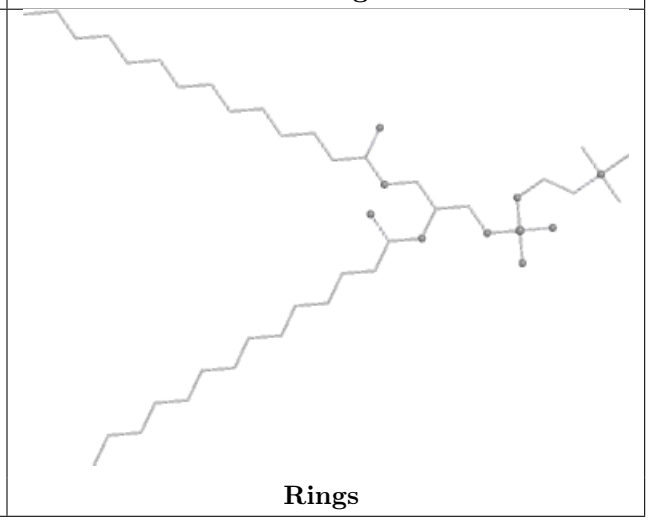
Bond lengths



Bond angles

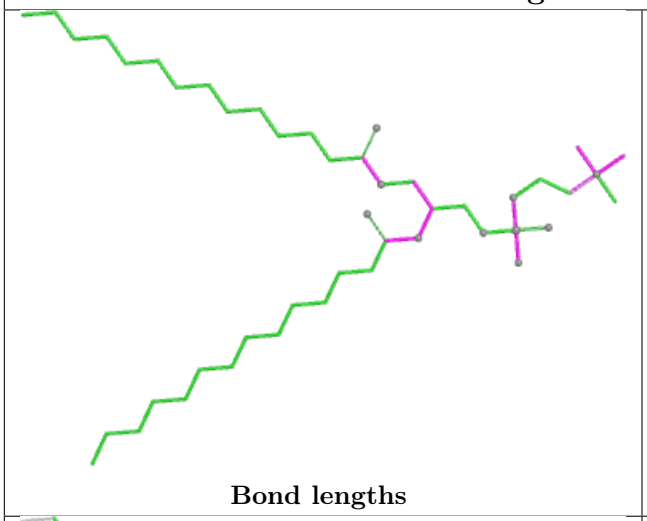


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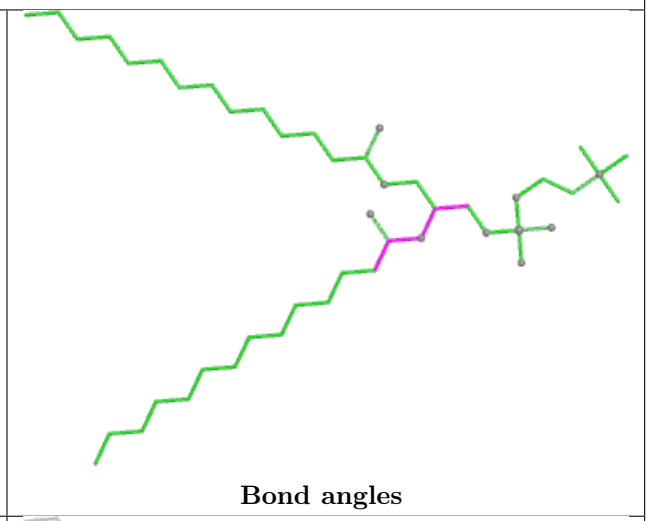


Rings

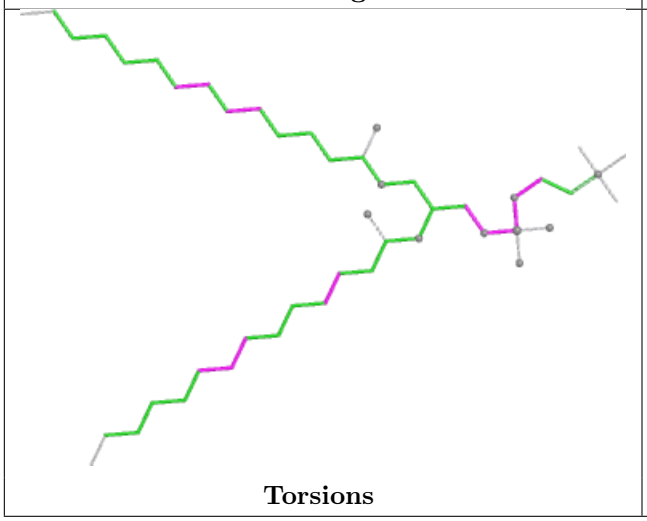
Ligand PX4 A 633



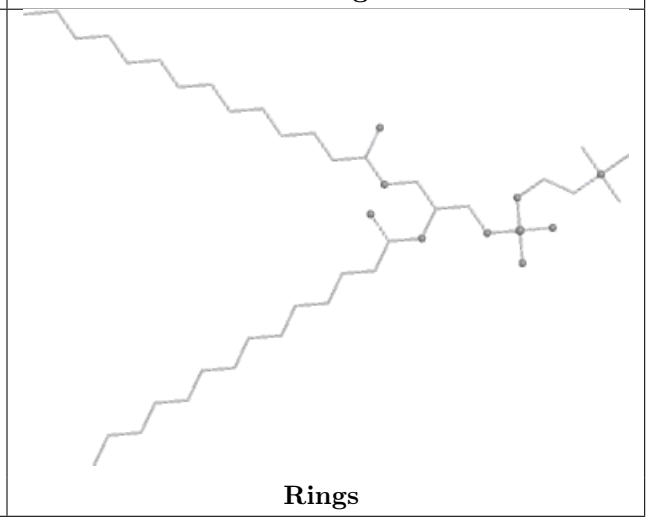
Bond lengths



Bond angles

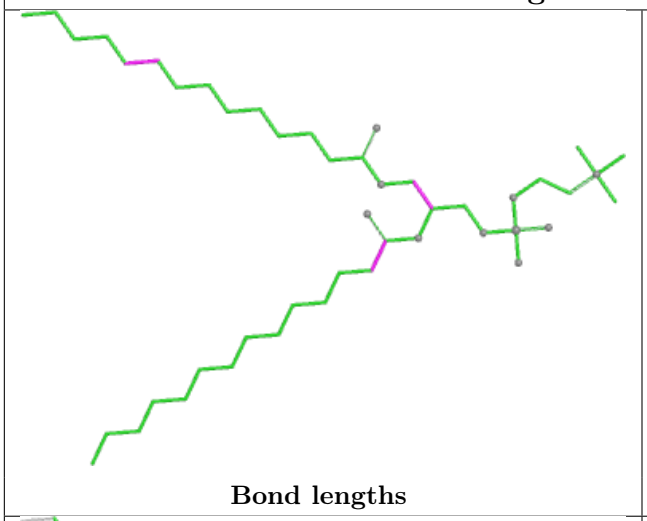


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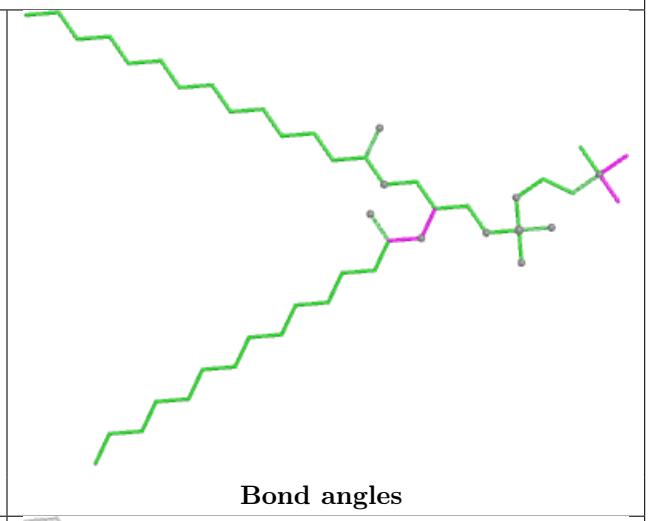


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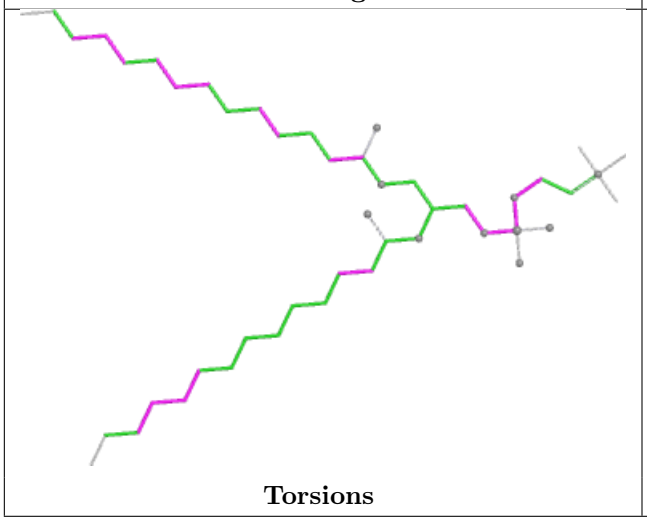
Ligand PX4 C 330



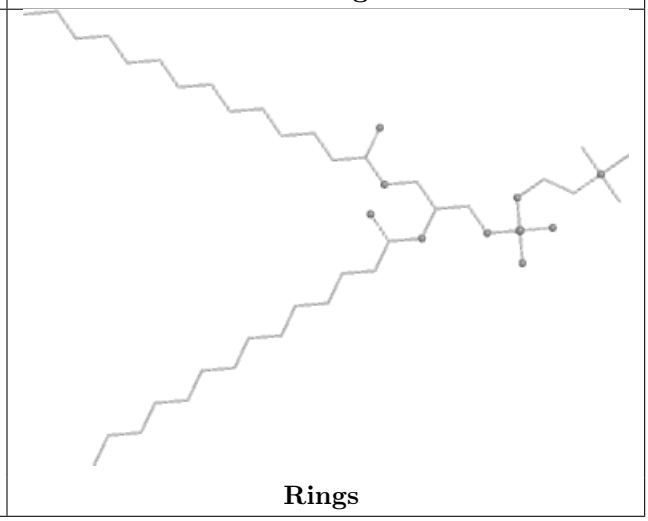
Bond lengths



Bond angles

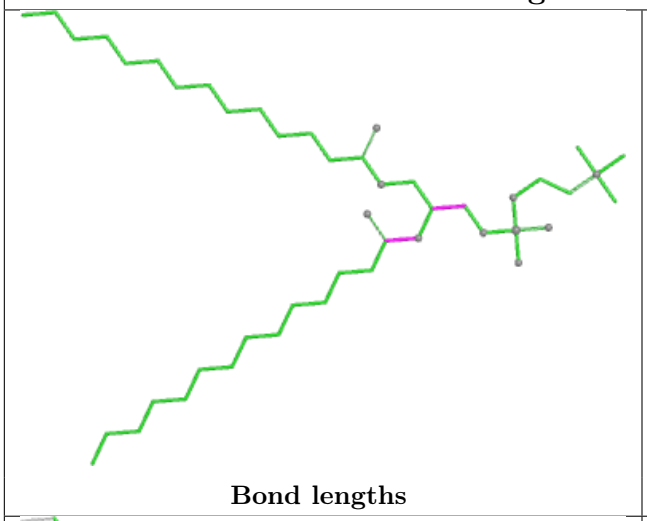


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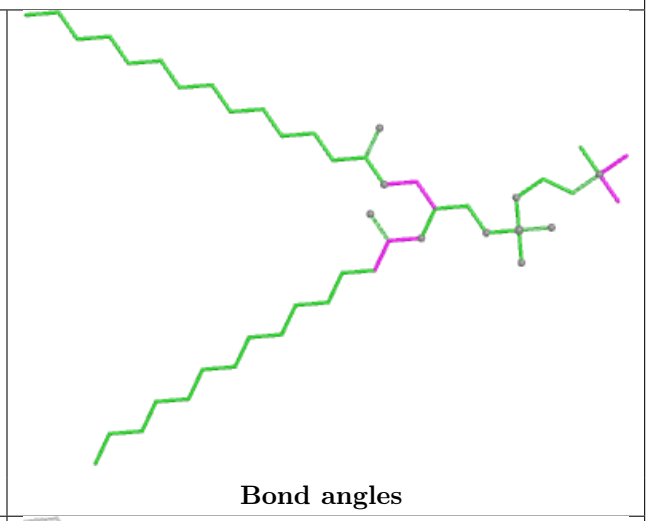


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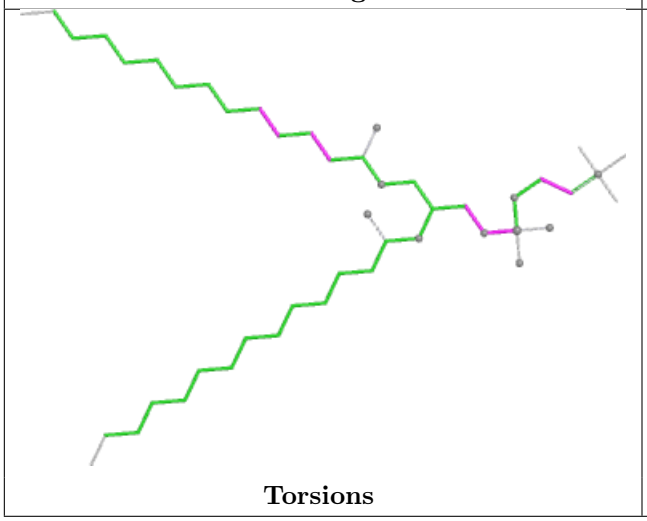
Ligand PX4 B 328



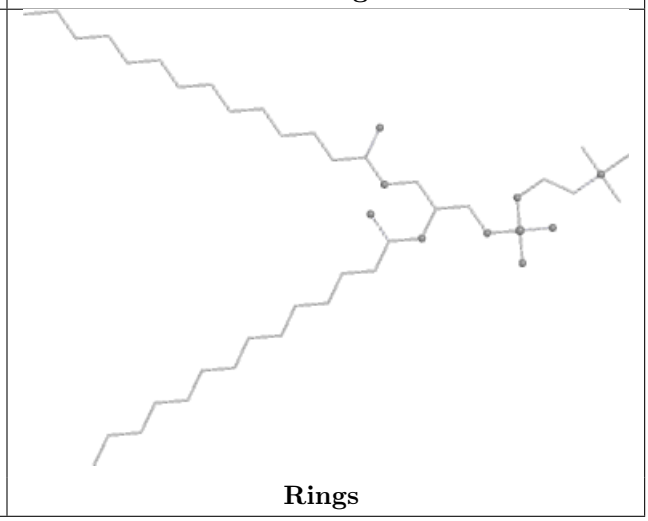
Bond lengths



Bond angles

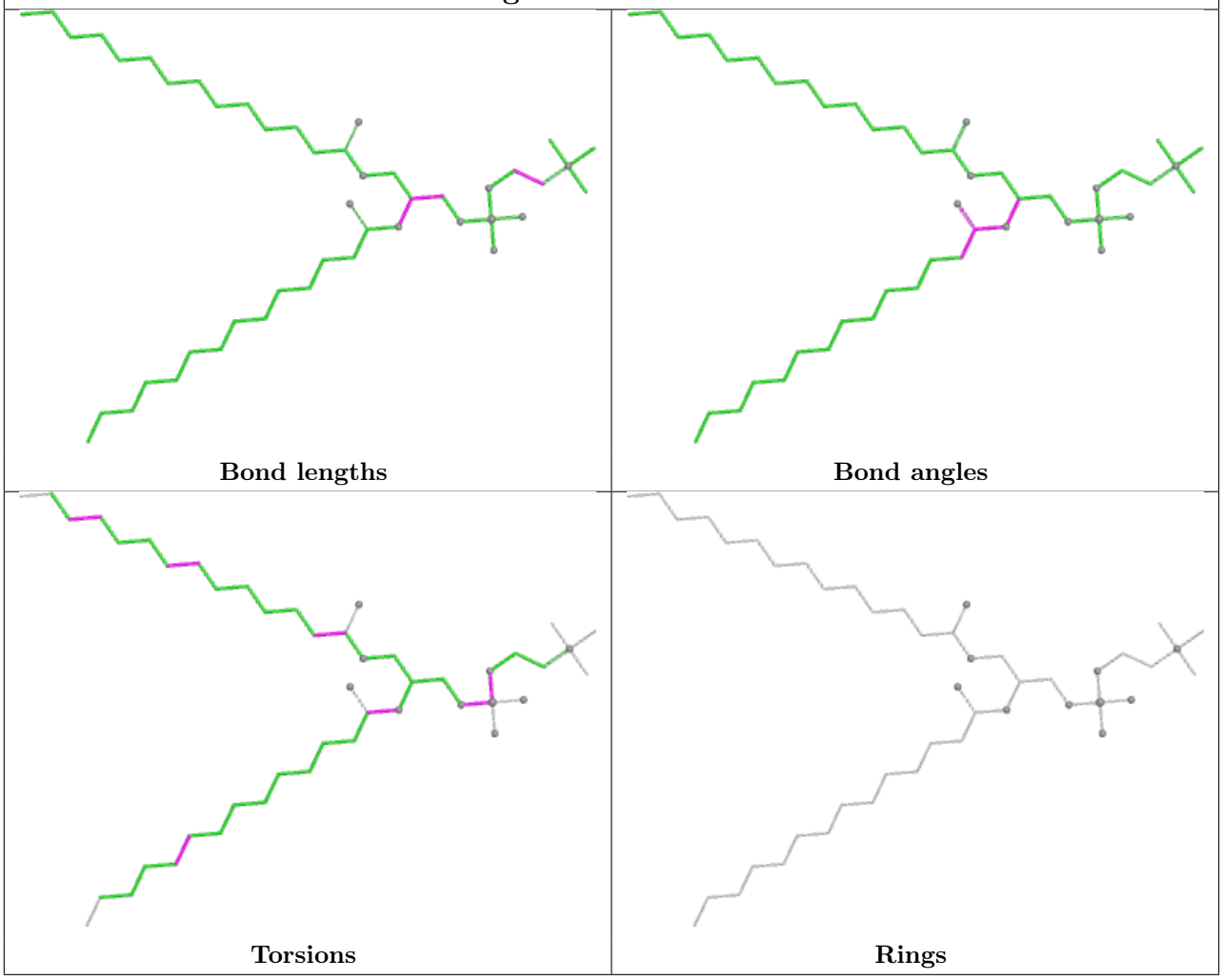


Torsions

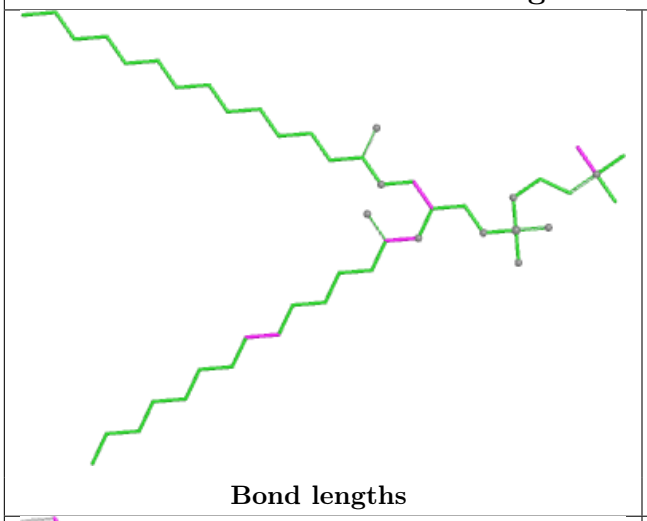


Rings

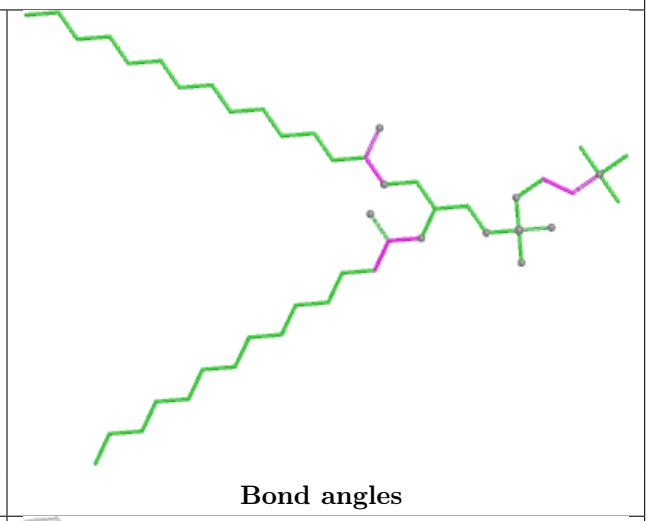
Ligand PX4 B 358



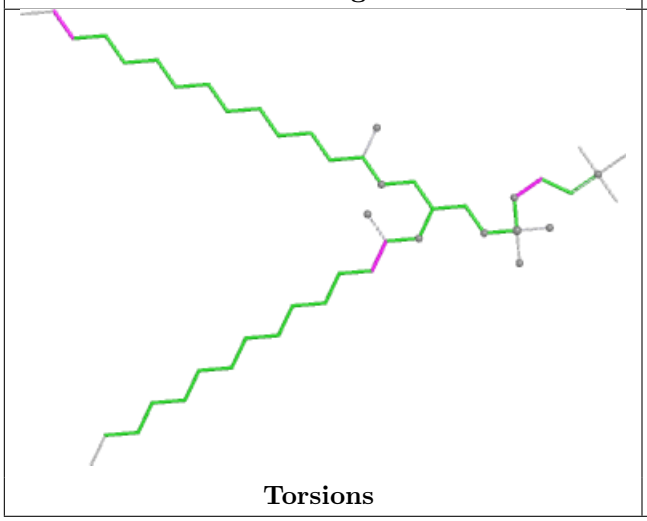
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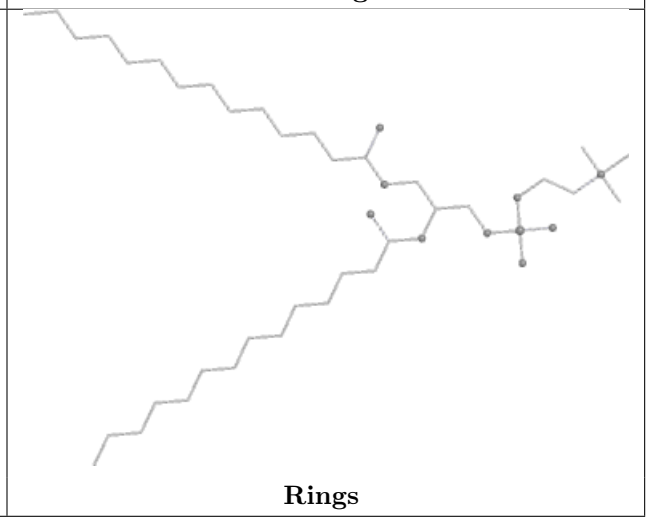
Bond lengths



Bond angles

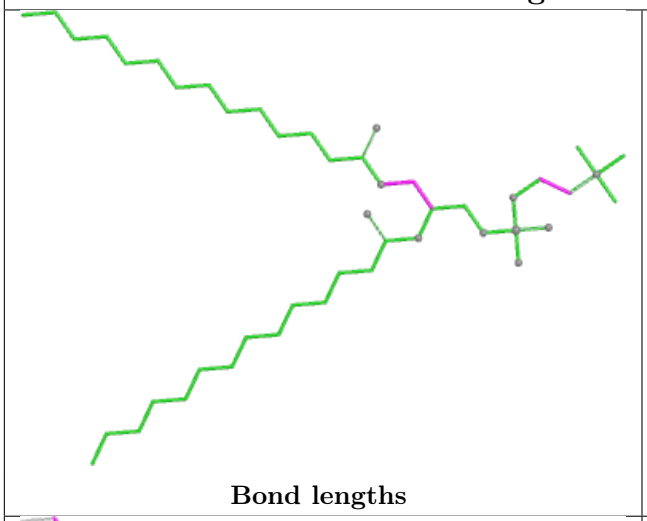


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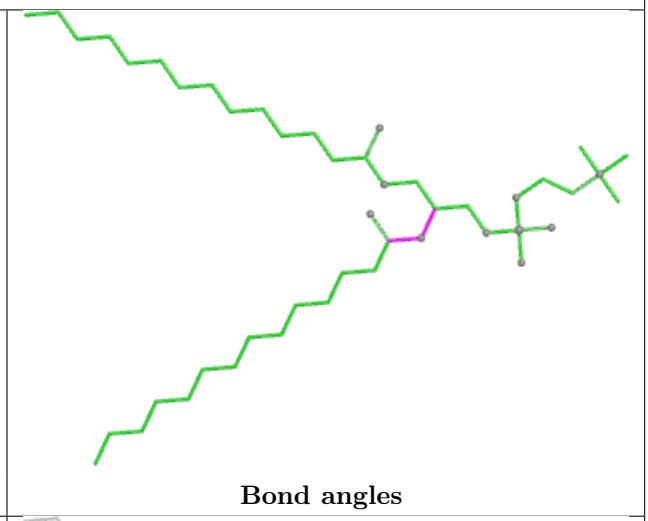


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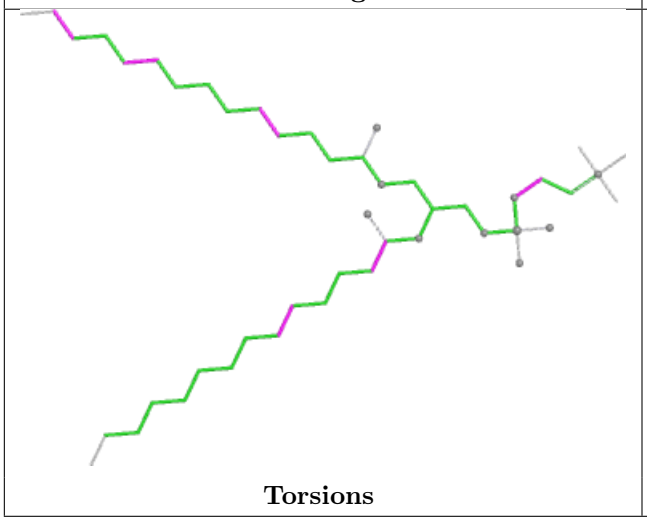
Ligand PX4 C 341



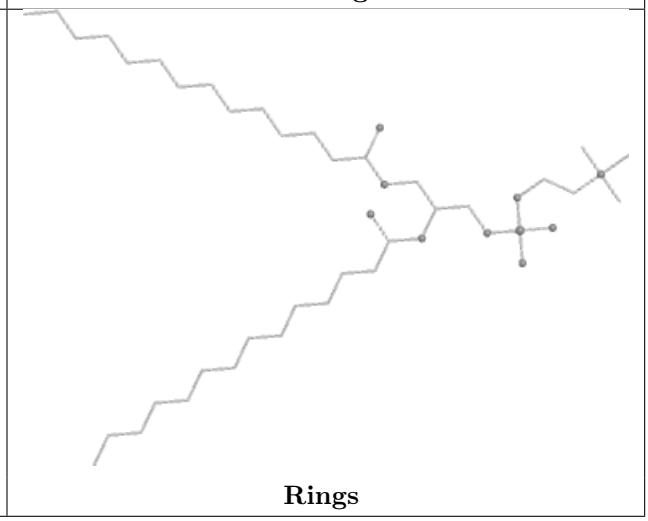
Bond lengths



Bond angles

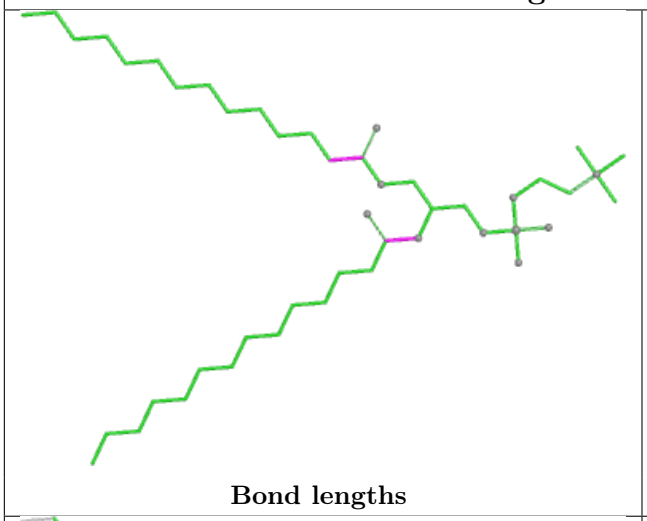


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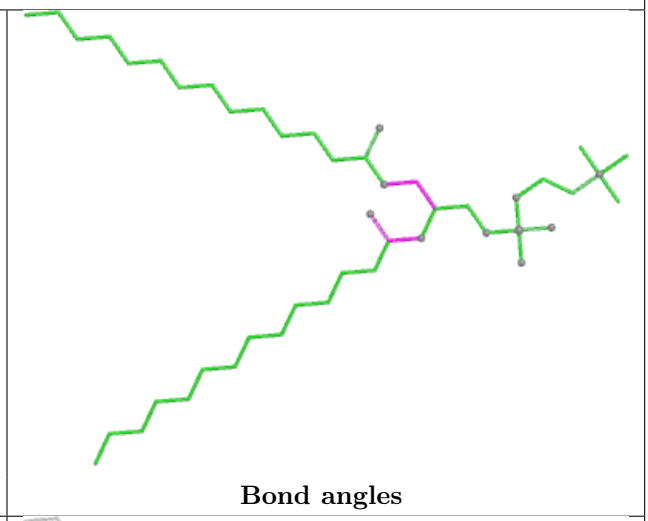


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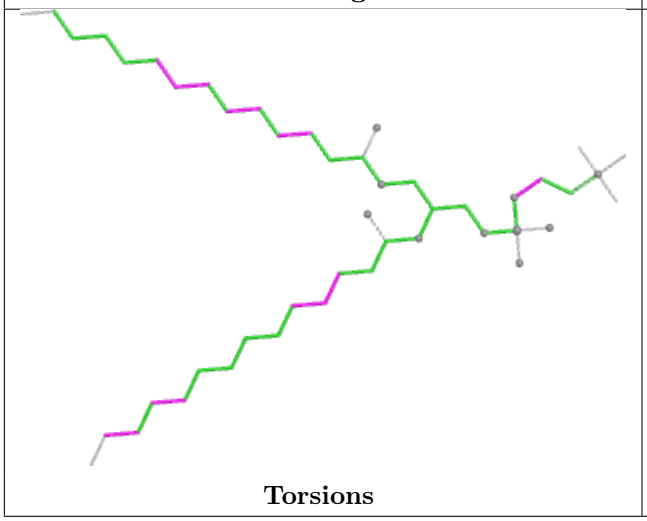
Ligand PX4 B 303



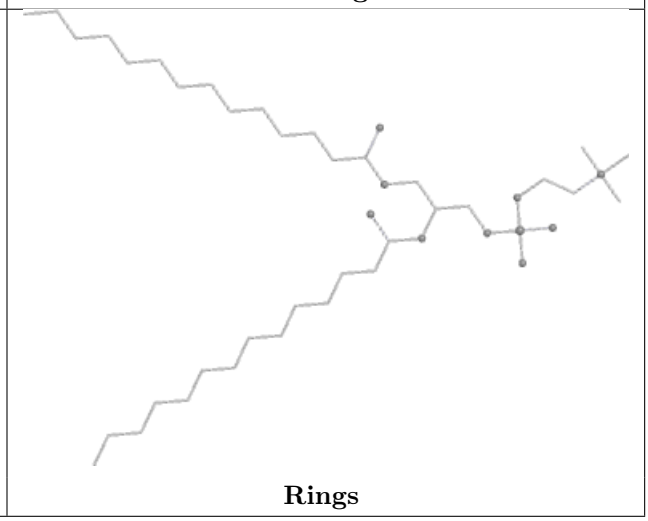
Bond lengths



Bond angles

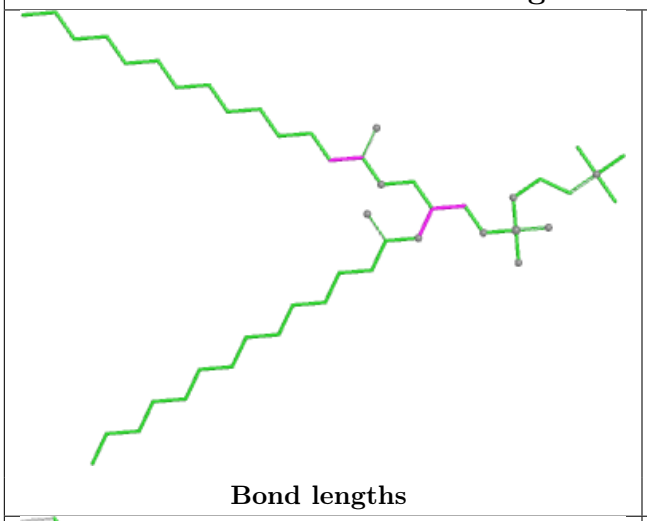


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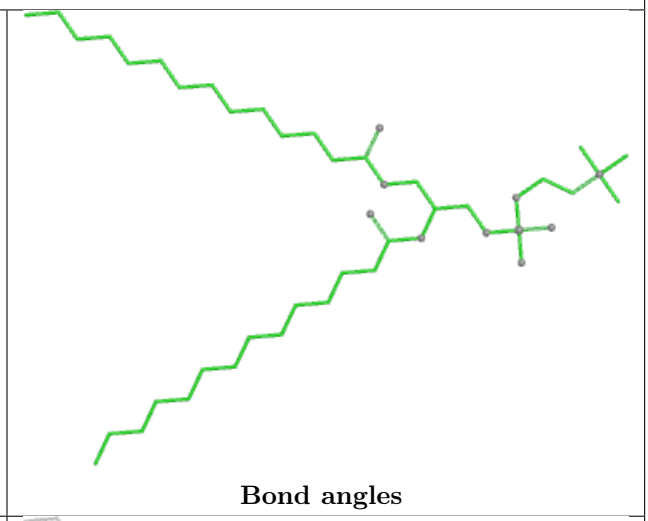


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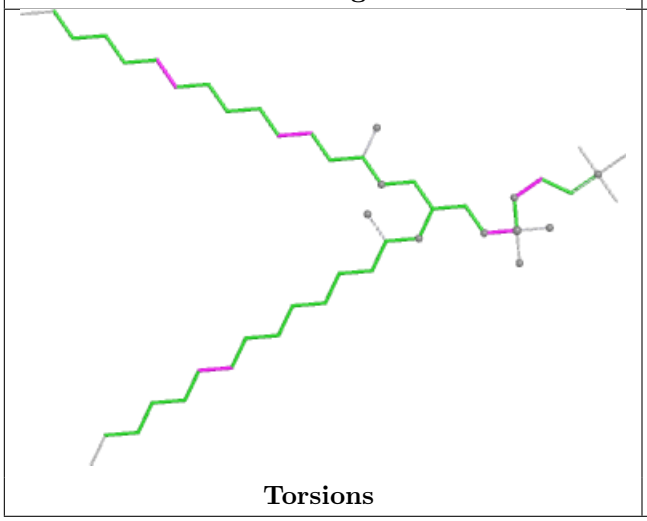
Ligand PX4 B 323



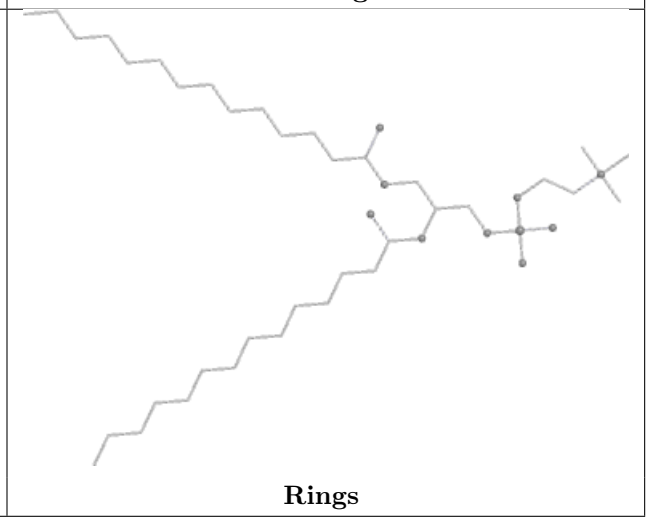
Bond lengths



Bond angles

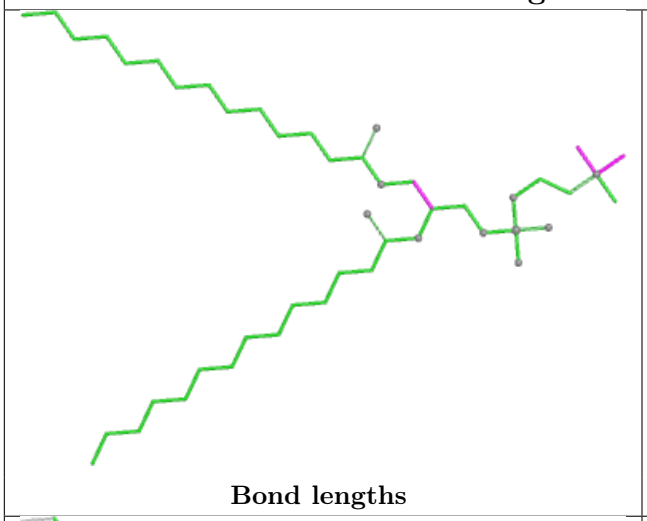


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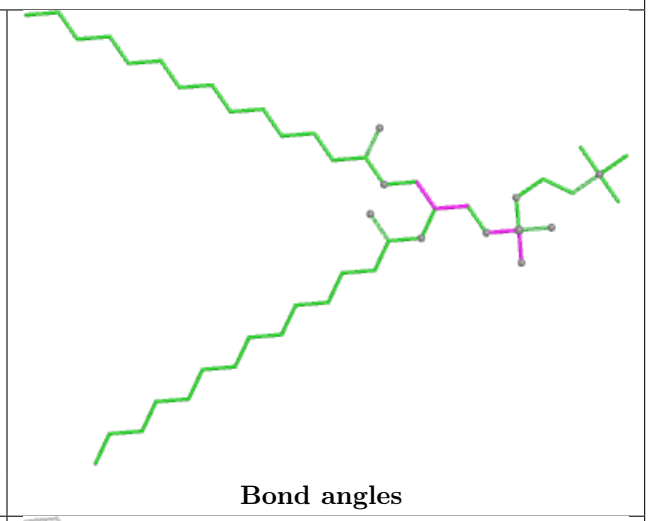


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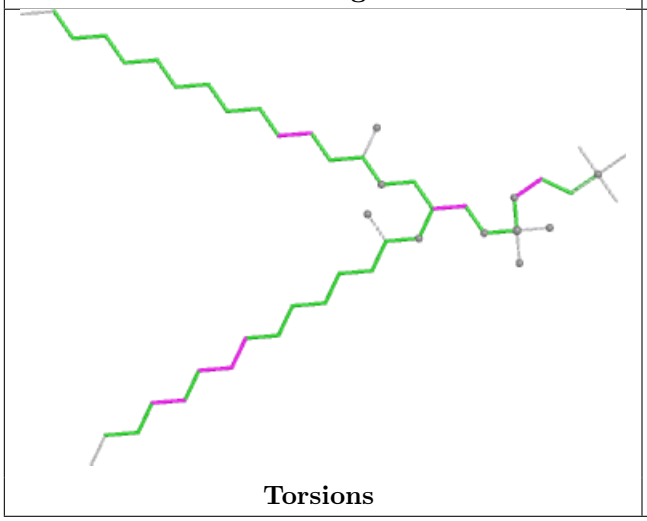
Ligand PX4 B 392



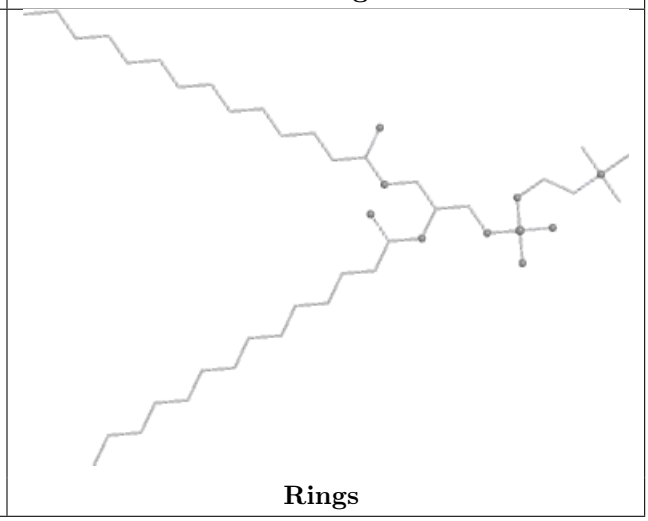
Bond lengths



Bond angles

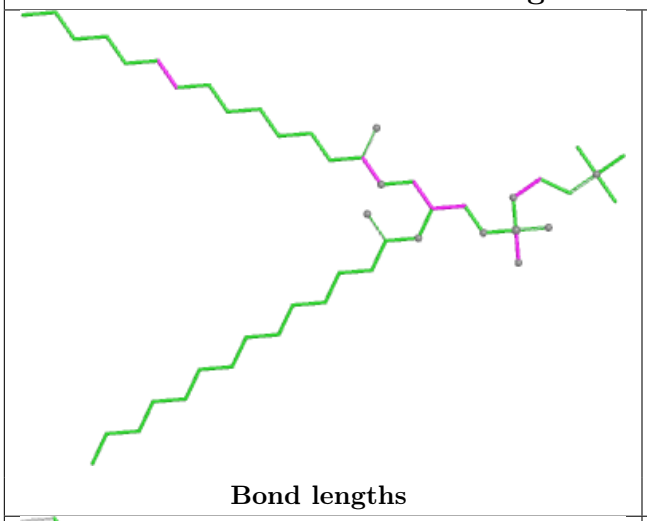


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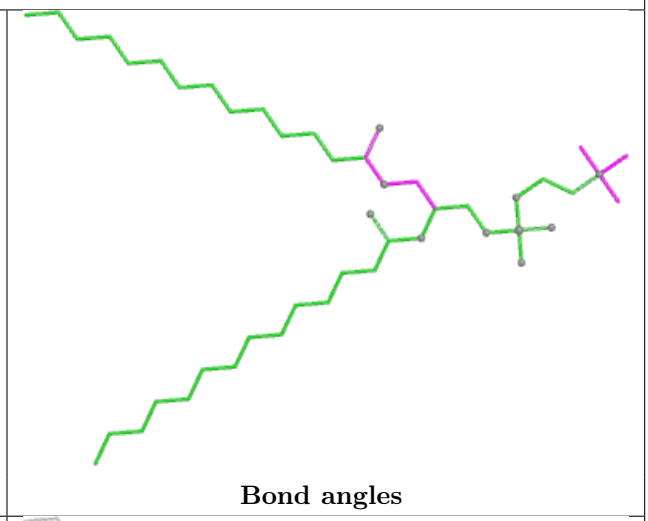


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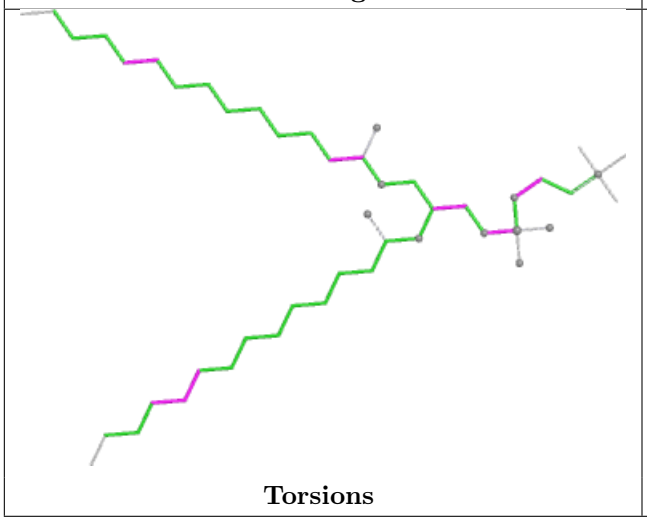
Ligand PX4 A 609



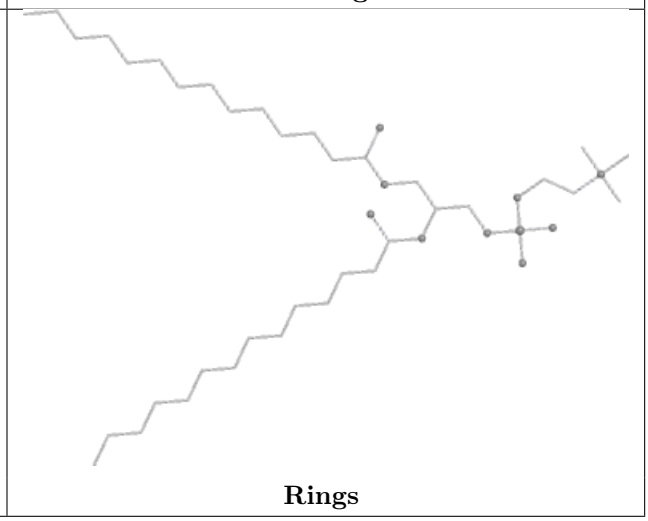
Bond lengths



Bond angles

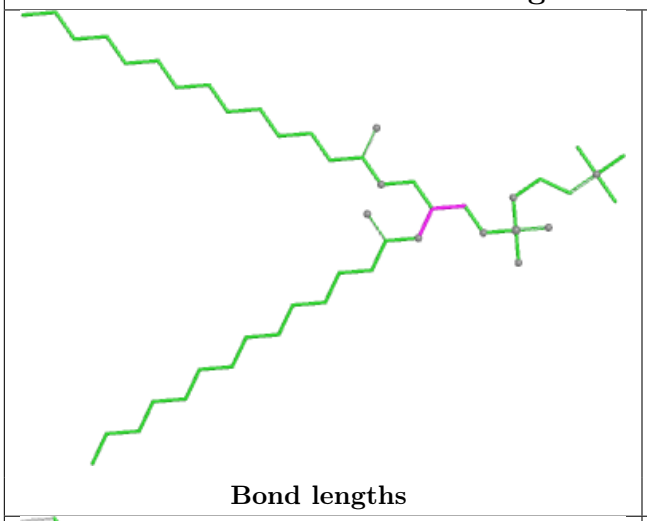


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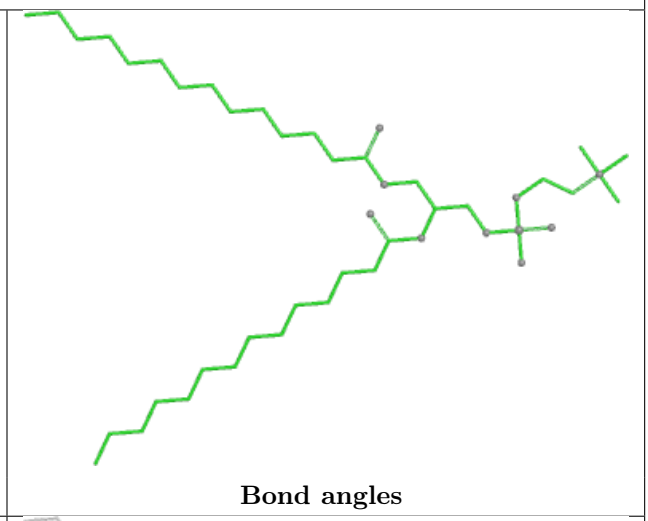


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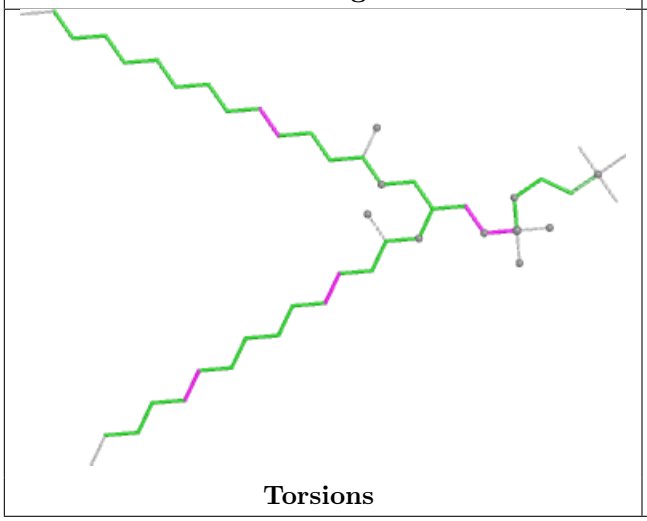
Ligand PX4 B 310



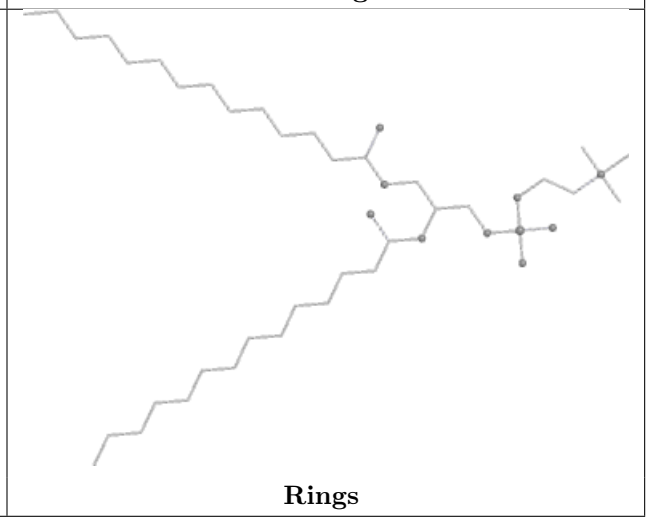
Bond lengths



Bond angles

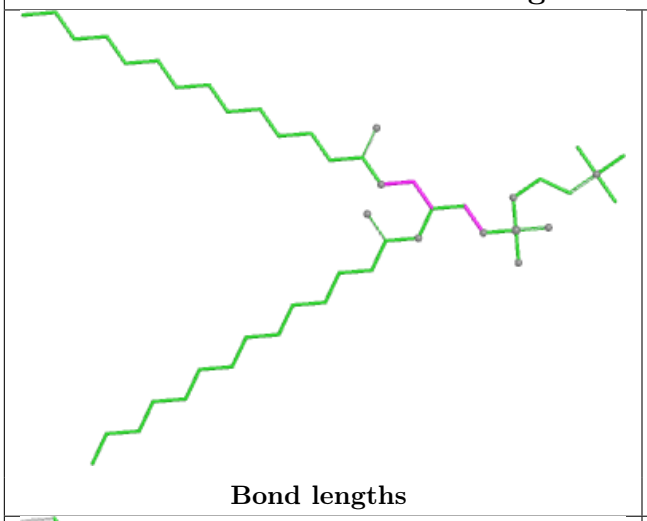


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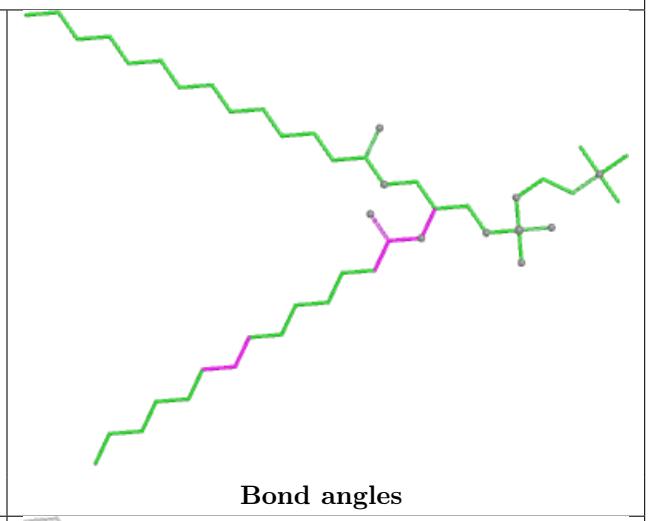


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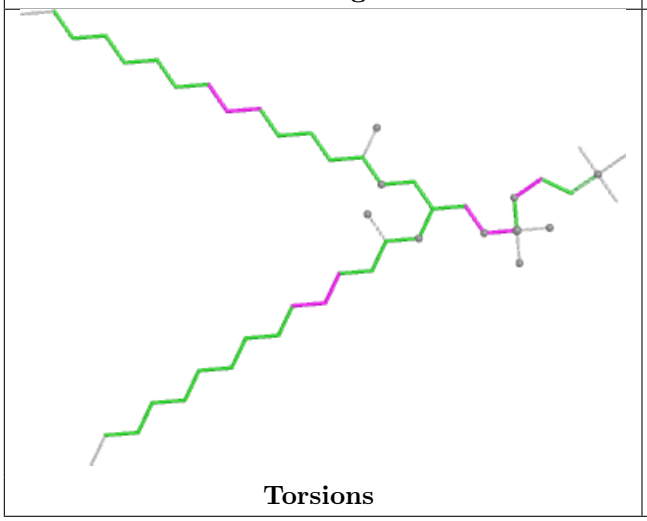
Ligand PX4 B 368



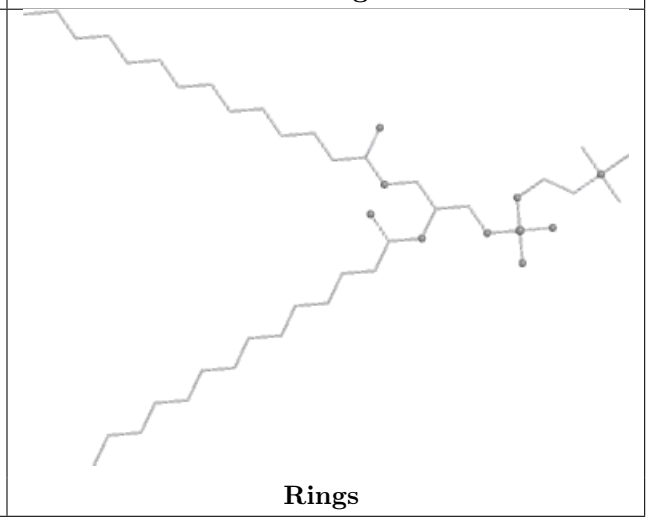
Bond lengths



Bond angles

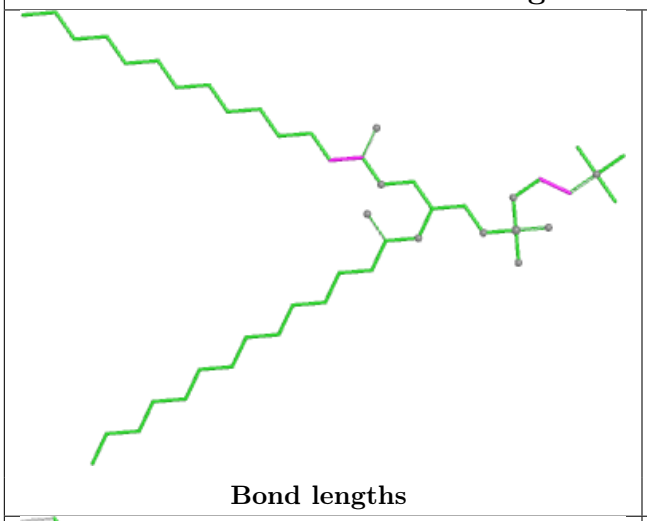


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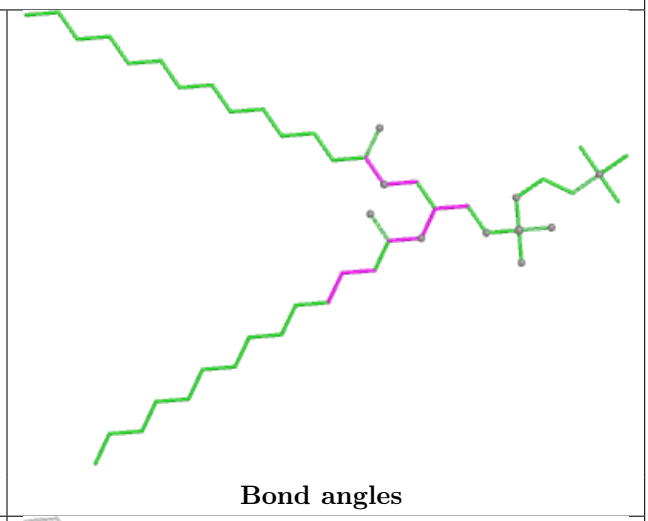


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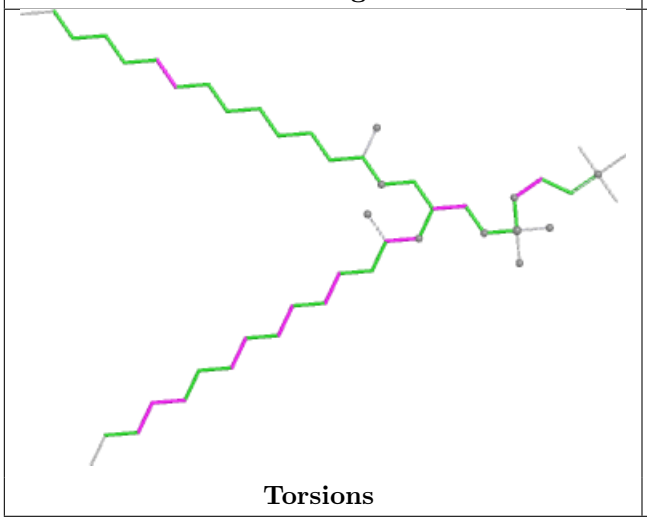
Ligand PX4 B 351



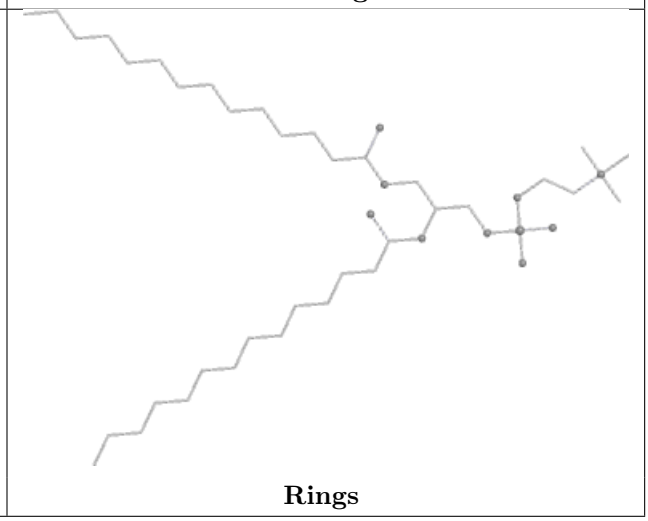
Bond lengths



Bond angles

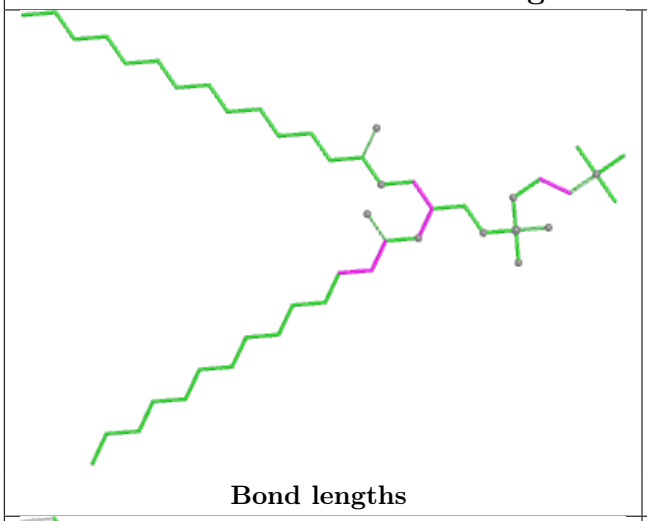


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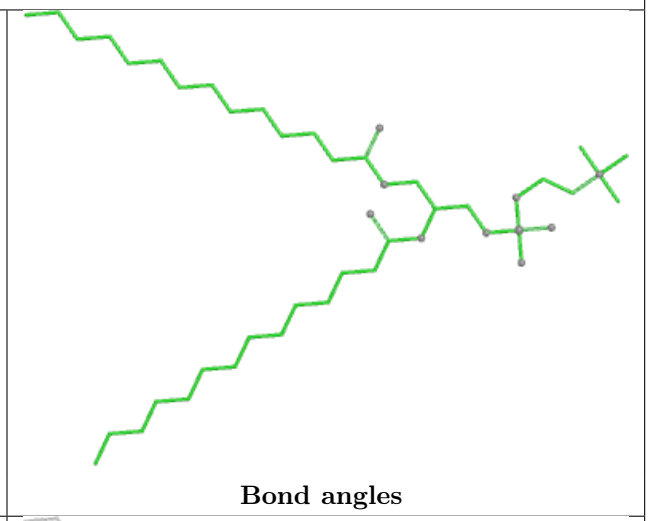


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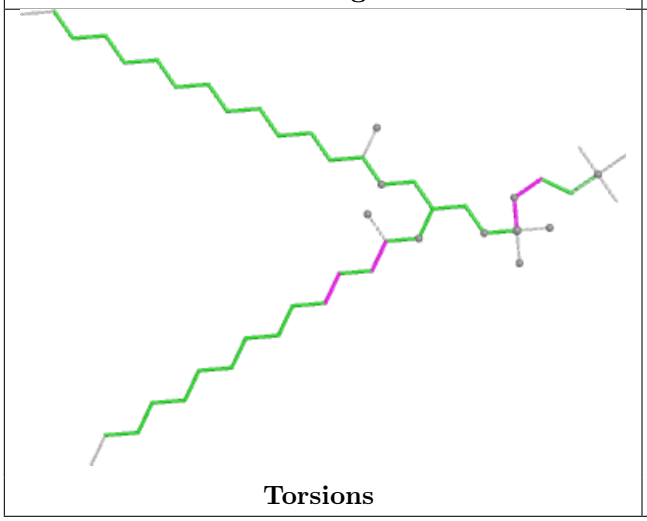
Ligand PX4 A 631



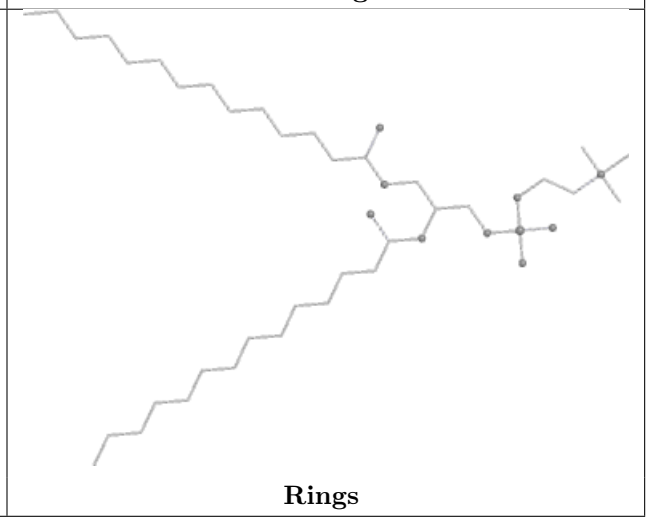
Bond lengths



Bond angles

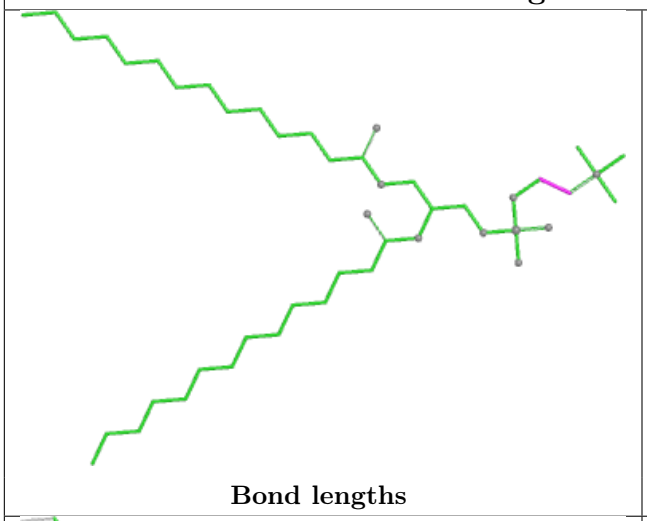


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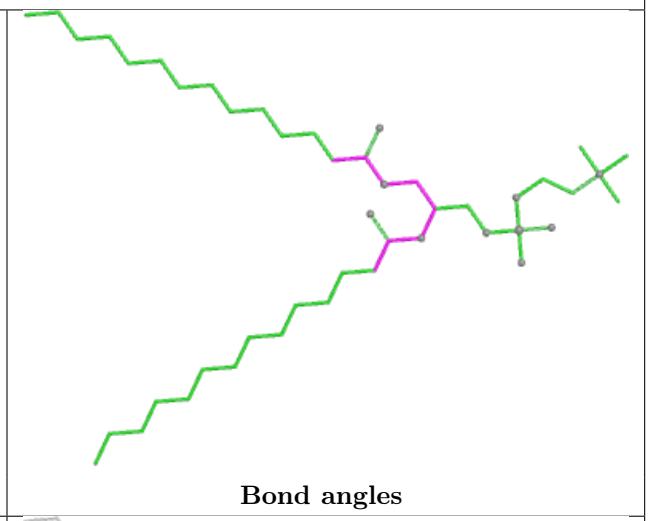


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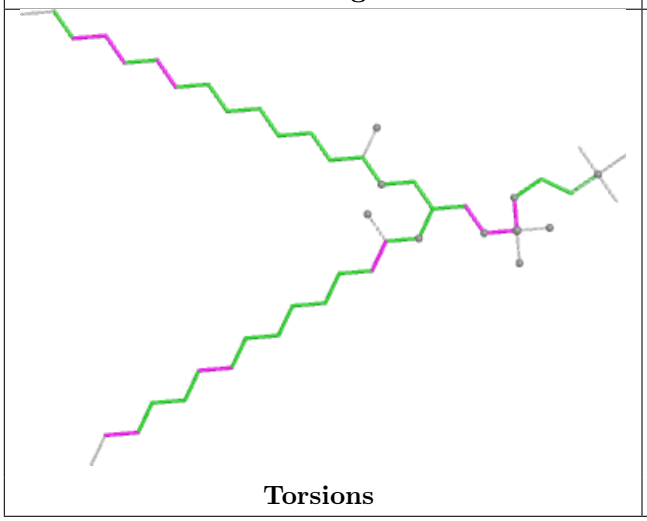
Ligand PX4 B 313



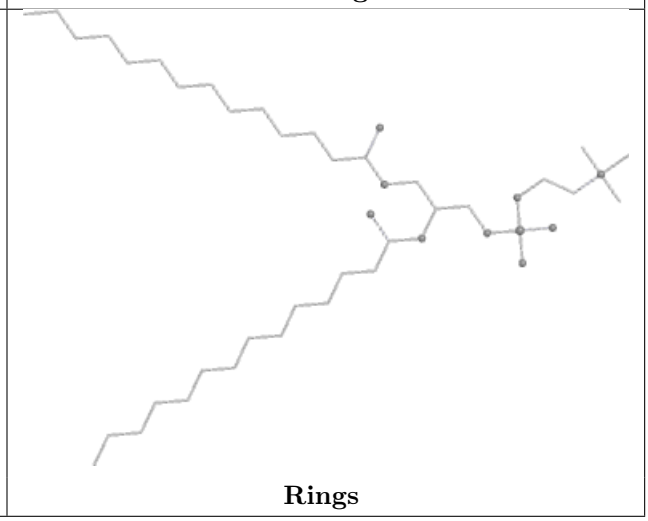
Bond lengths



Bond angles

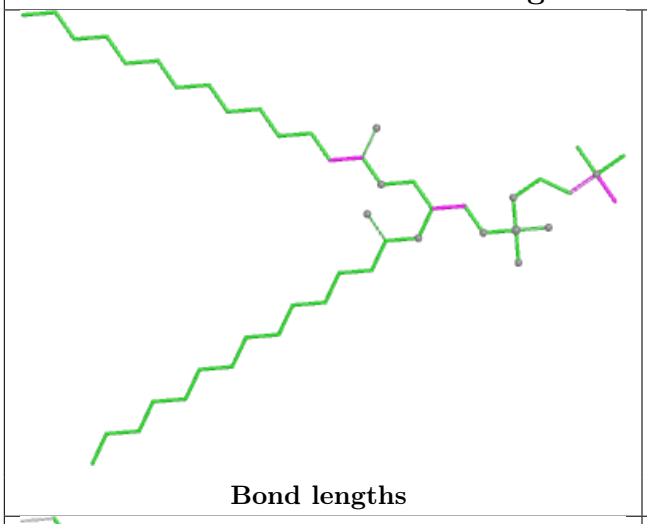


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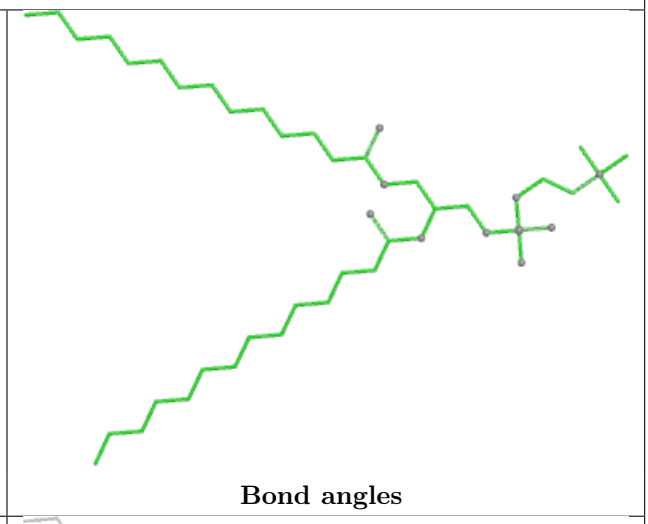


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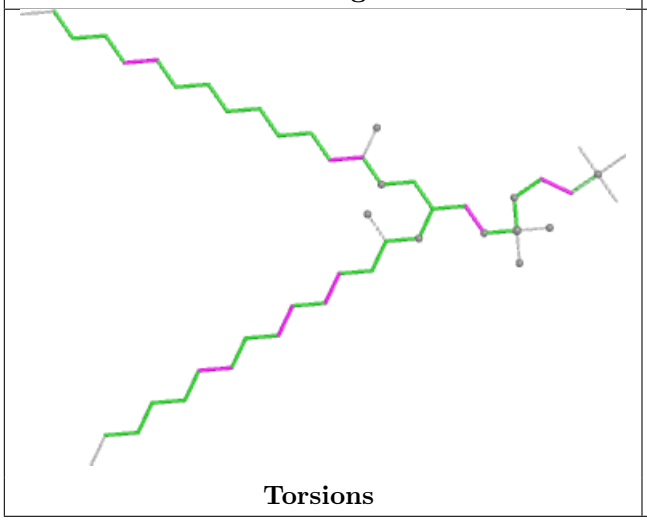
Ligand PX4 A 629



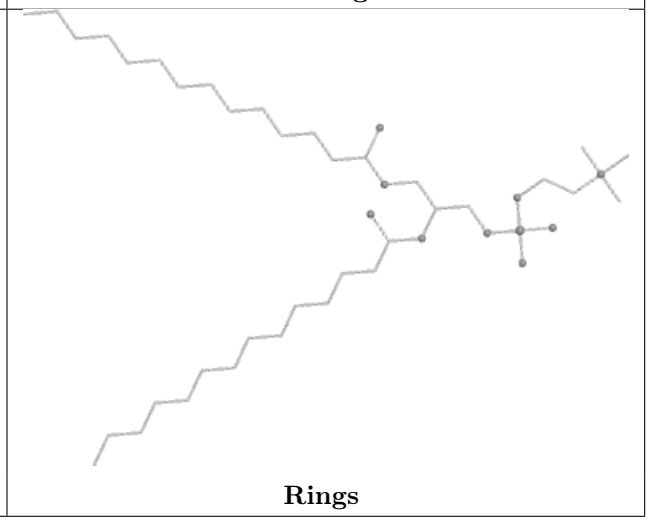
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Bond angles

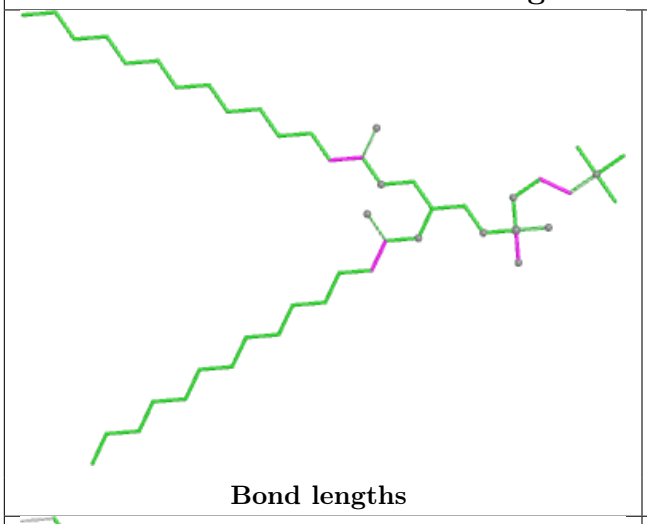


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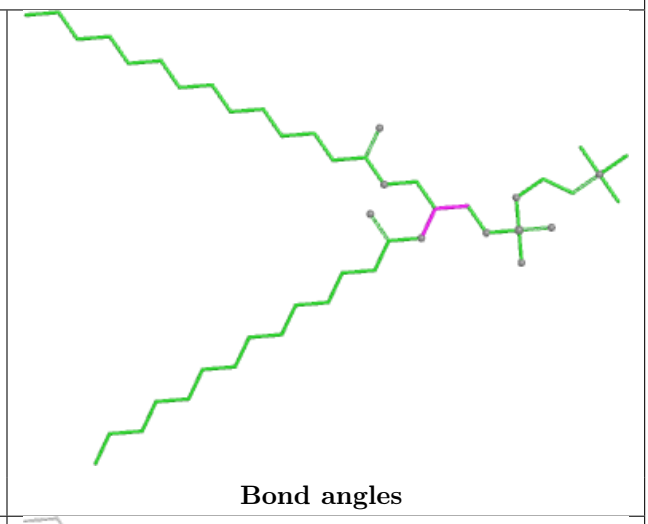


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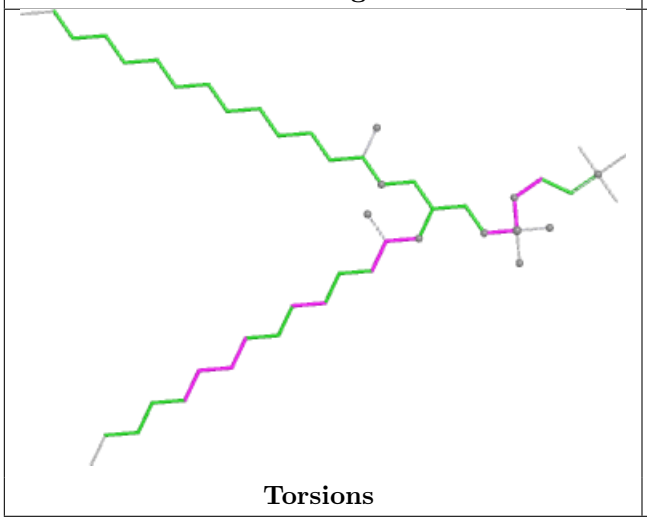
Ligand PX4 C 314



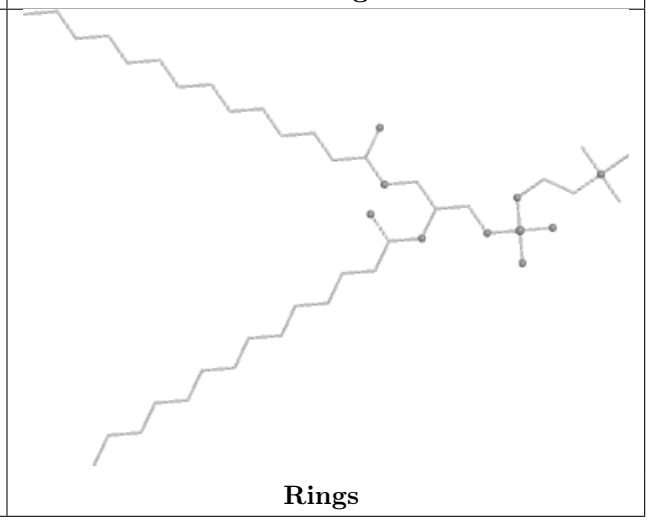
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Bond angles

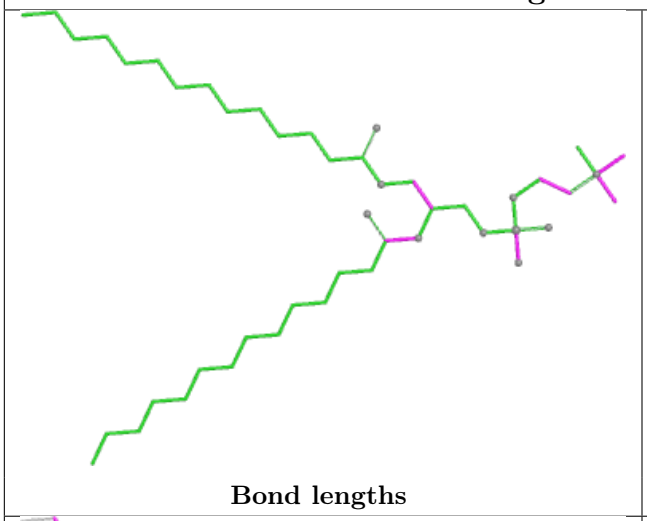


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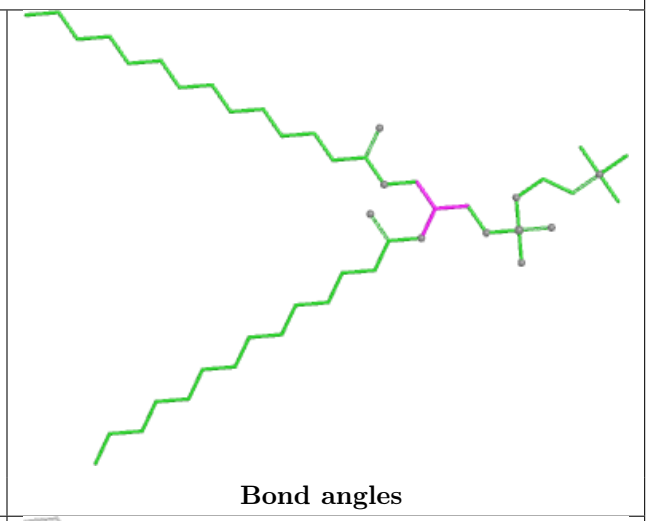


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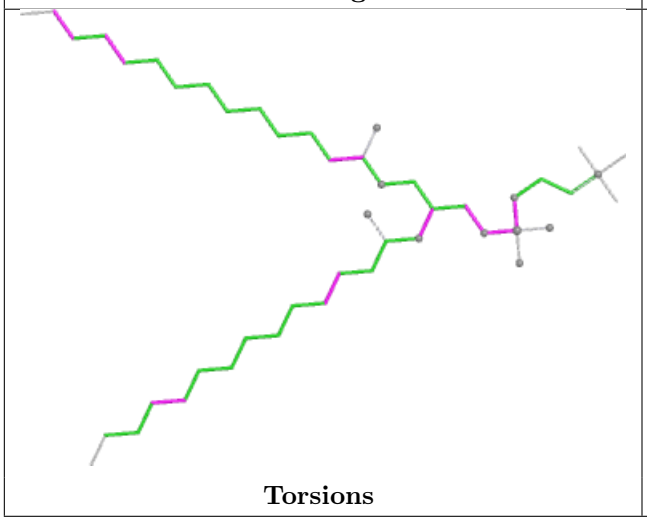
Ligand PX4 B 376



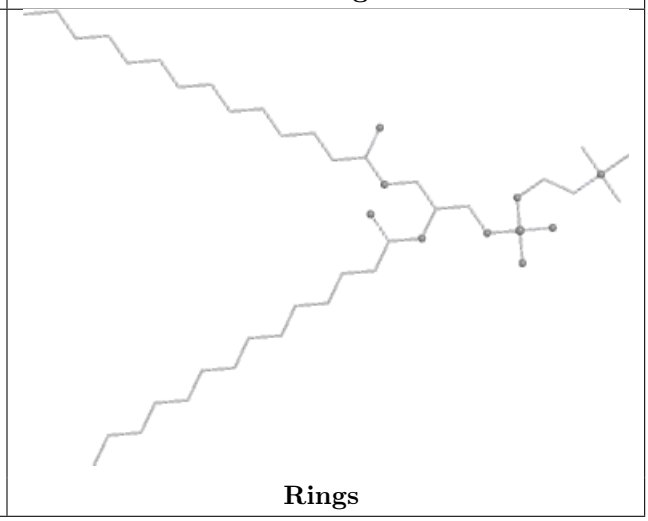
Bond lengths



Bond angles

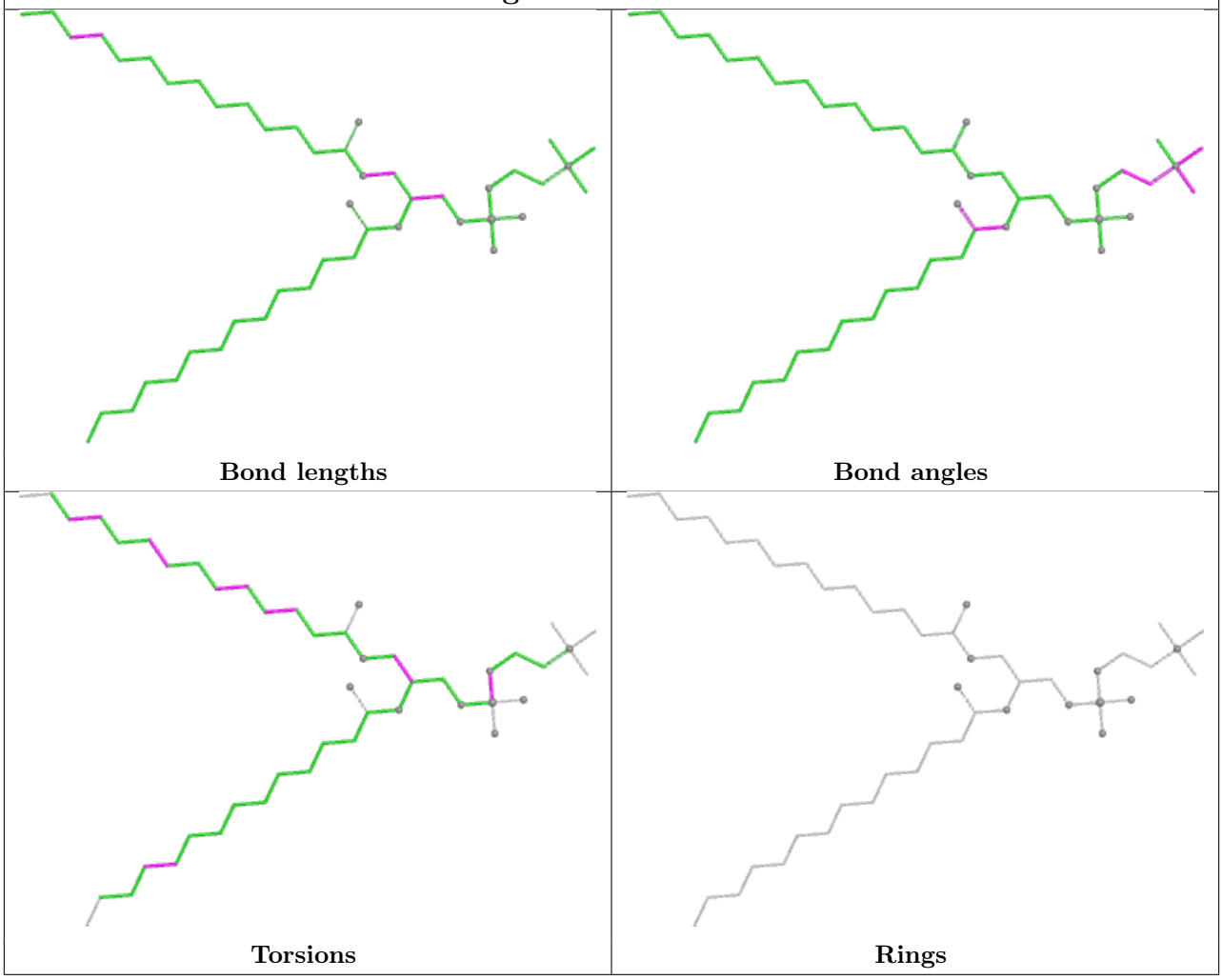


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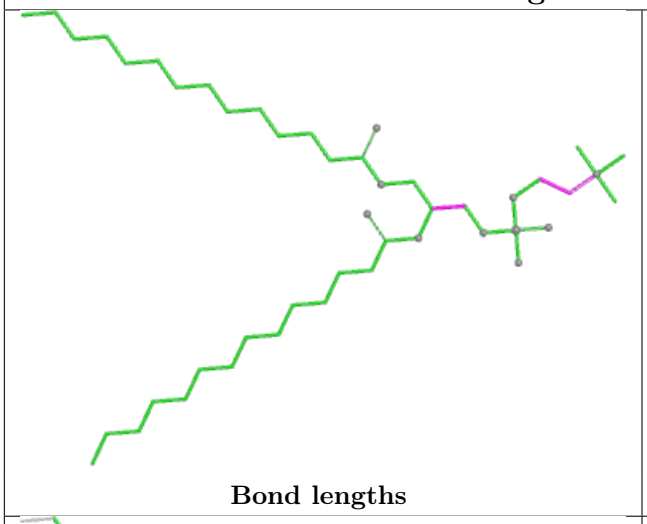


Rings

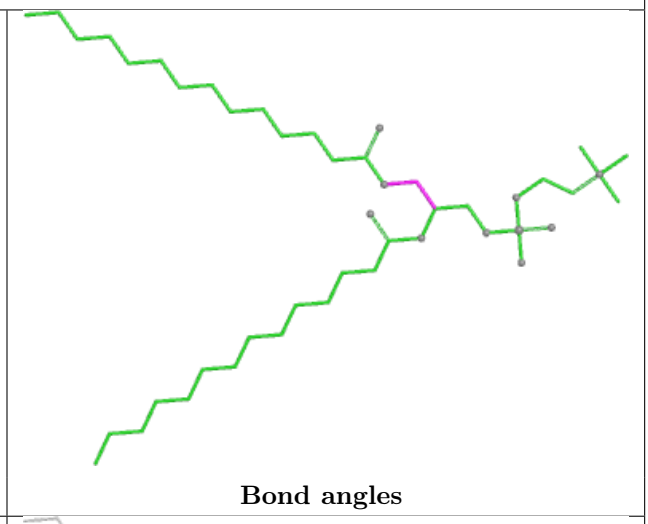
Ligand PX4 C 362



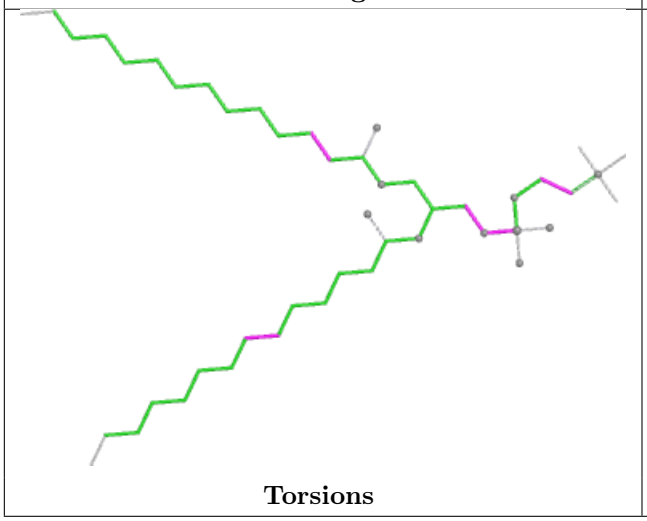
Ligand PX4 C 344



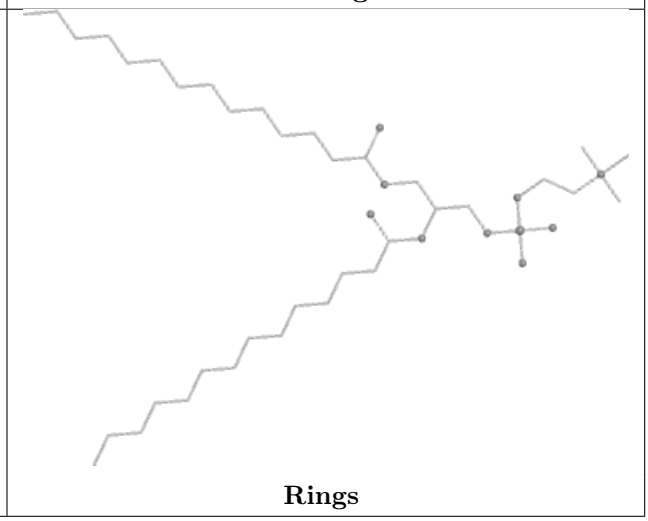
Bond lengths



Bond angles

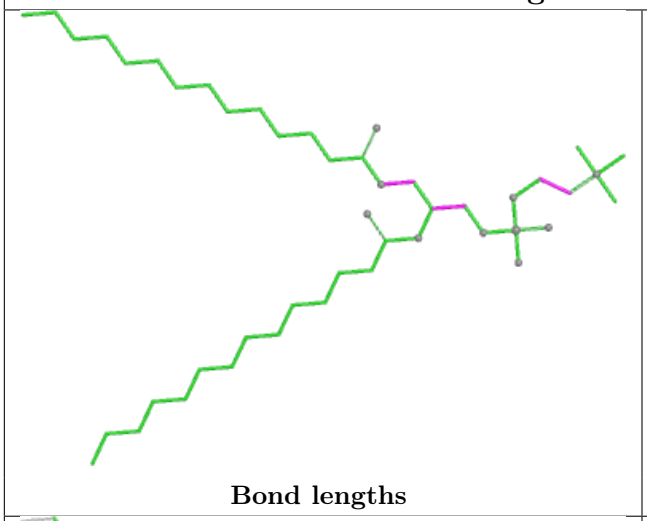


Torsions

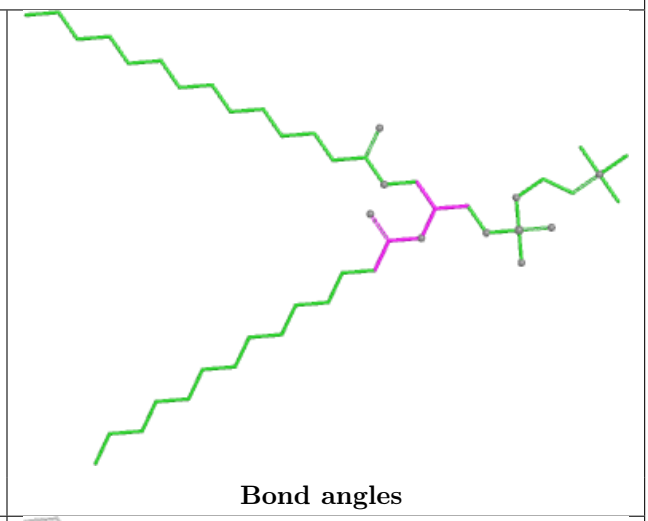


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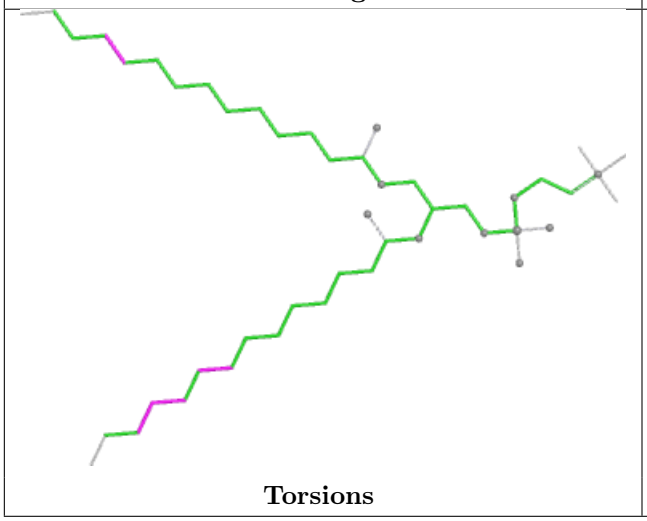
Ligand PX4 A 613



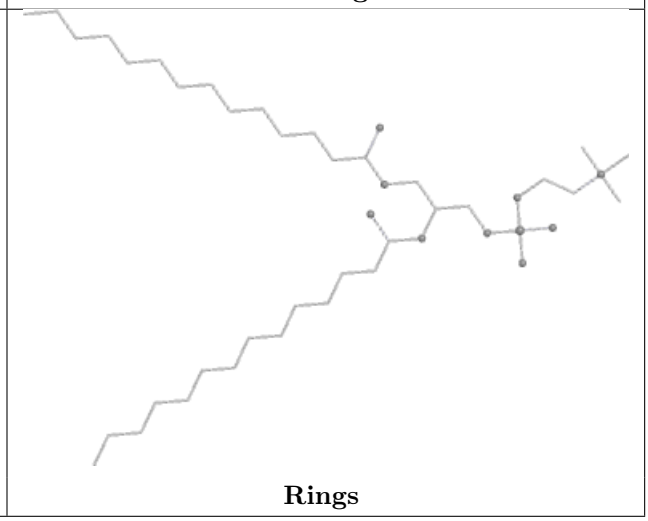
Bond lengths



Bond angles

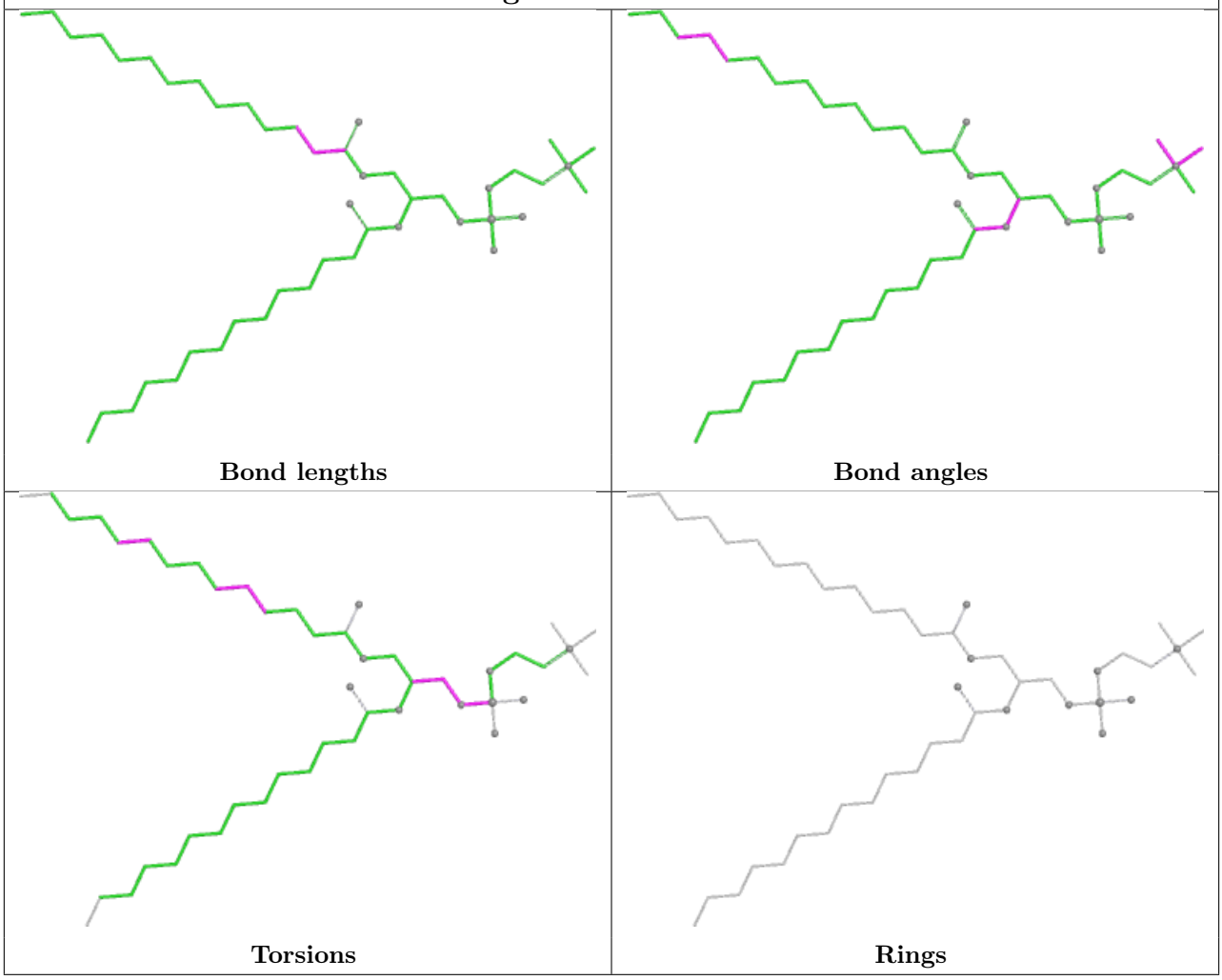


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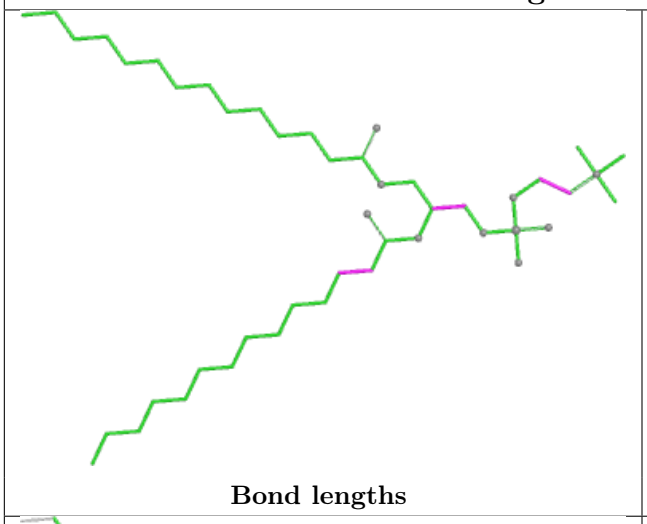


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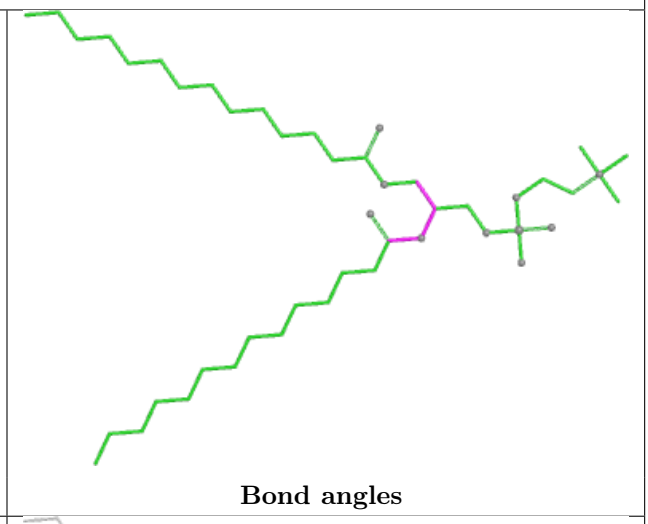
Ligand PX4 B 318



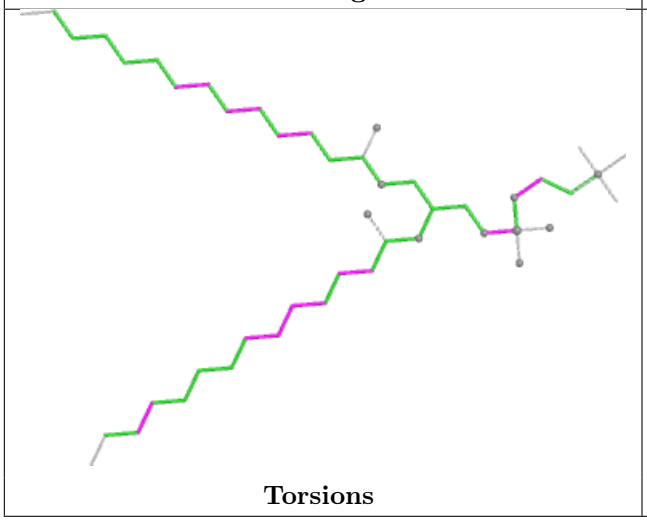
Ligand PX4 C 340



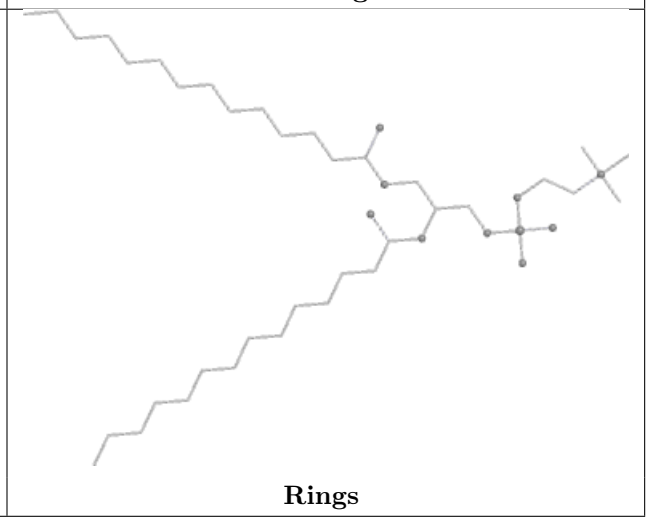
Bond lengths



Bond angles

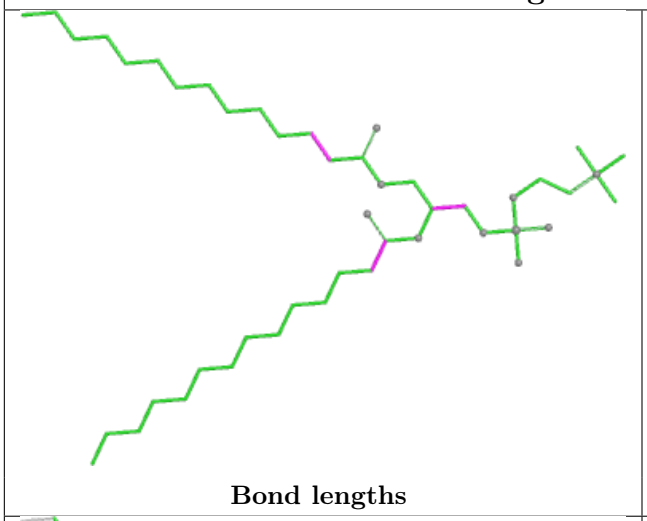


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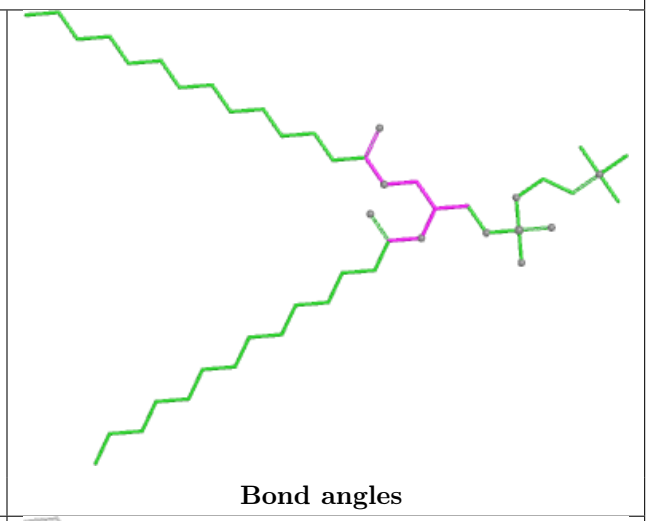


Rings

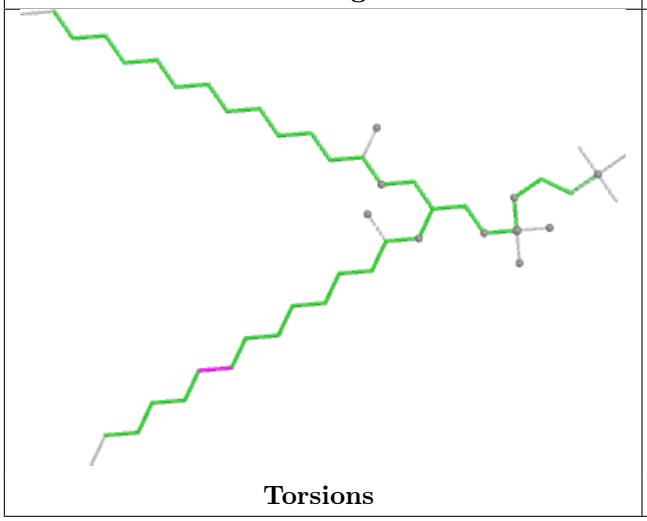
Ligand PX4 A 648



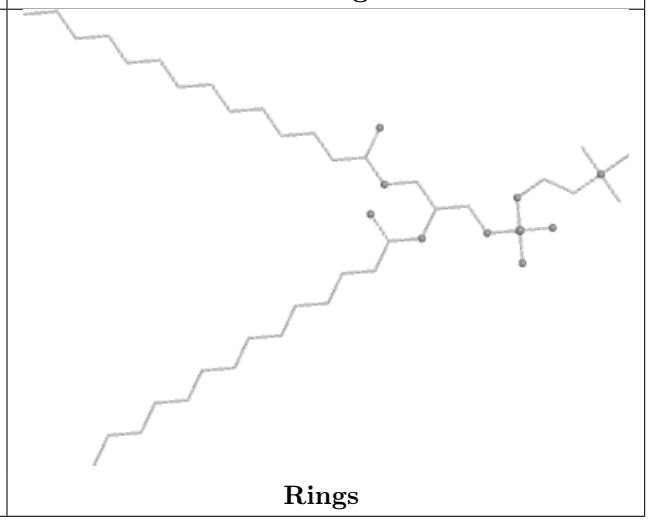
Bond lengths



Bond angles

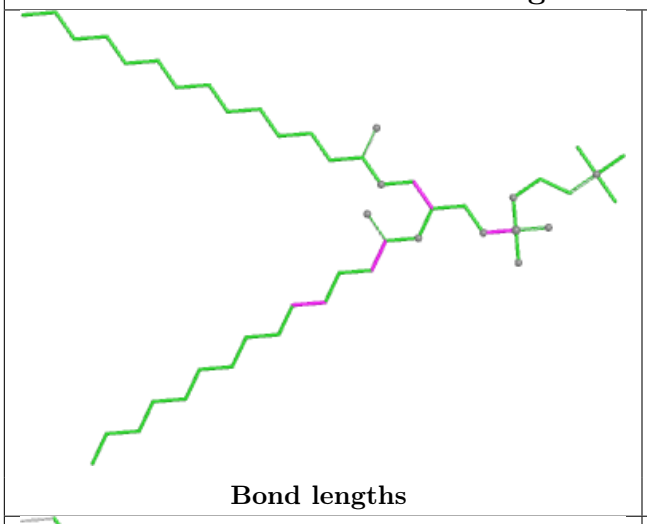


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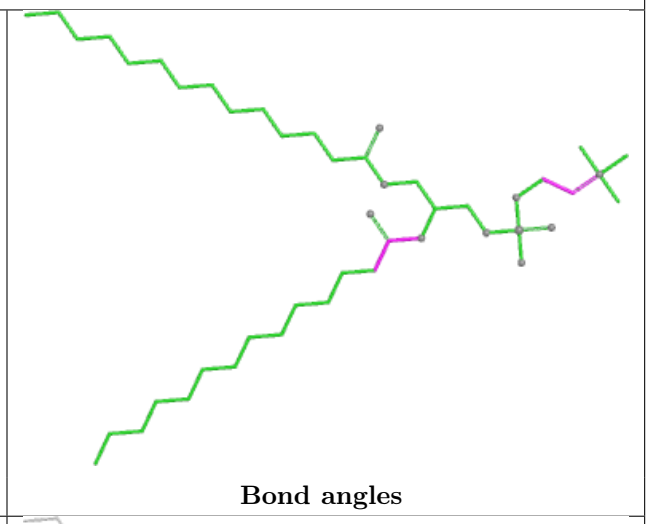


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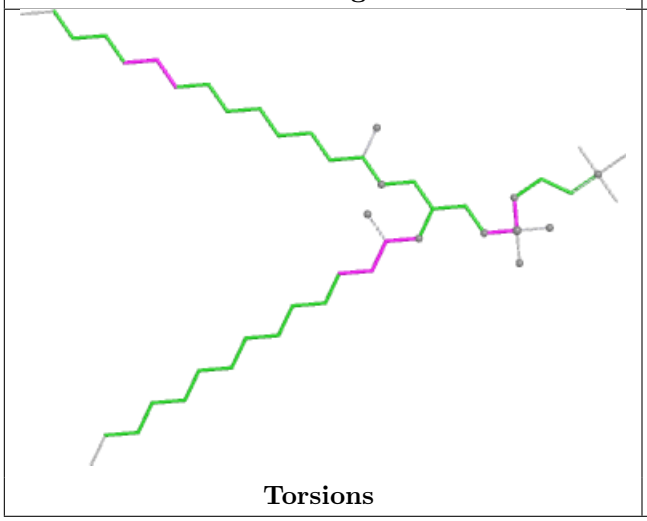
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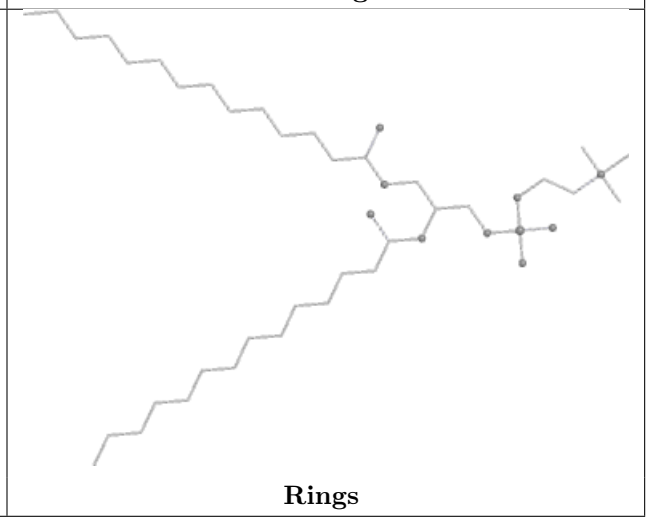
Bond lengths



Bond angles

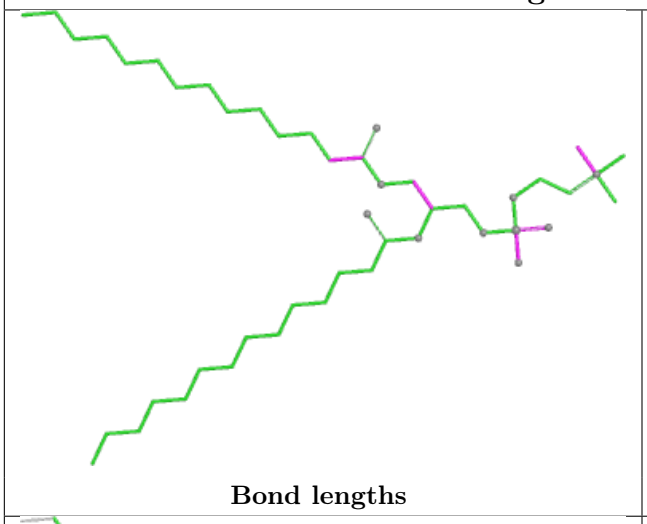


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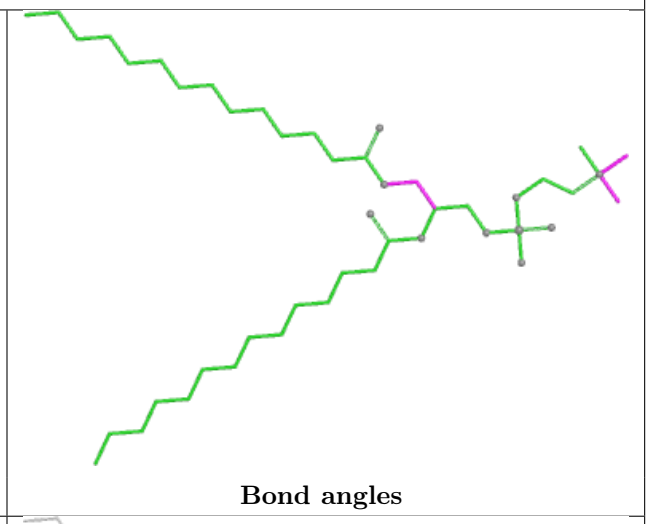


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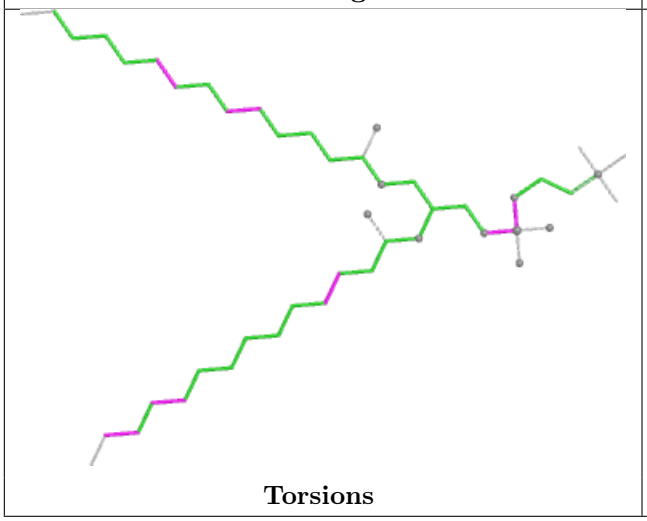
Ligand PX4 C 342



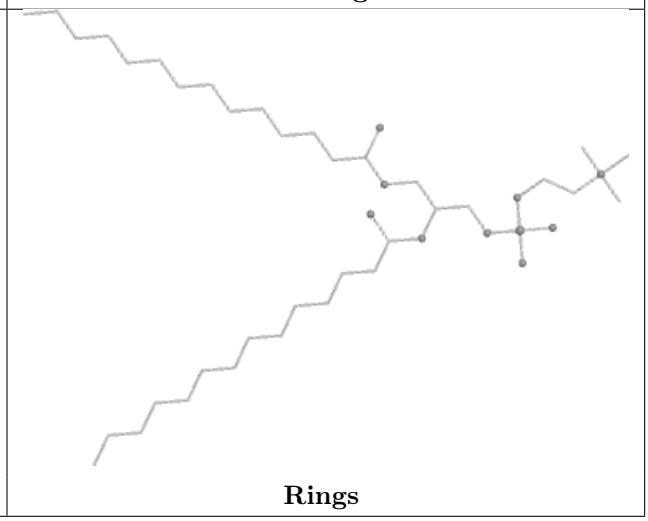
Bond lengths



Bond angles

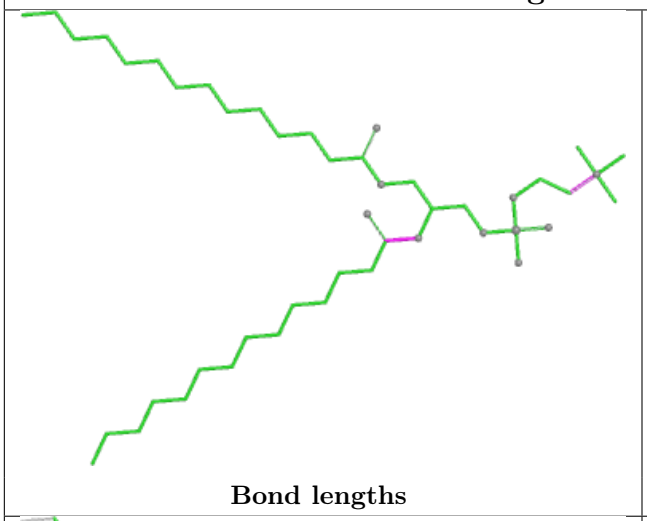


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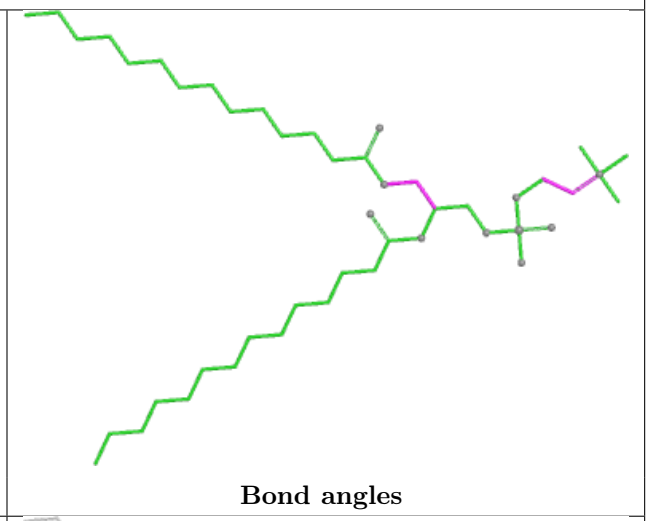


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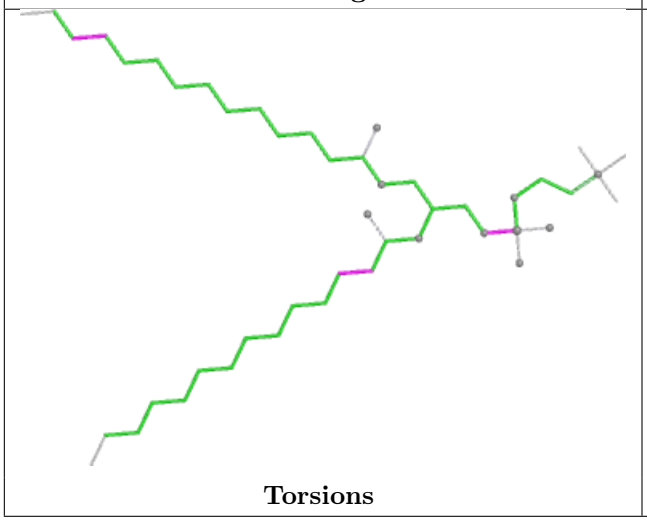
Ligand PX4 A 630



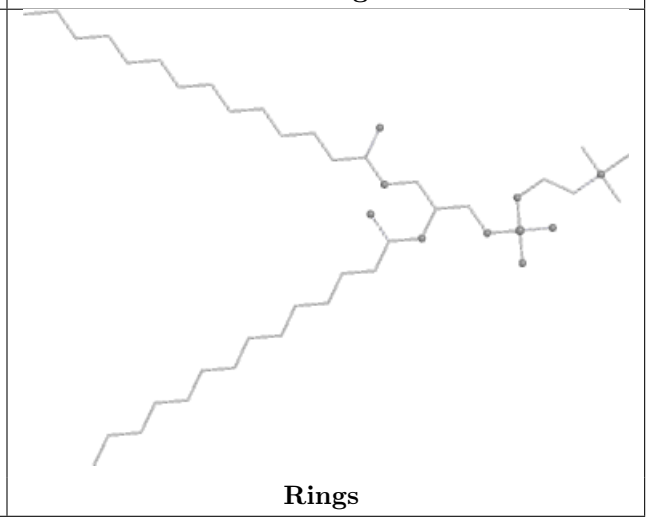
Bond lengths



Bond angles

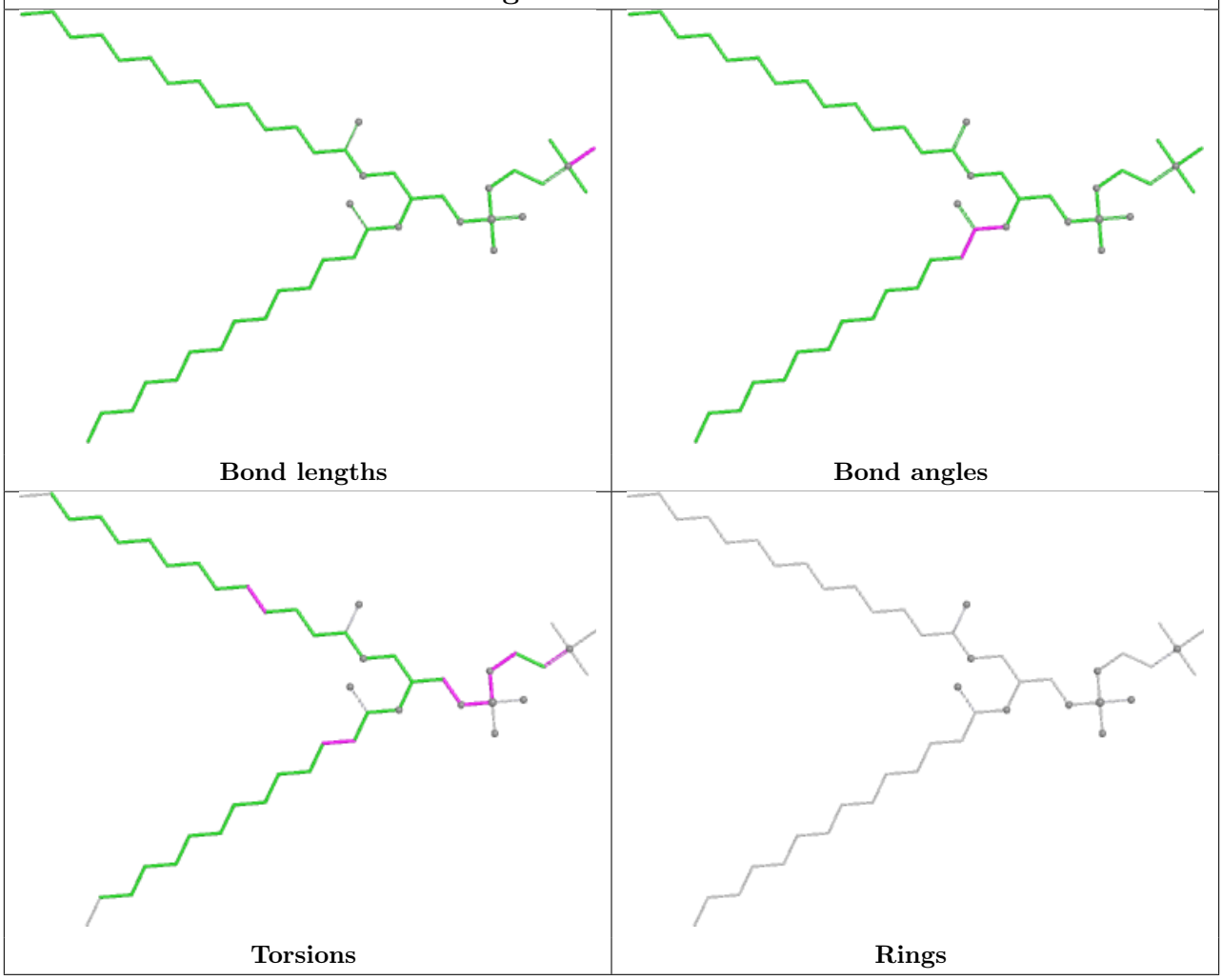


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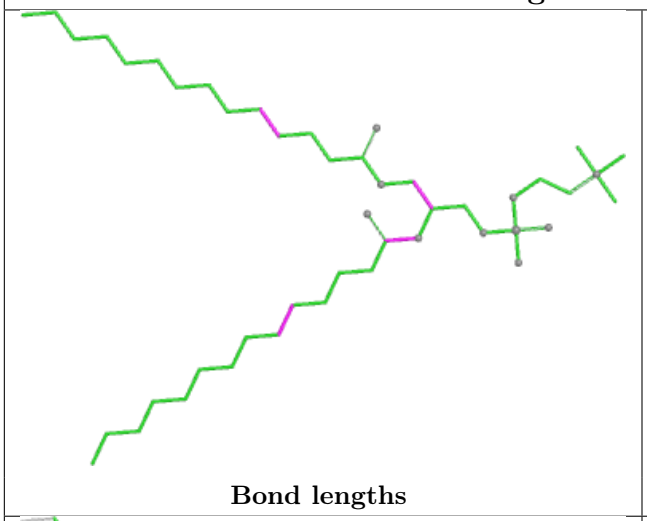


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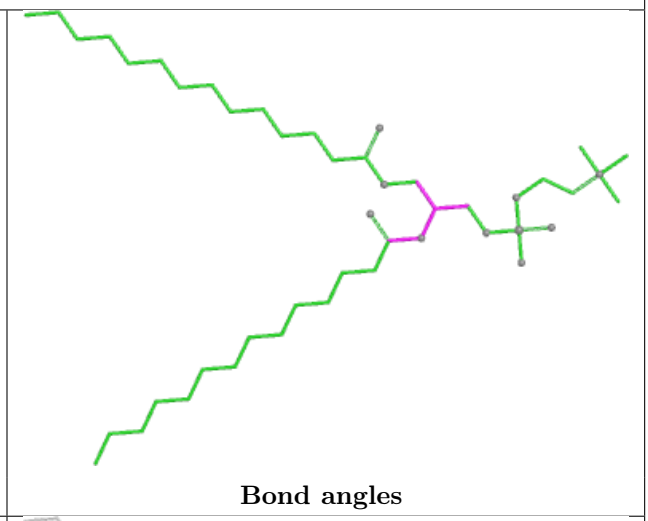
Ligand PX4 C 349



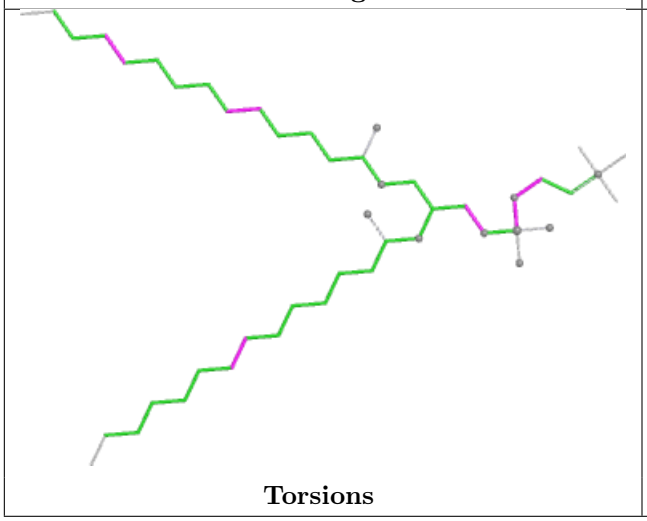
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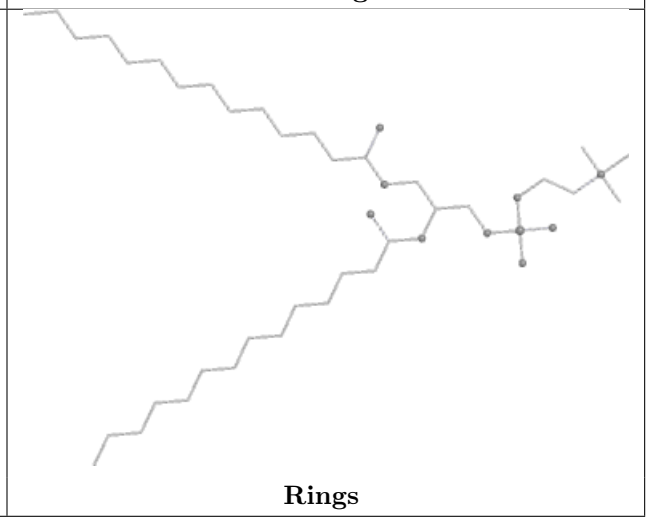
Bond lengths



Bond angles

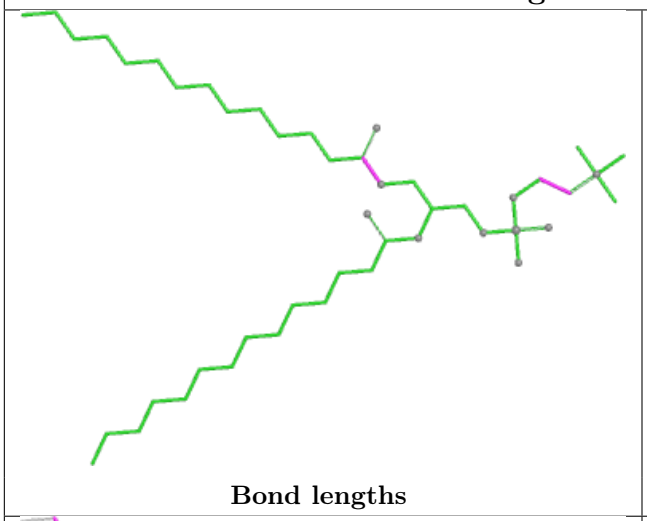


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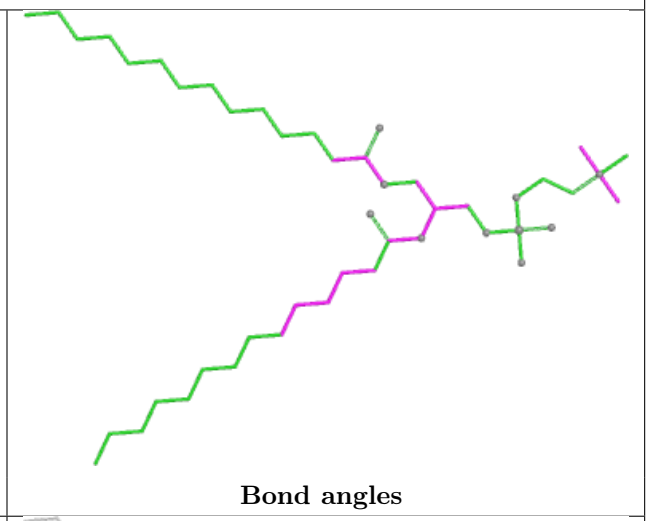


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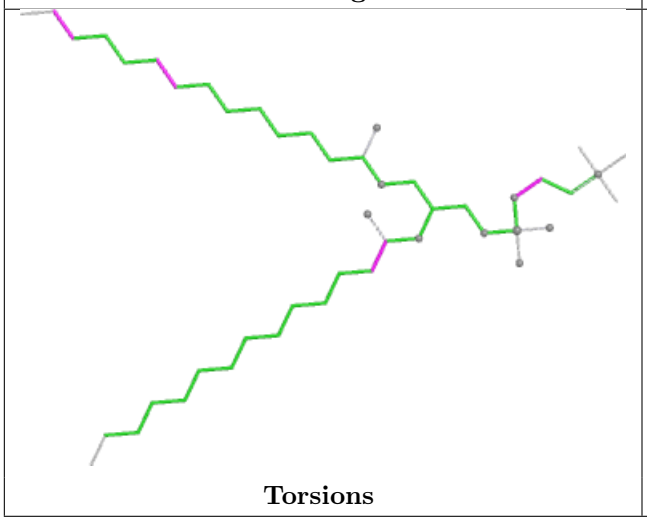
Ligand PX4 B 374



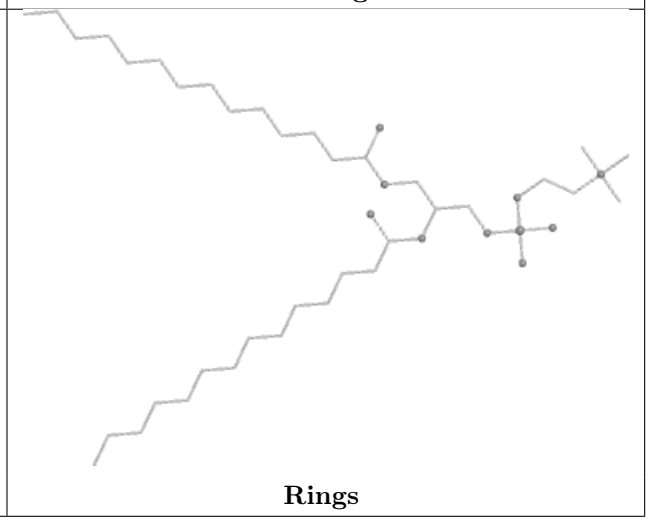
Bond lengths



Bond angles

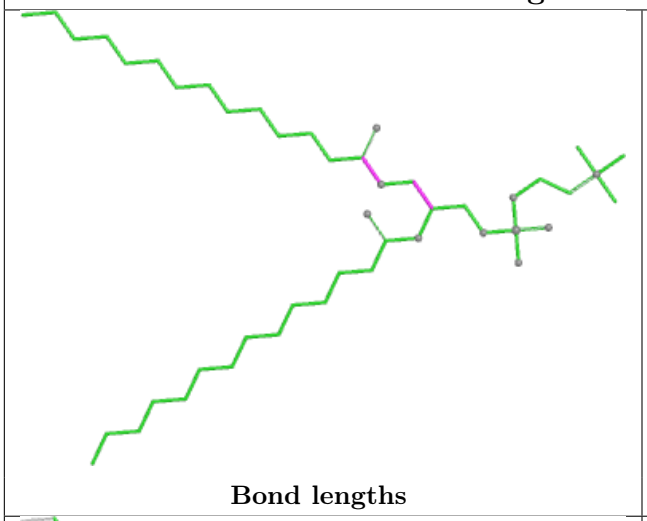


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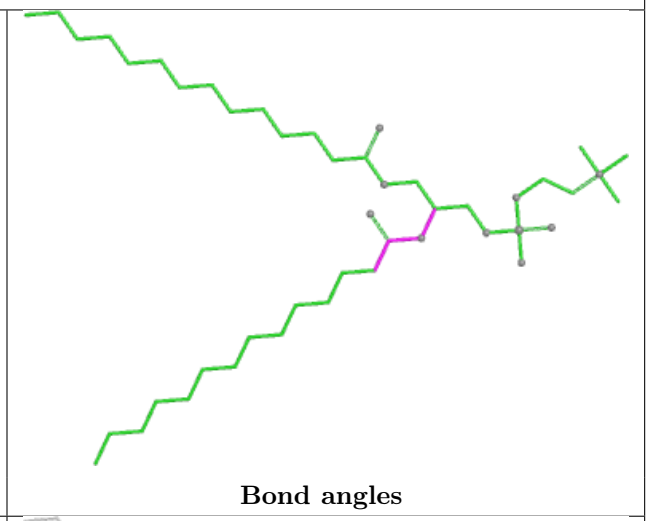


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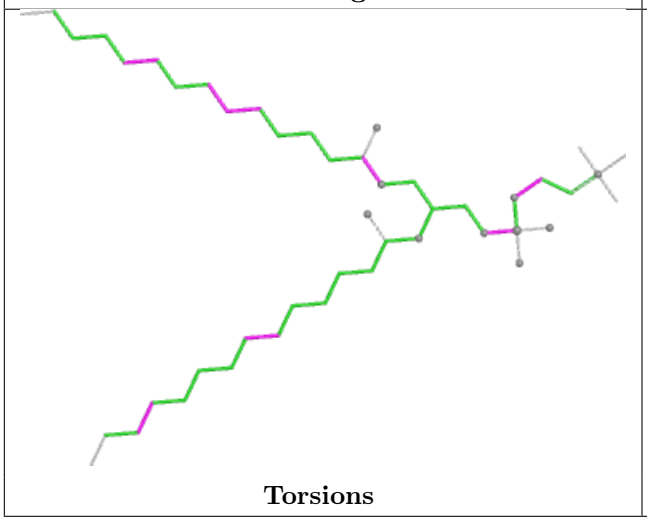
Ligand PX4 A 611



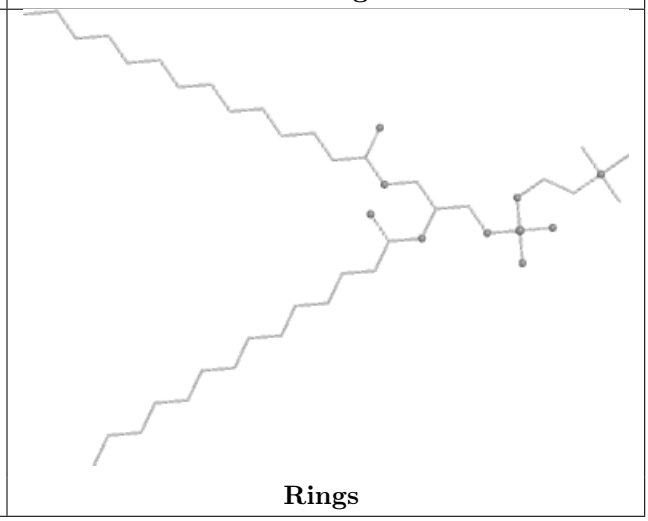
Bond lengths



Bond angles

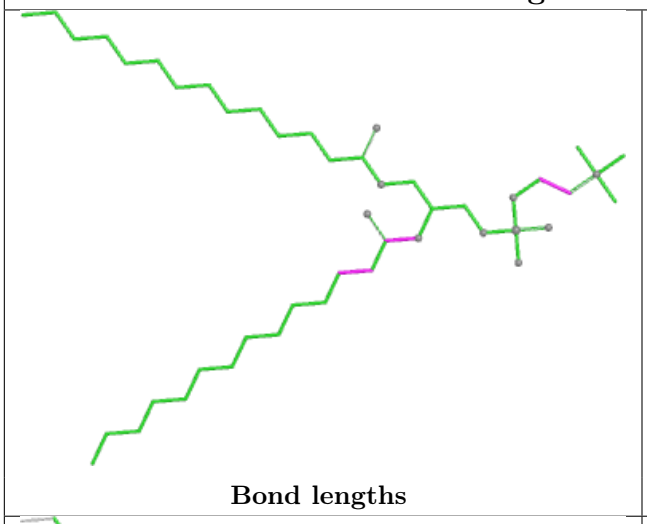


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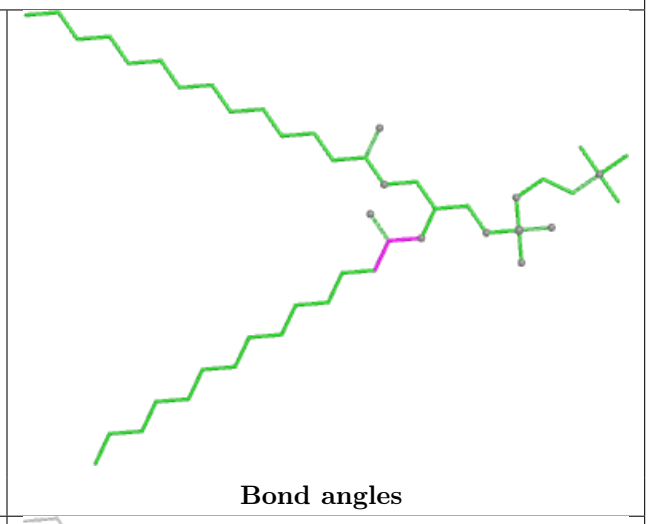


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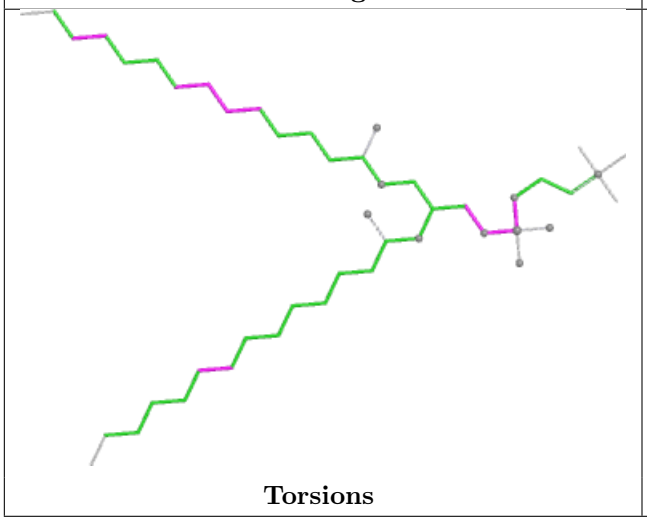
Ligand PX4 C 315



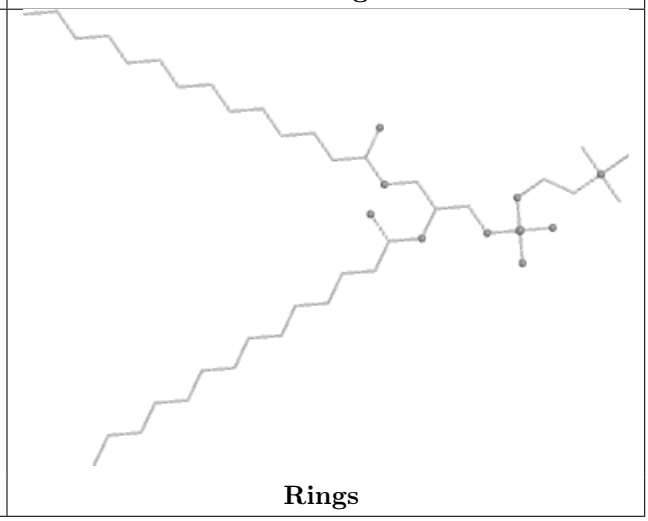
Bond lengths



Bond angles

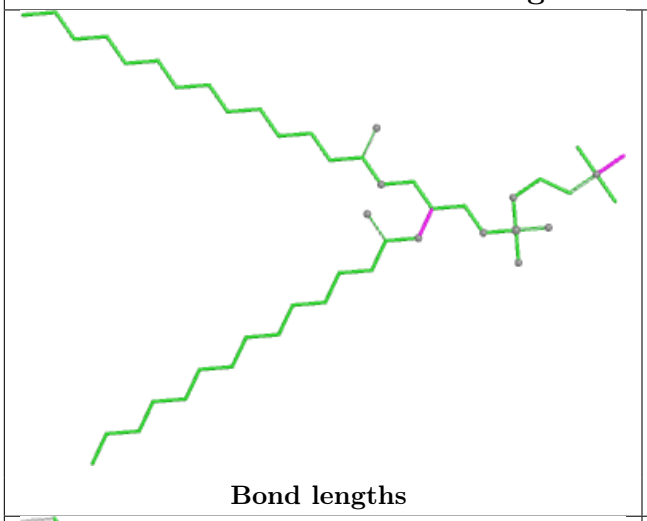


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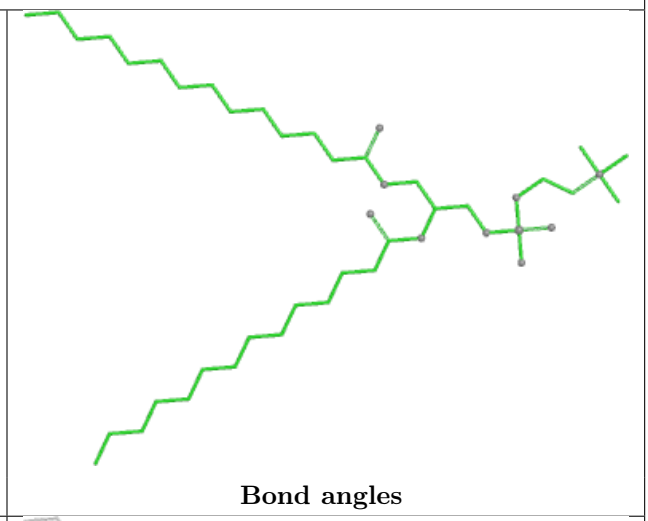


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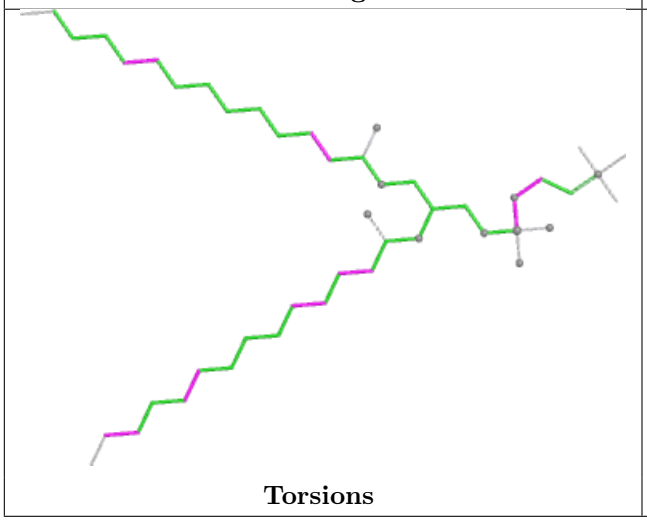
Ligand PX4 A 640



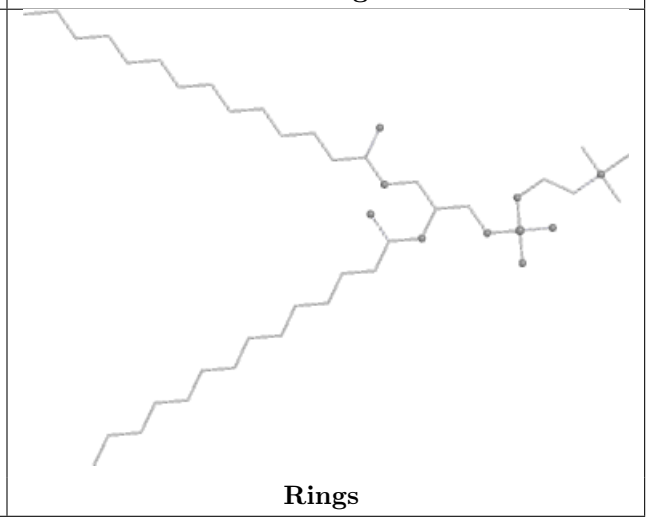
Bond lengths



Bond angles

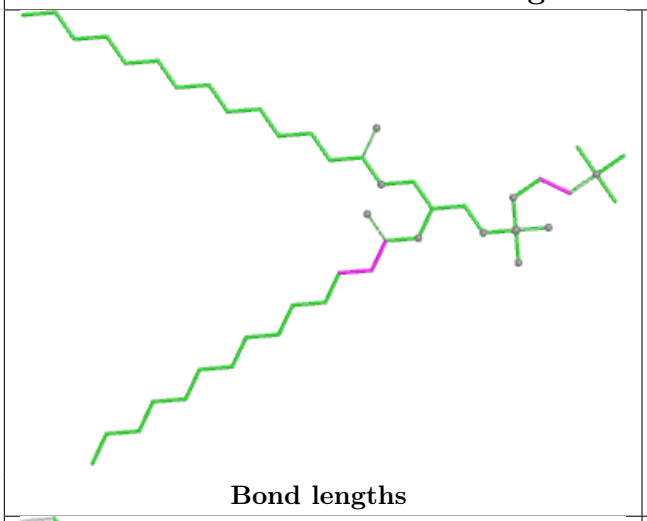


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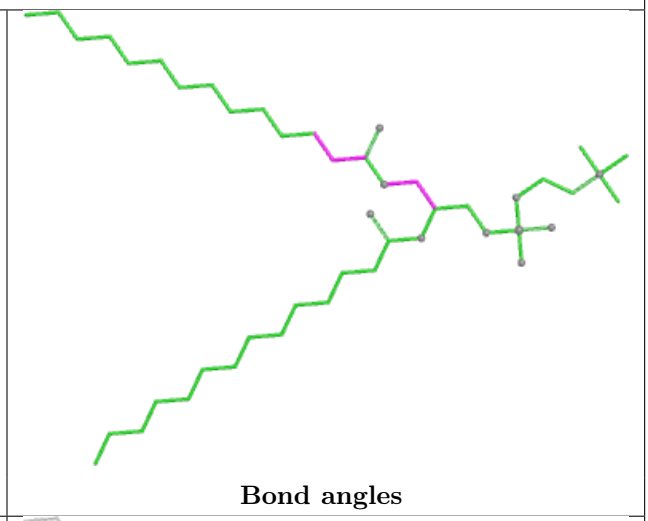


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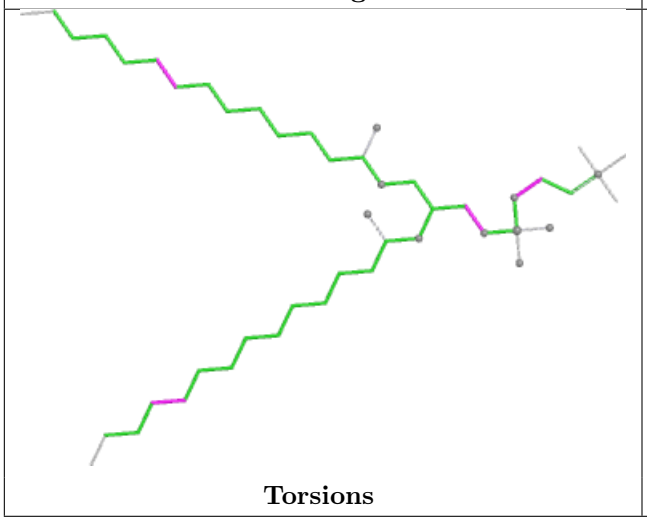
Ligand PX4 C 326



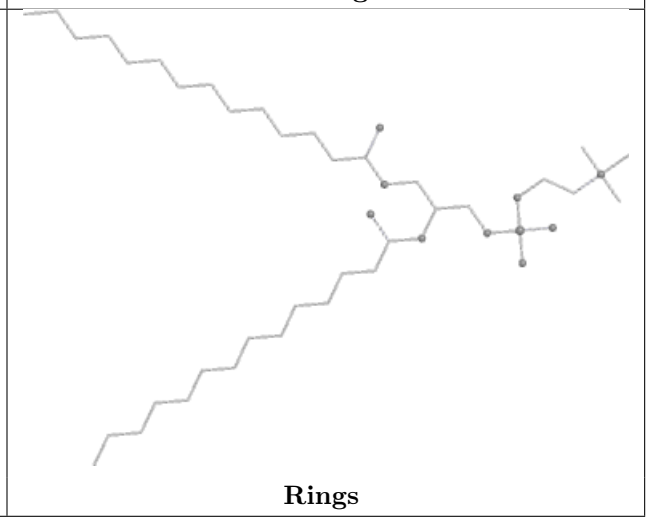
Bond lengths



Bond angles

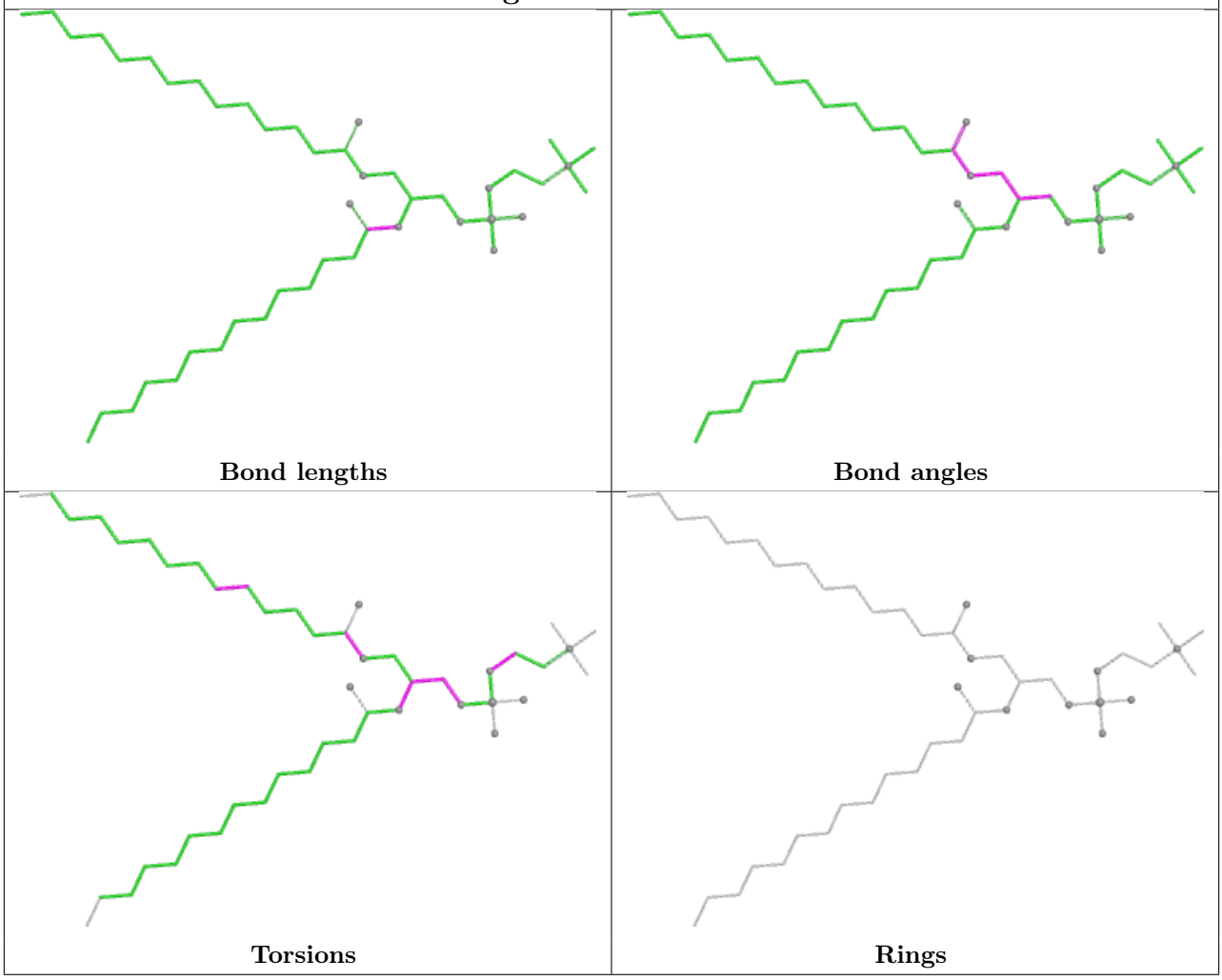


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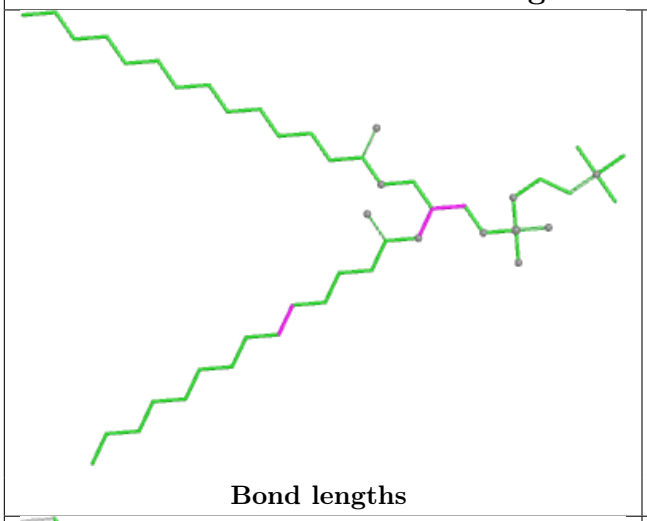


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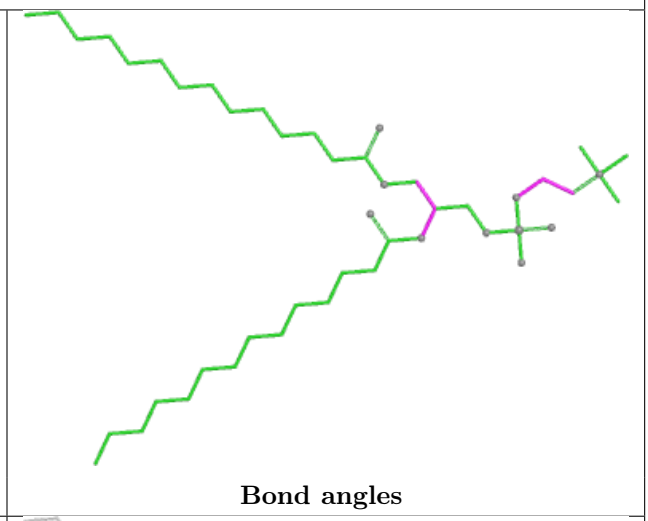
Ligand PX4 B 343



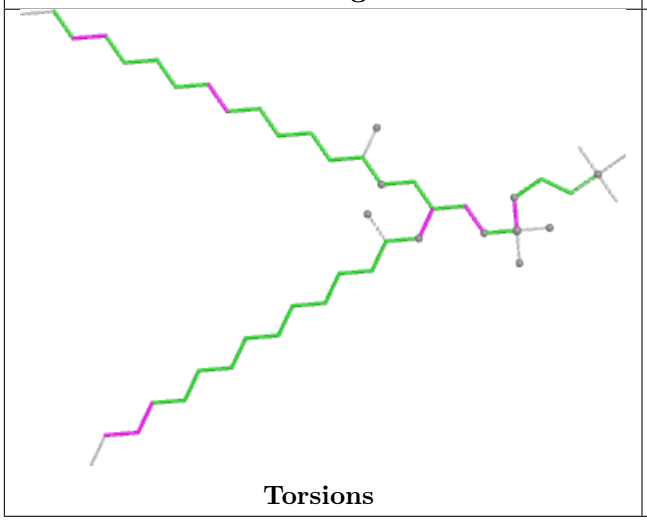
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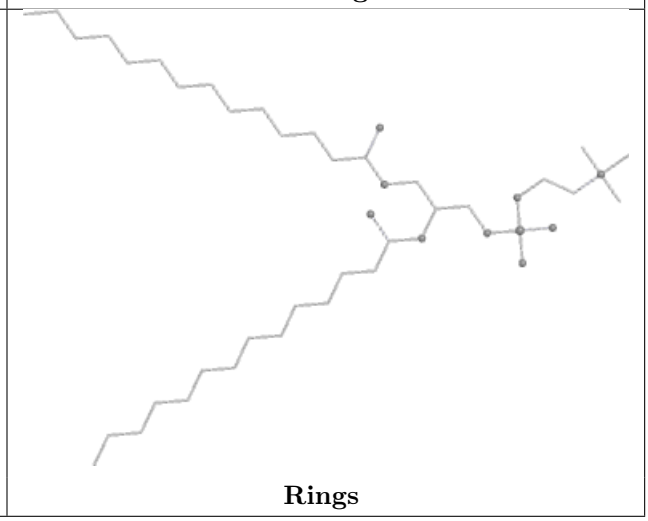
Bond lengths



Bond angles

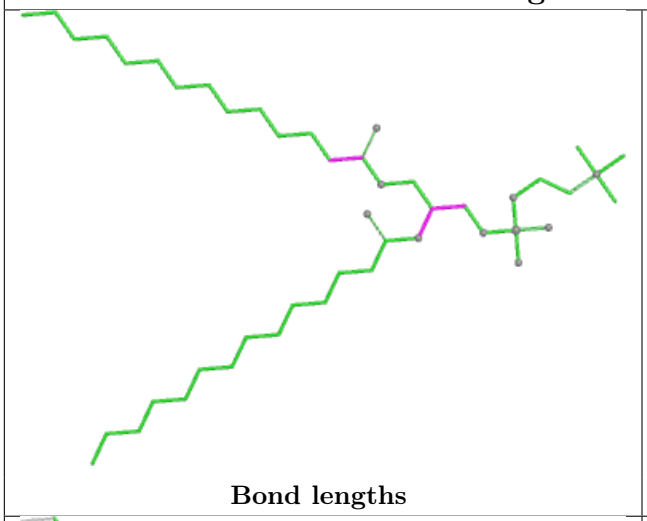


Torsions

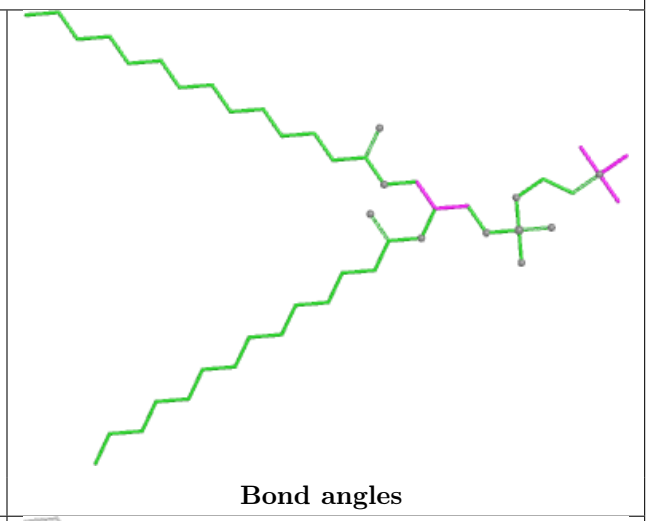


Rings

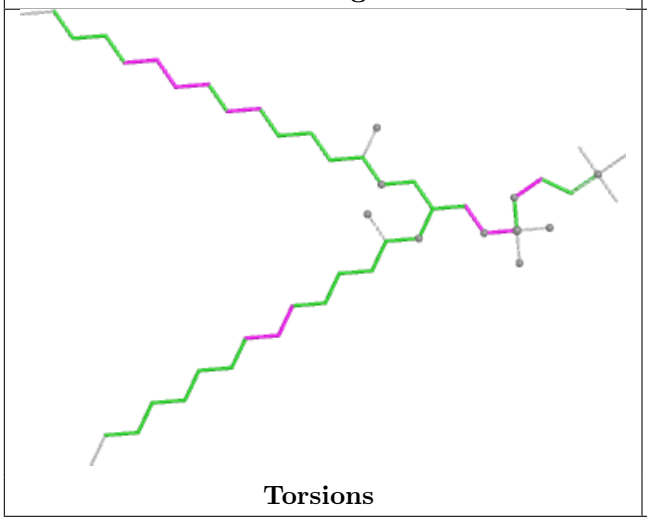
Ligand PX4 C 312



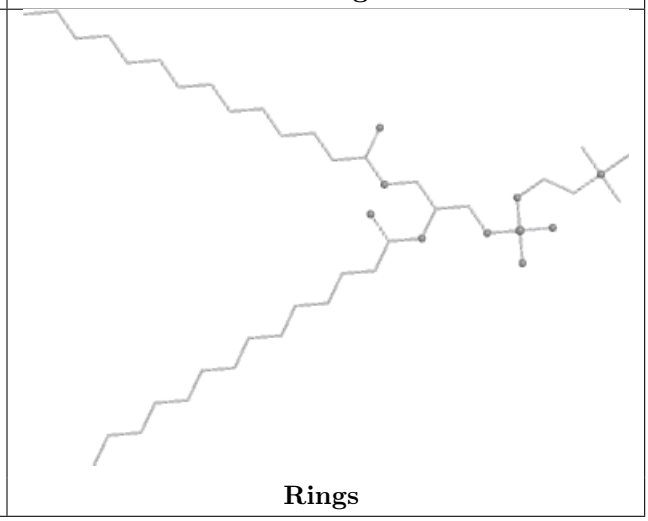
Bond lengths



Bond angles

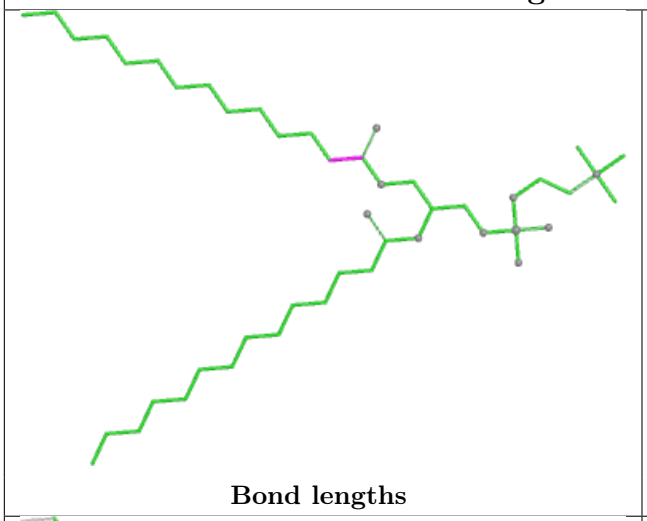


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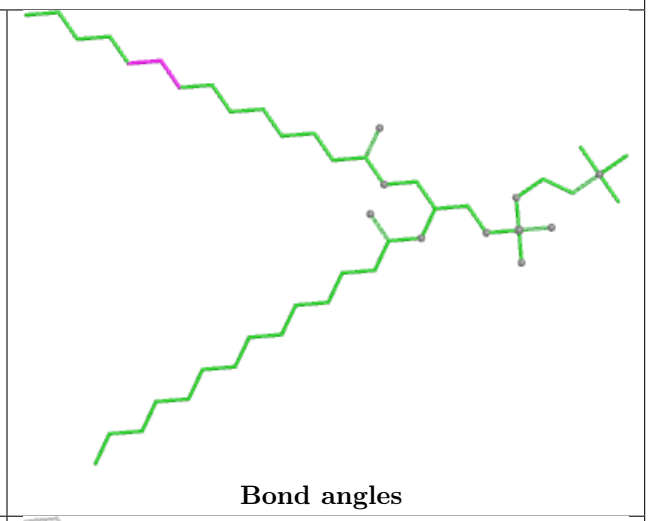


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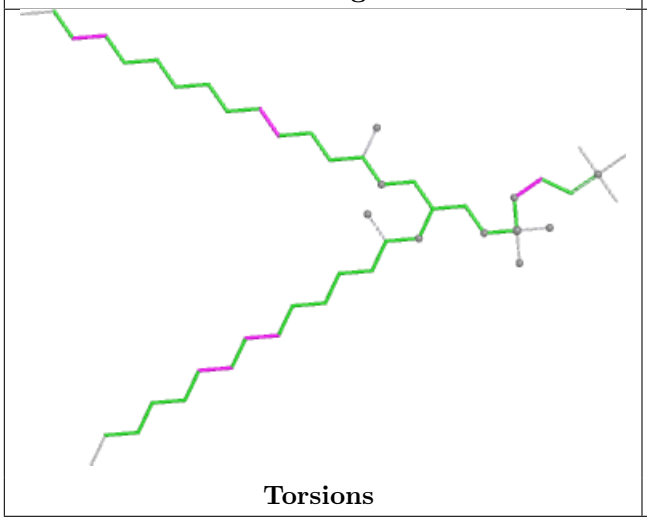
Ligand PX4 C 366



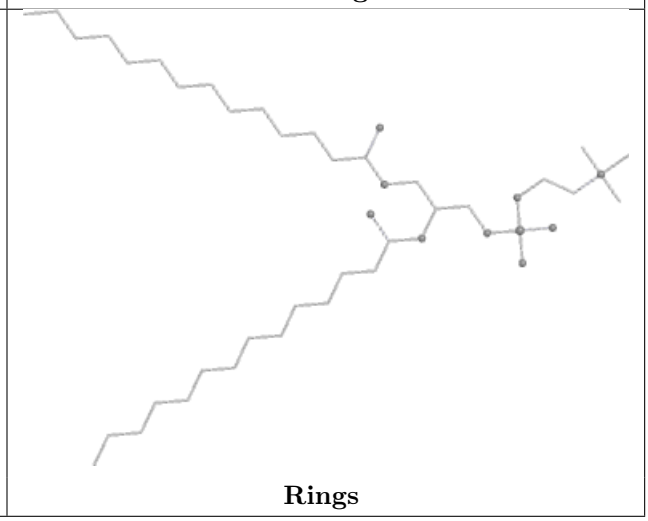
Bond lengths



Bond angles

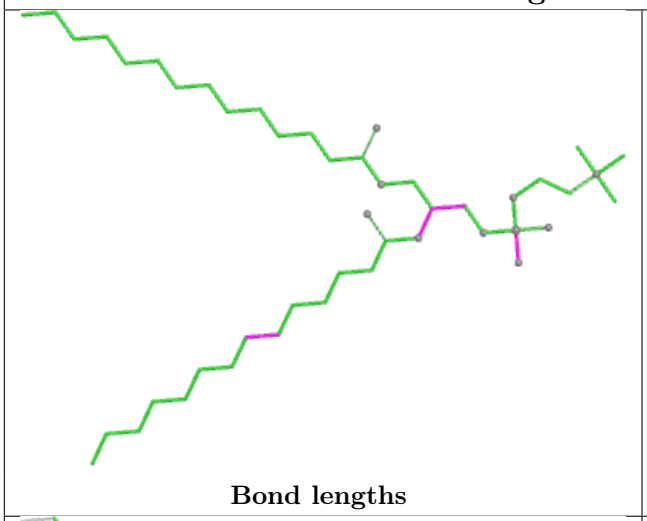


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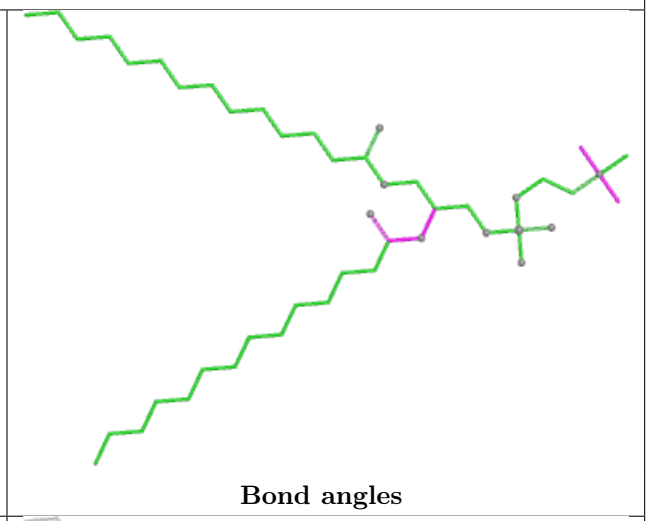


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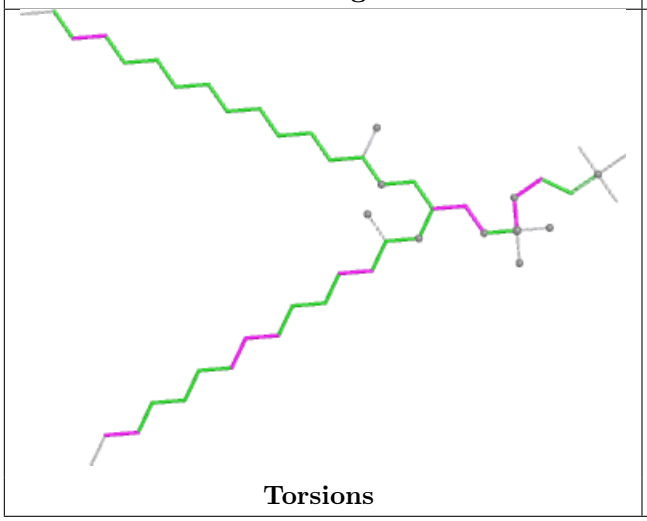
Ligand PX4 B 378



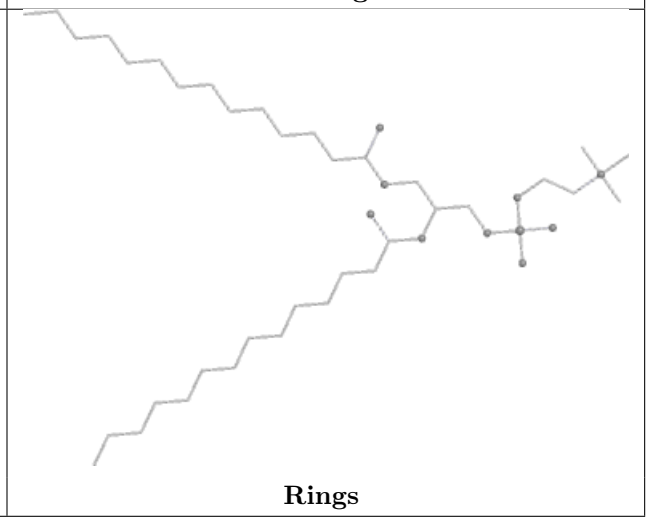
Bond lengths



Bond angles

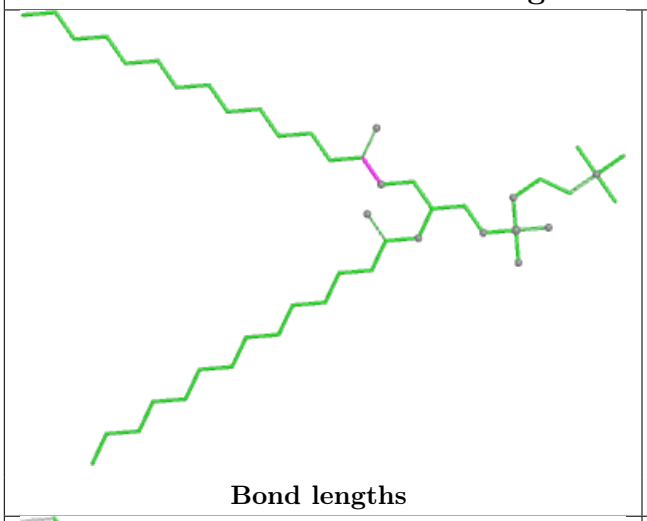


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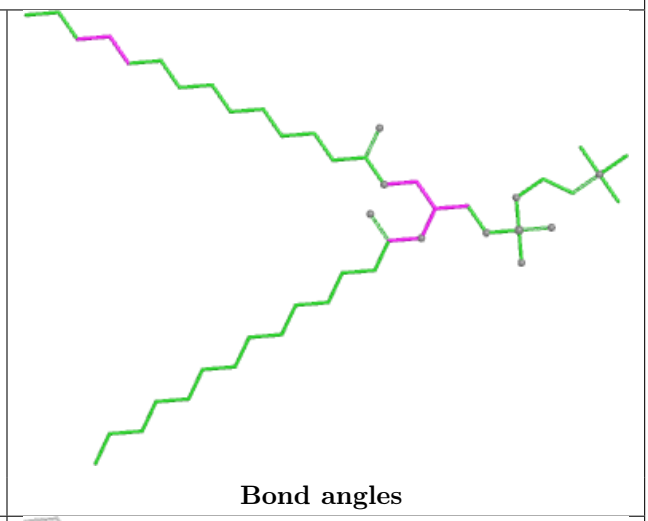


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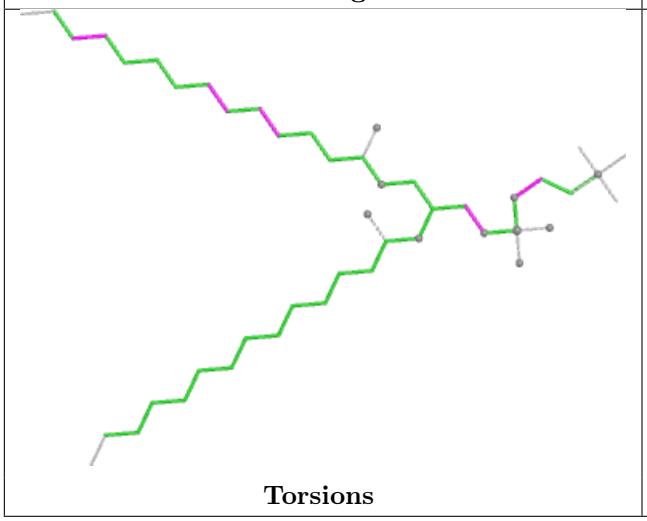
Ligand PX4 C 318



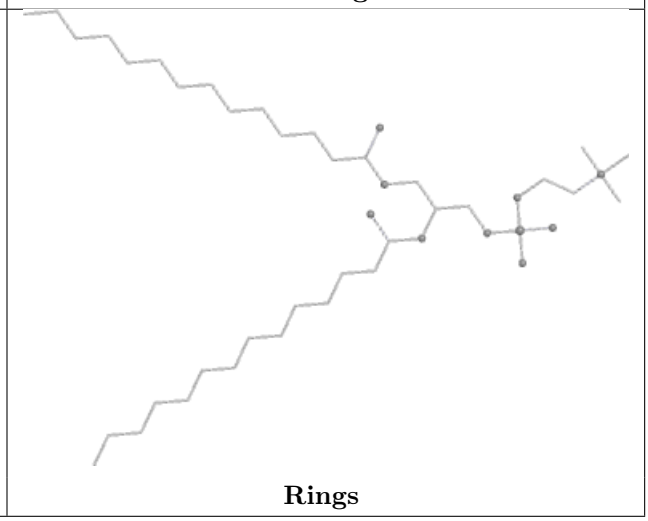
Bond lengths



Bond angles

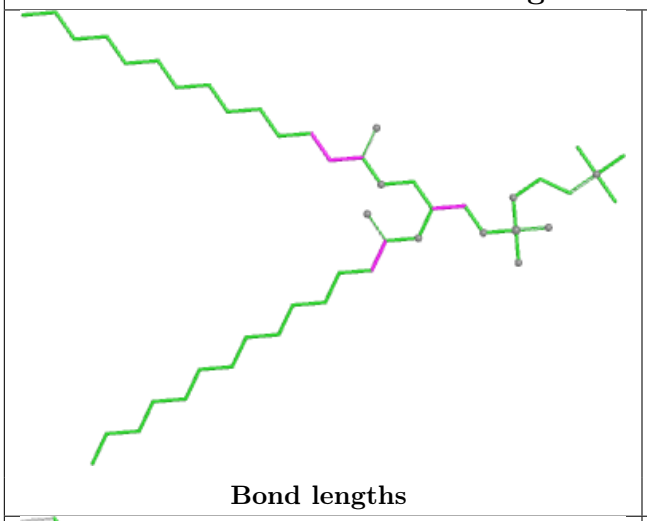


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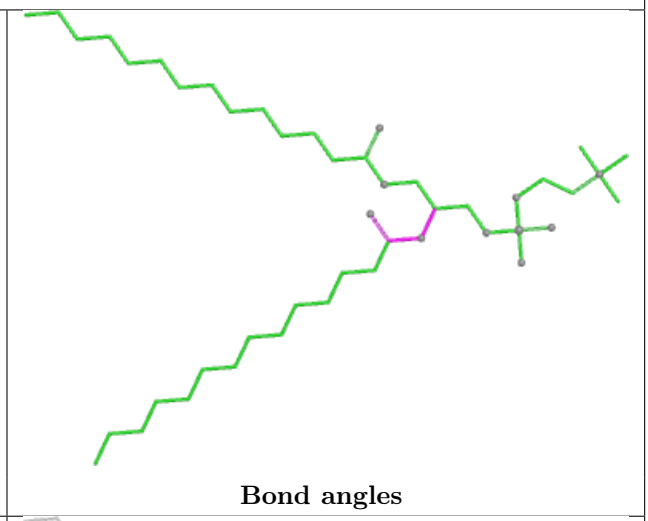


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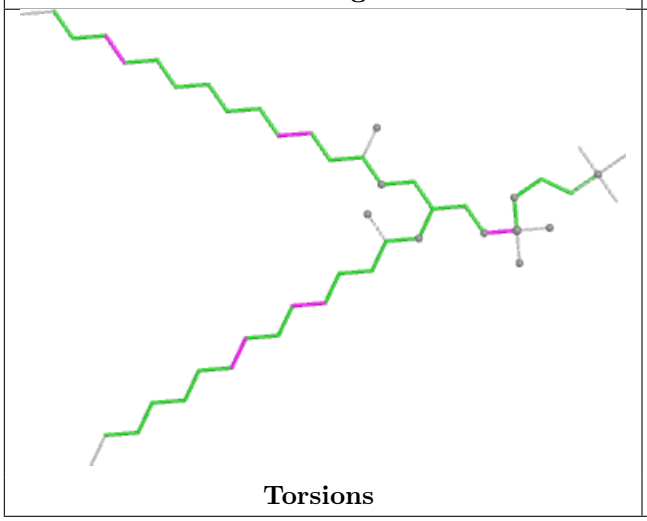
Ligand PX4 A 634



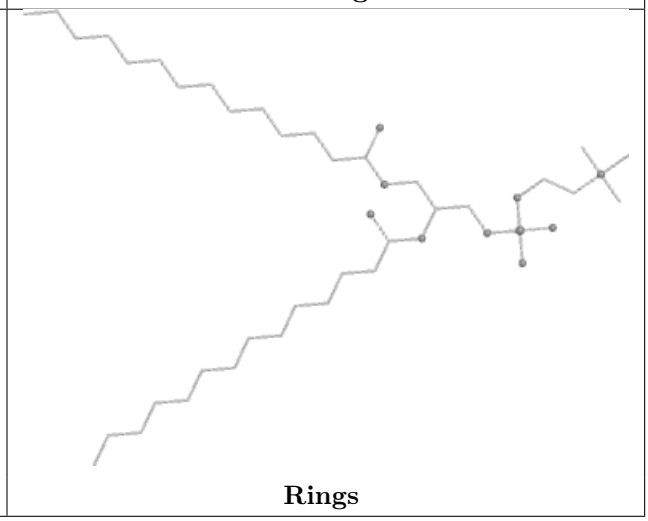
Bond lengths



Bond angles

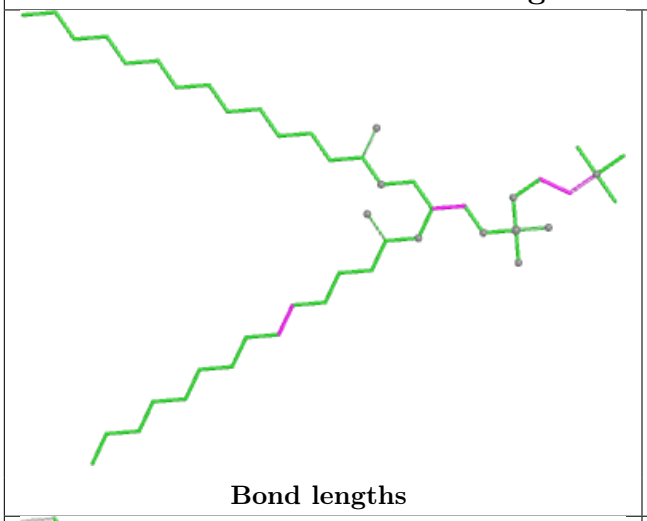


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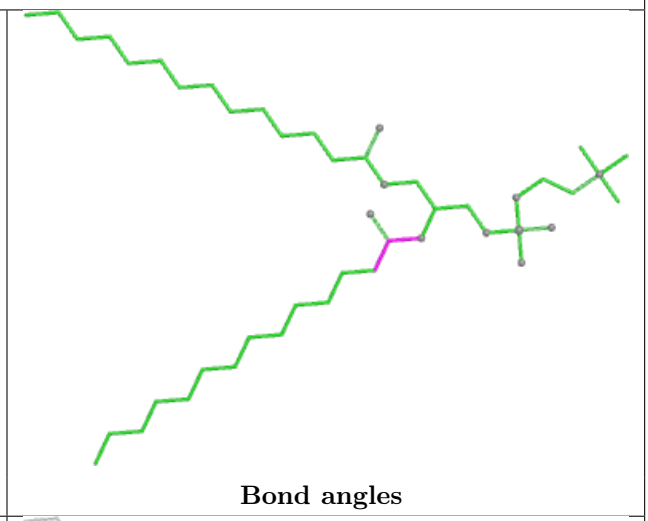


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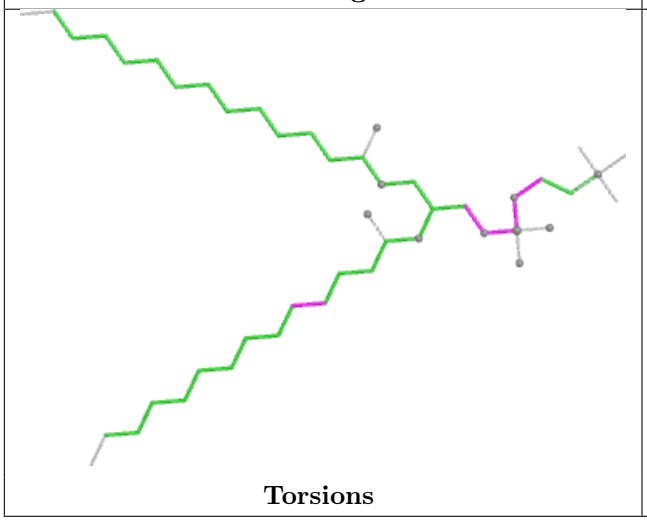
Ligand PX4 B 373



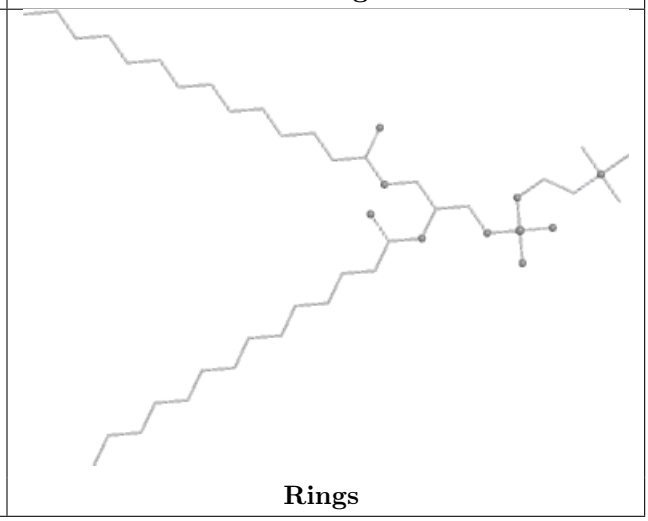
Bond lengths



Bond angles

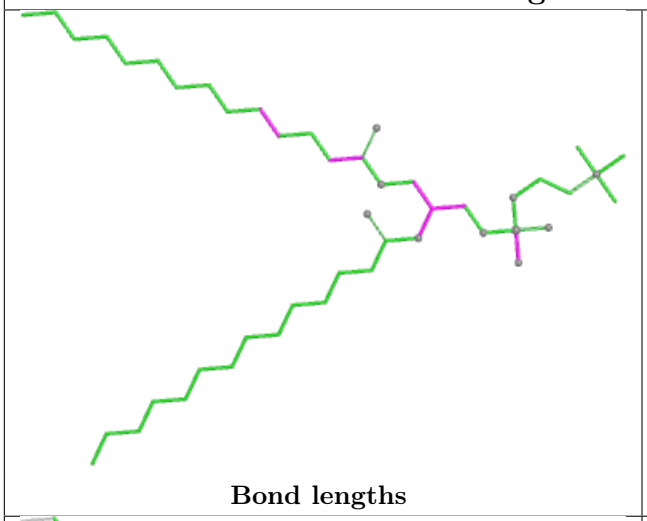


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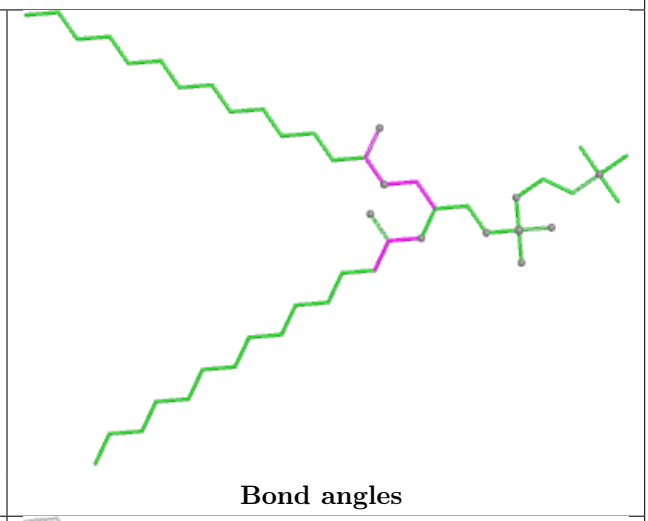


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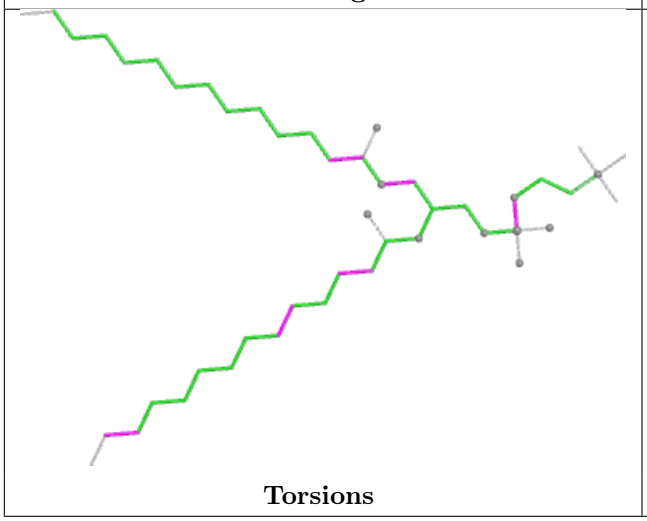
Ligand PX4 B 387



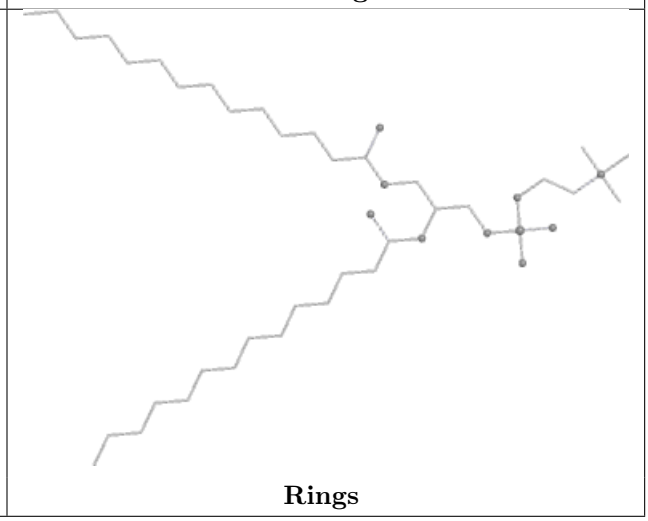
Bond lengths



Bond angles

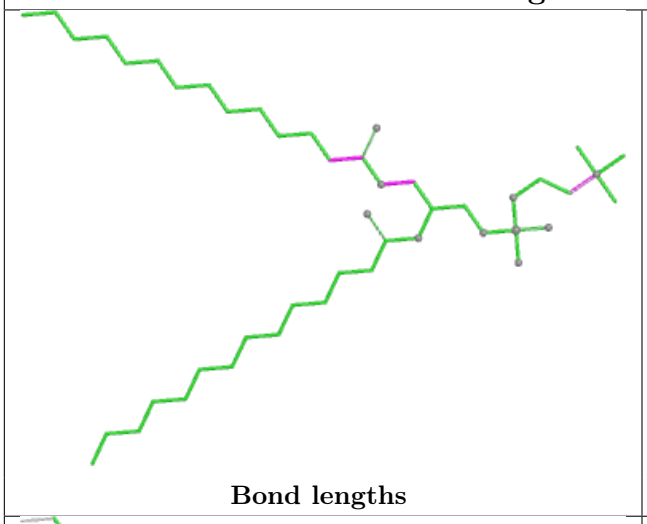


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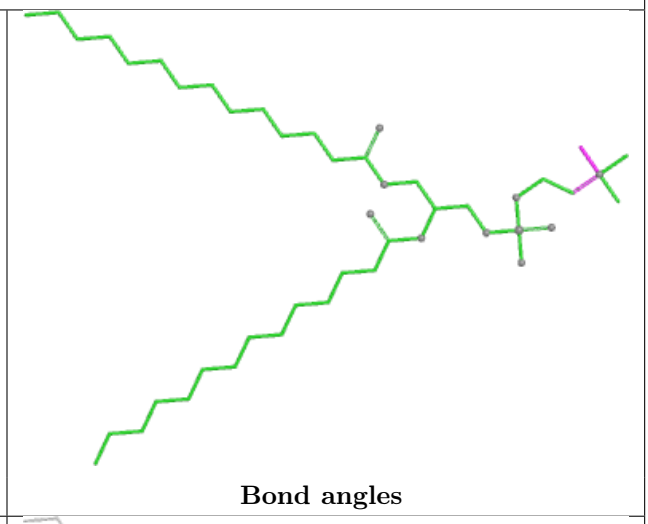


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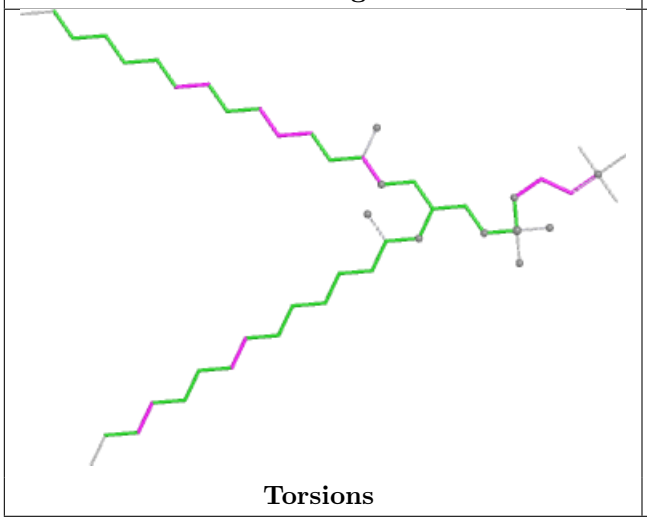
Ligand PX4 B 362



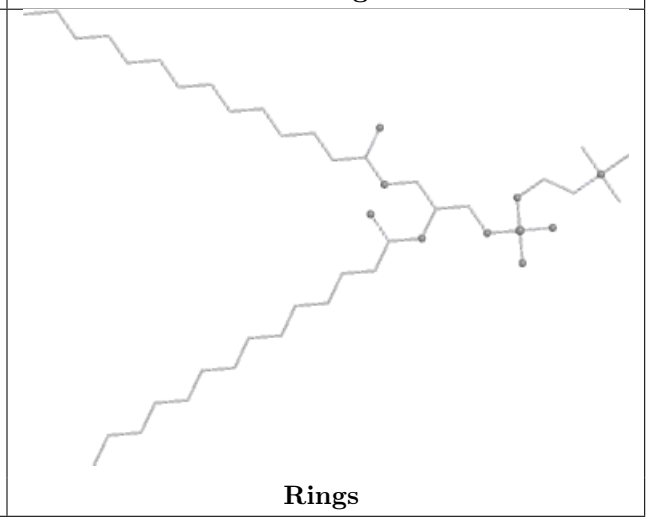
Bond lengths



Bond angles

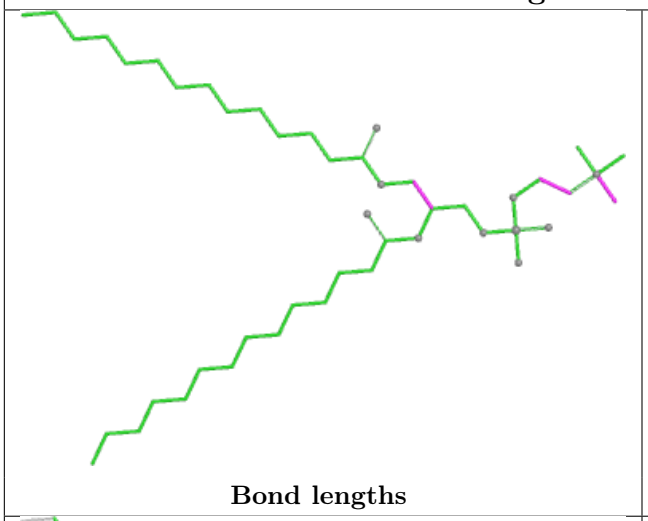


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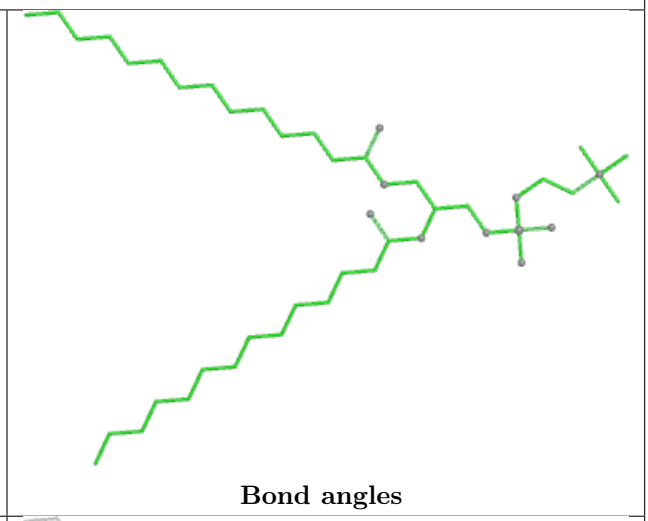


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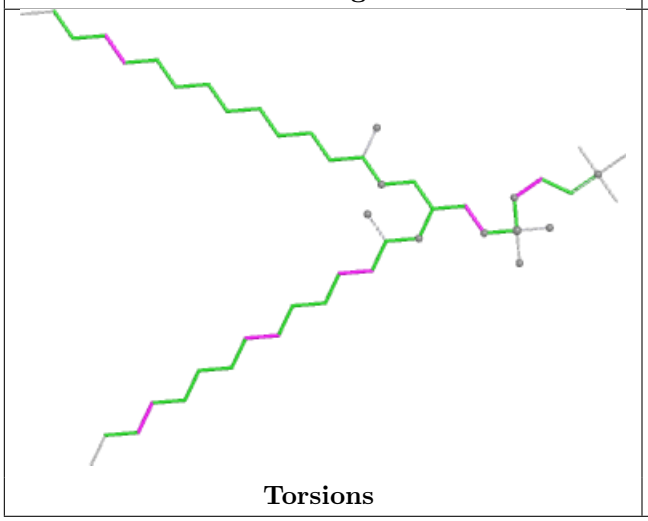
Ligand PX4 B 320



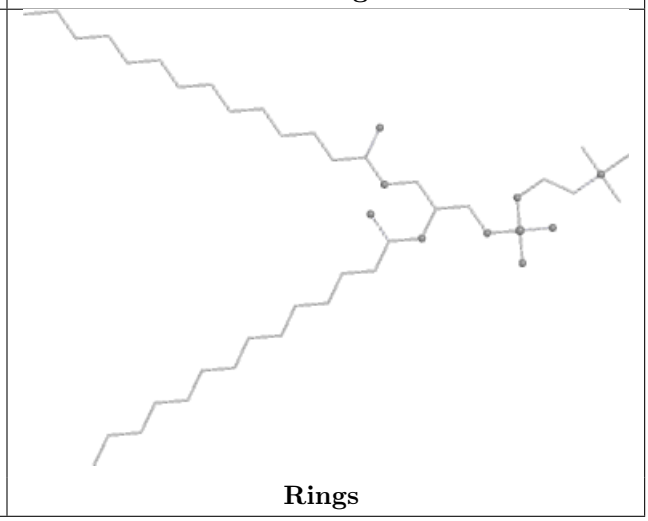
Bond lengths



Bond angles

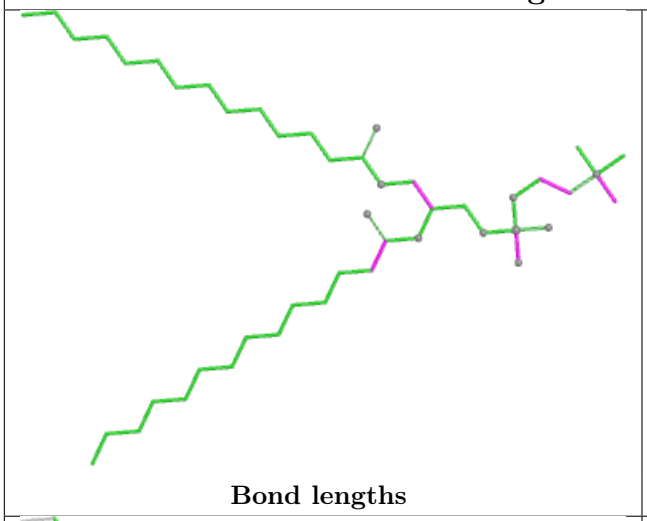


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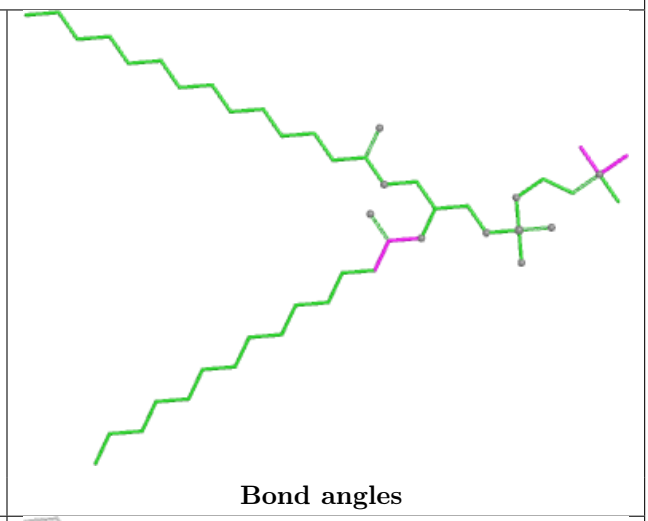


Rings

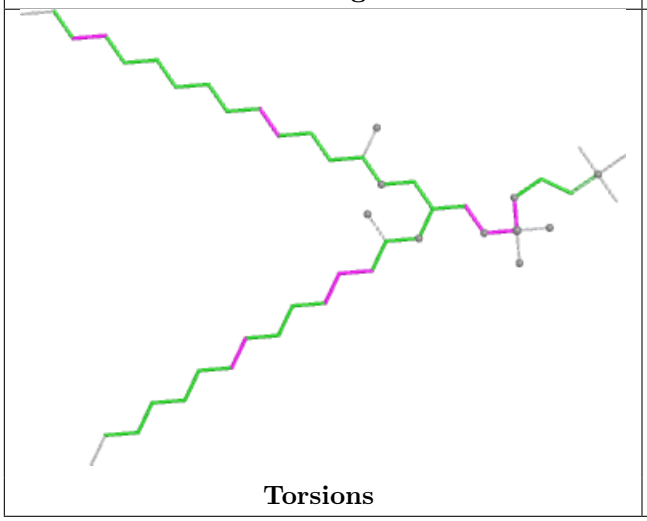
Ligand PX4 C 355



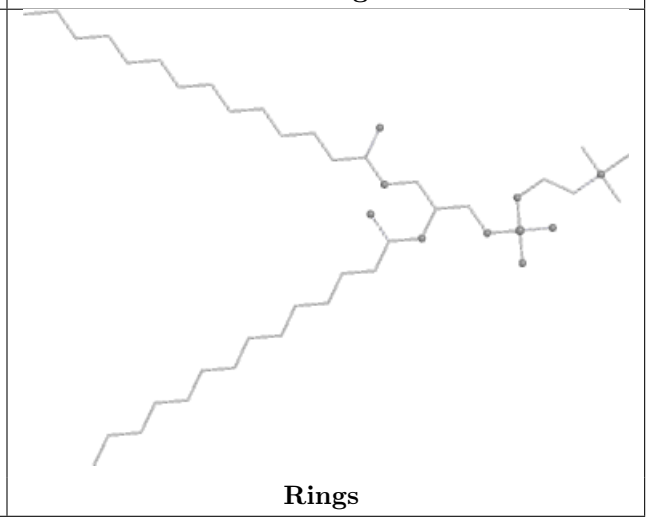
Bond lengths



Bond angles

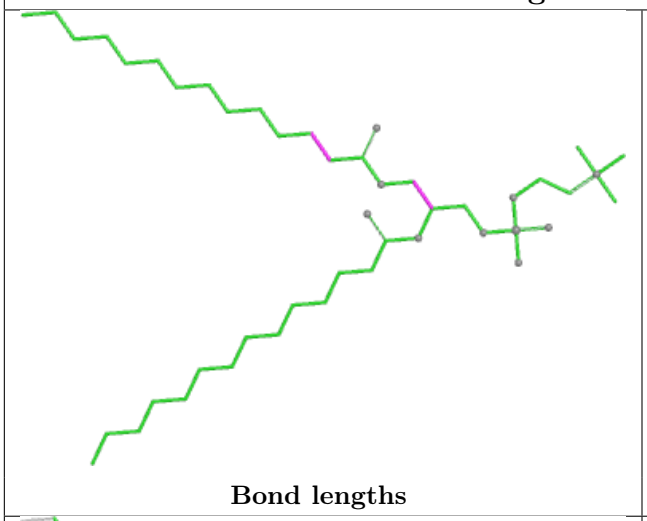


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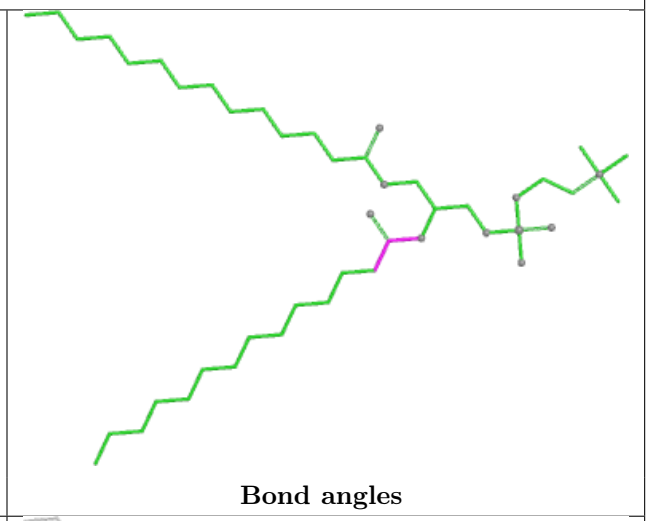


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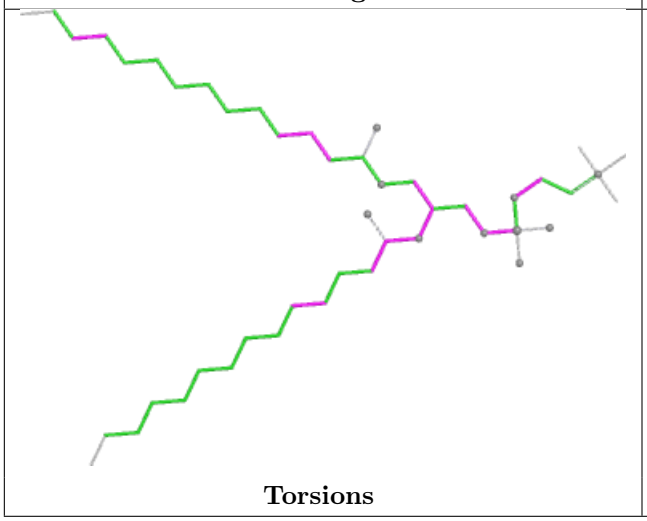
Ligand PX4 B 364



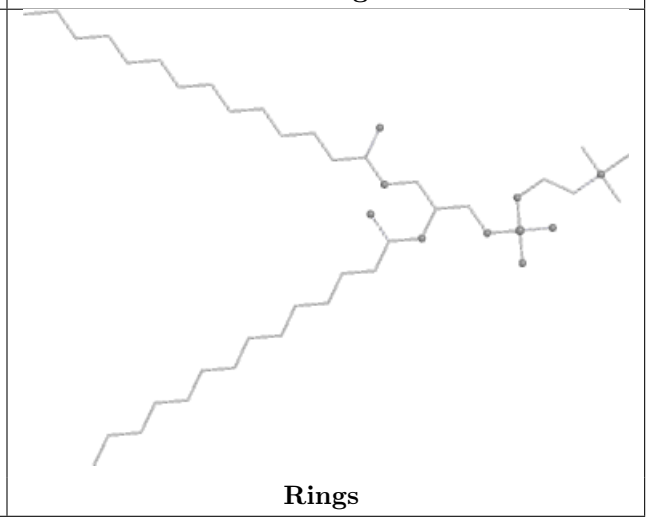
Bond lengths



Bond angles

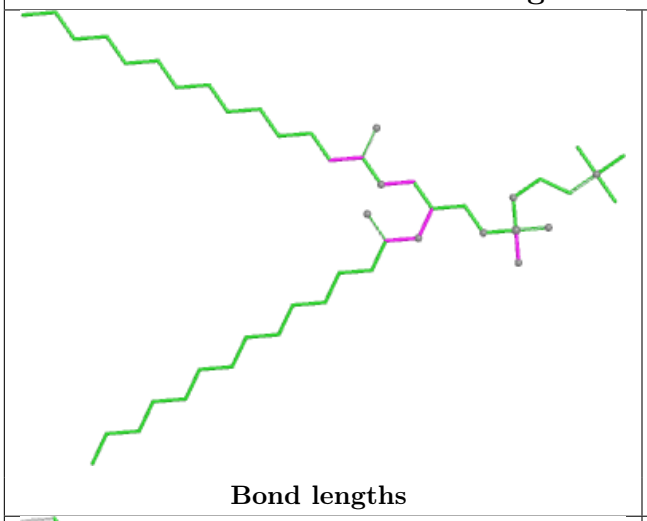


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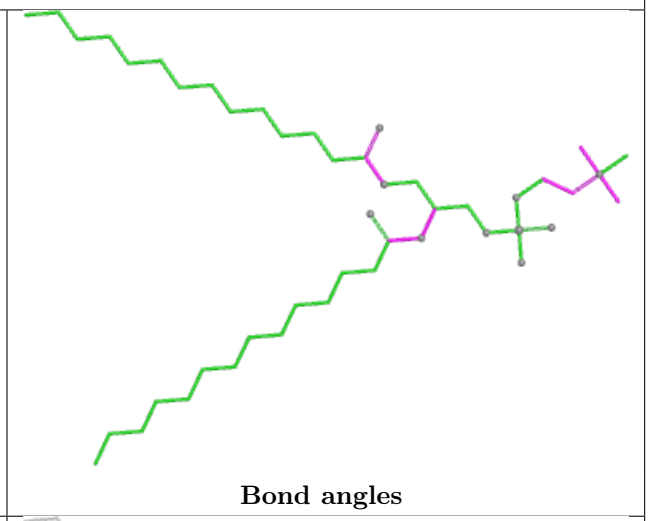


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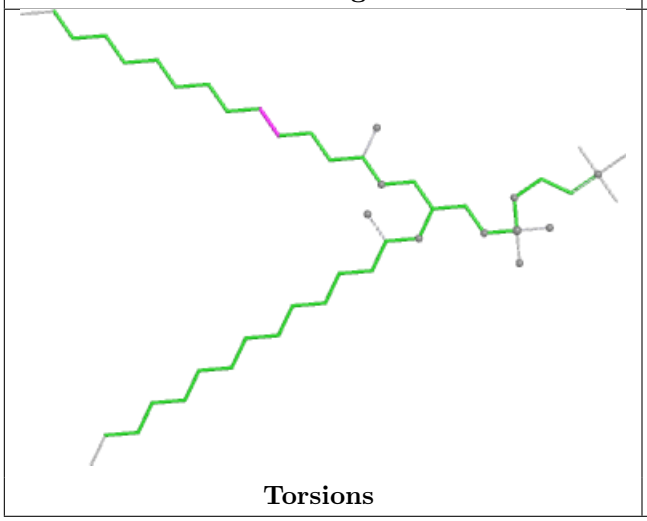
Ligand PX4 A 610



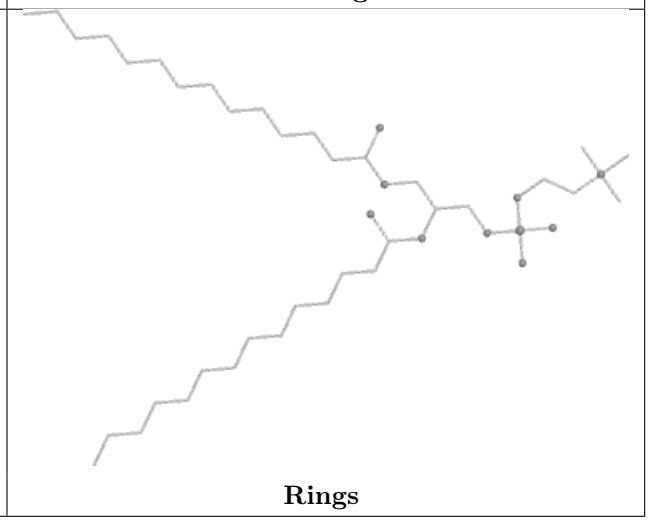
Bond lengths



Bond angles

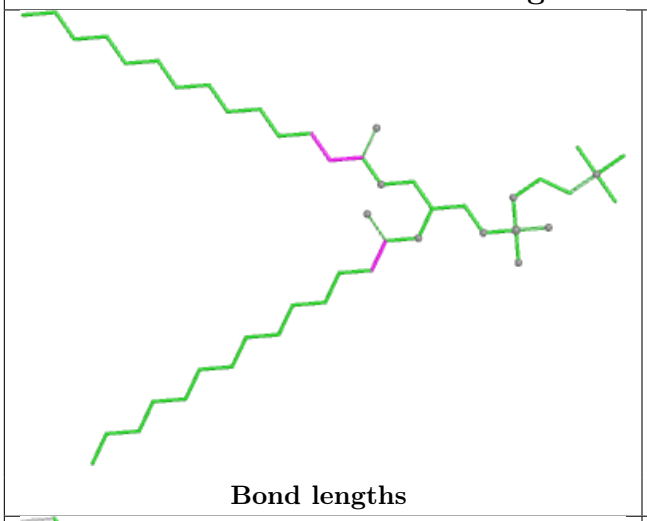


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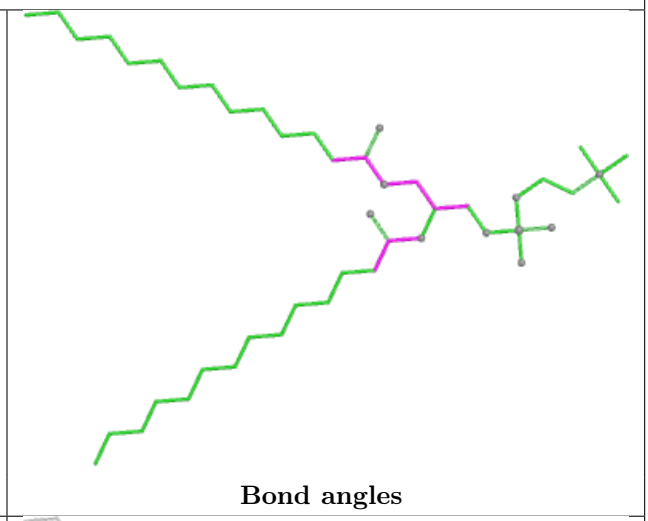


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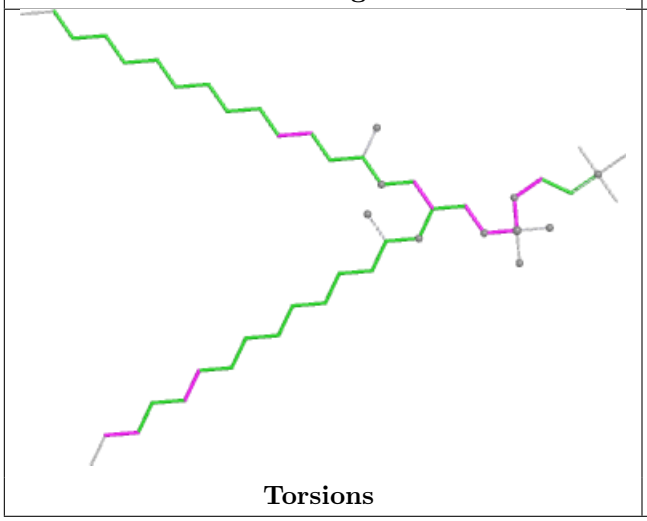
Ligand PX4 A 618



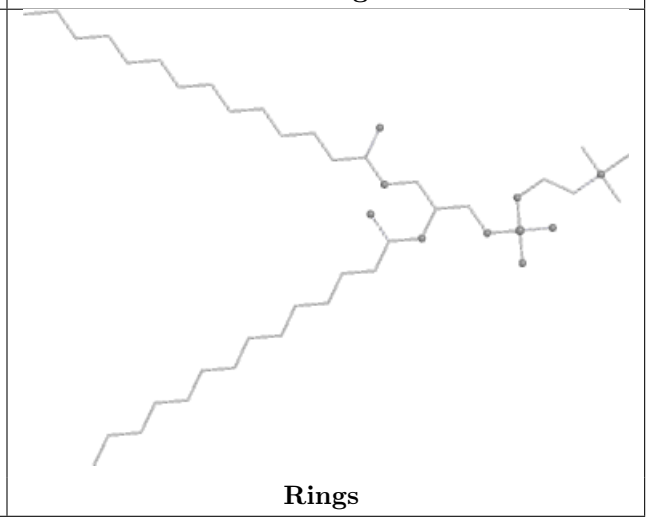
Bond lengths



Bond angles

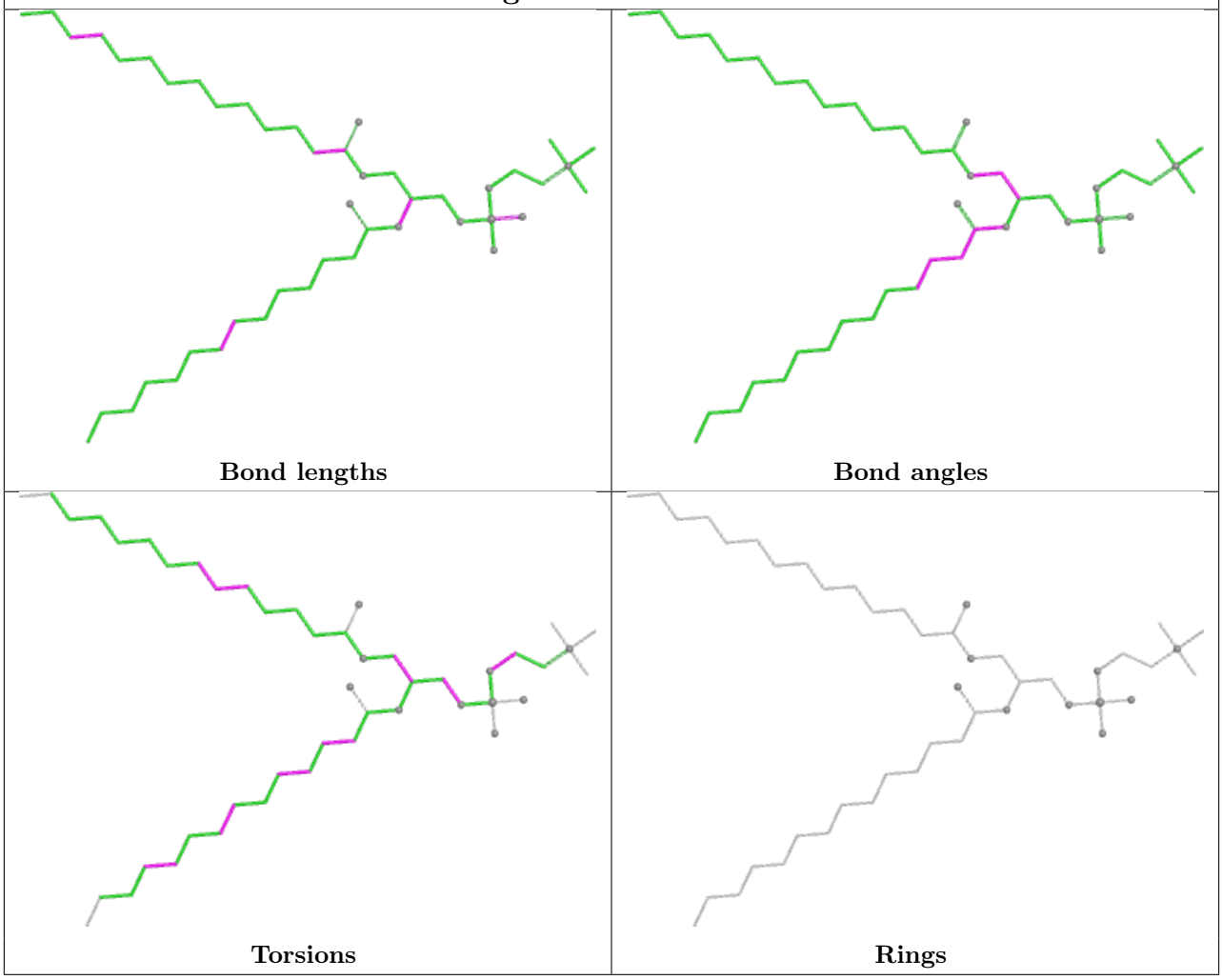


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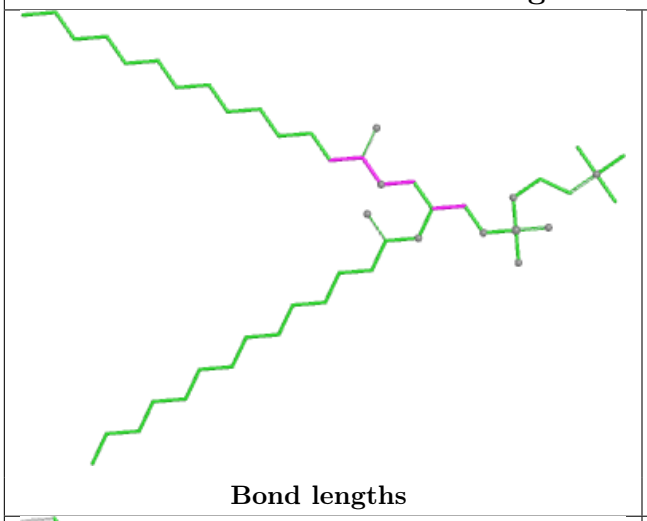


Rings

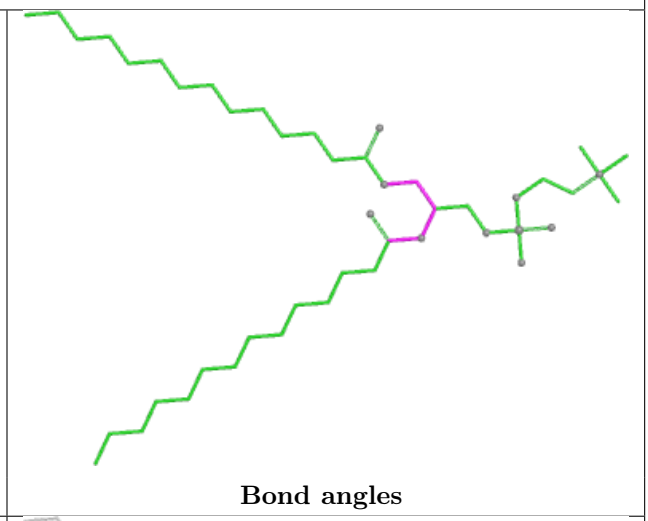
Ligand PX4 B 391



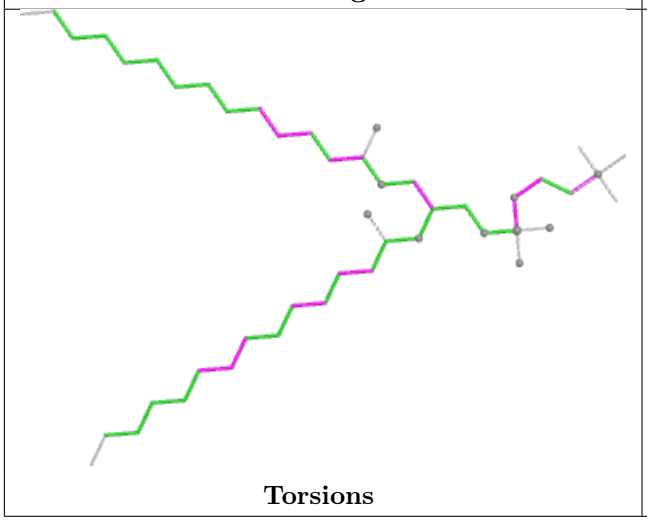
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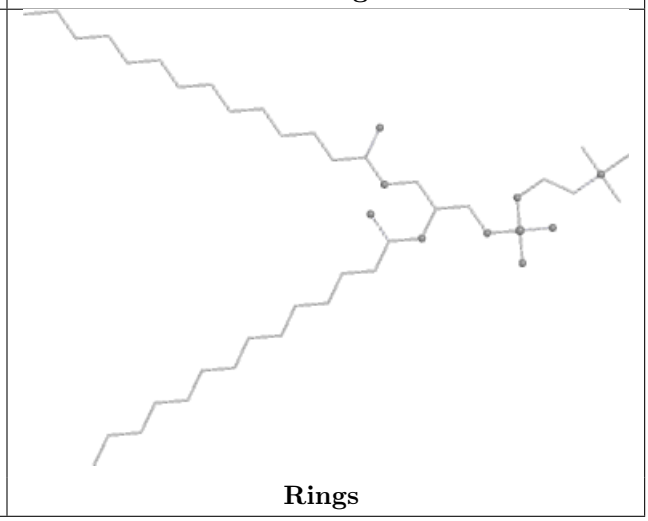
Bond lengths



Bond angles

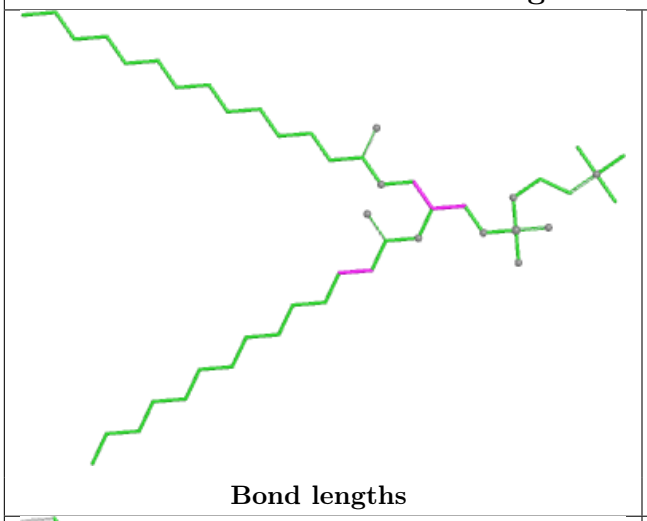


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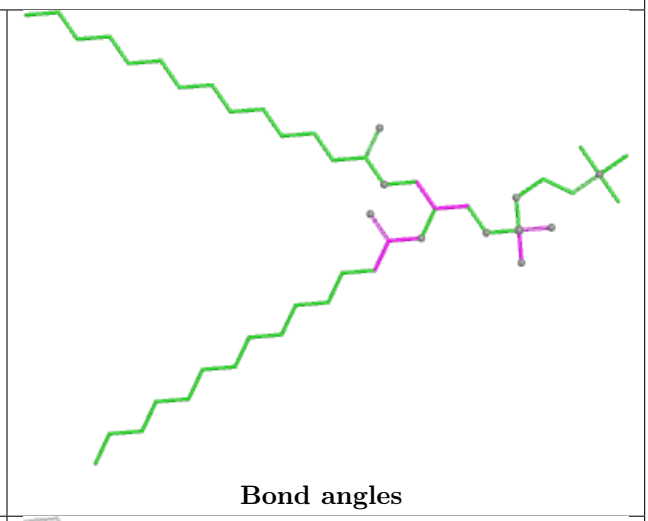


Rings

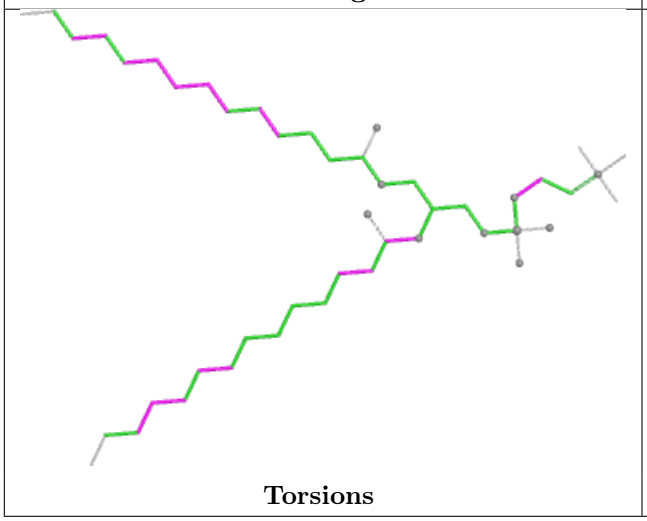
Ligand PX4 C 343



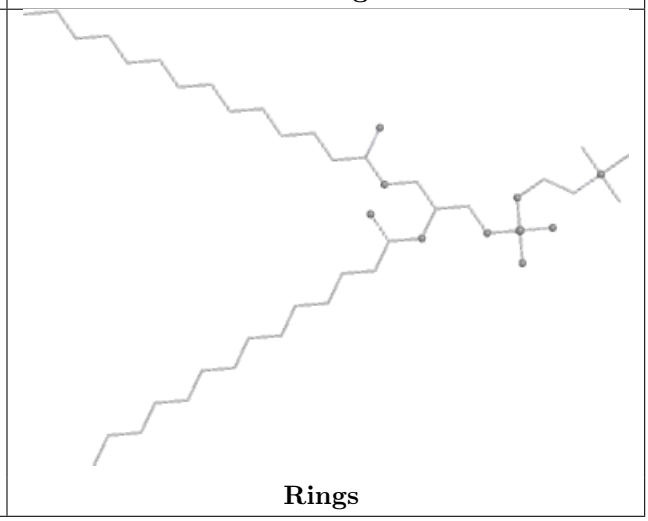
Bond lengths



Bond angles

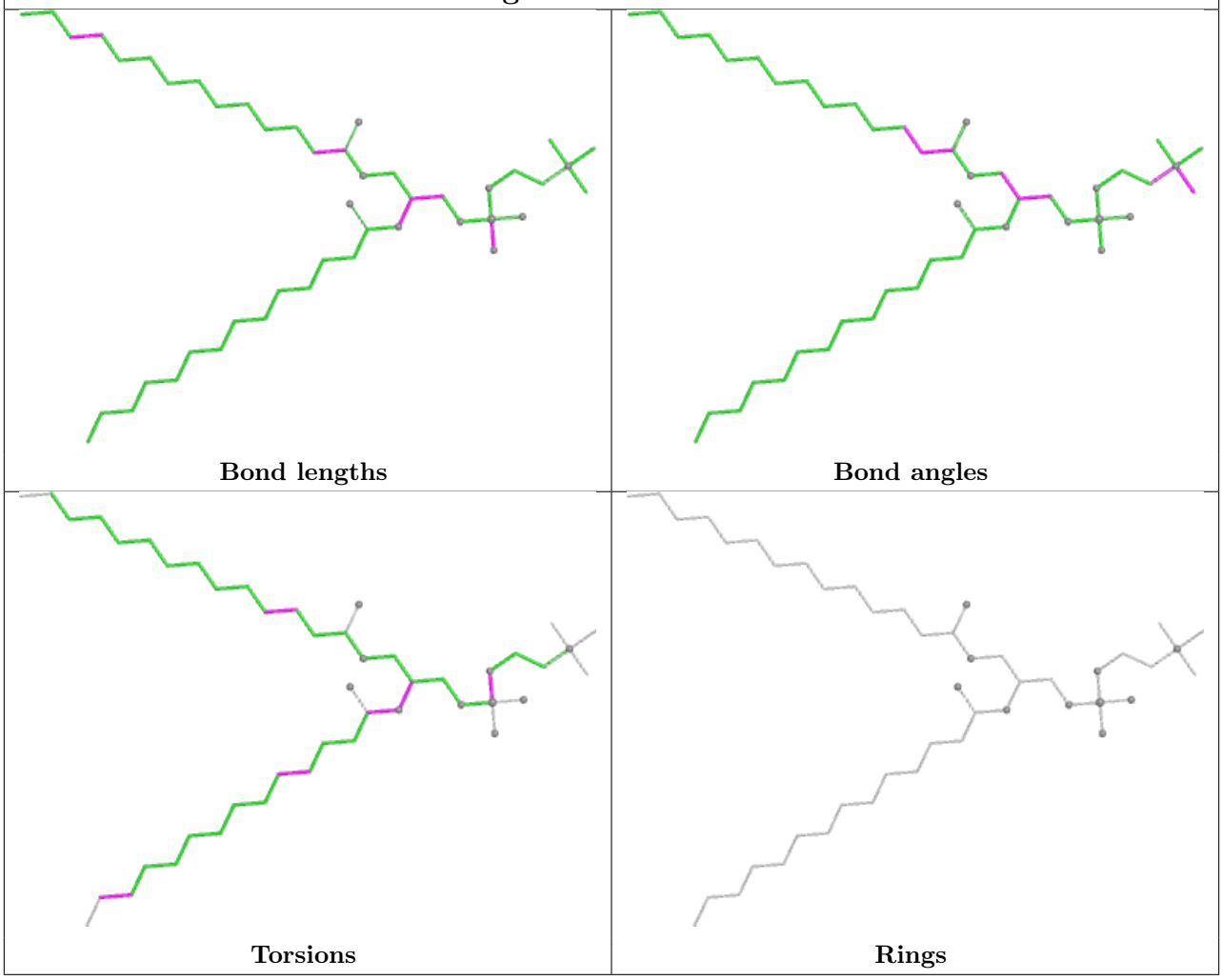


Torsions

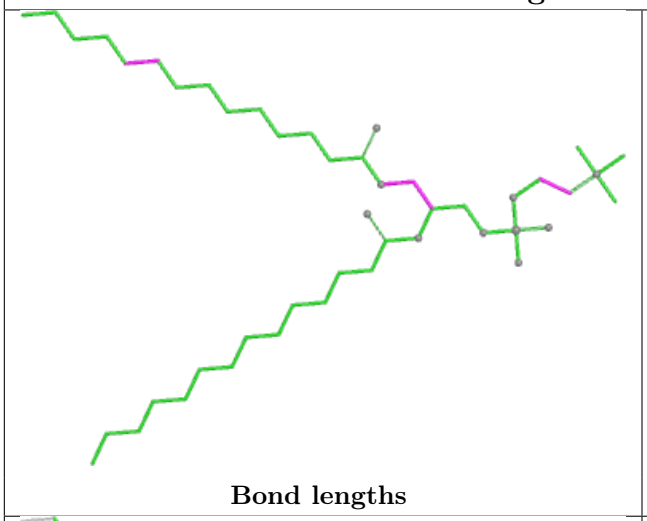


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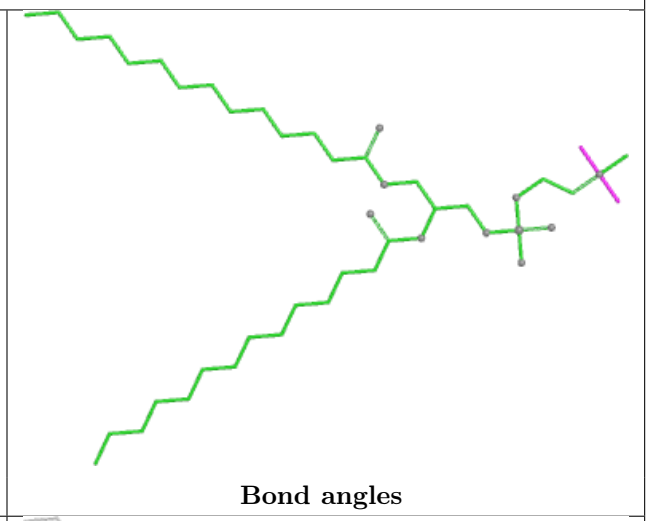
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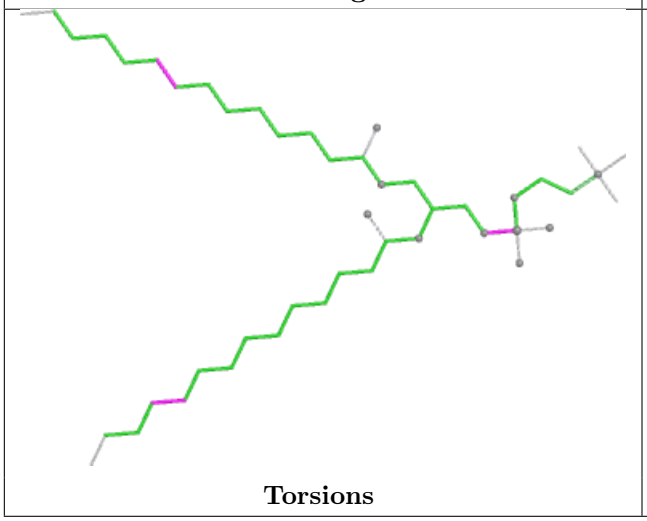
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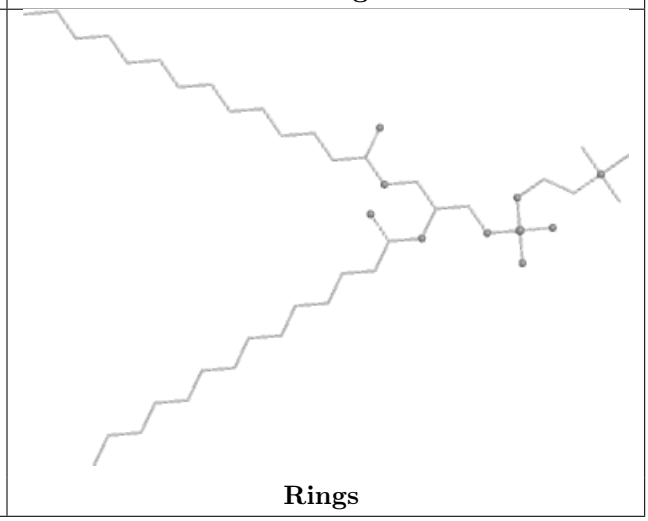
Bond lengths



Bond angles

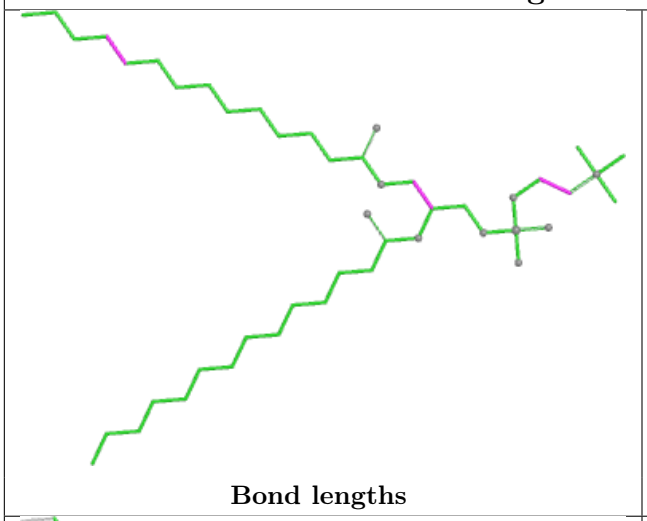


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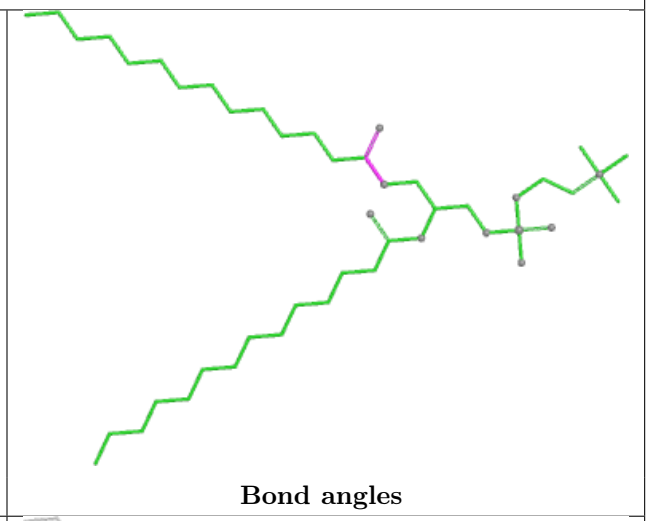


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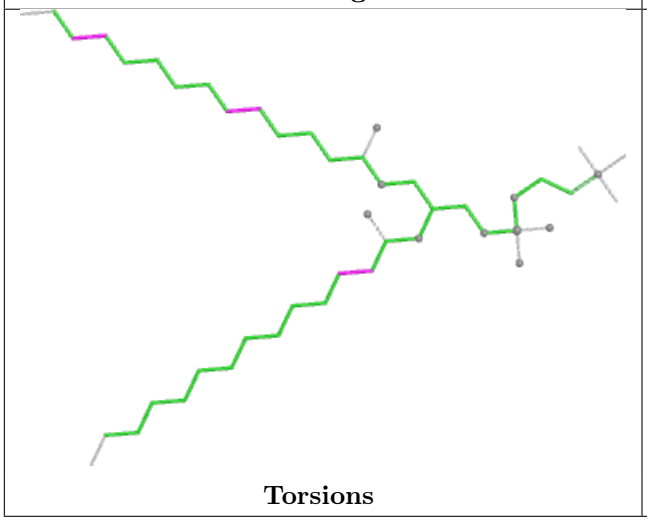
Ligand PX4 A 625



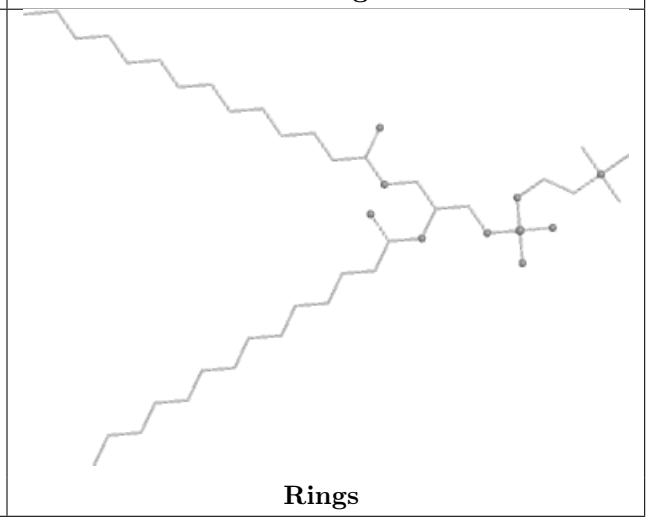
Bond lengths



Bond angles

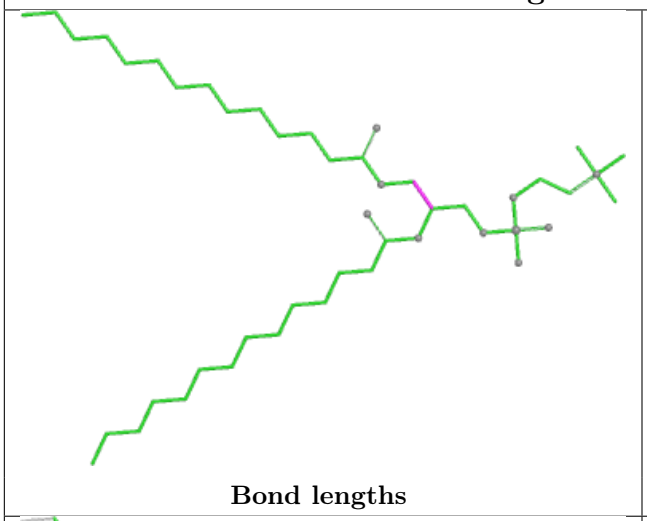


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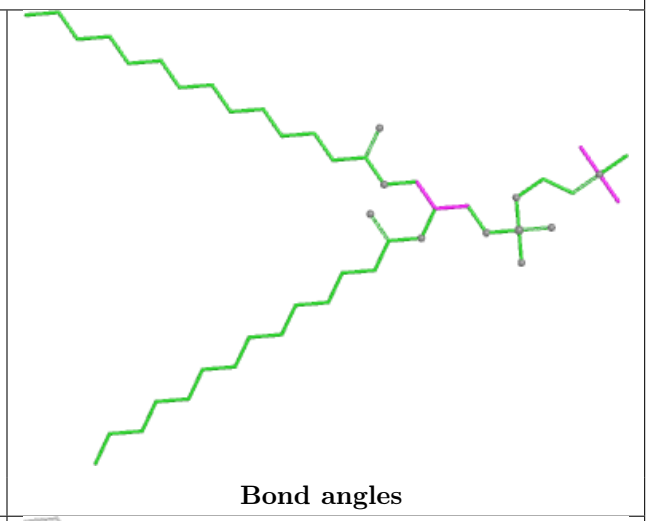


Rings

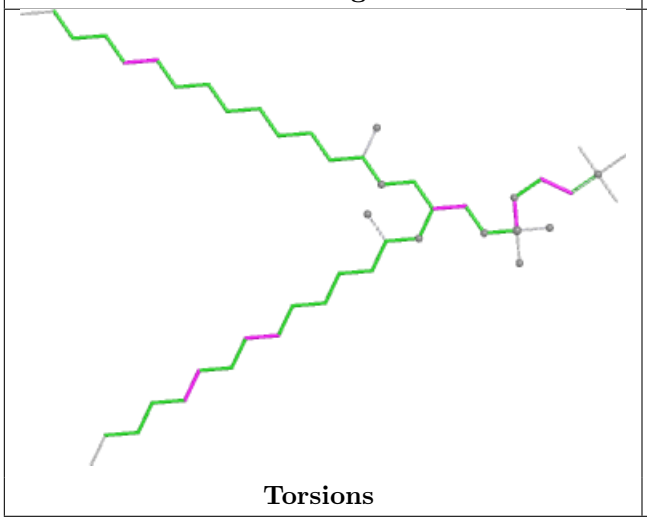
Ligand PX4 A 605



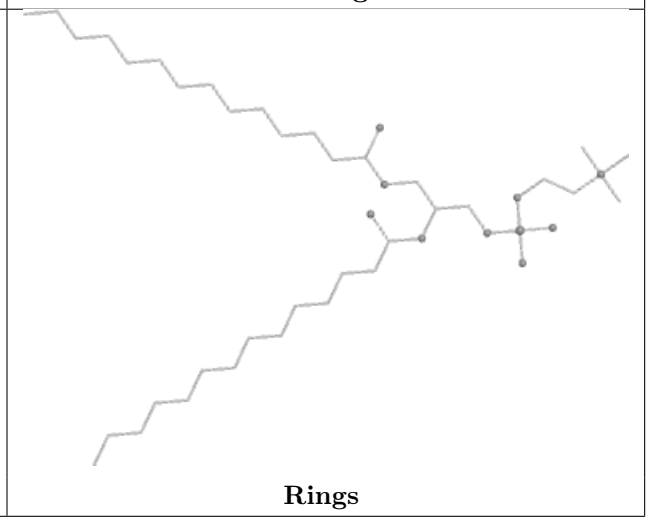
Bond lengths



Bond angles

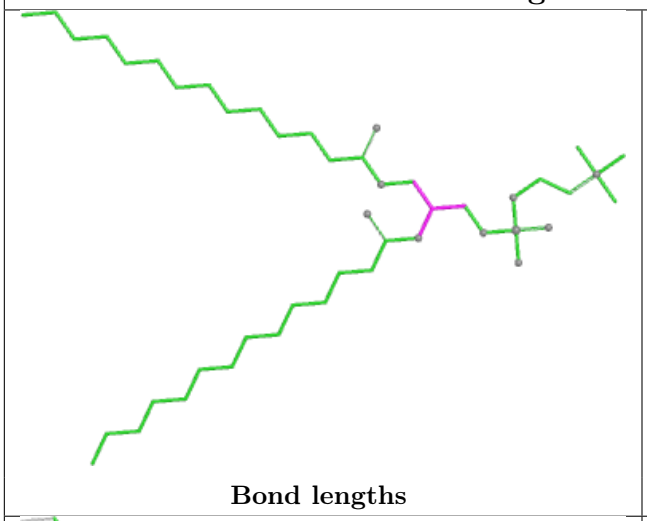


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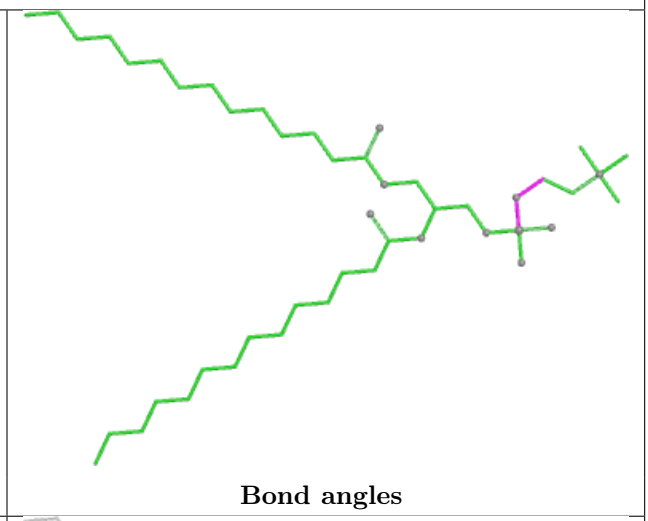


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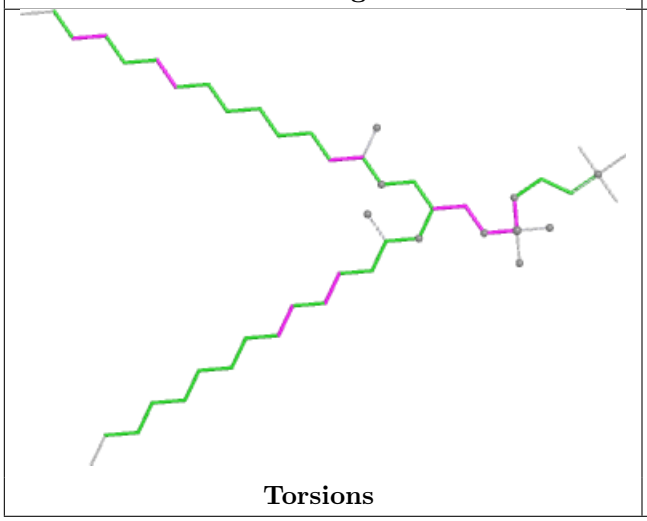
Ligand PX4 B 354



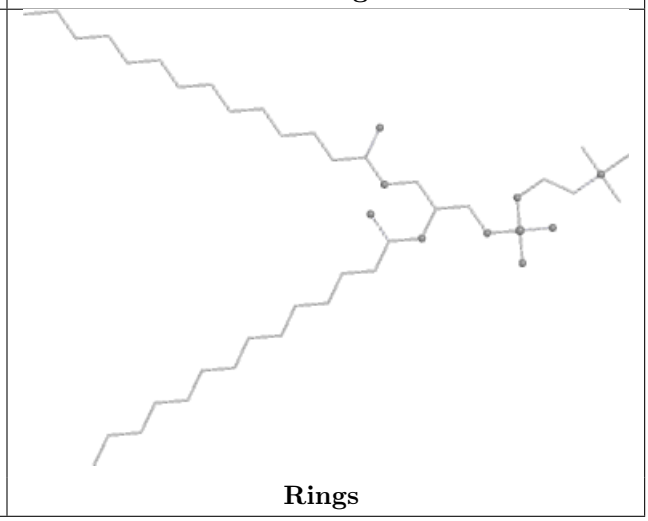
Bond lengths



Bond angles

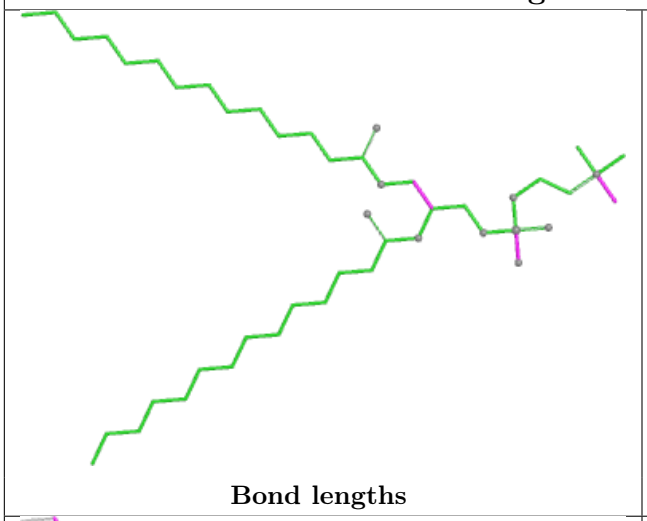


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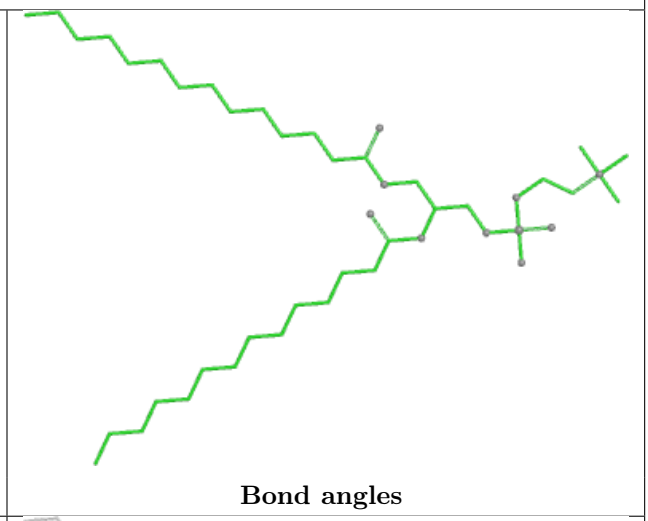


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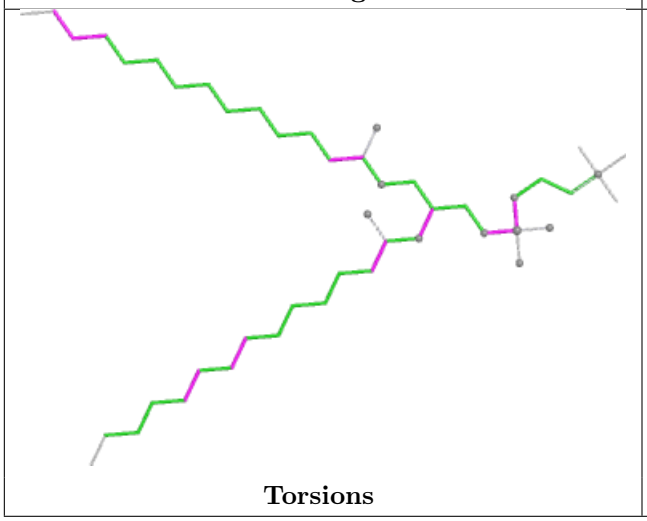
Ligand PX4 B 308



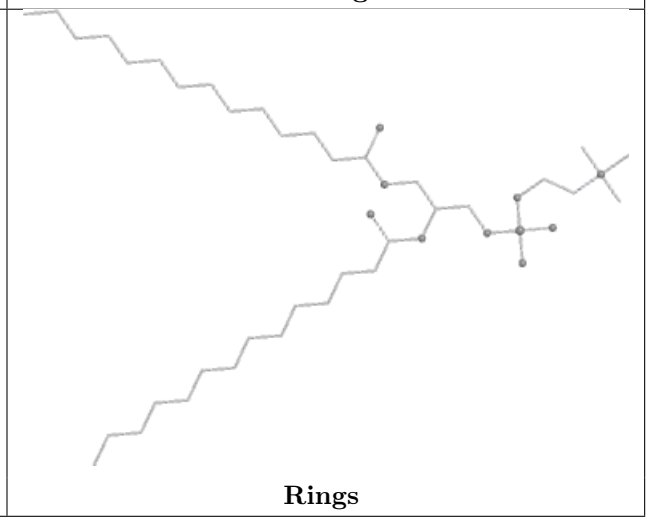
Bond lengths



Bond angles

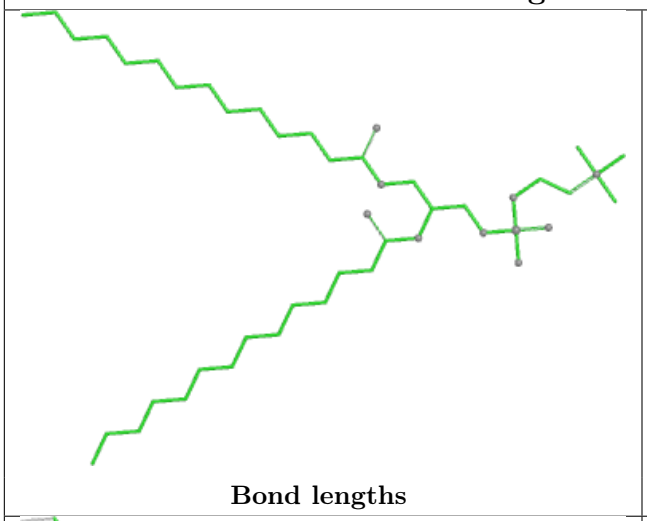


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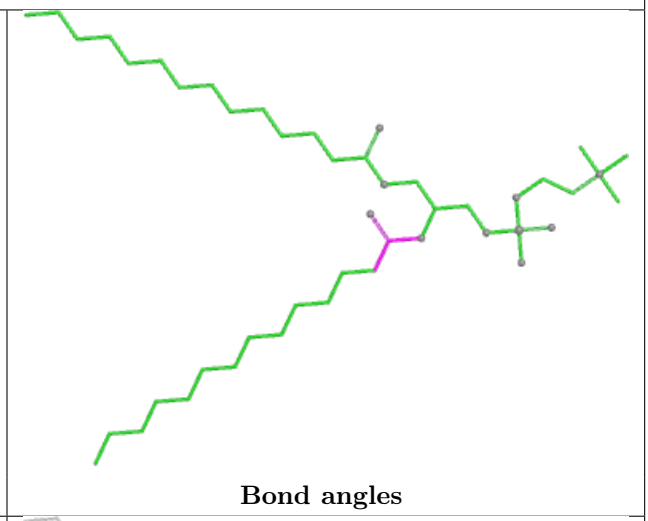


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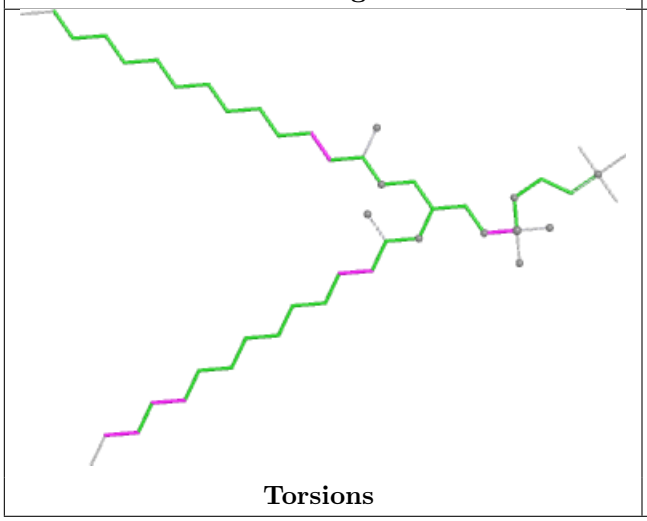
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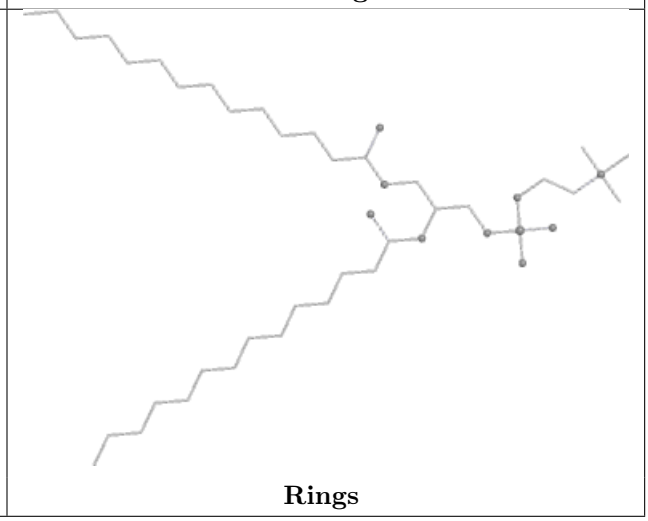
Bond lengths



Bond angles

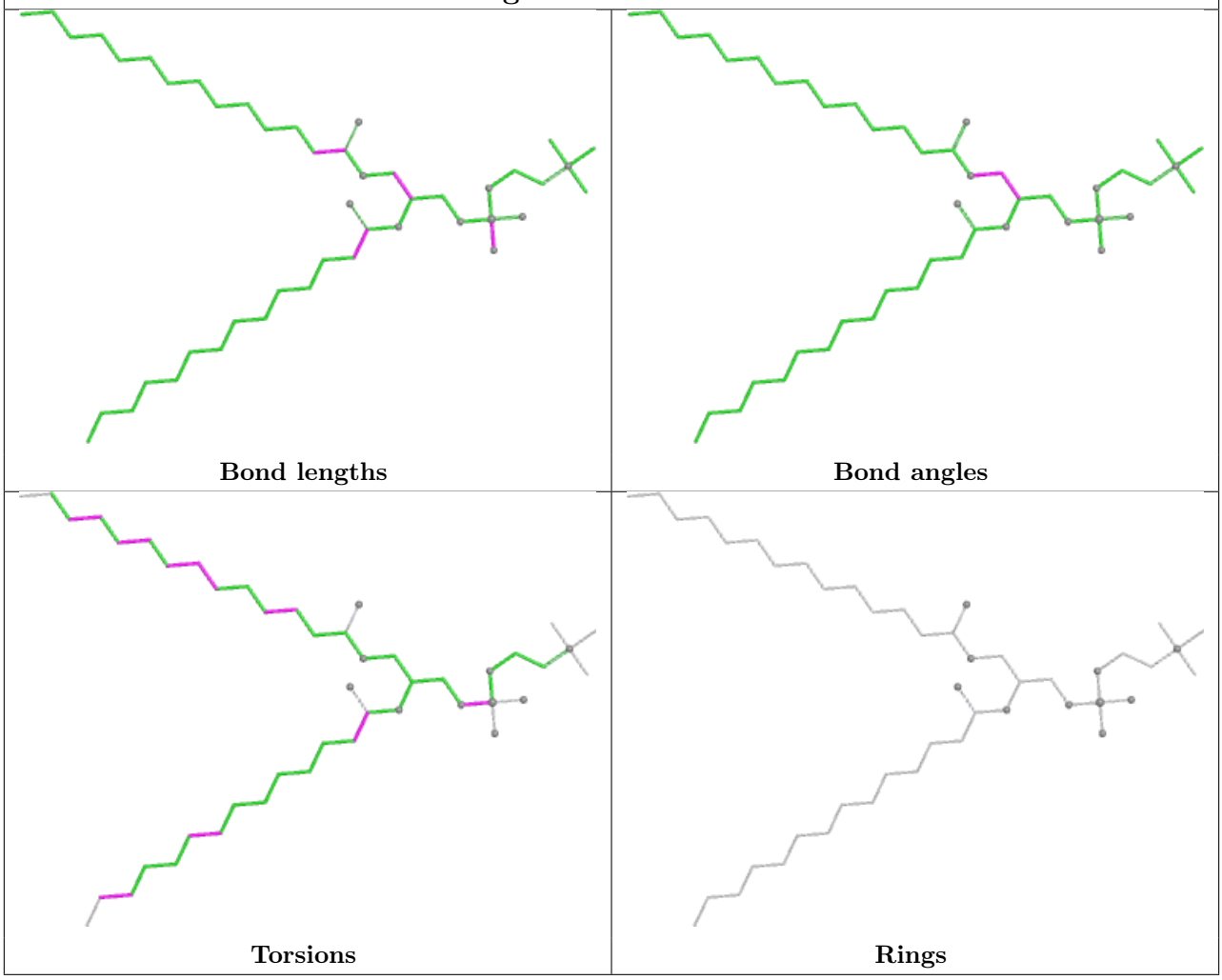


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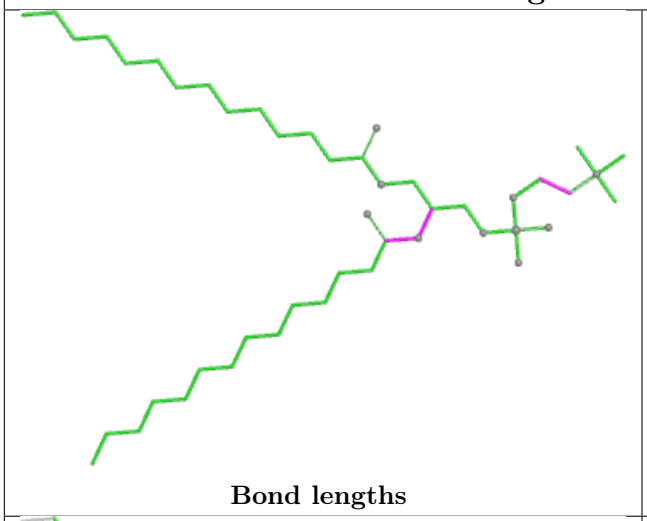


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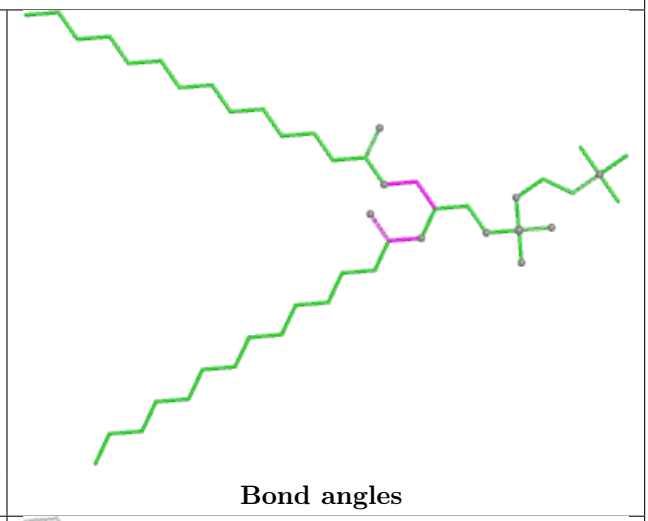
Ligand PX4 B 361



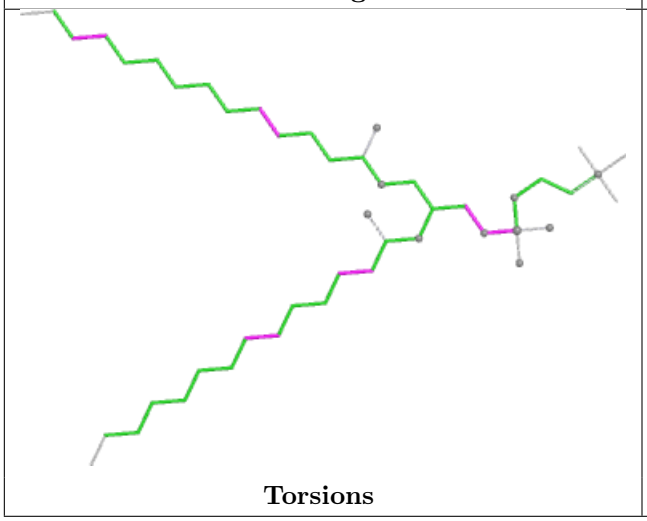
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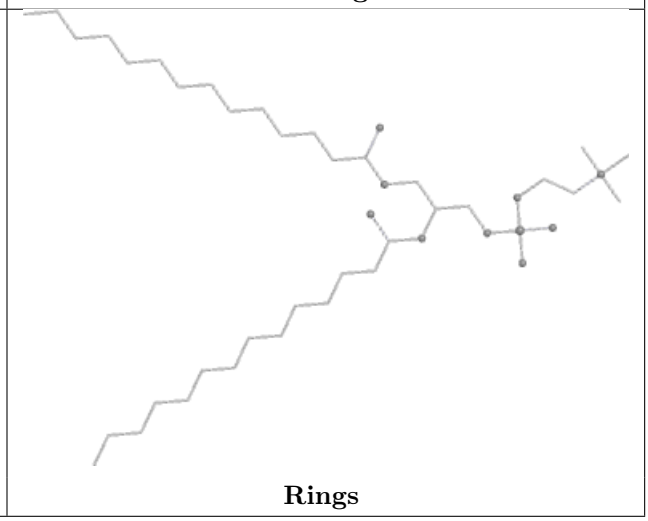
Bond lengths



Bond angles

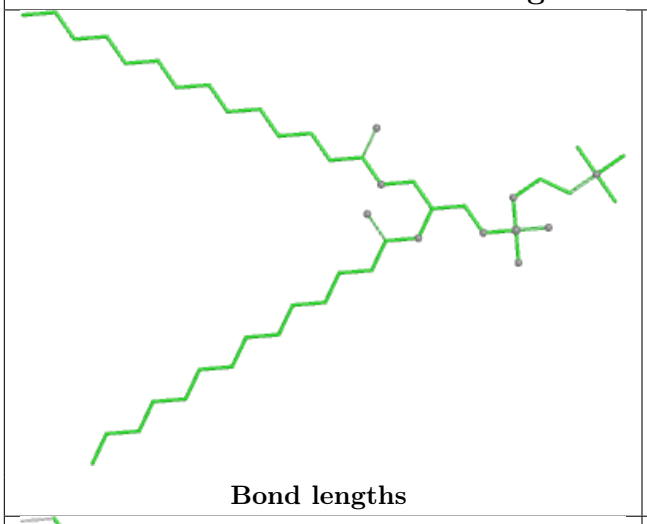


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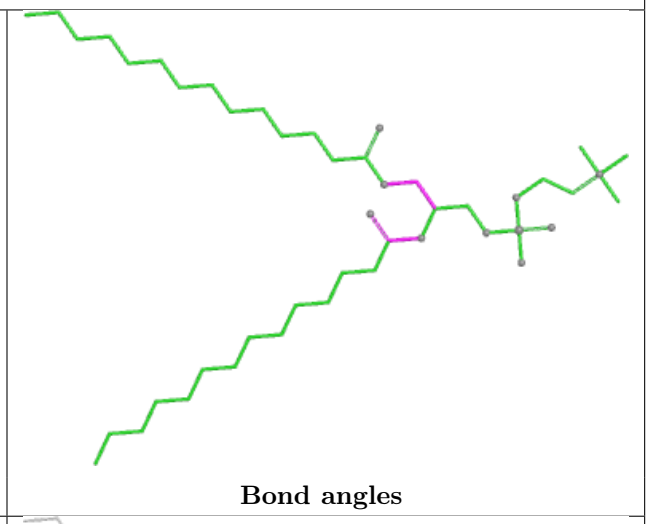


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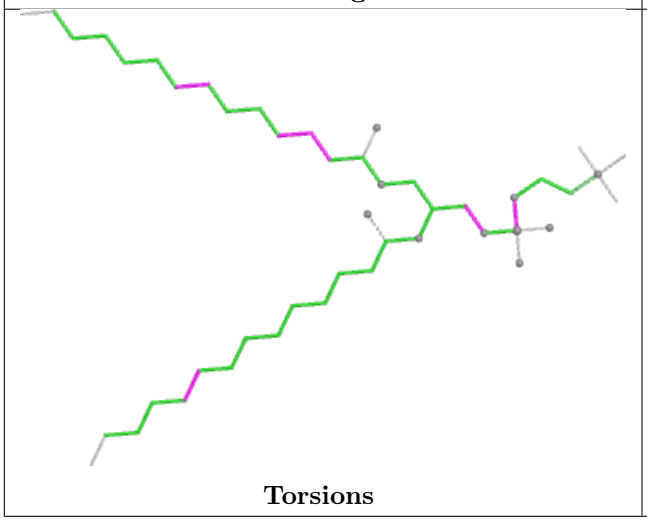
Ligand PX4 A 621



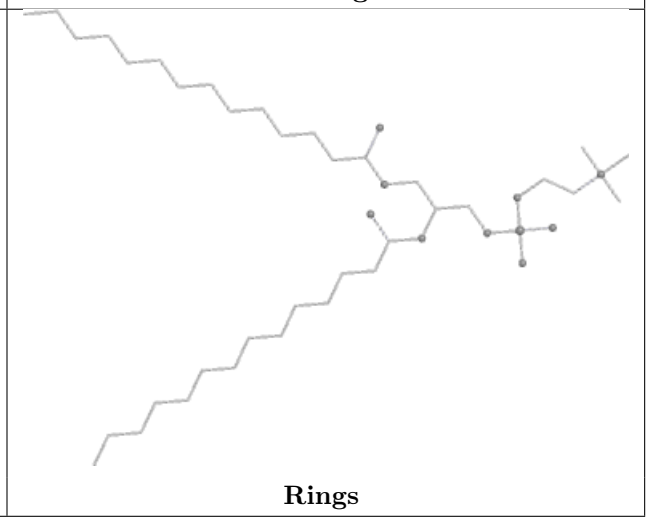
Bond lengths



Bond angles

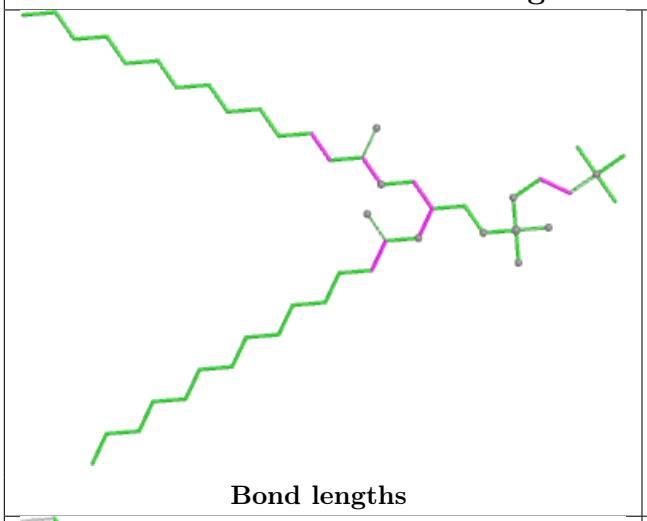


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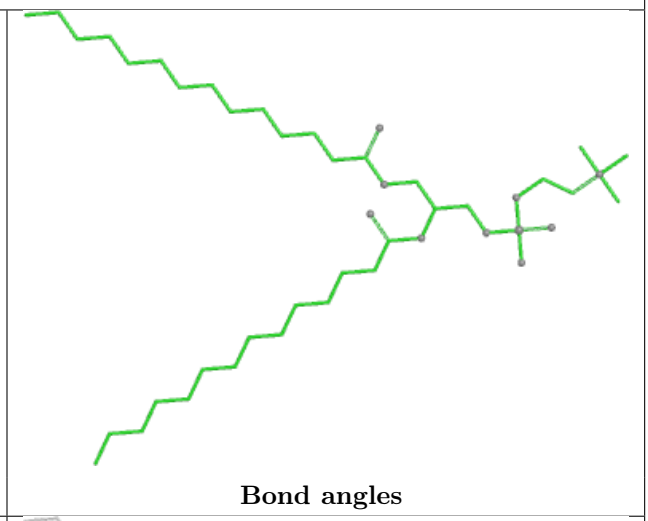


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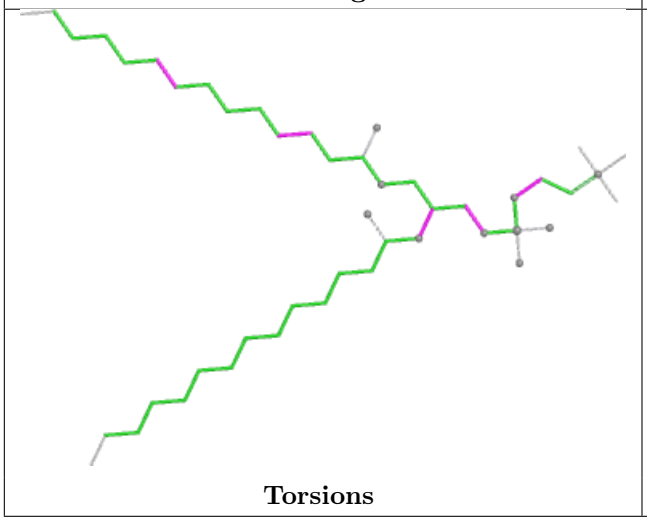
Ligand PX4 C 336



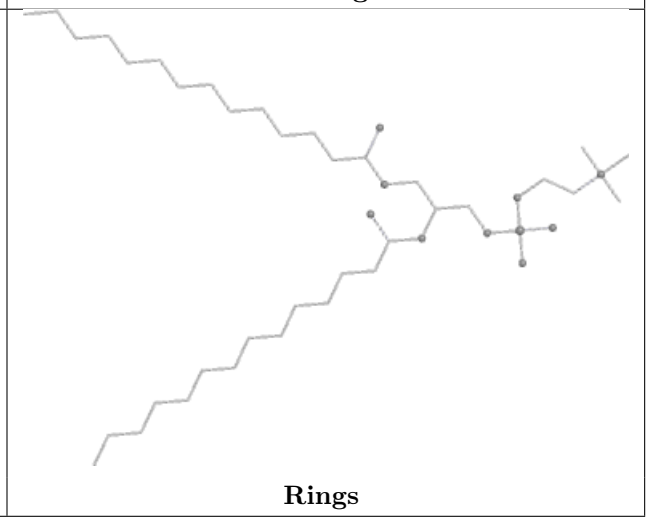
Bond lengths



Bond angles

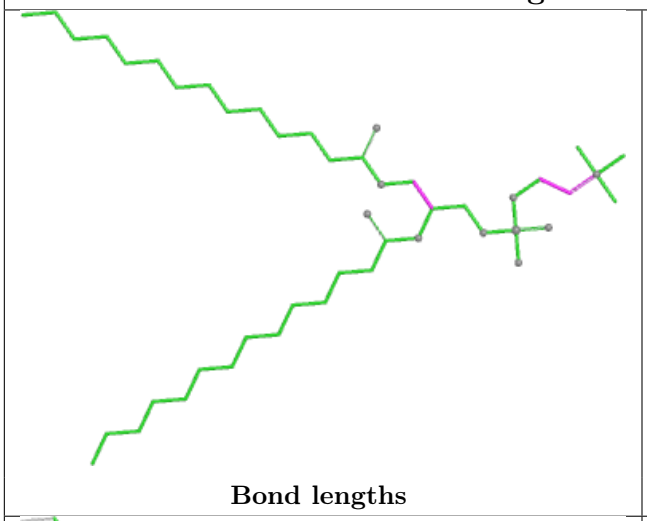


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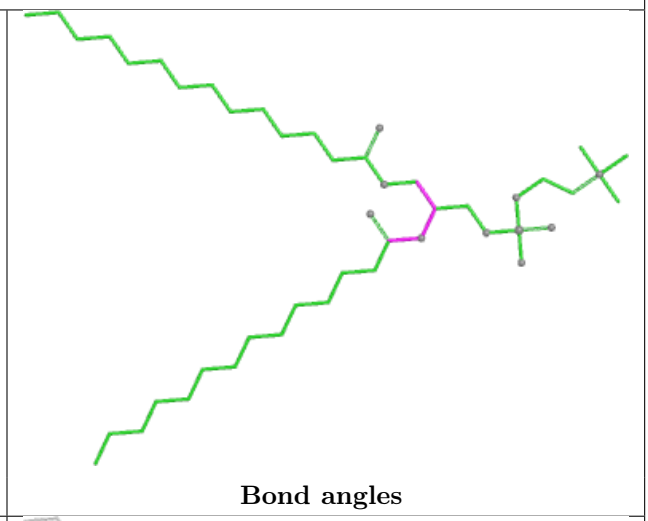


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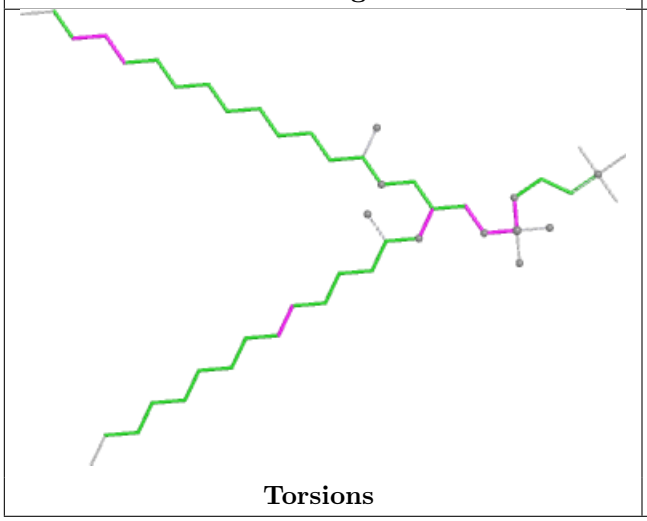
Ligand PX4 A 606



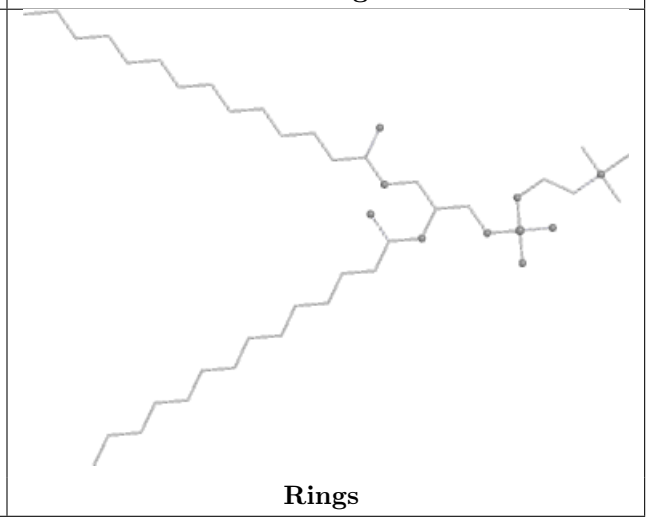
Bond lengths



Bond angles

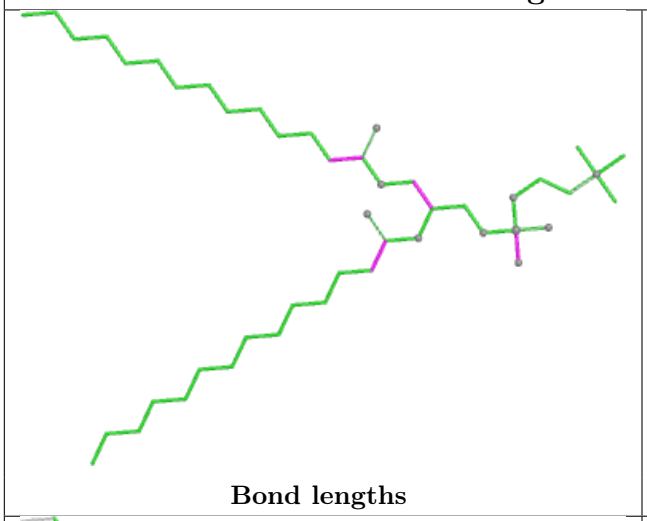


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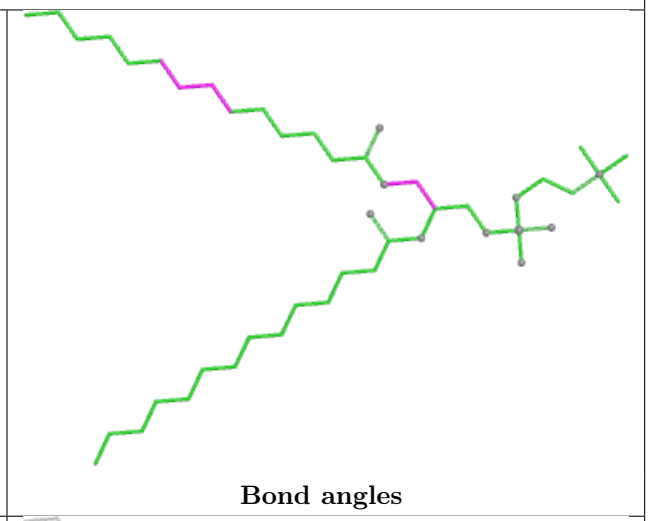


Rings

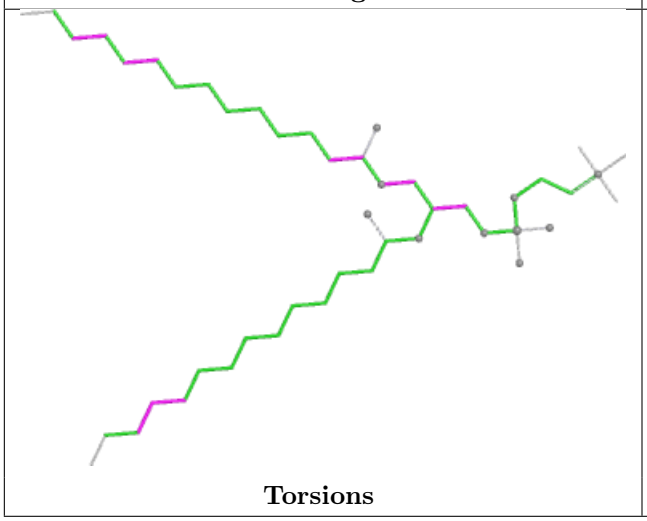
Ligand PX4 A 646



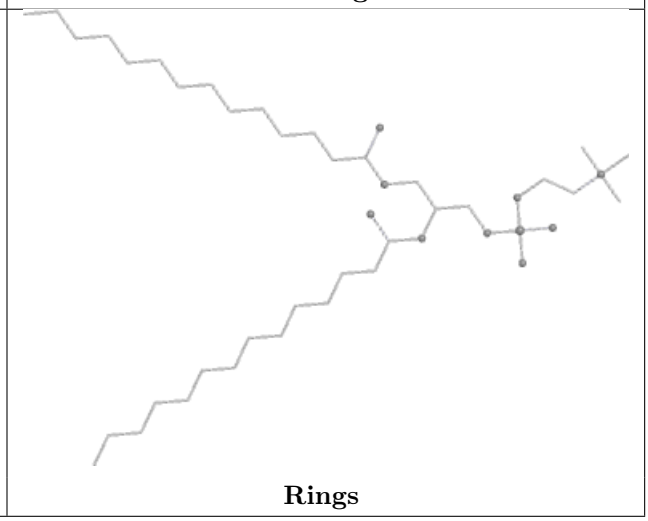
Bond lengths



Bond angles

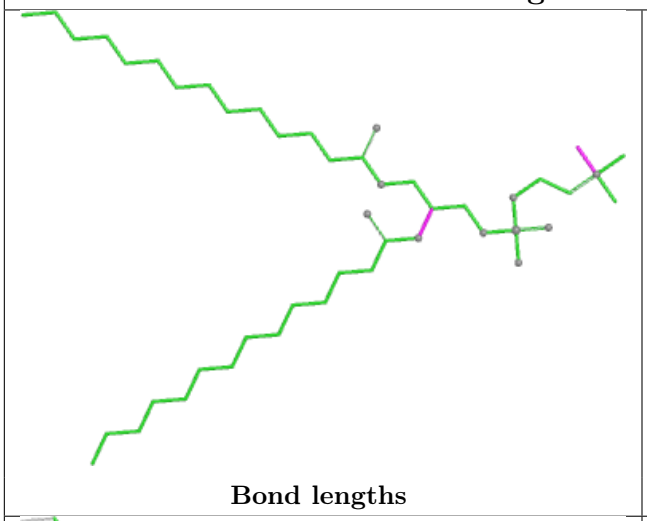


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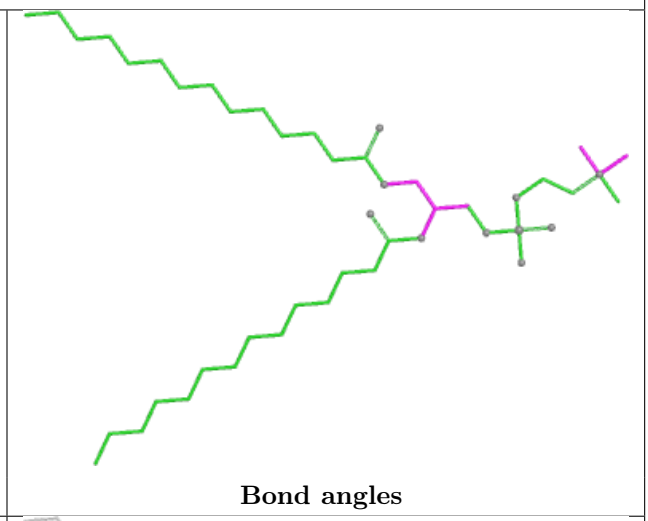


Rings

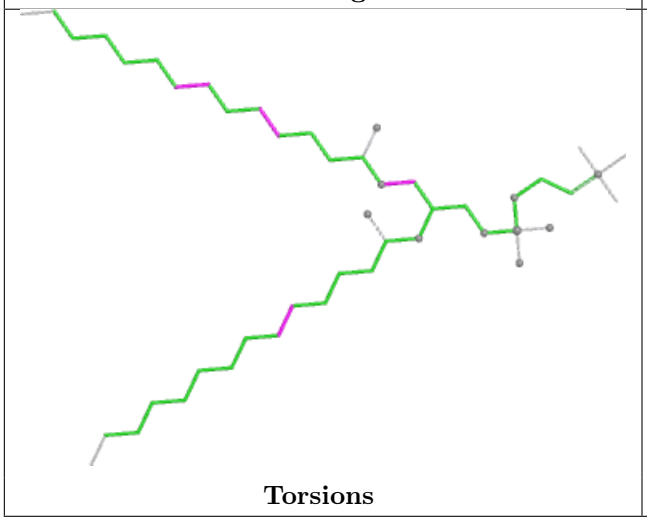
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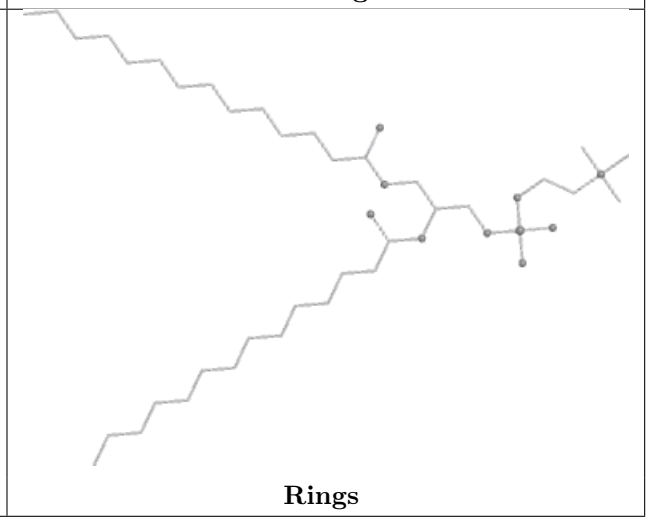
Bond lengths



Bond angles

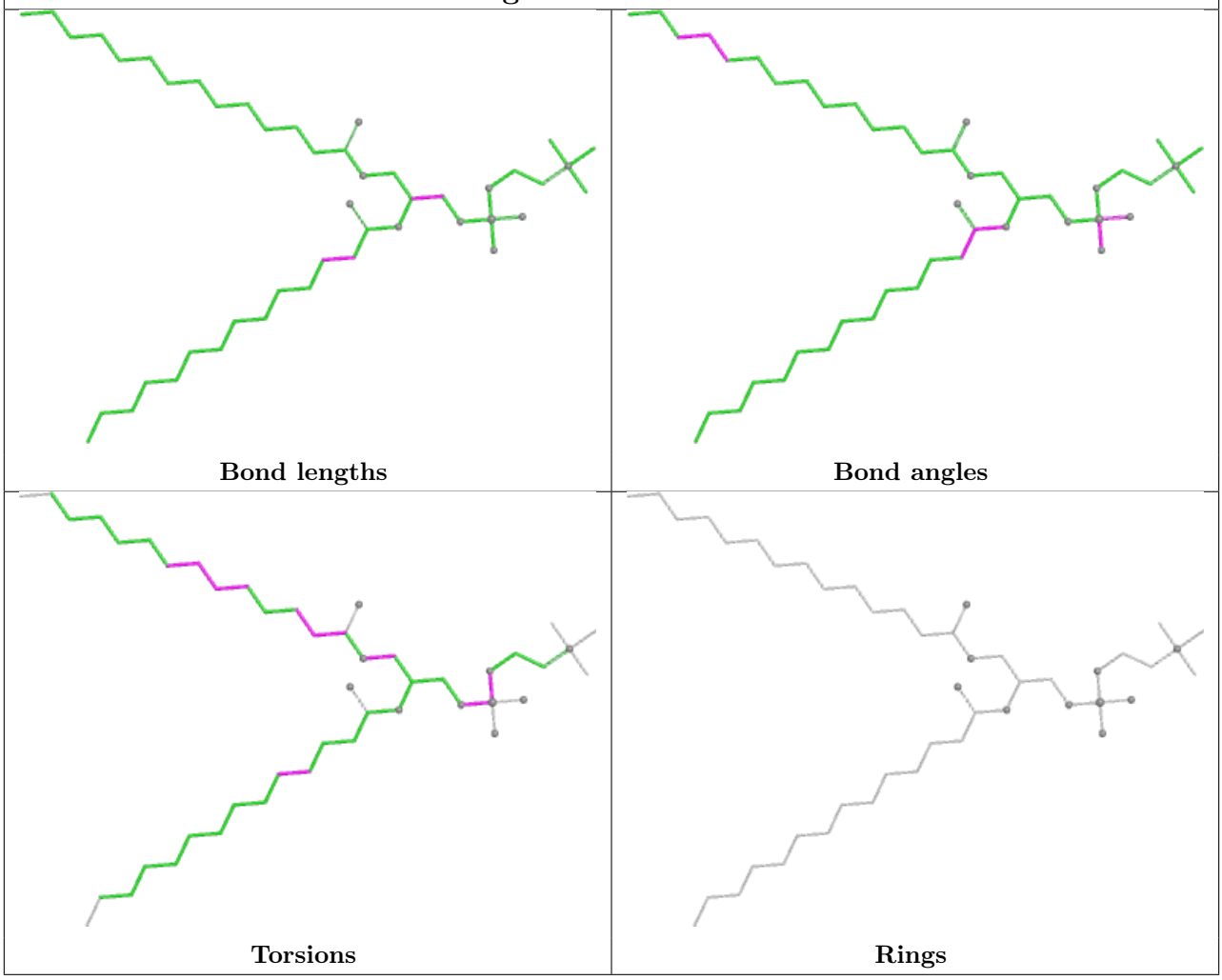


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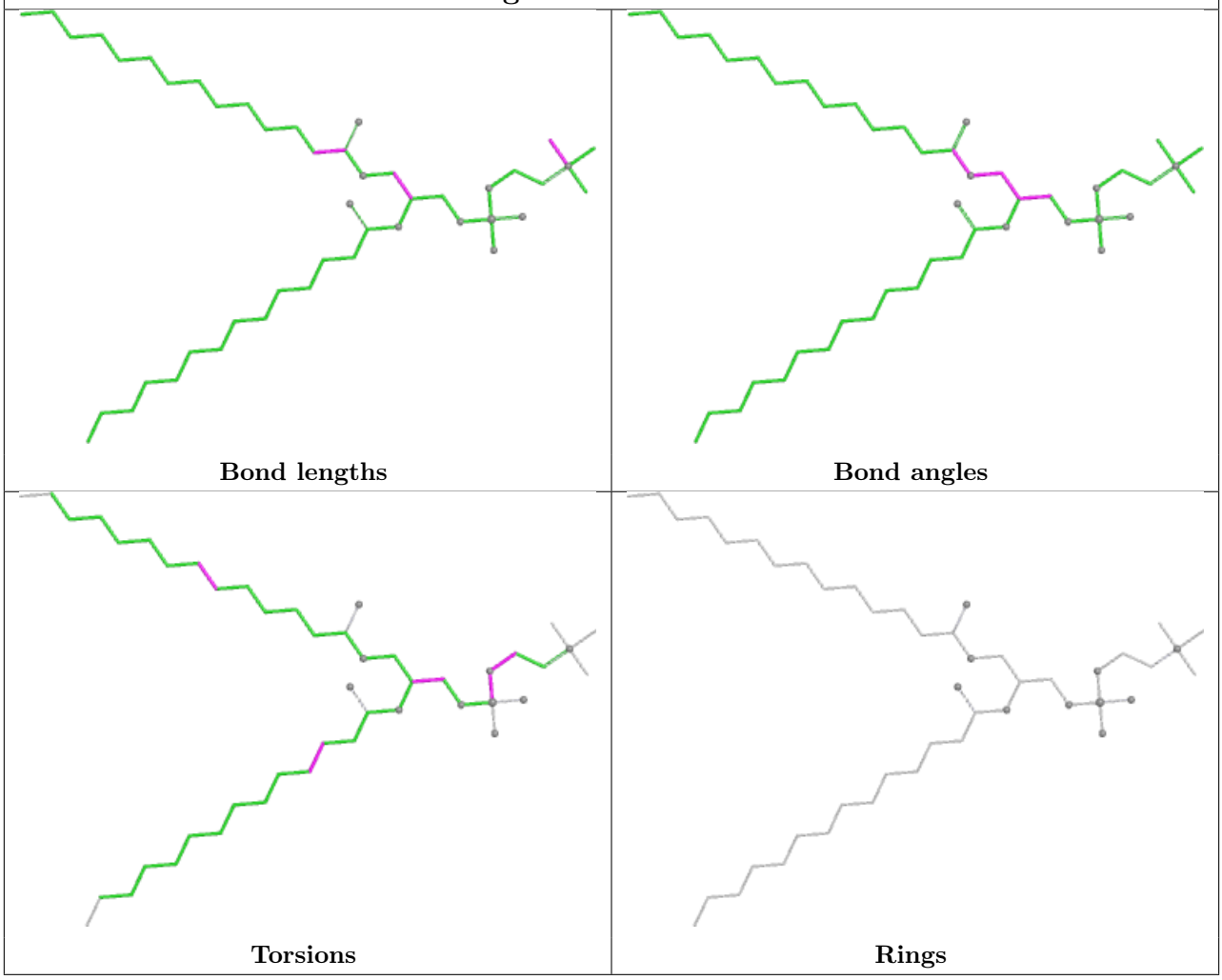


Rings

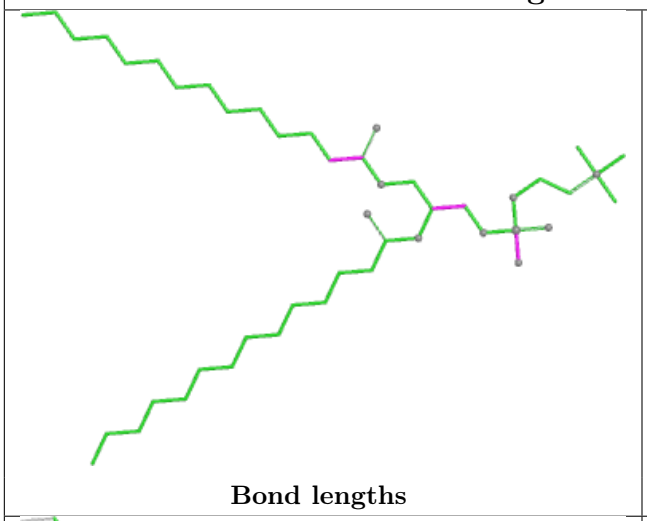
Ligand PX4 C 367



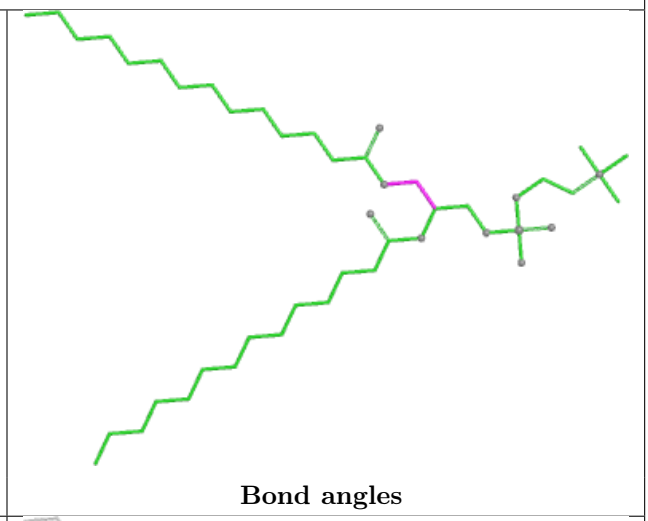
Ligand PX4 B 363



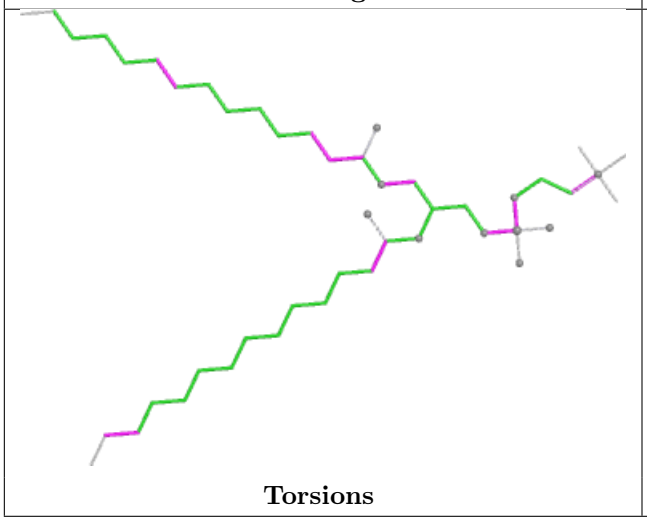
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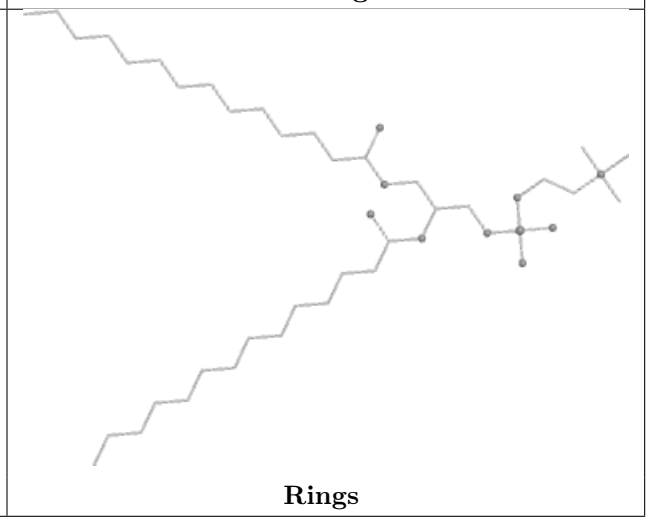
Bond lengths



Bond angles

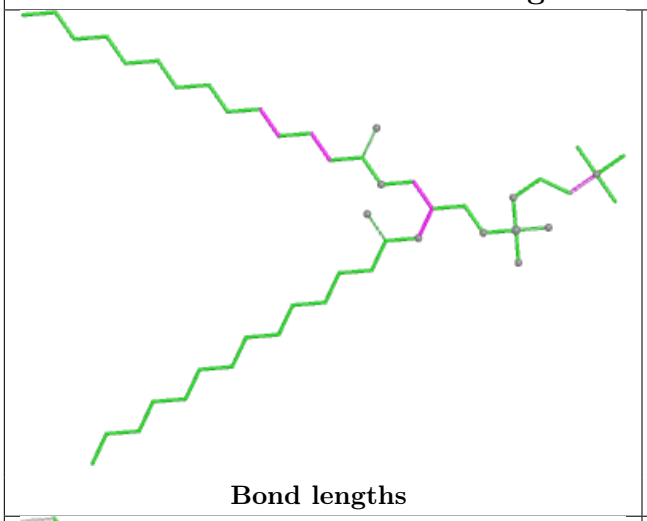


Torsions

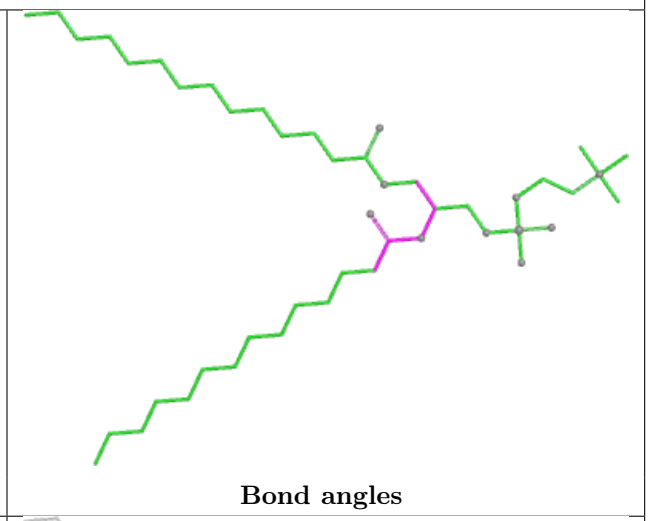


Rings

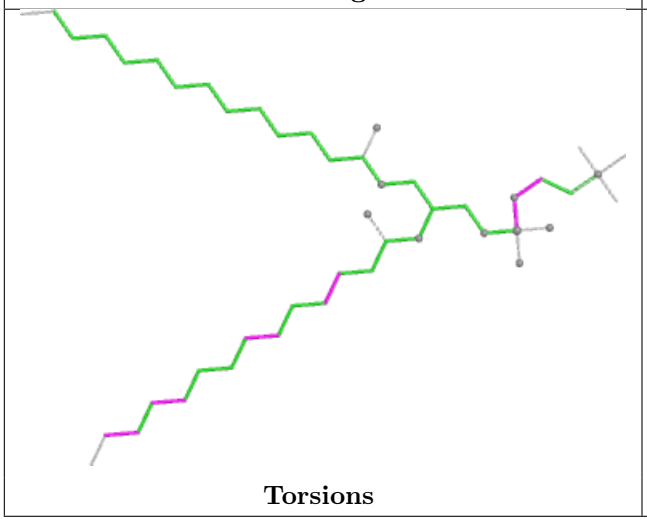
Ligand PX4 A 603



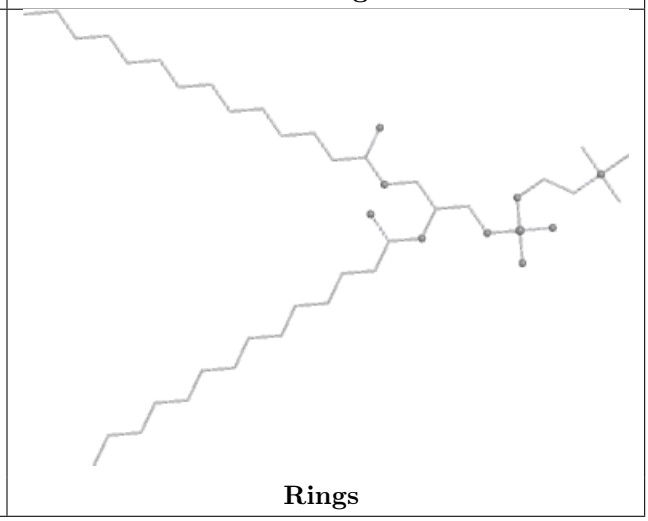
Bond lengths



Bond angles

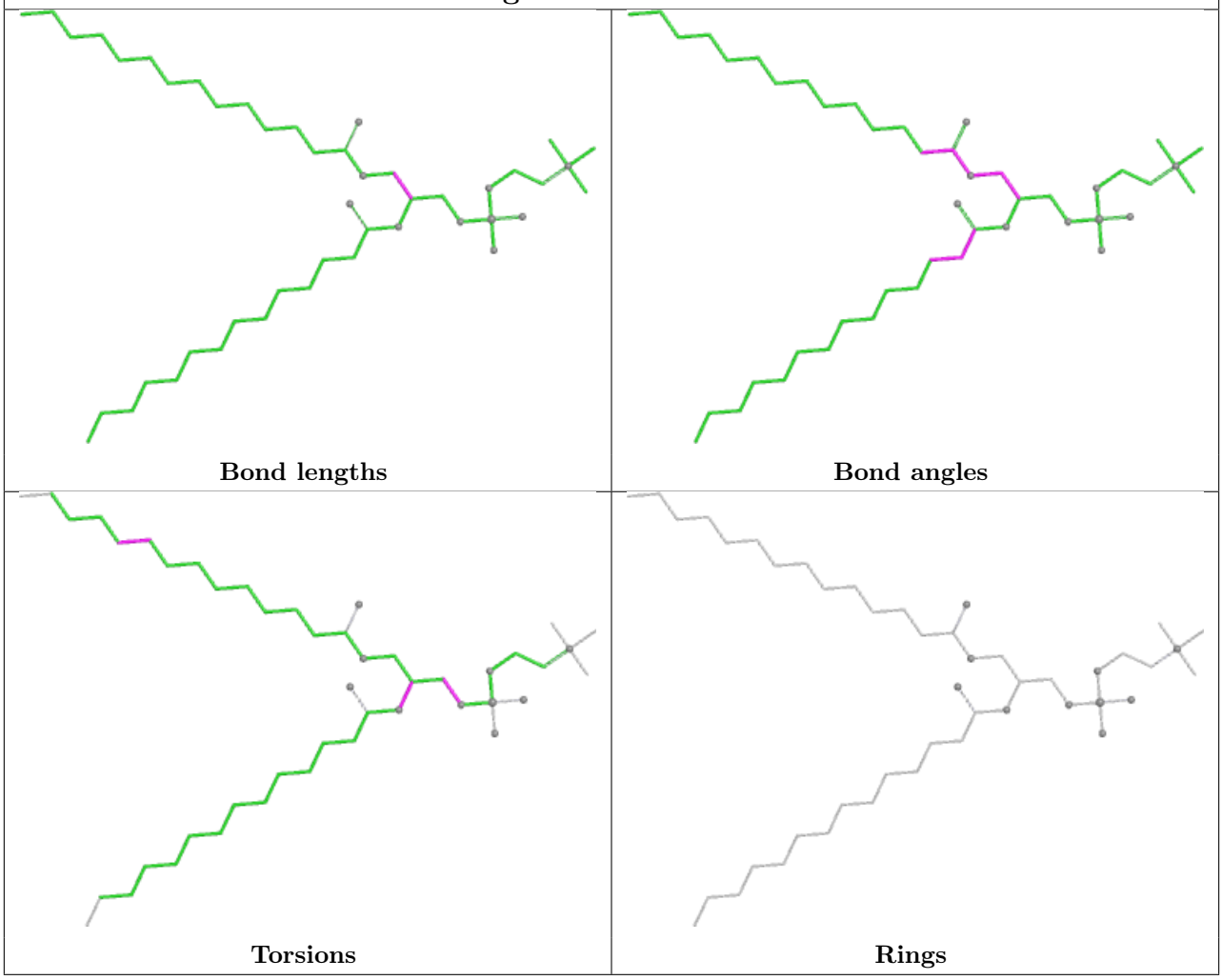


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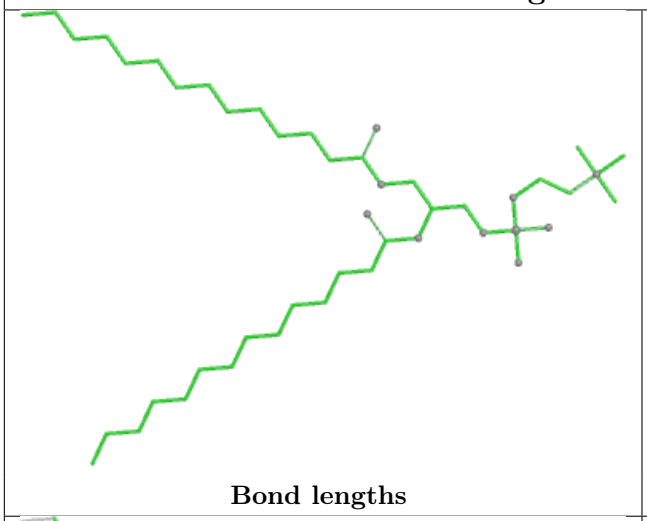


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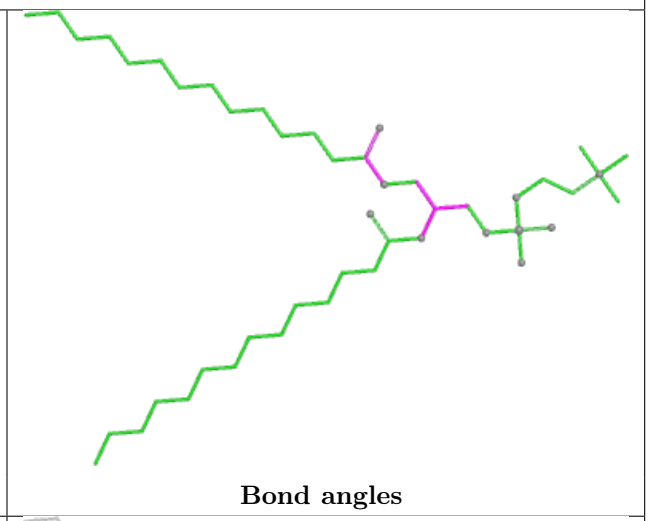
Ligand PX4 B 369



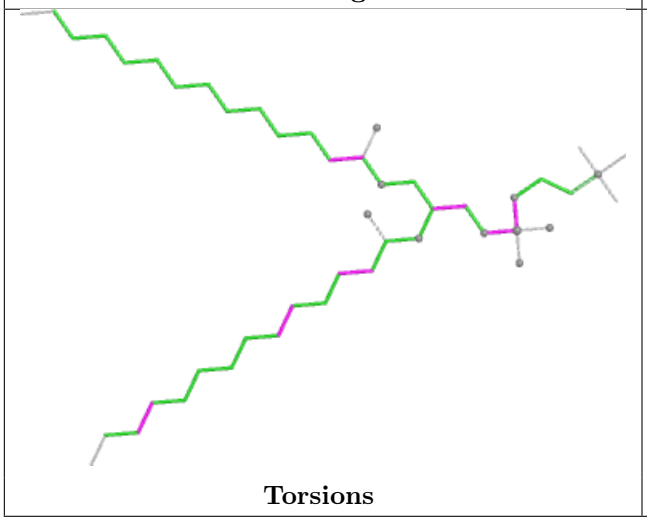
Ligand PX4 B 365



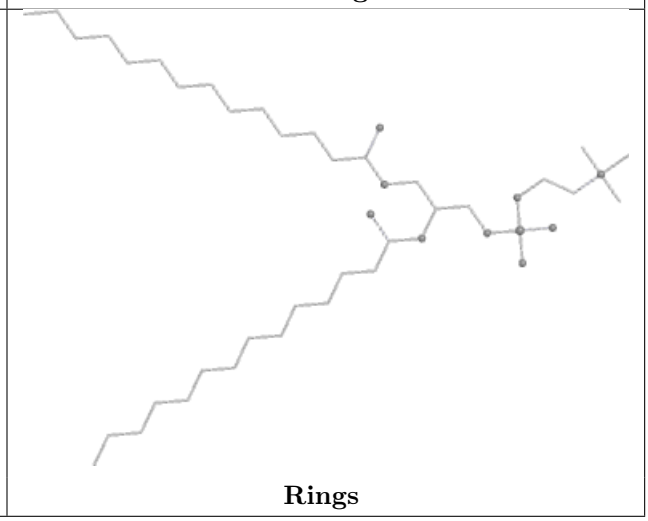
Bond lengths



Bond angles

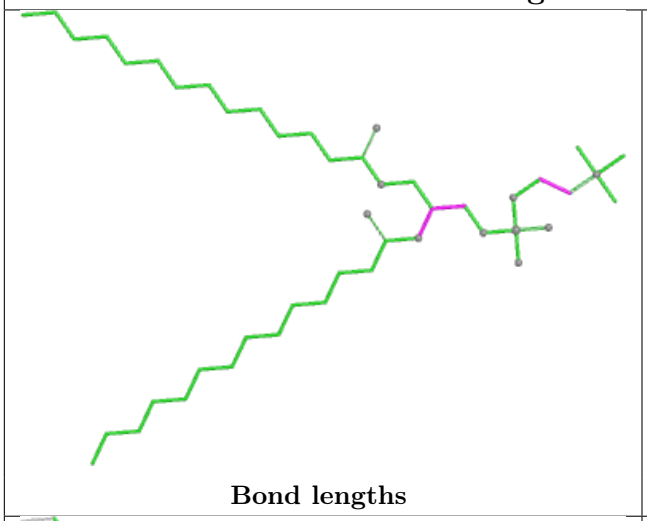


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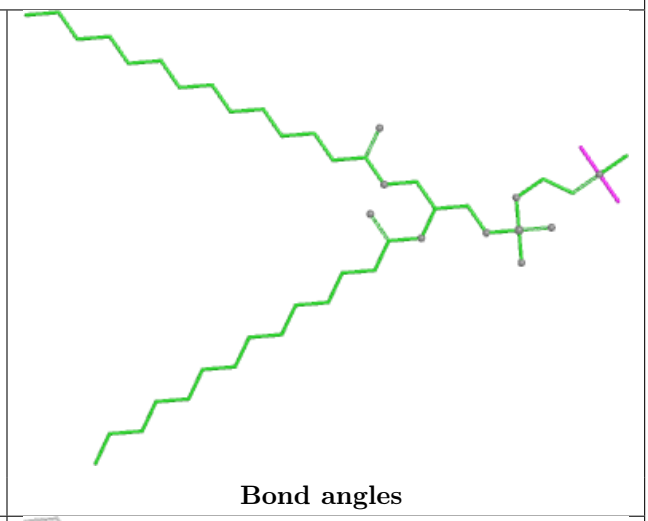


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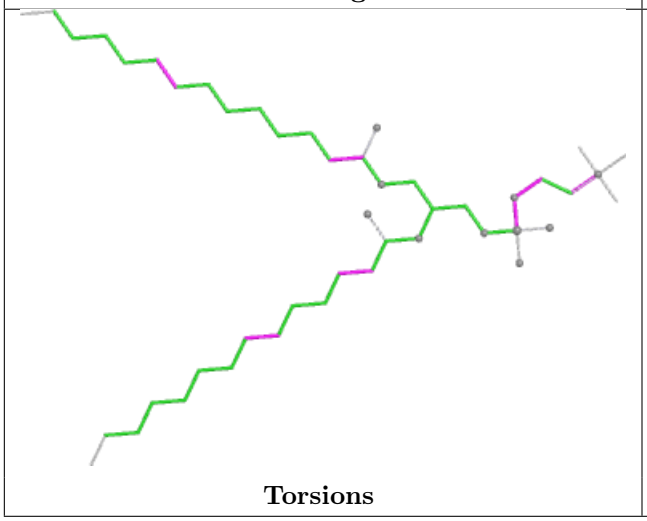
Ligand PX4 A 626



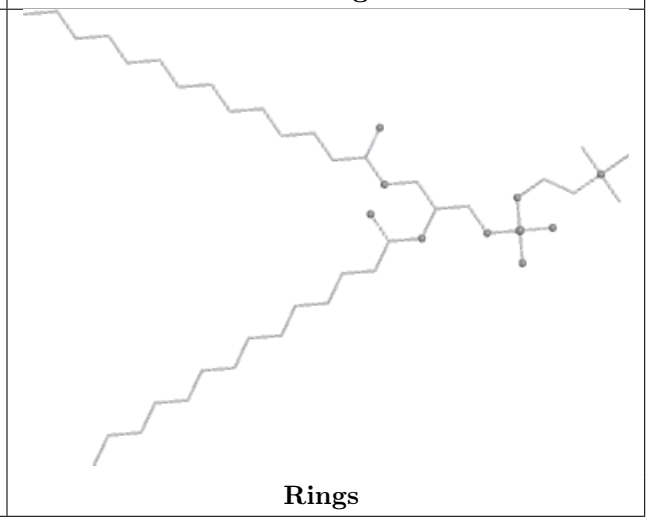
Bond lengths



Bond angles

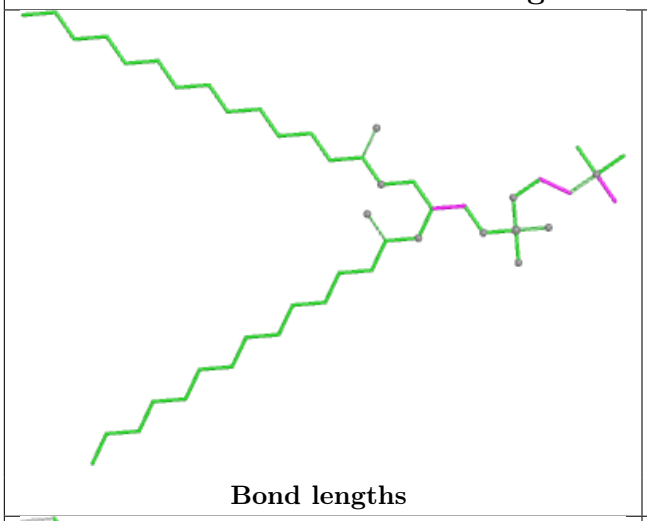


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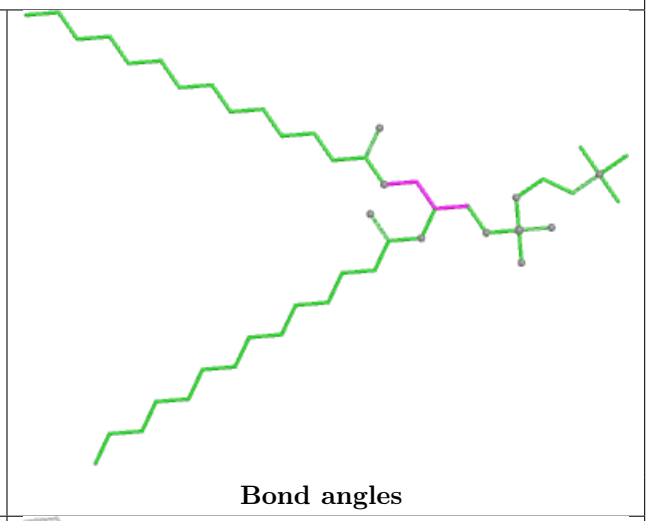


Rings

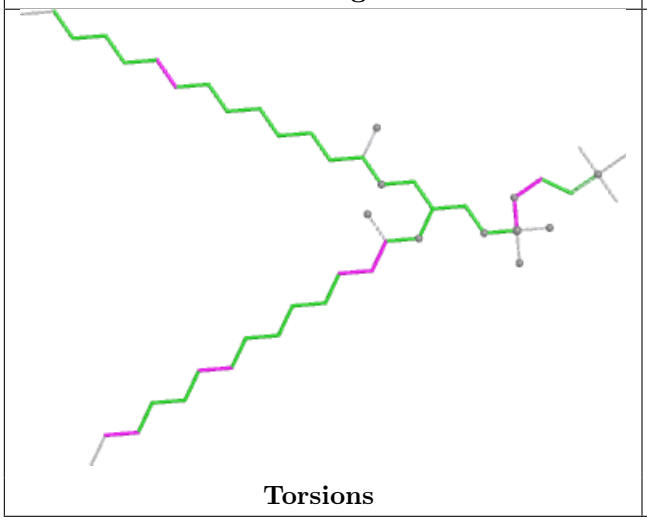
Ligand PX4 A 624



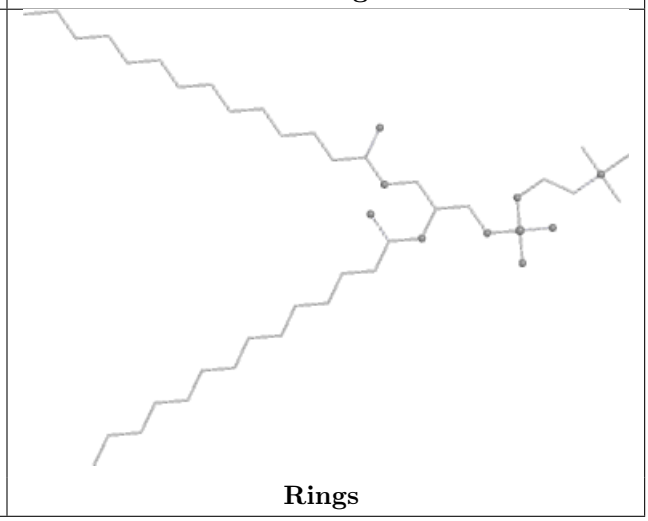
Bond lengths



Bond angles

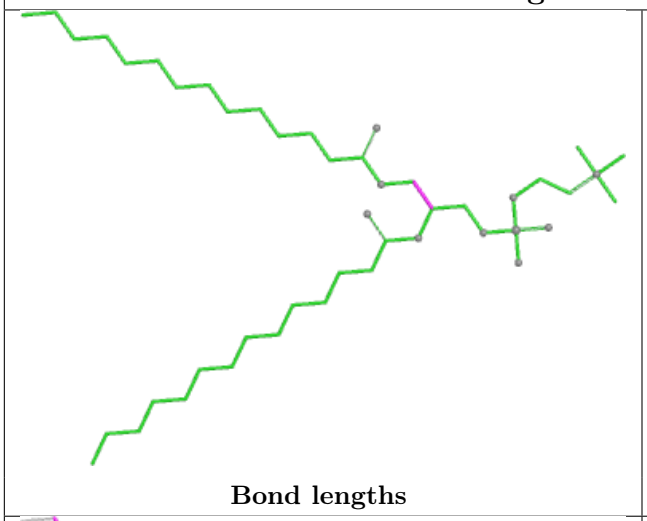


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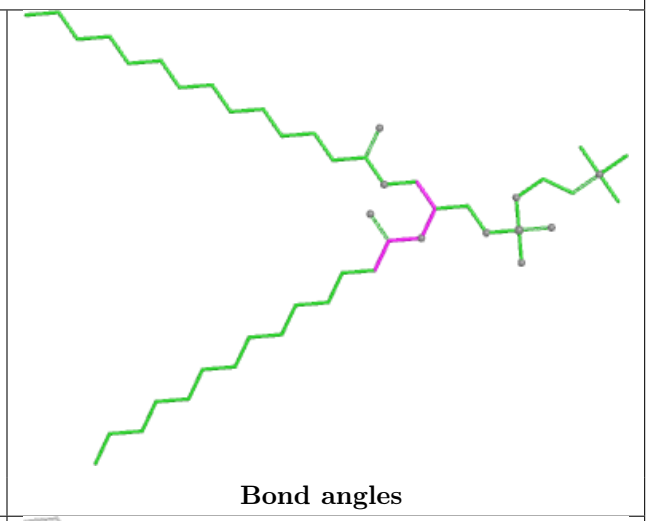


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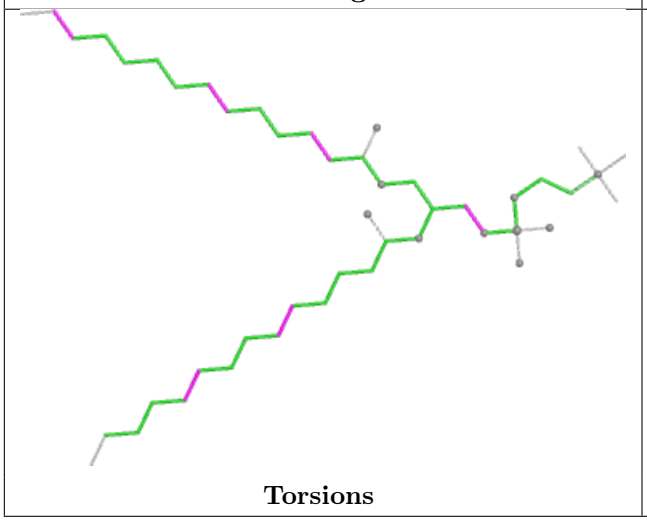
Ligand PX4 A 628



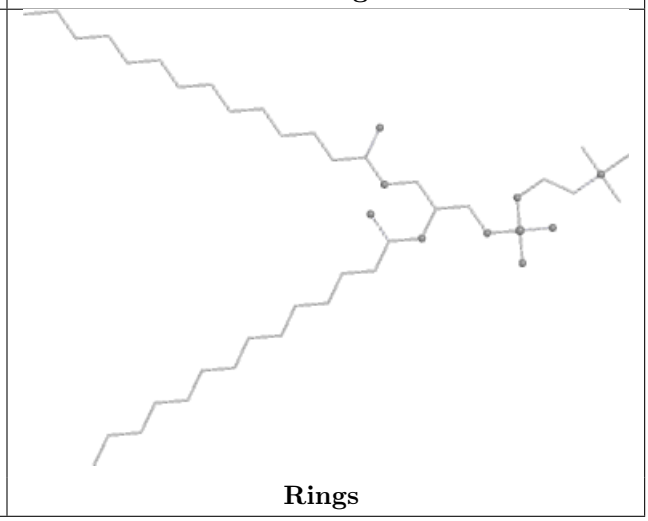
Bond lengths



Bond angles

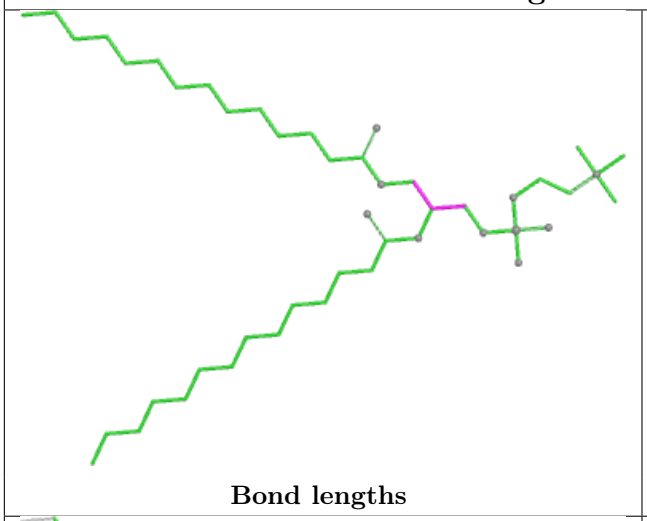


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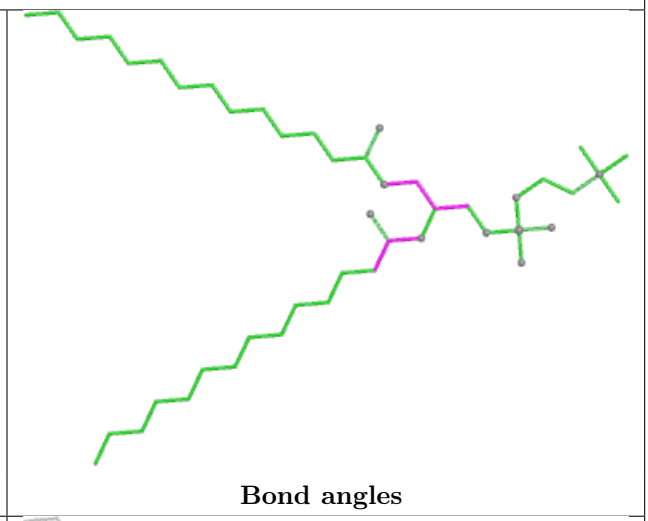


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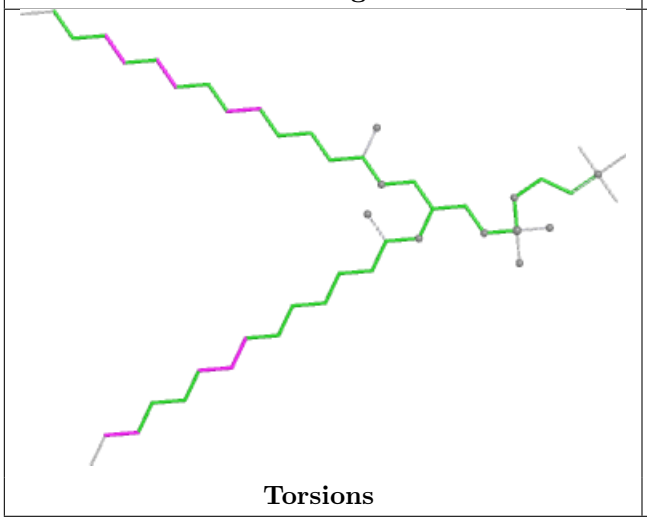
Ligand PX4 B 317



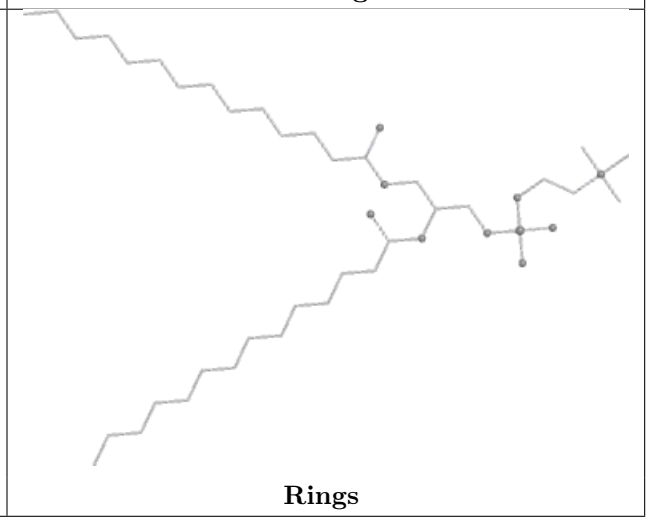
Bond lengths



Bond angles

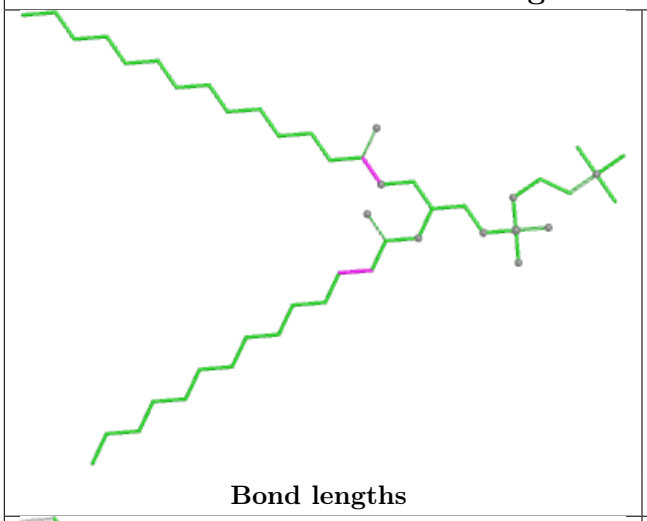


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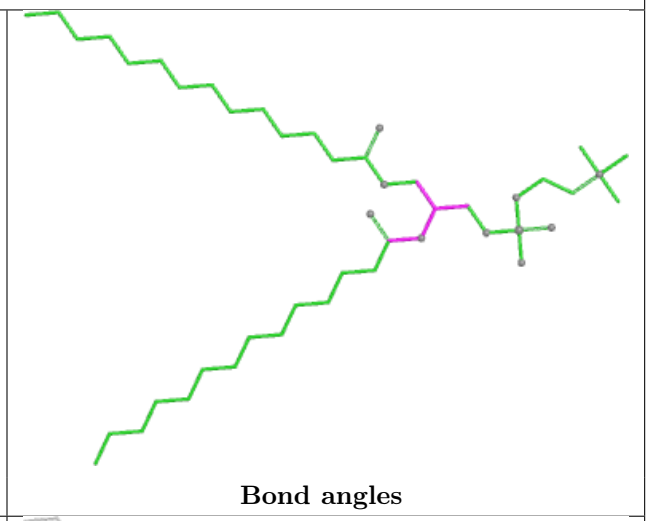


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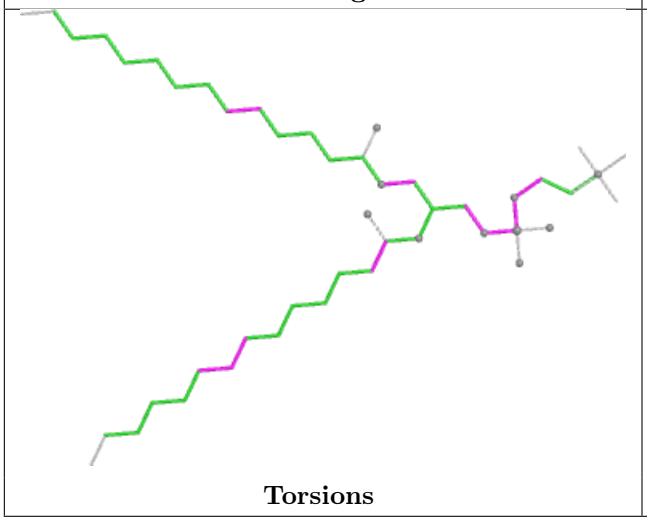
Ligand PX4 C 334



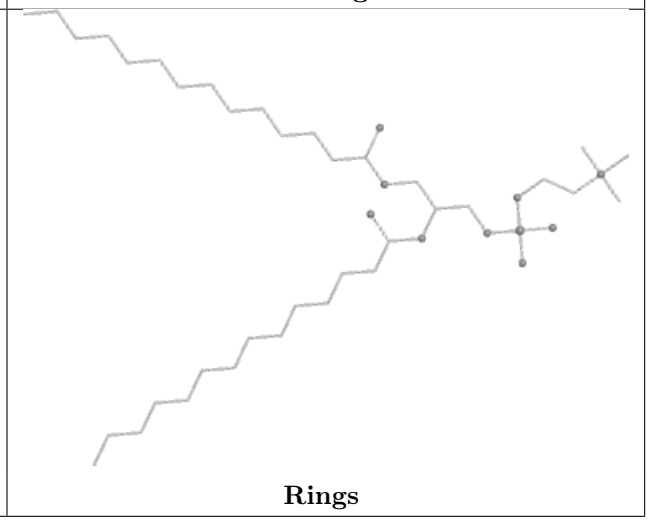
Bond lengths



Bond angles

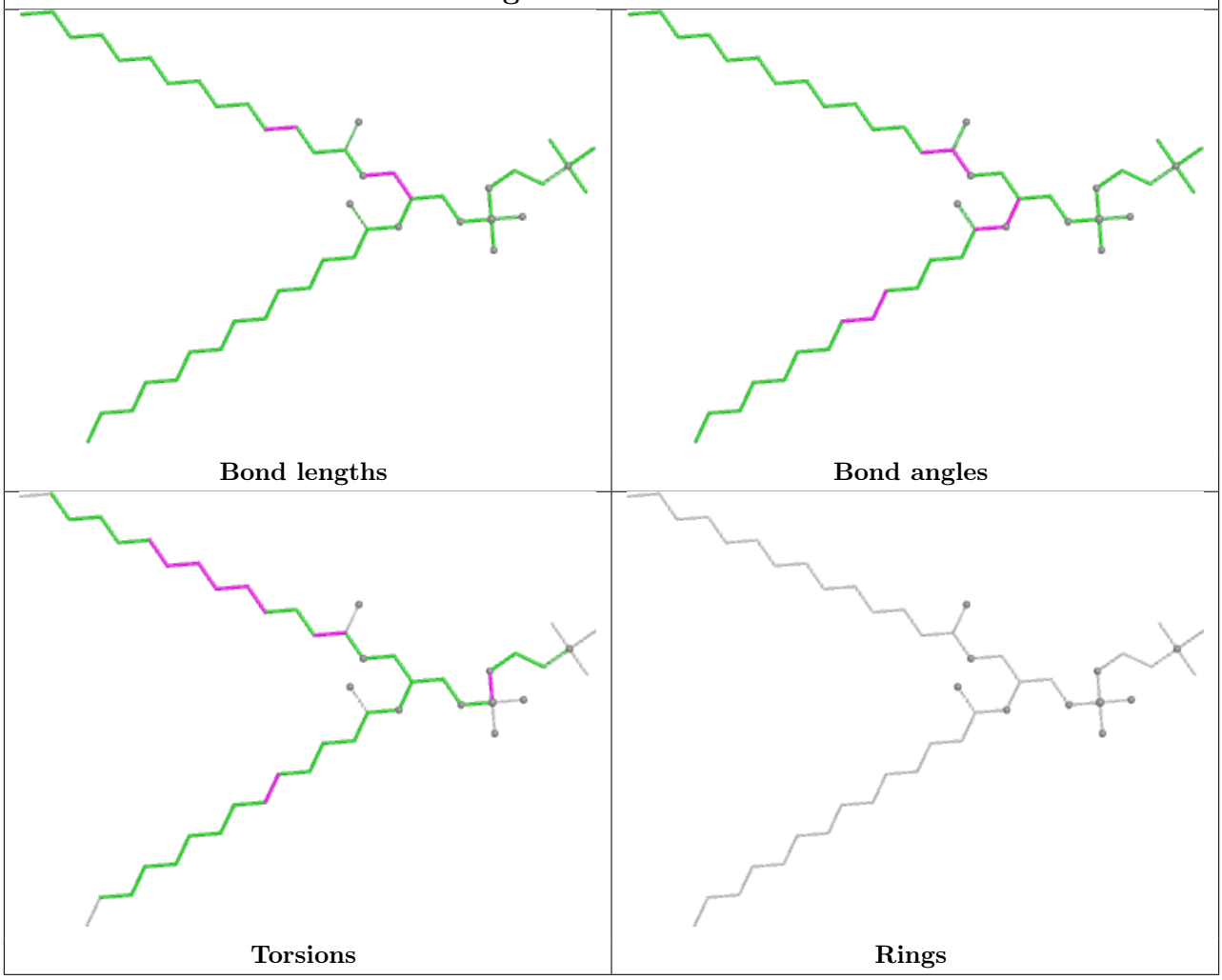


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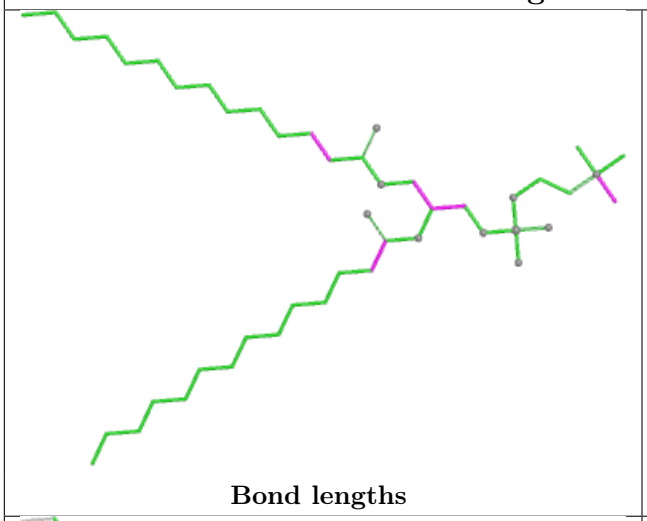


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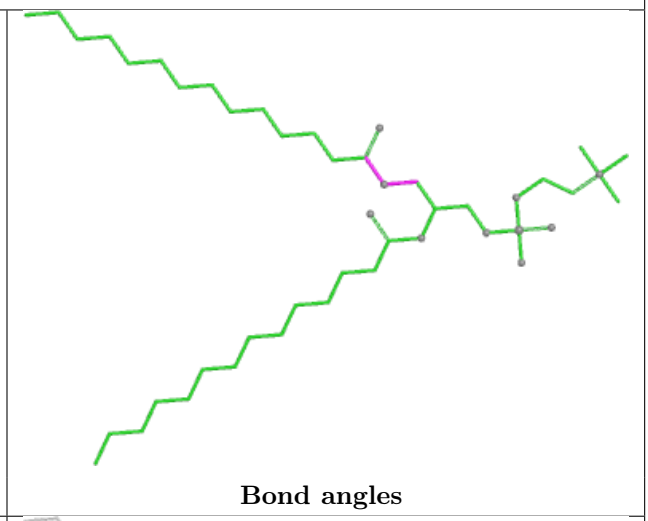
Ligand PX4 B 389



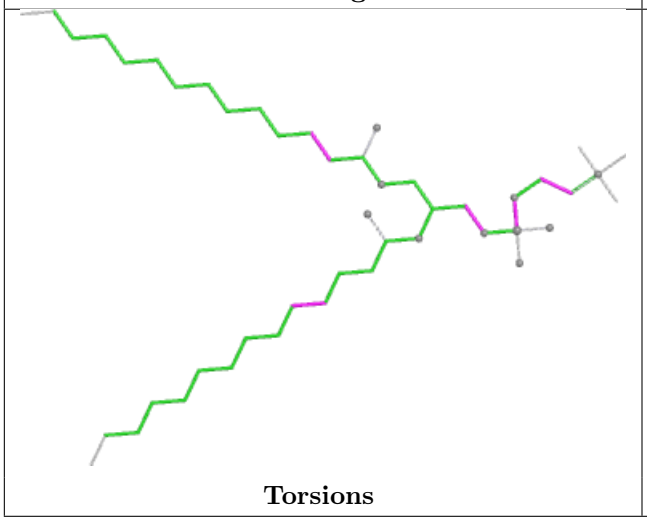
Ligand PX4 A 614



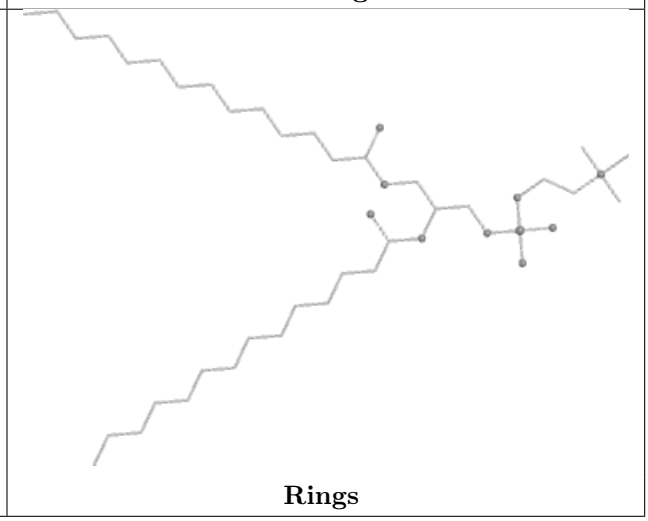
Bond lengths



Bond angles

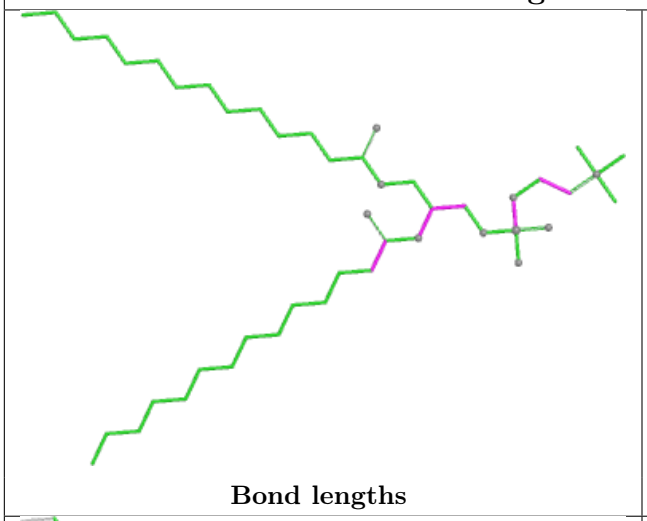


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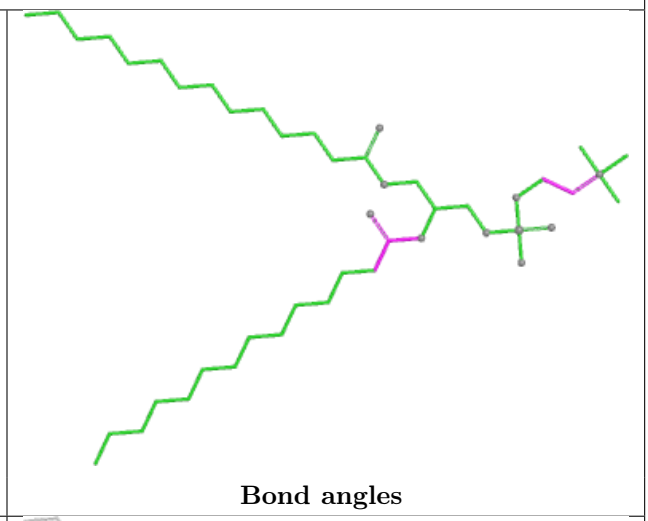


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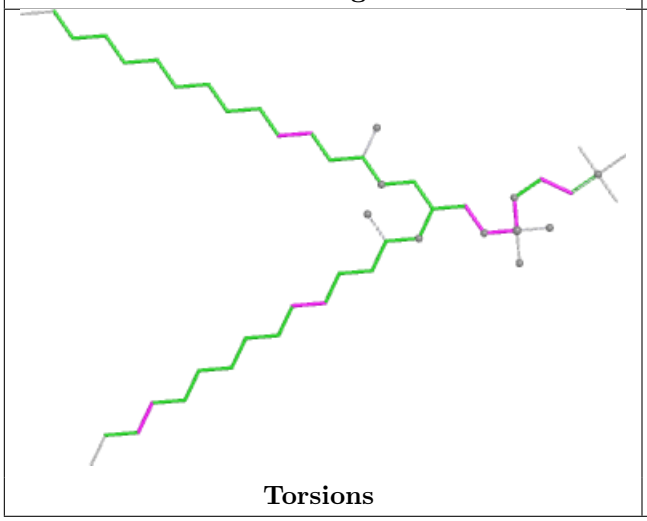
Ligand PX4 C 347



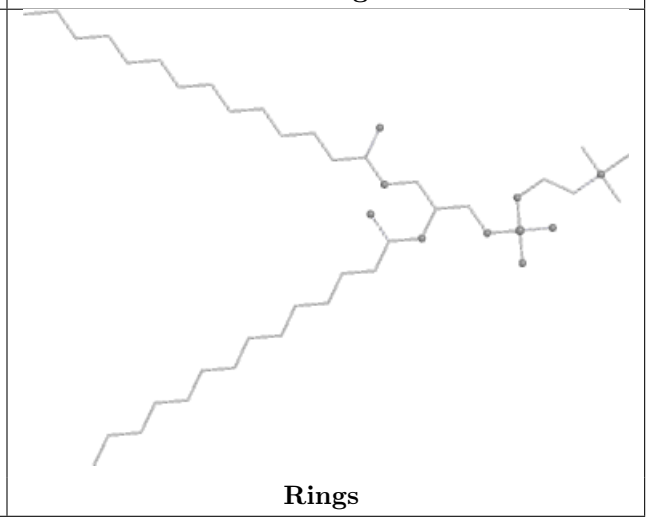
Bond lengths



Bond angles

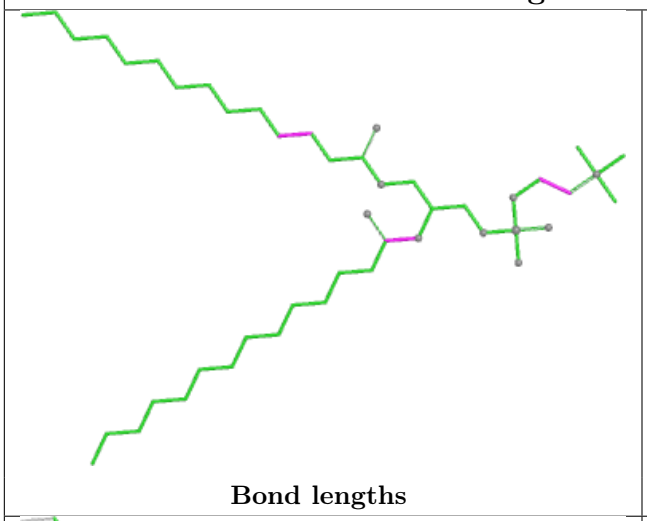


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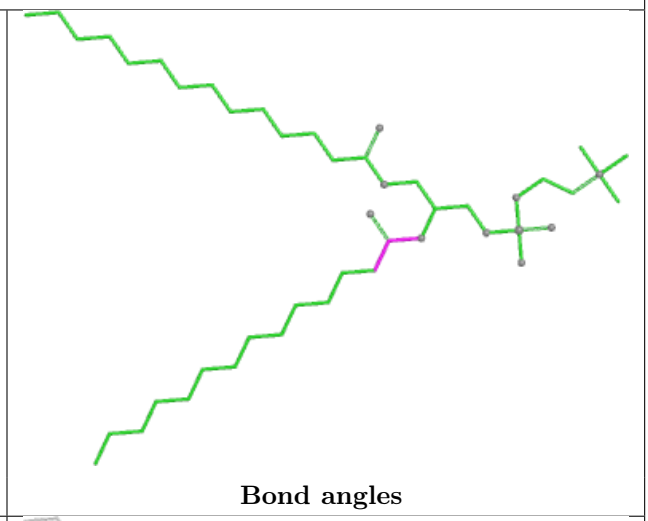


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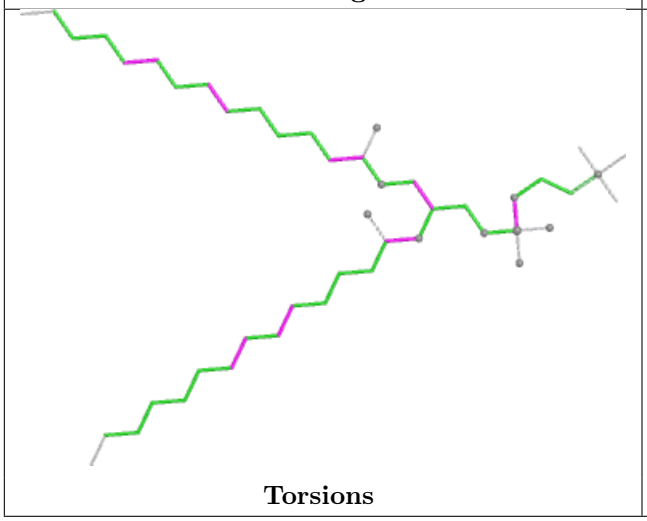
Ligand PX4 C 327



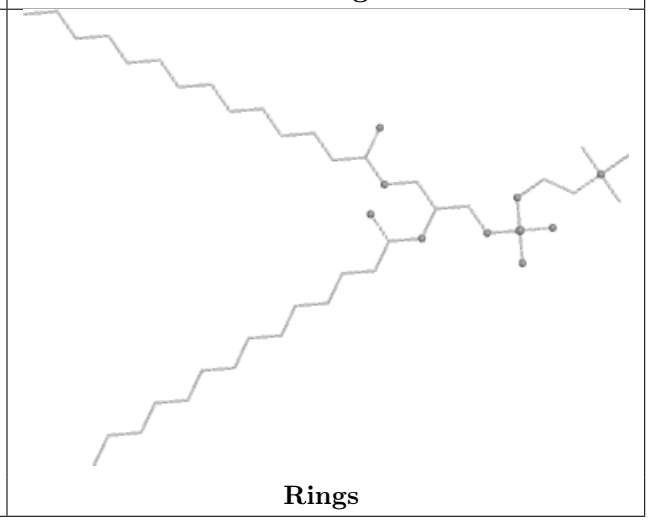
Bond lengths



Bond angles

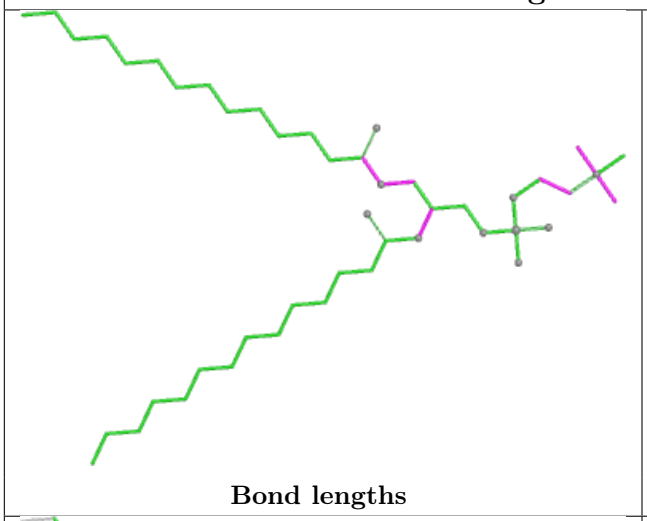


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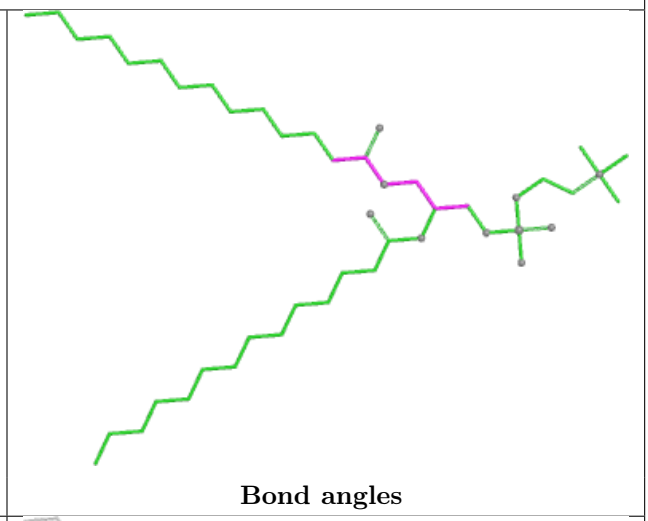


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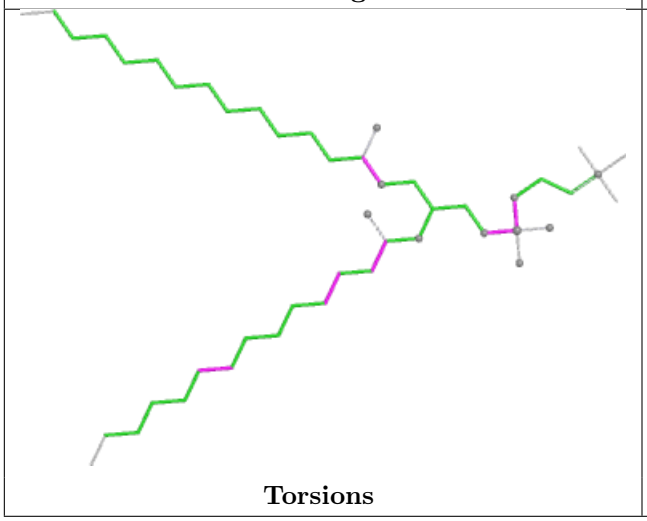
Ligand PX4 B 380



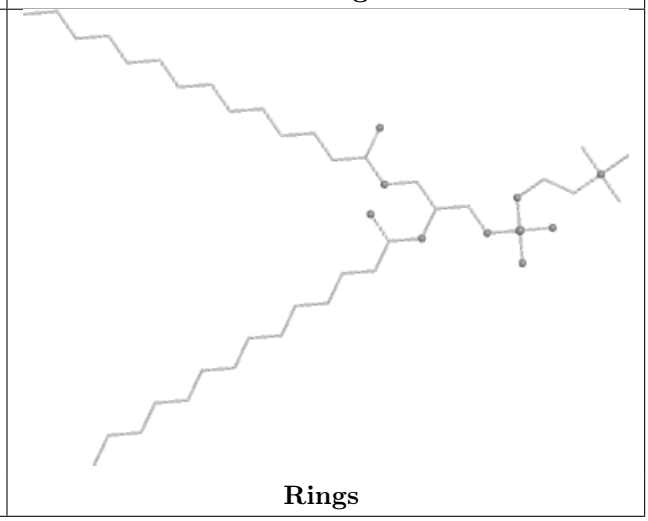
Bond lengths



Bond angles

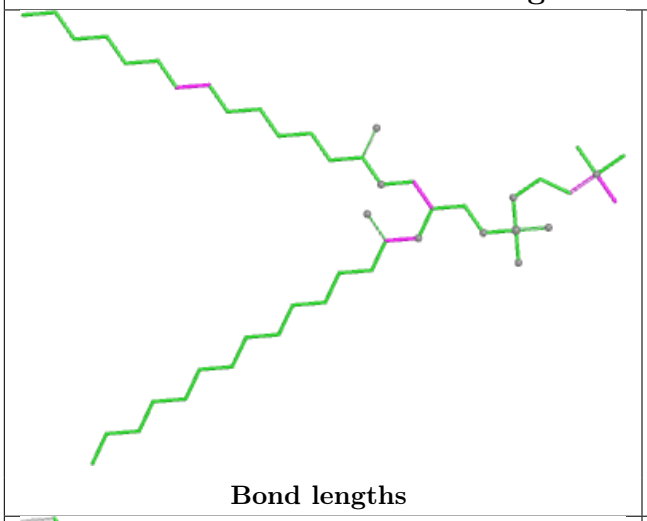


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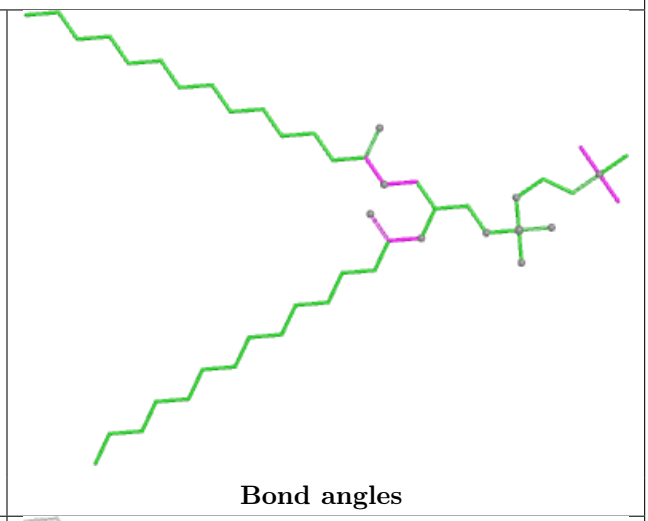


Rings

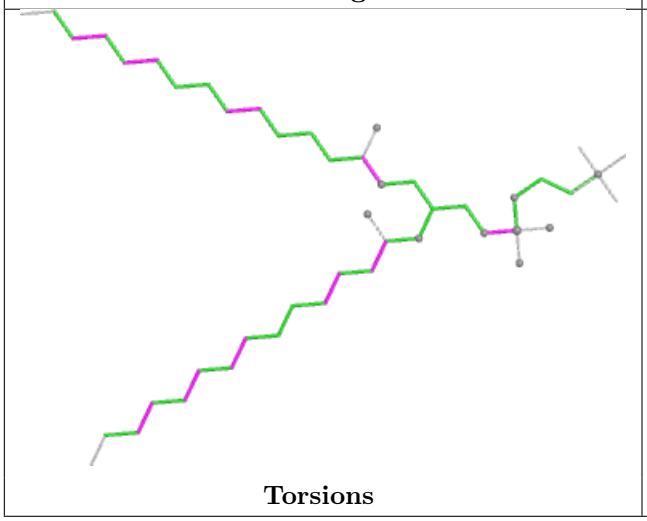
Ligand PX4 C 322



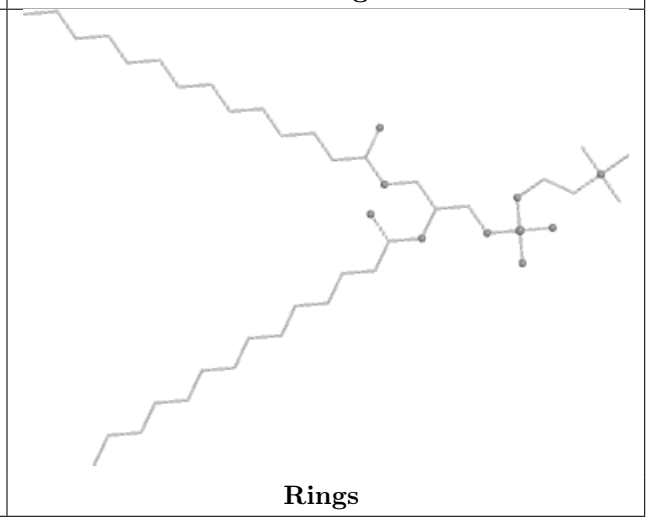
Bond lengths



Bond angles

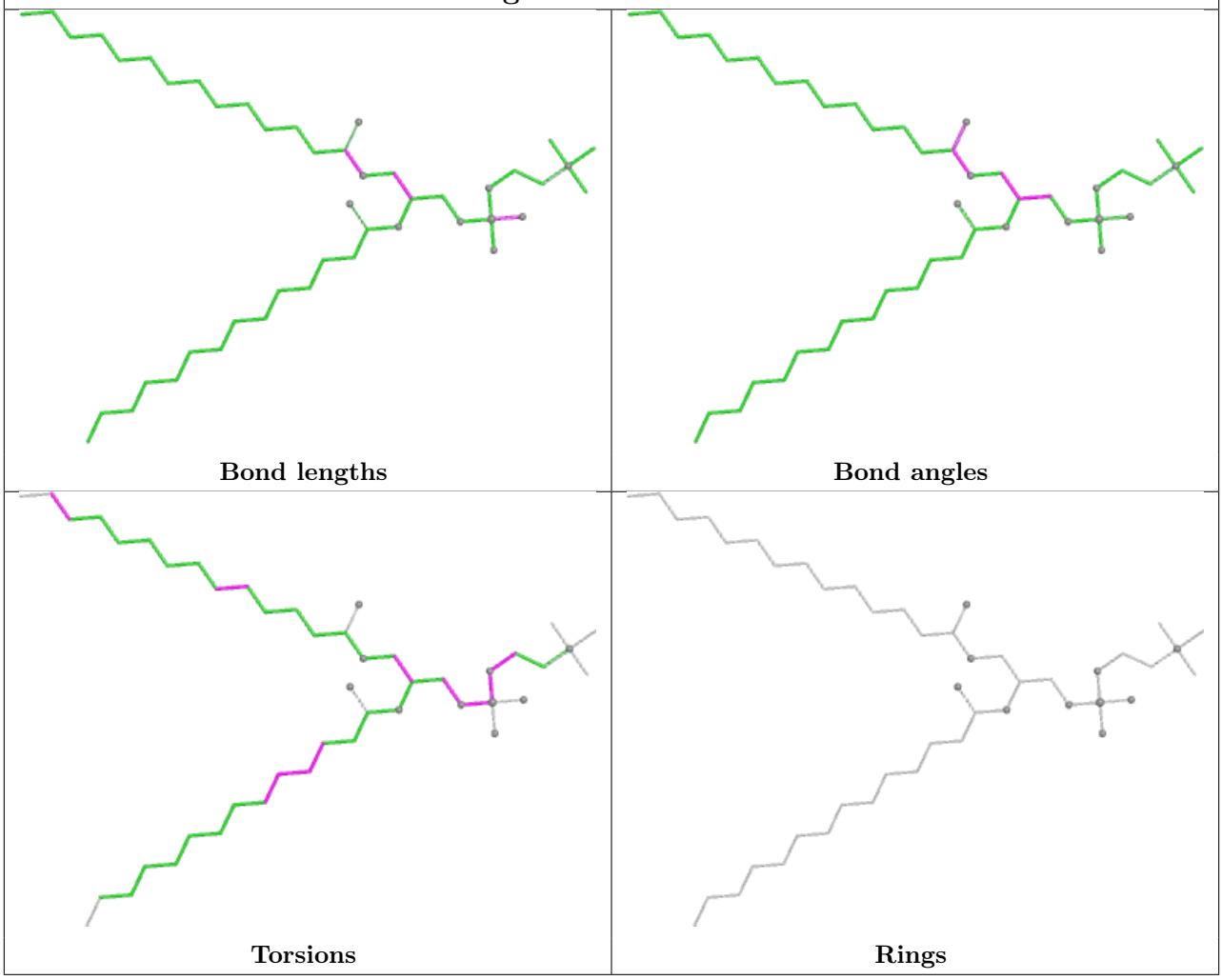


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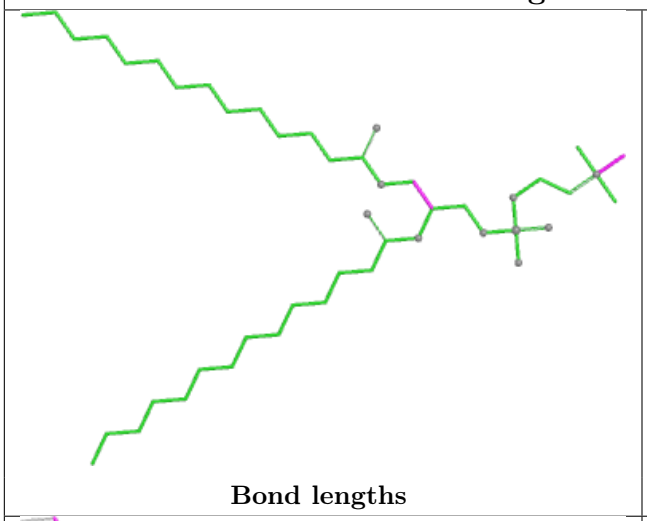


Rings

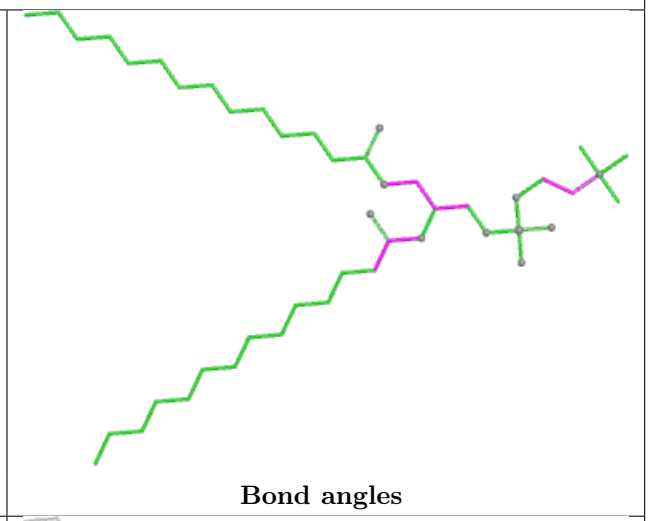
Ligand PX4 B 331



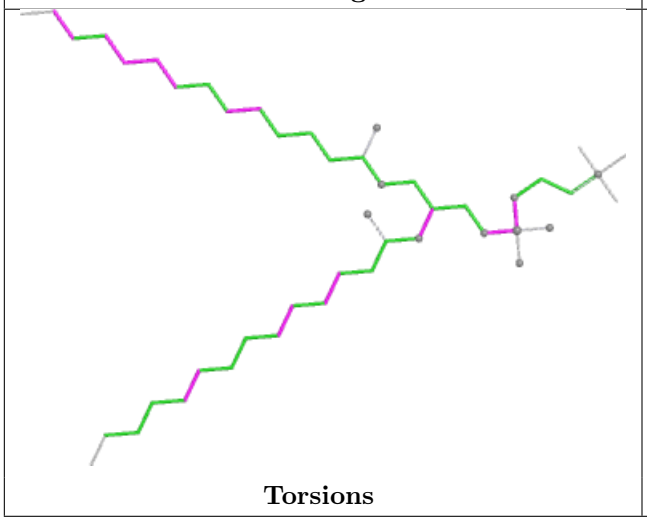
Ligand PX4 B 325



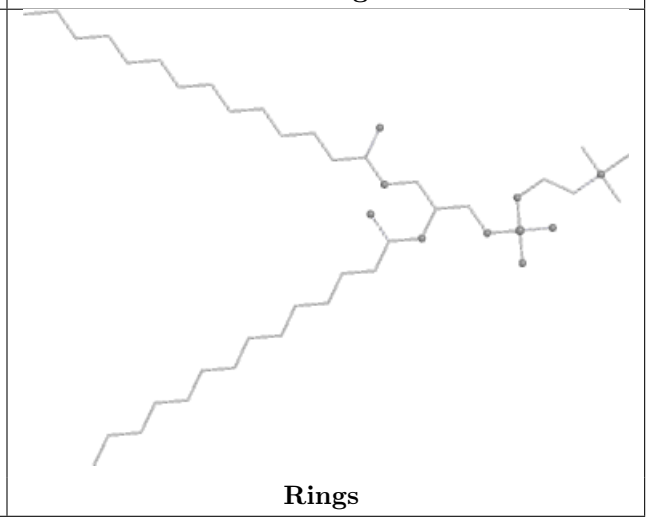
Bond lengths



Bond angles

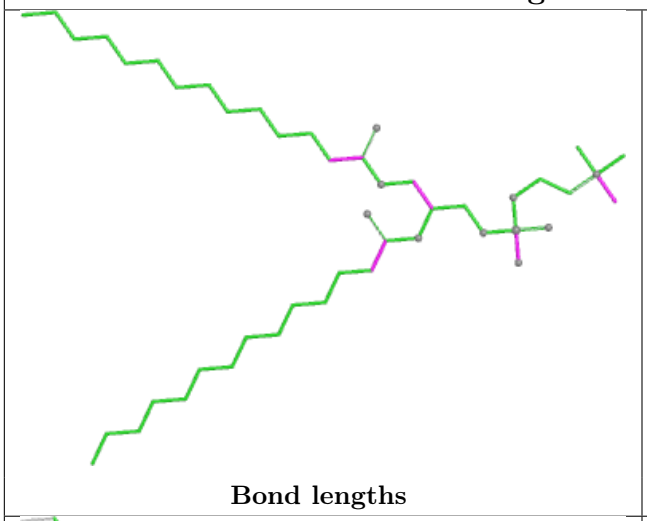


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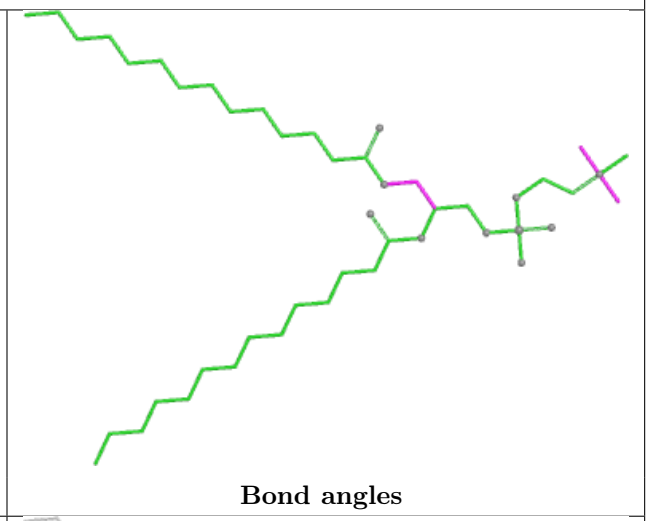


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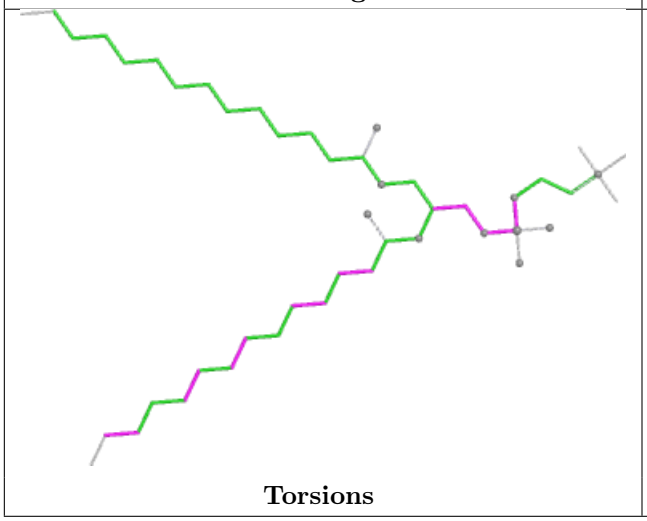
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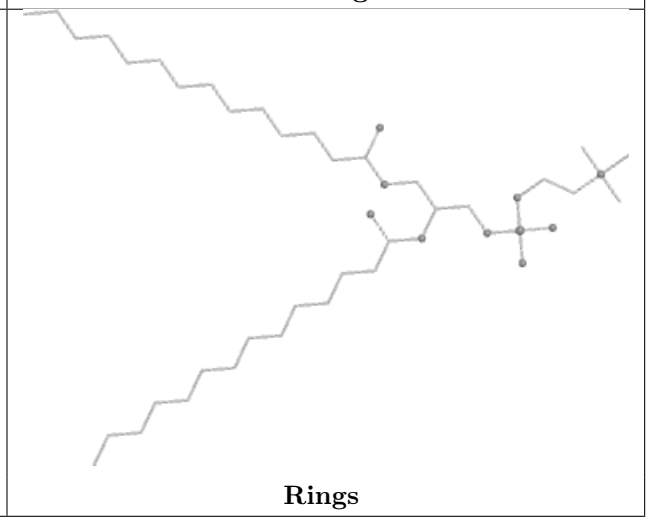
Bond lengths



Bond angles

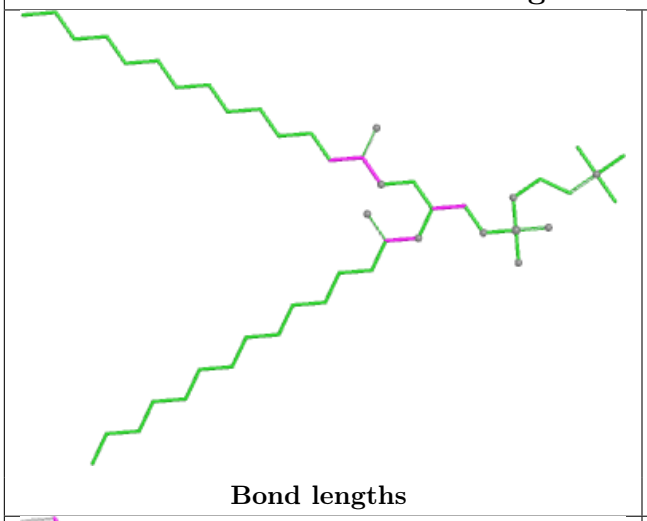


Torsions

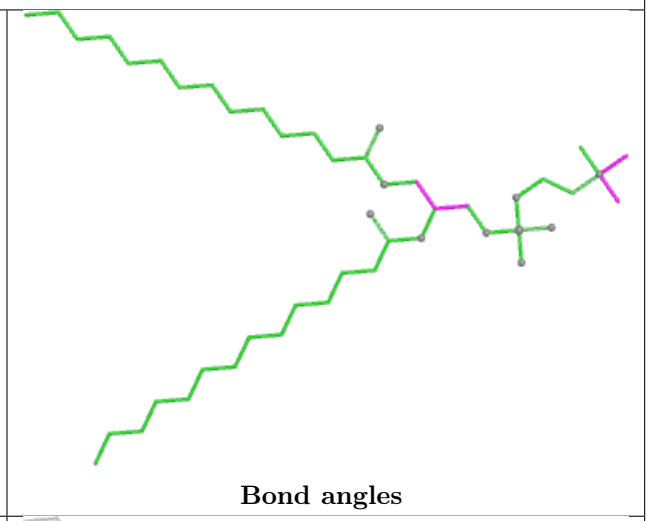


Rings

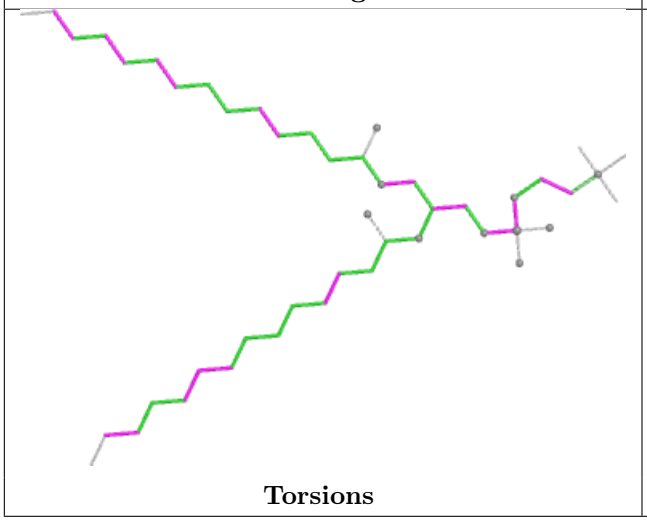
Ligand PX4 B 307



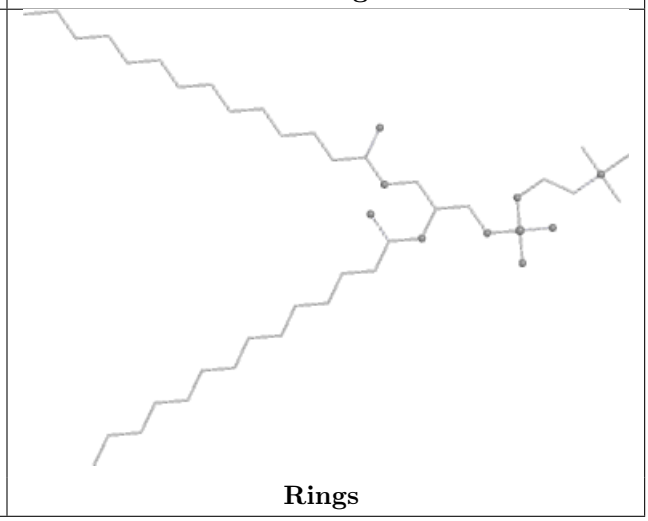
Bond lengths



Bond angles

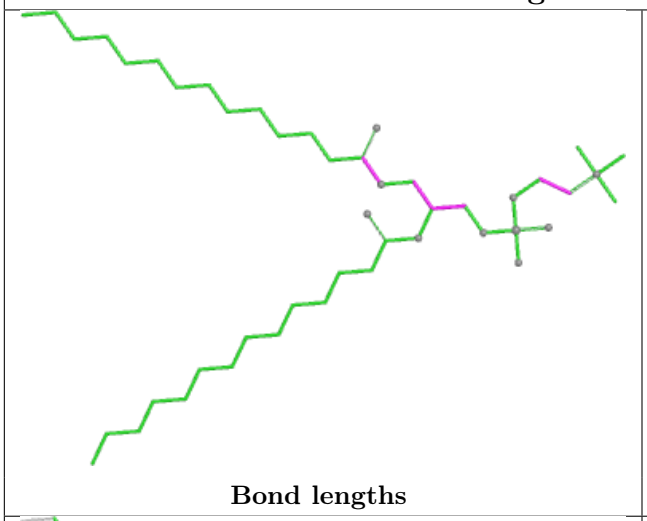


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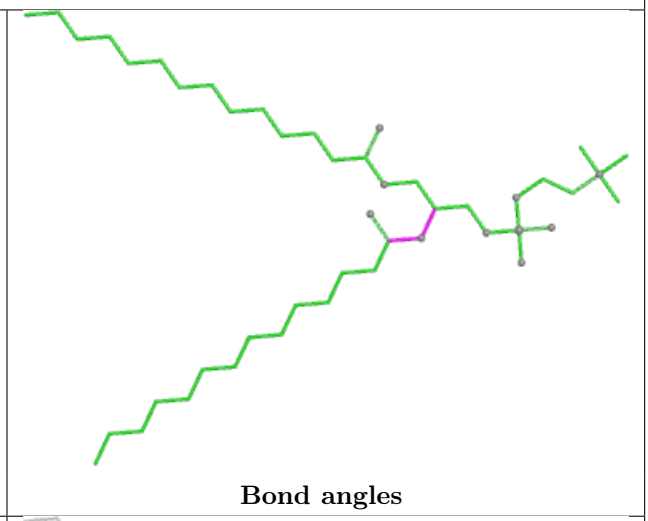


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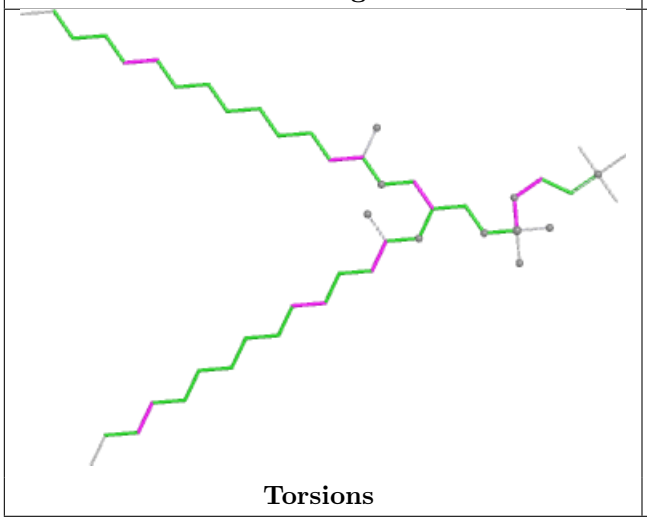
Ligand PX4 C 304



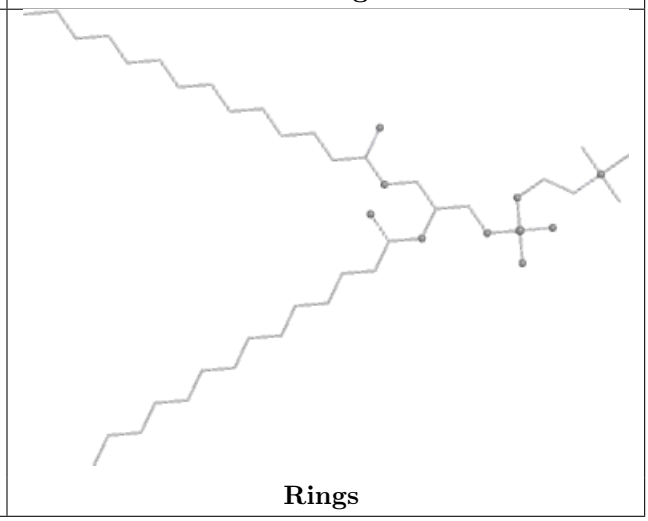
Bond lengths



Bond angles

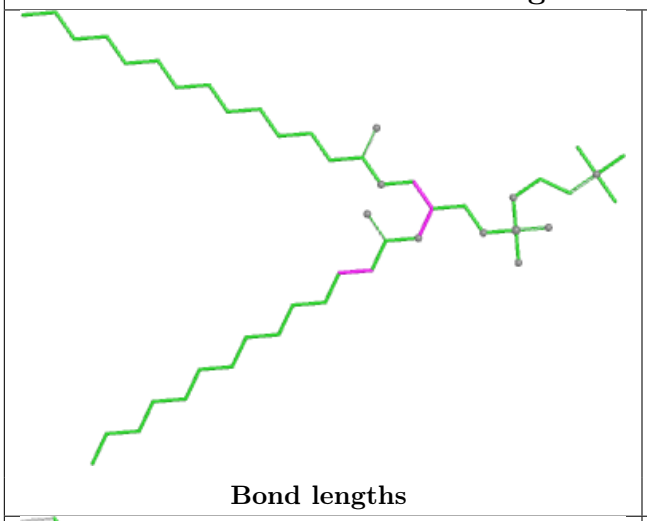


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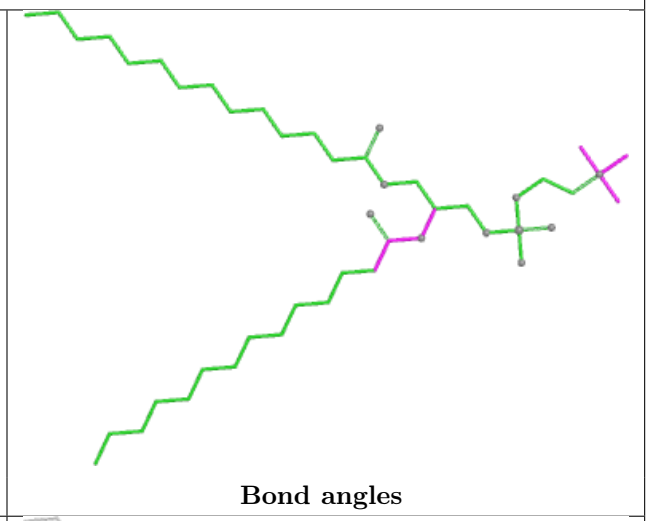


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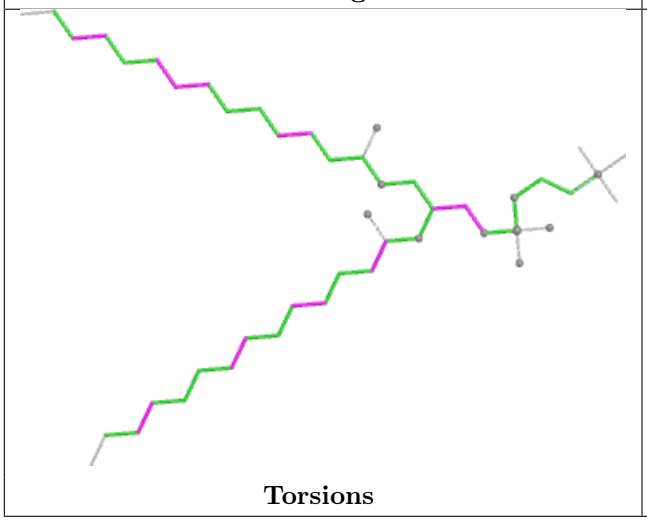
Ligand PX4 B 324



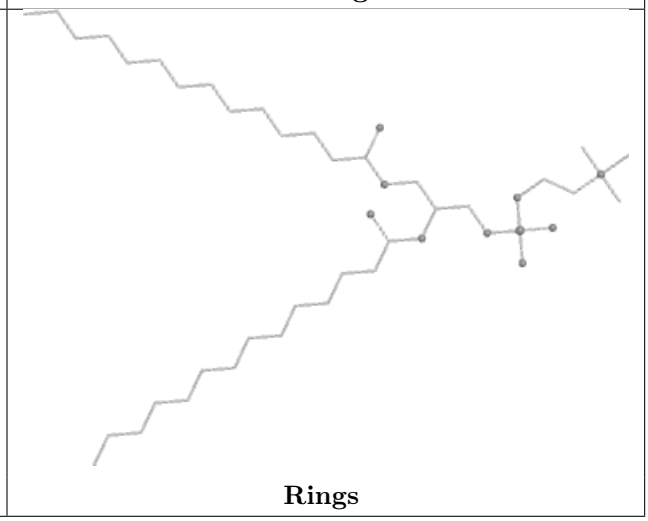
Bond lengths



Bond angles

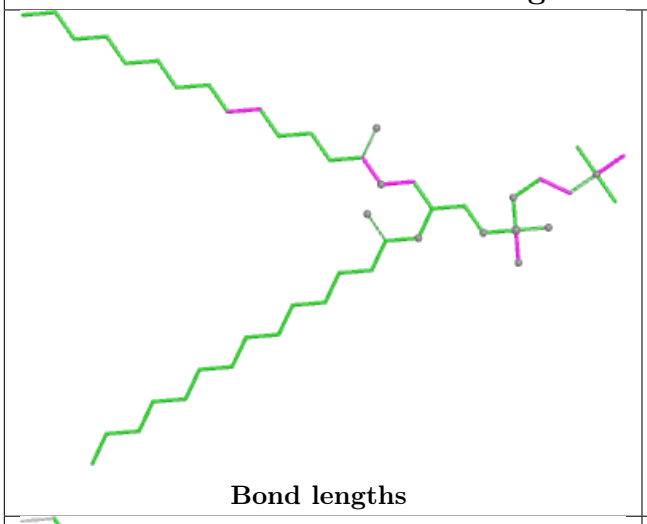


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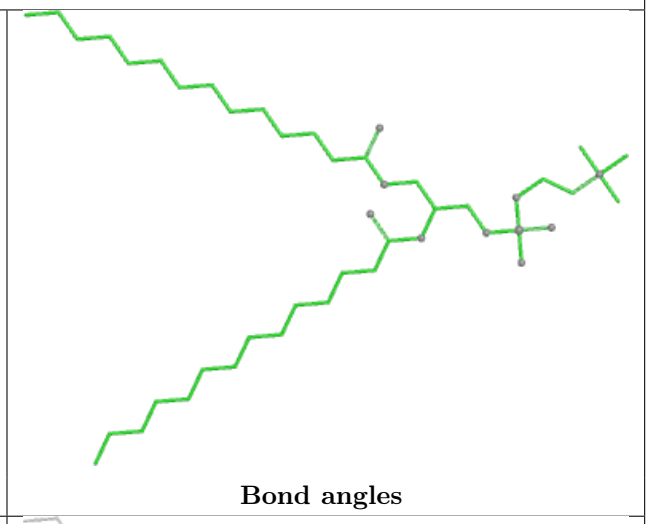


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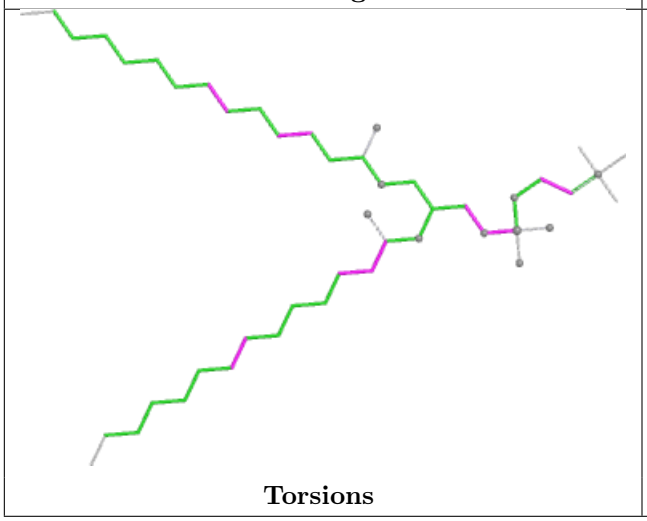
Ligand PX4 B 311



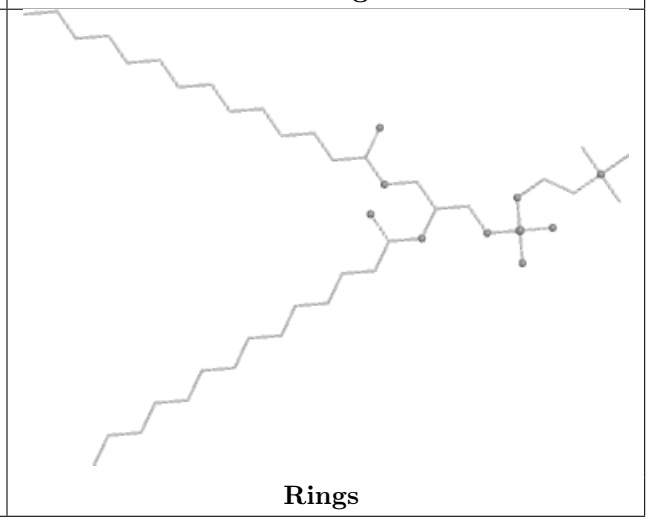
Bond lengths



Bond angles

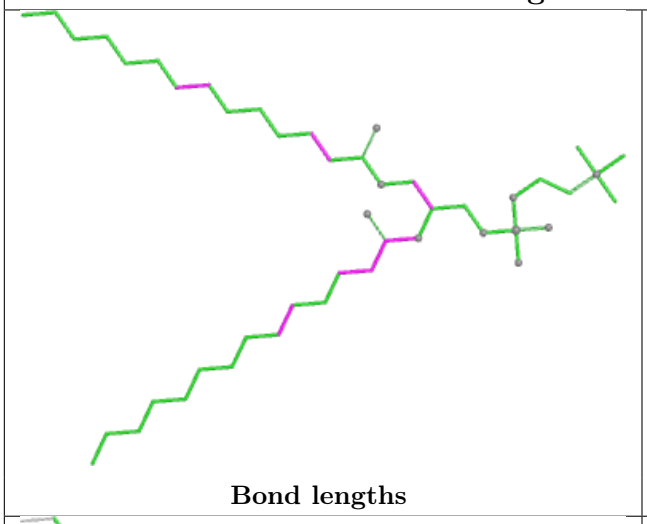


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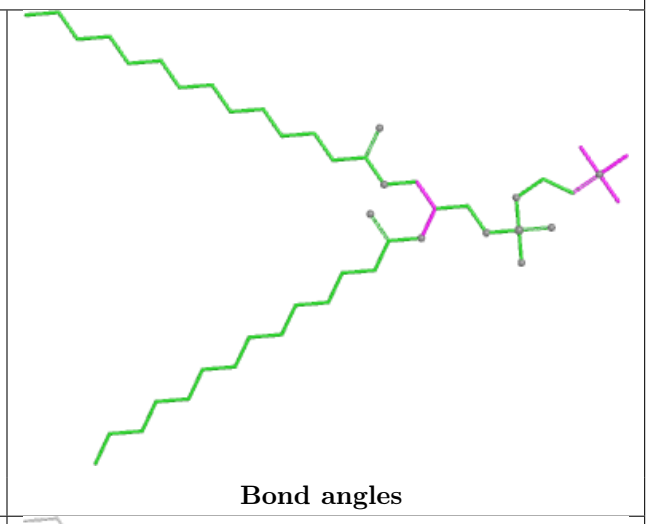


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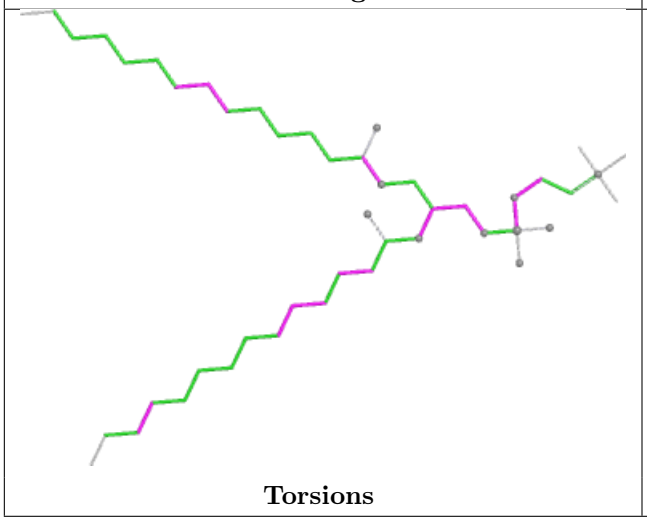
Ligand PX4 A 644



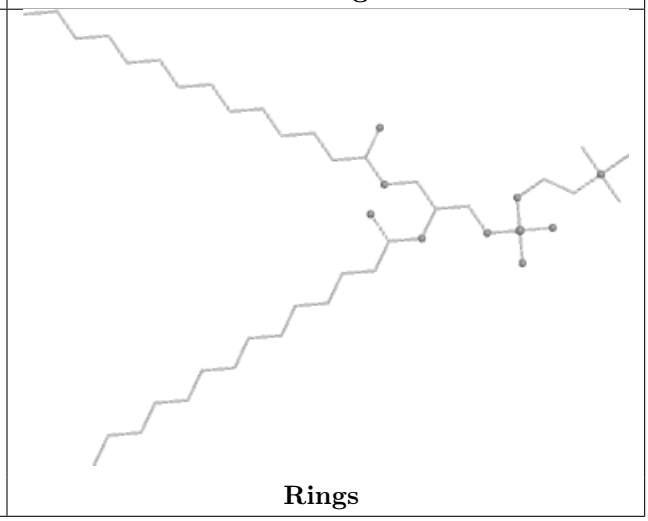
Bond lengths



Bond angles

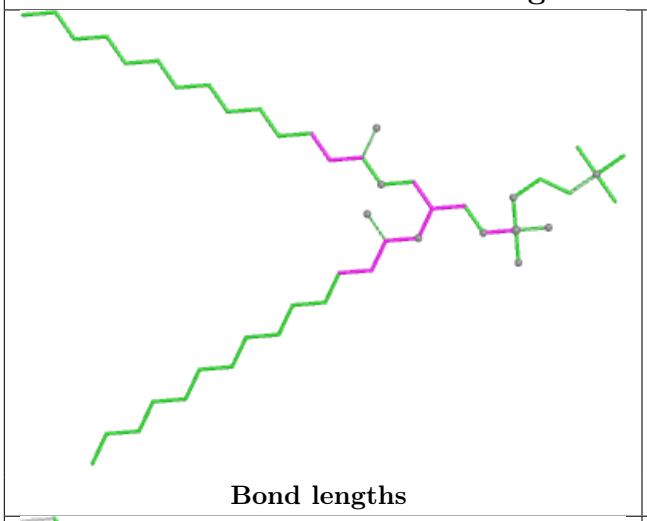


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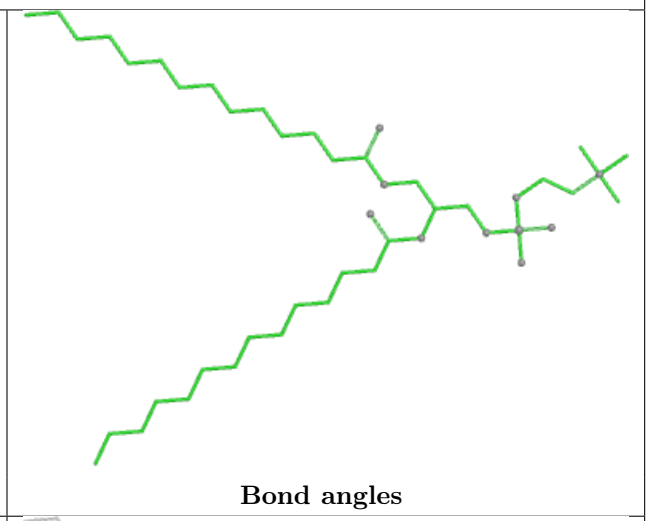


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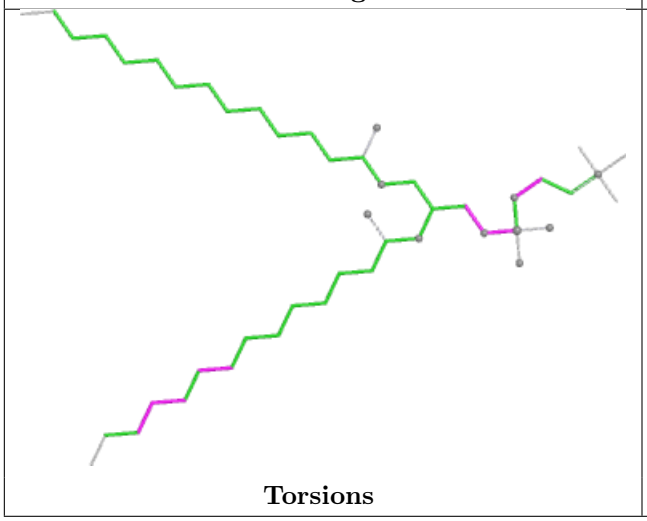
Ligand PX4 B 350



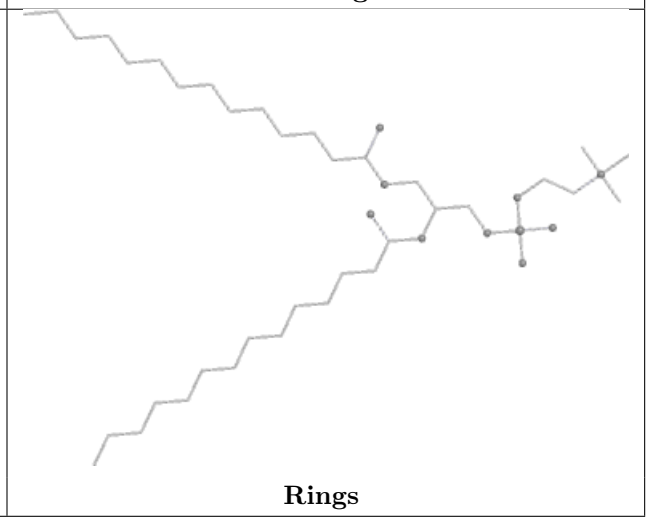
Bond lengths



Bond angles

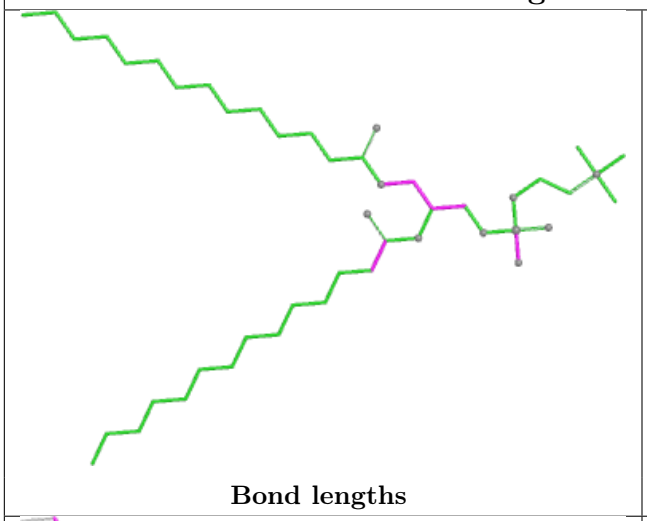


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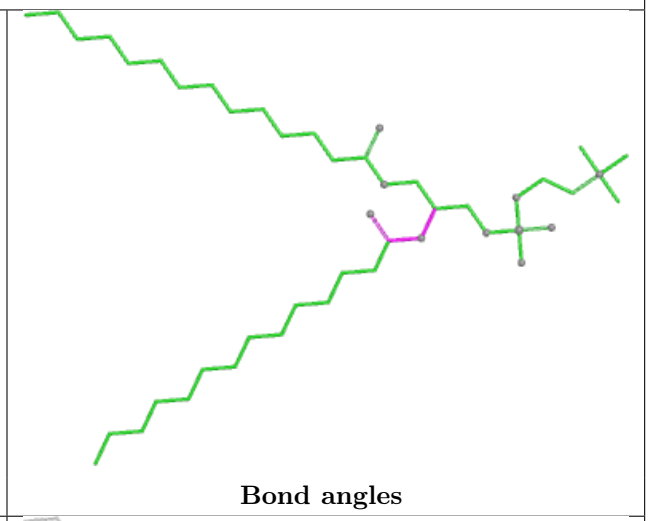


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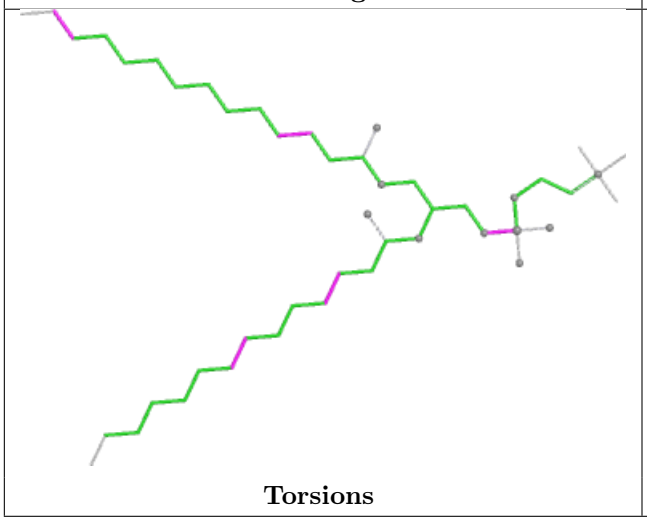
Ligand PX4 B 316



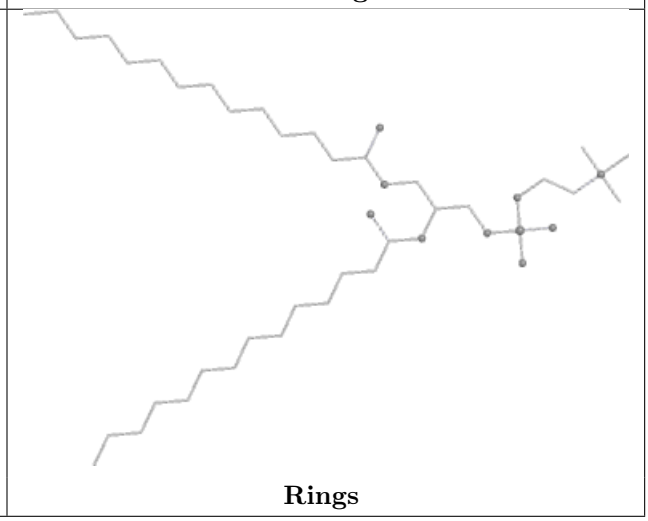
Bond lengths



Bond angles

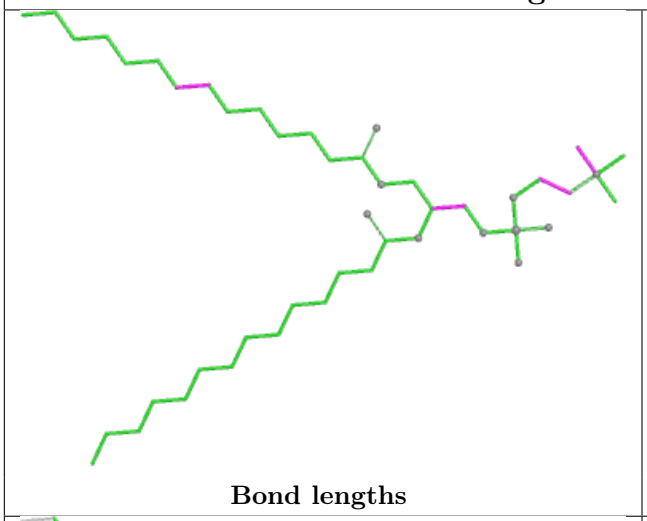


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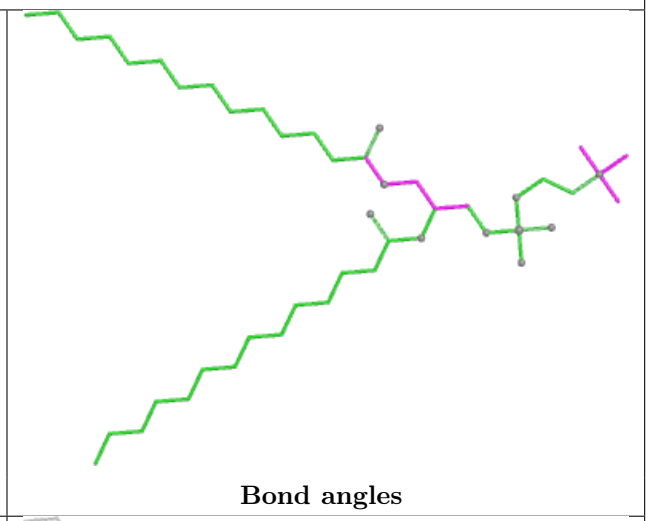


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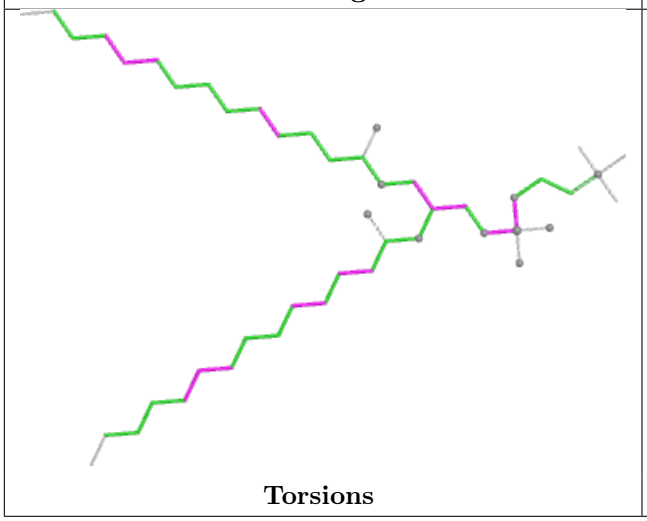
Ligand PX4 B 359



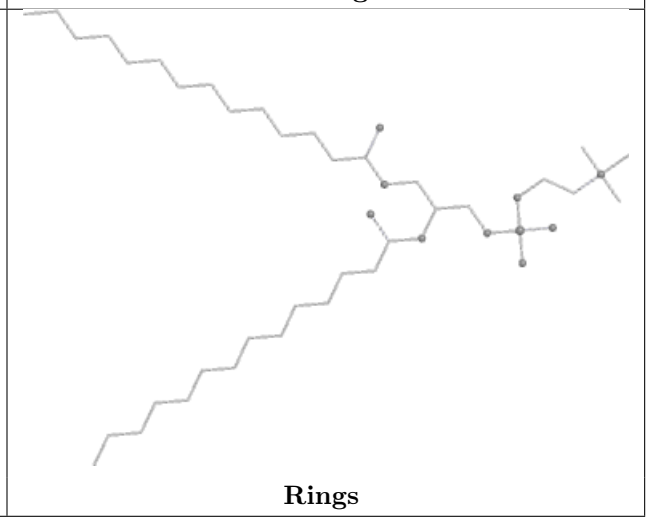
Bond lengths



Bond angles

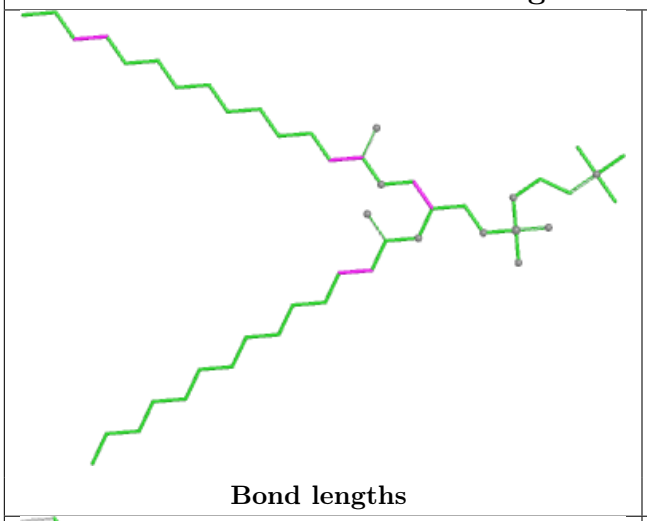


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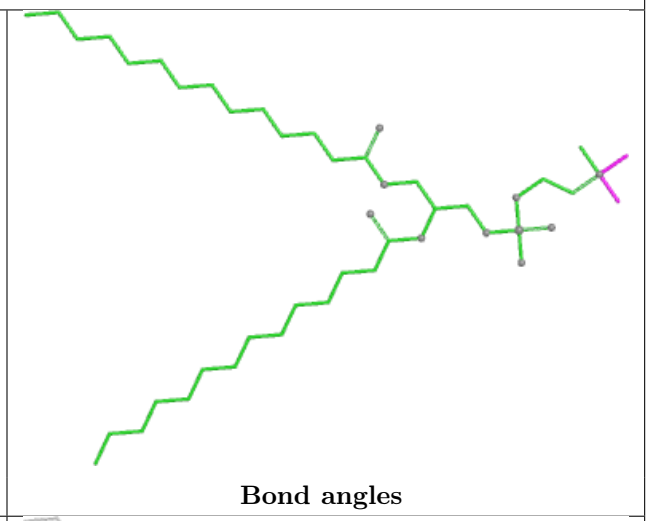


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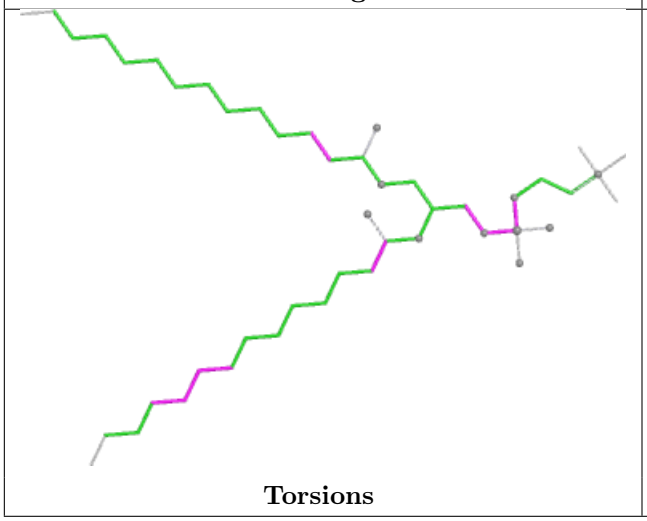
Ligand PX4 B 330



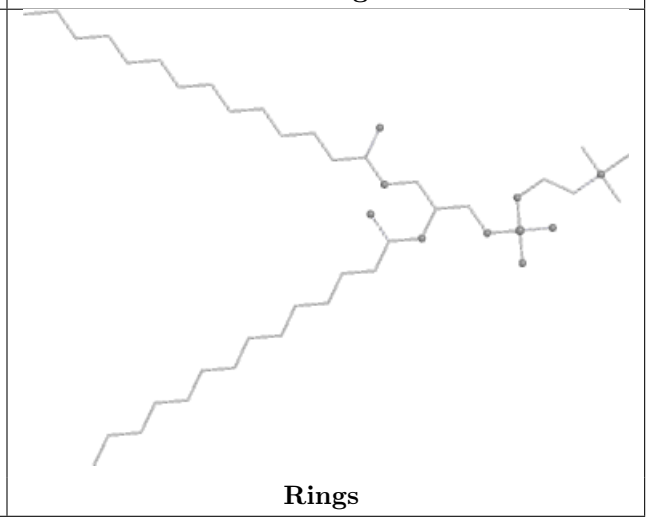
Bond lengths



Bond angles

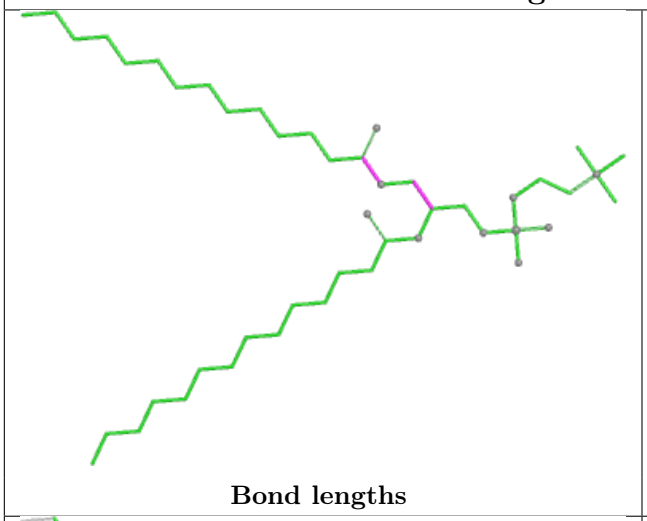


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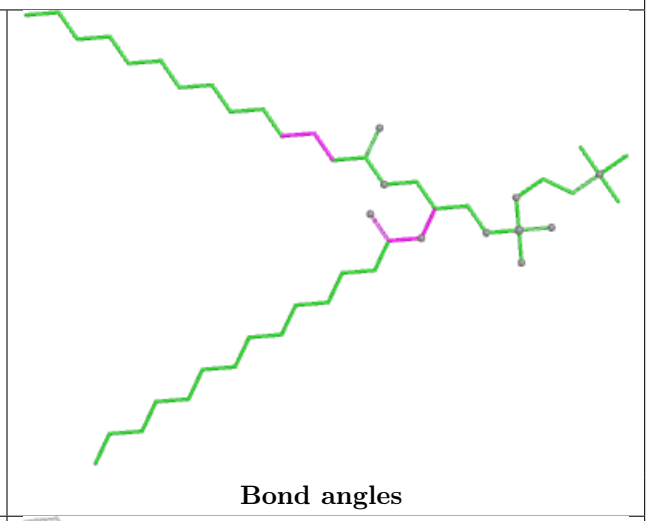


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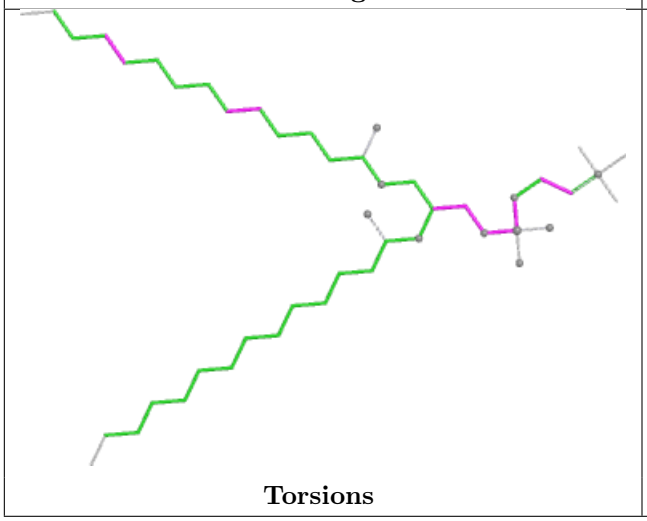
Ligand PX4 B 337



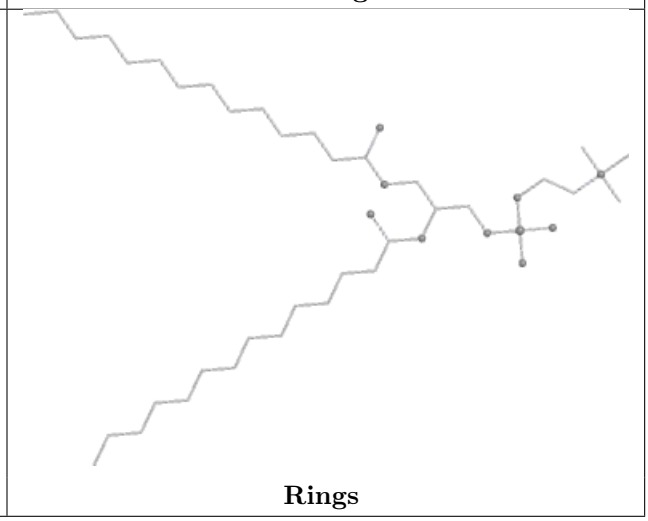
Bond lengths



Bond angles

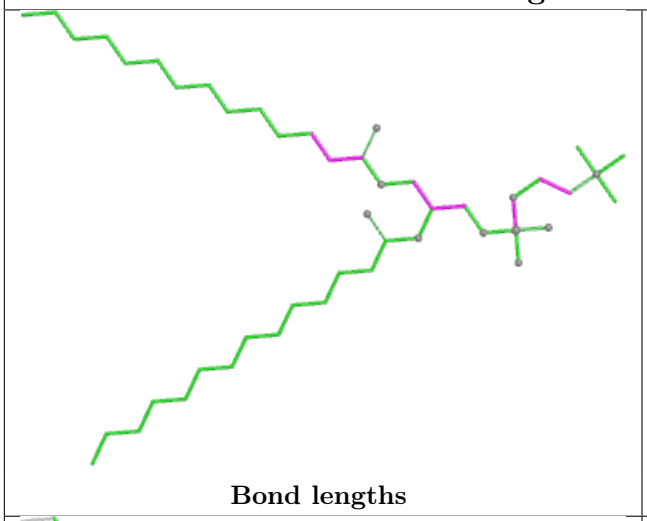


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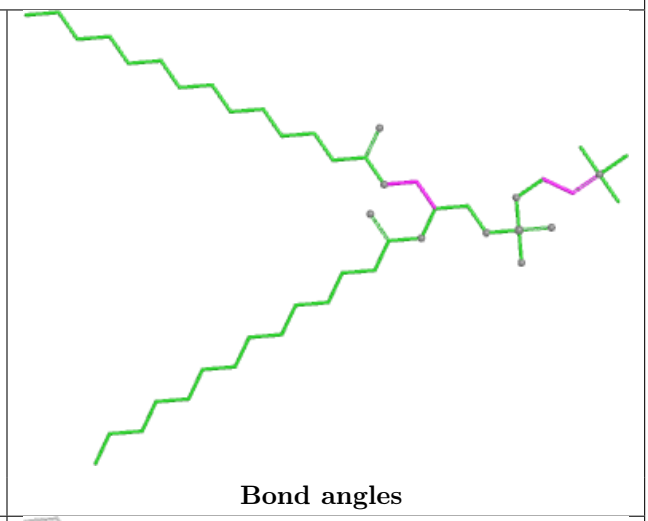


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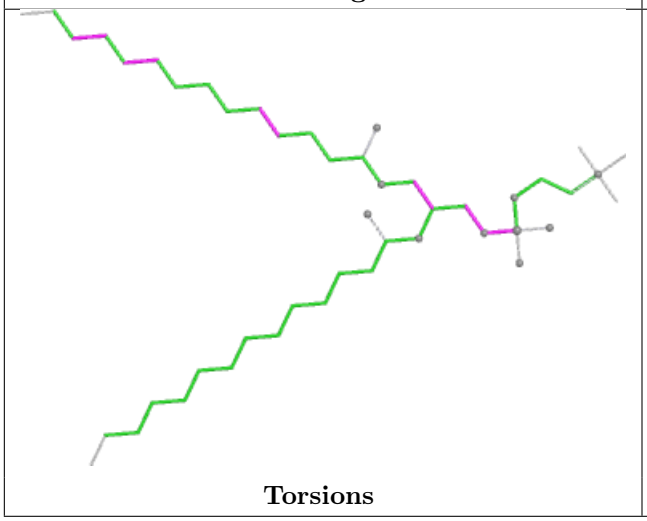
Ligand PX4 C 323



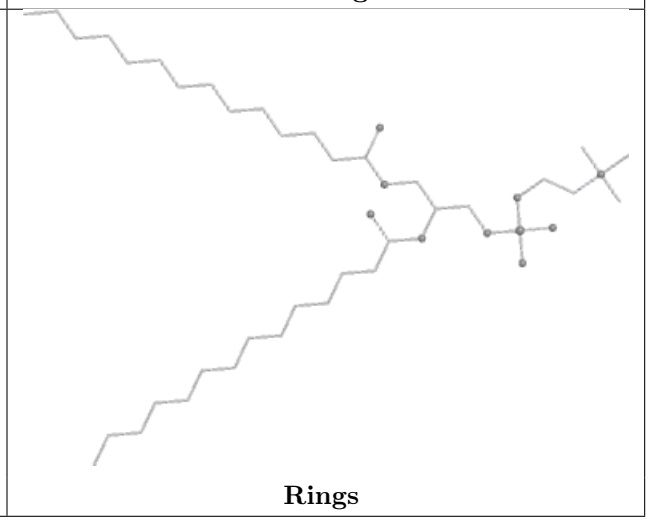
Bond lengths



Bond angles

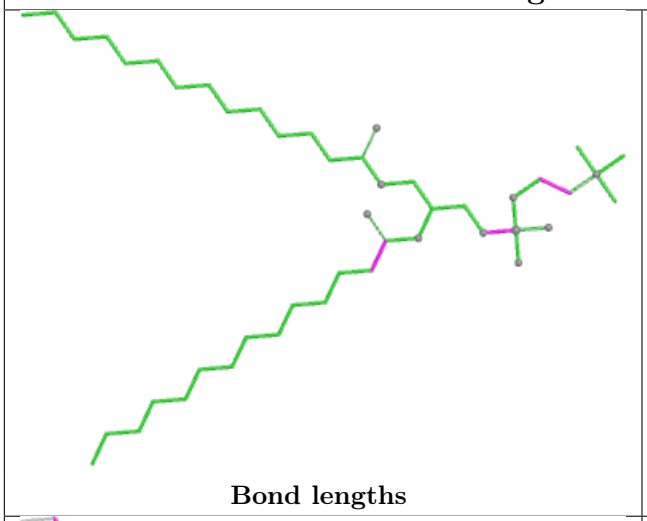


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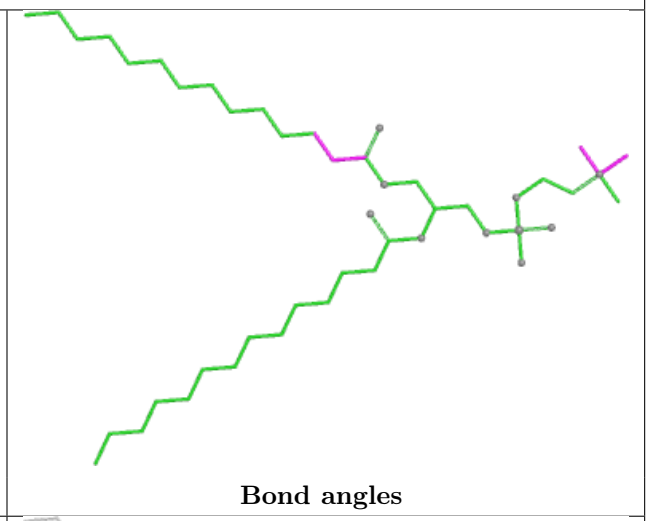


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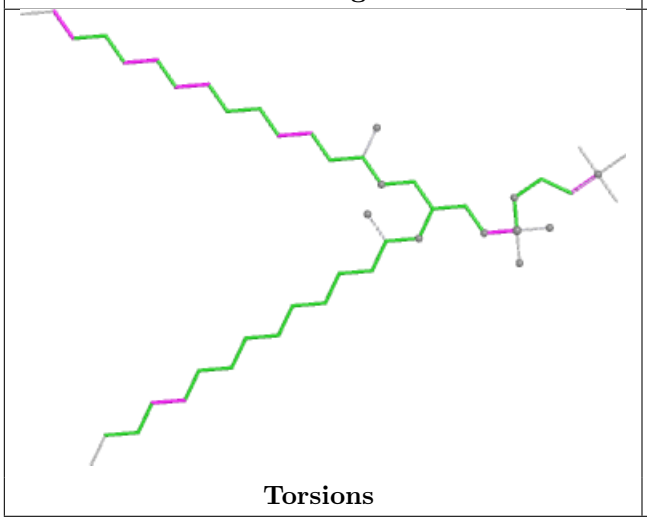
Ligand PX4 A 619



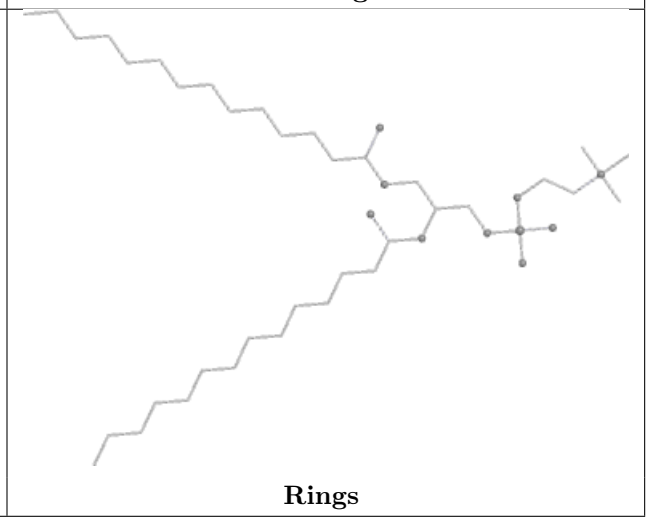
Bond lengths



Bond angles

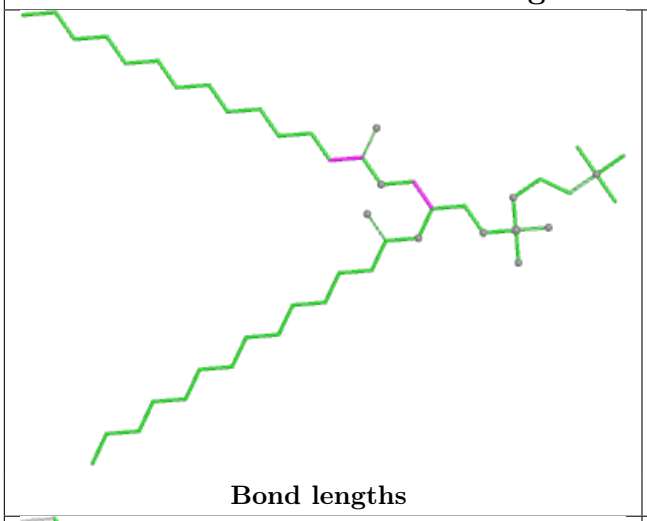


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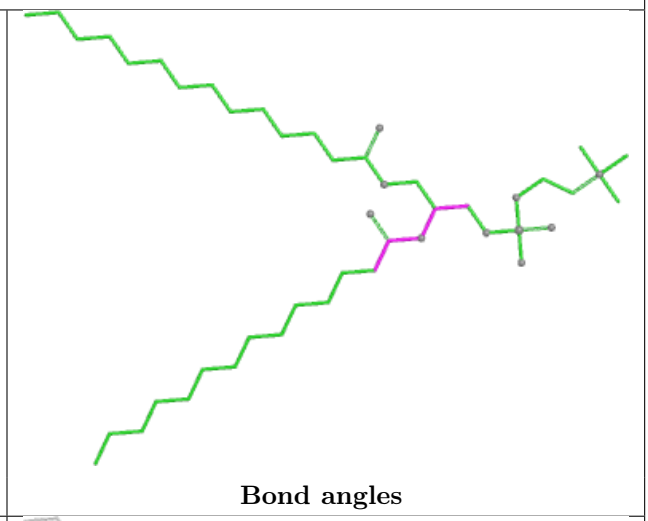


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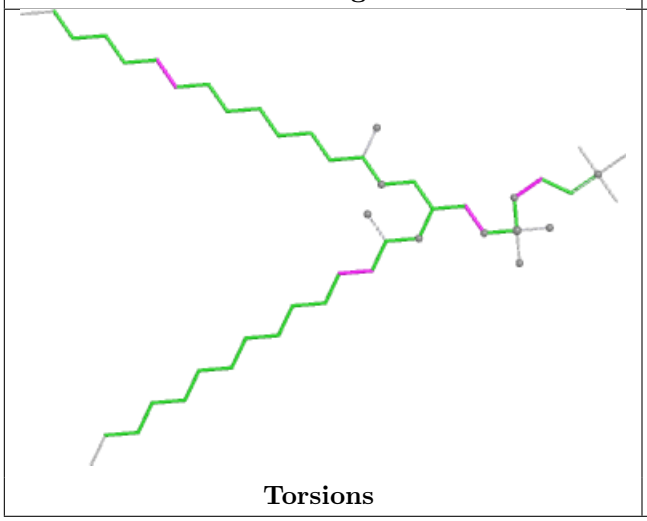
Ligand PX4 B 347



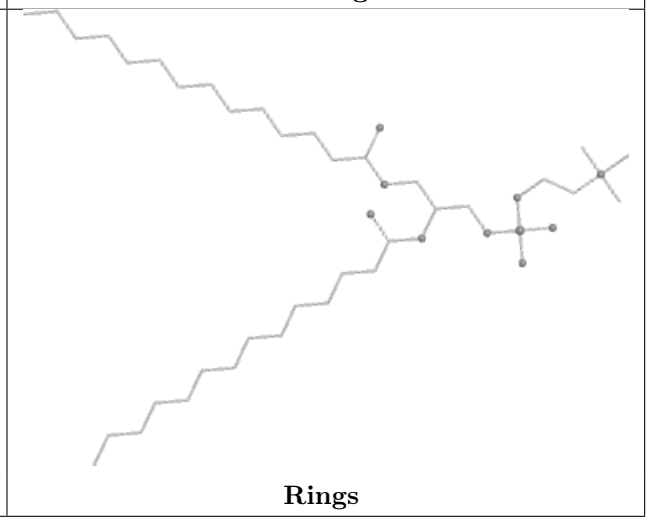
Bond lengths



Bond angles

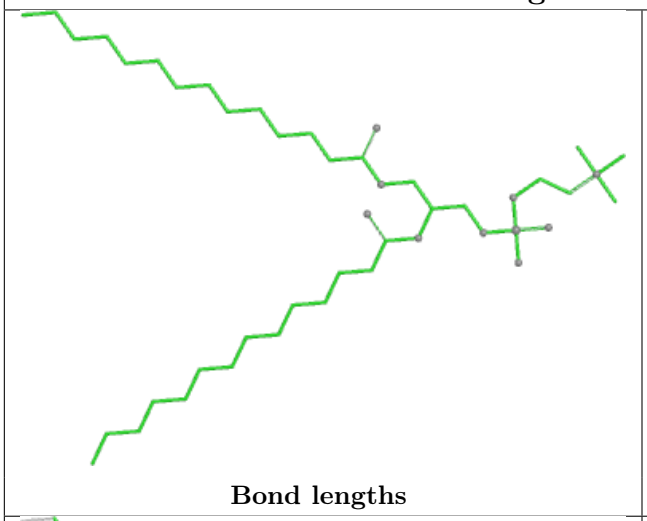


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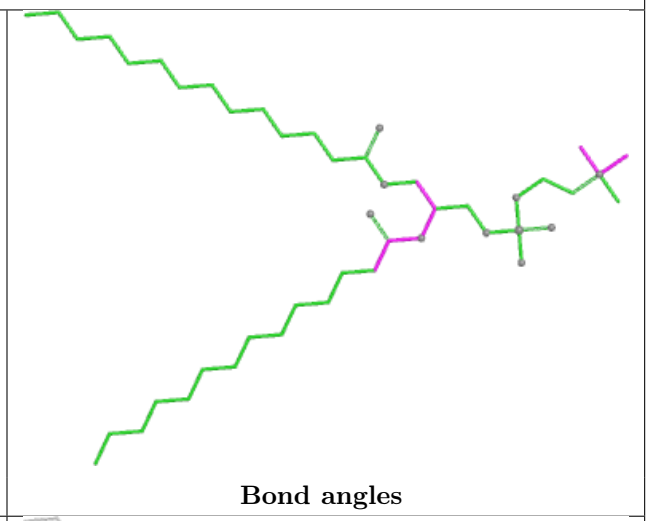


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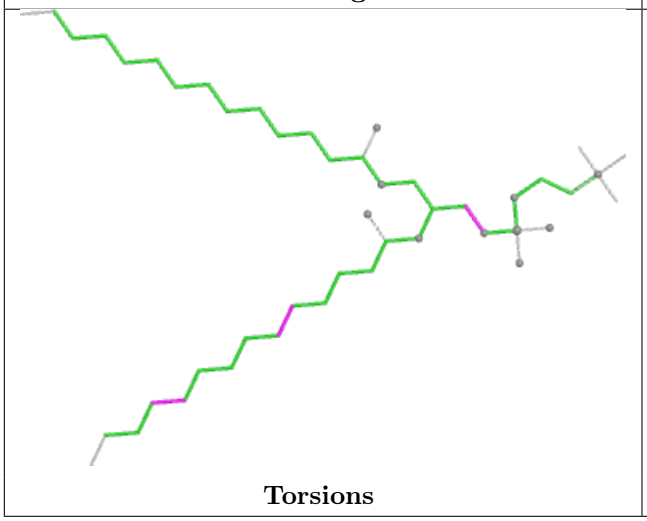
Ligand PX4 B 353



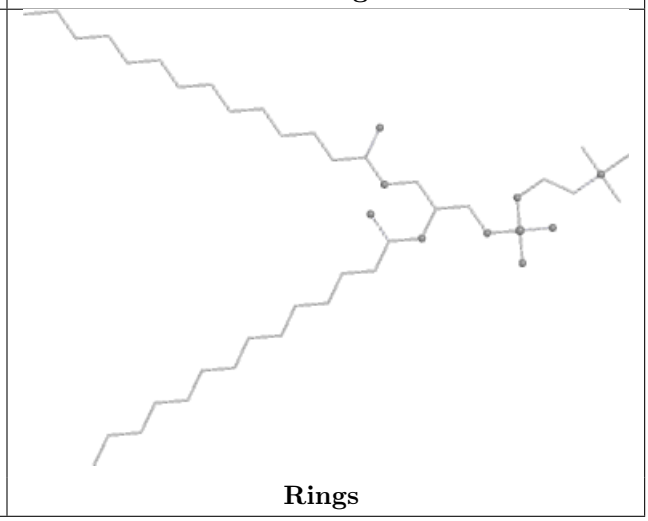
Bond lengths



Bond angles

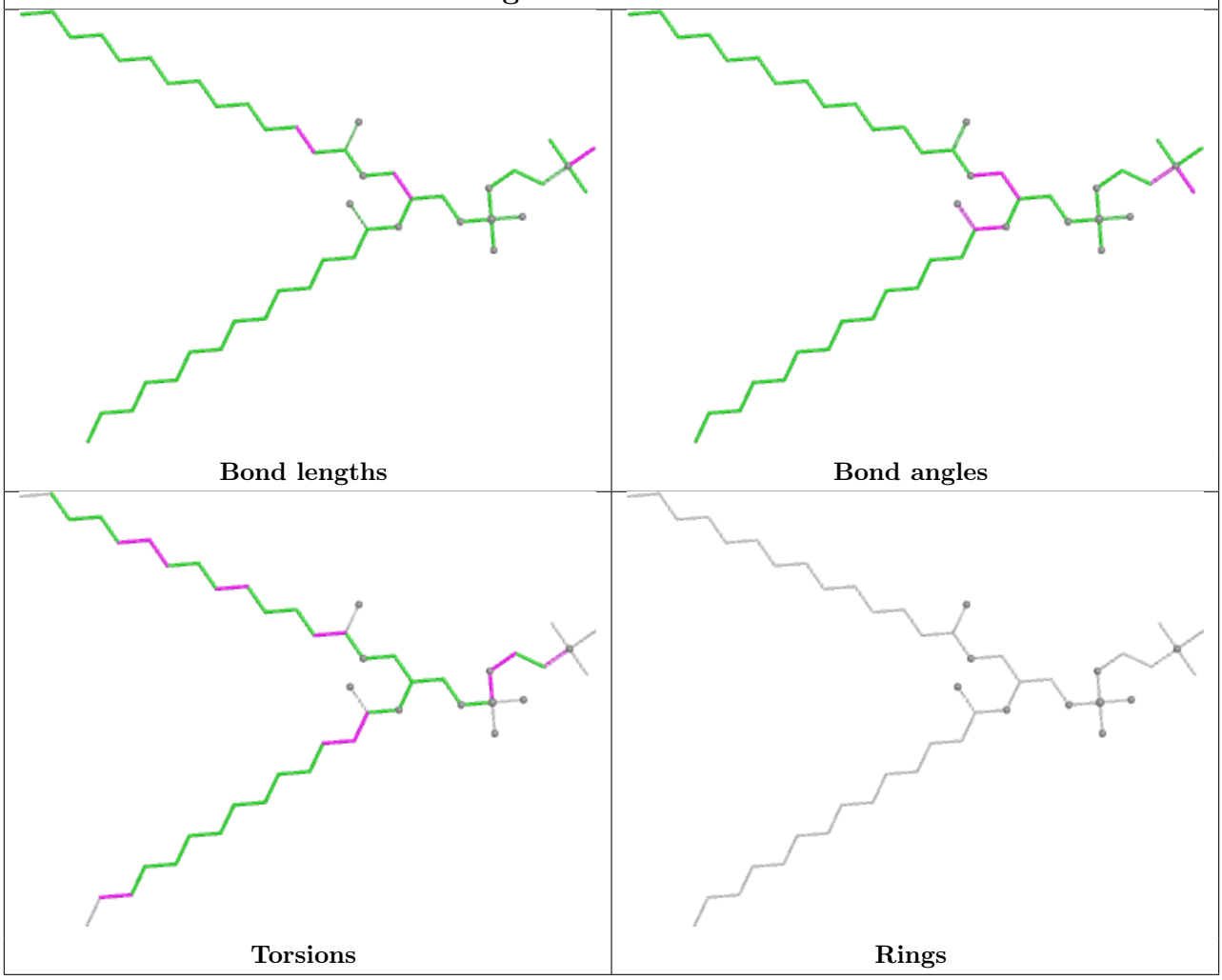


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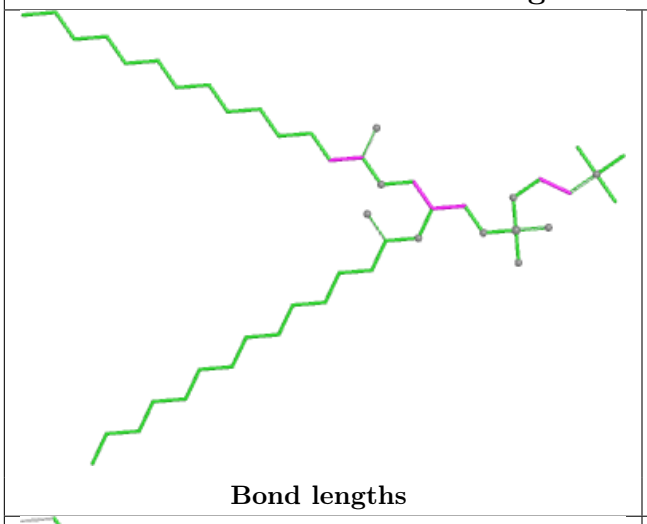


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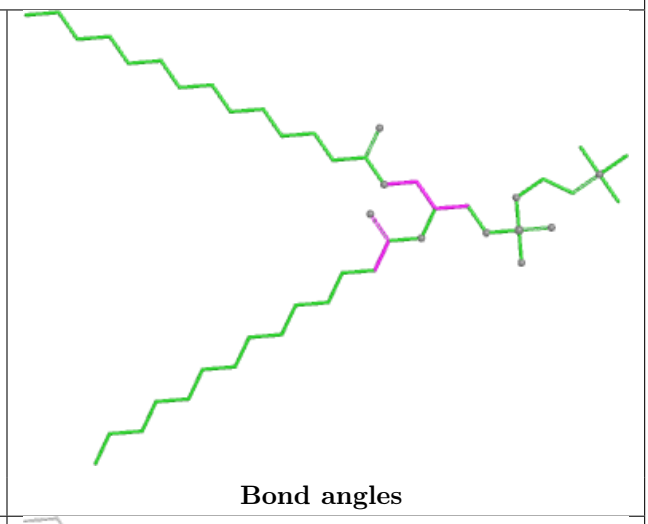
Ligand PX4 C 360



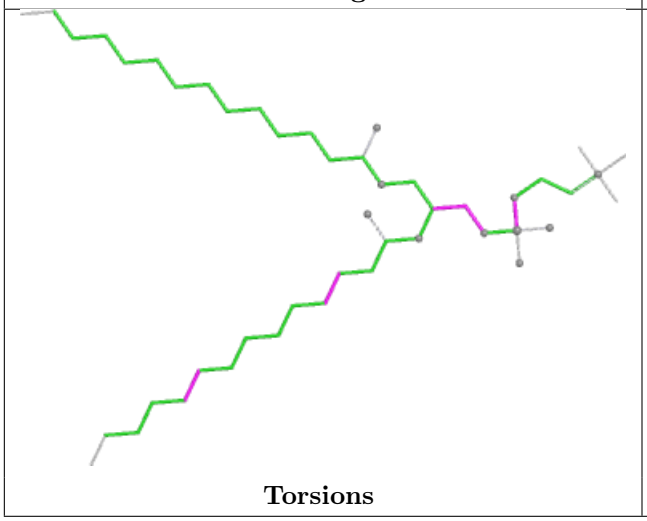
Ligand PX4 B 341



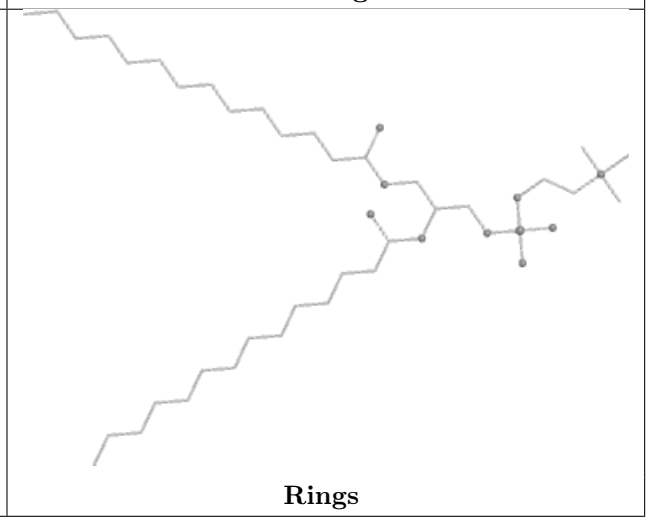
Bond lengths



Bond angles

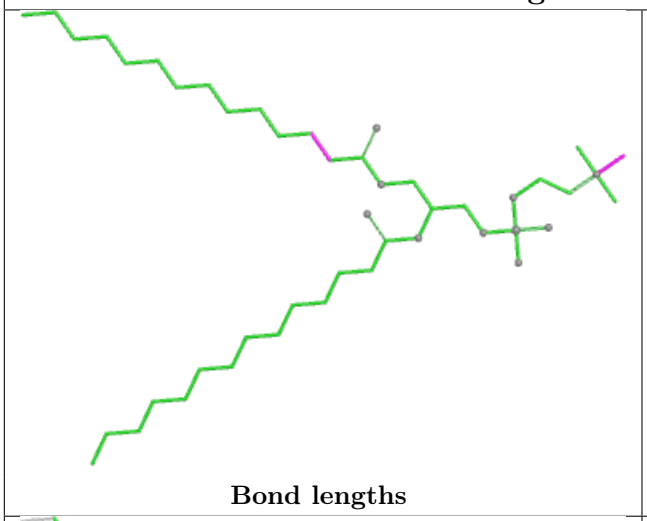


Torsions

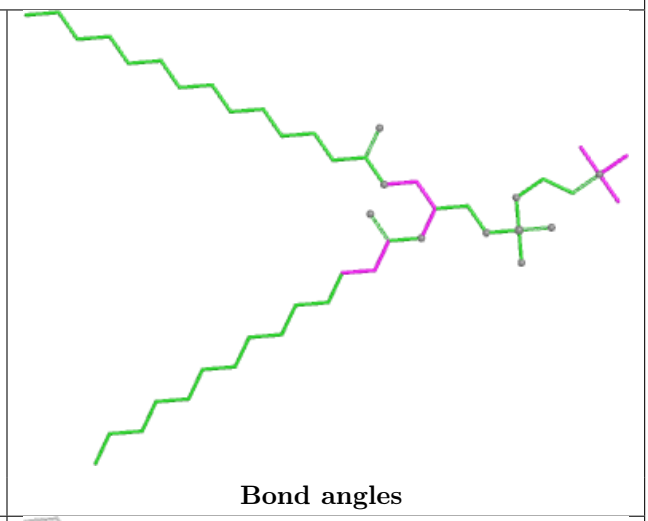


Rings

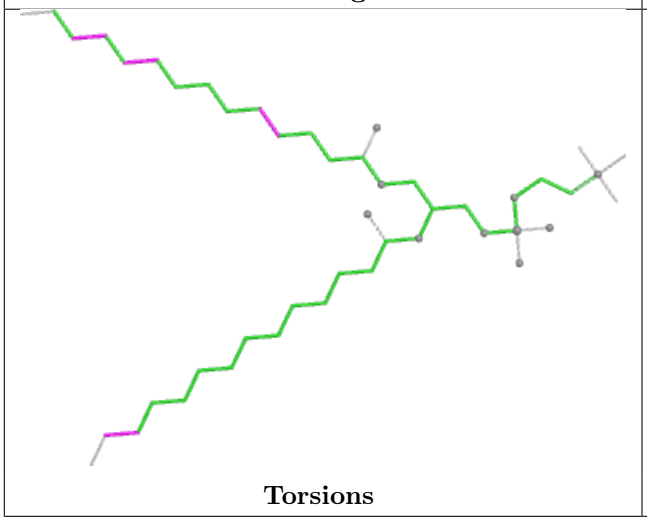
Ligand PX4 C 332



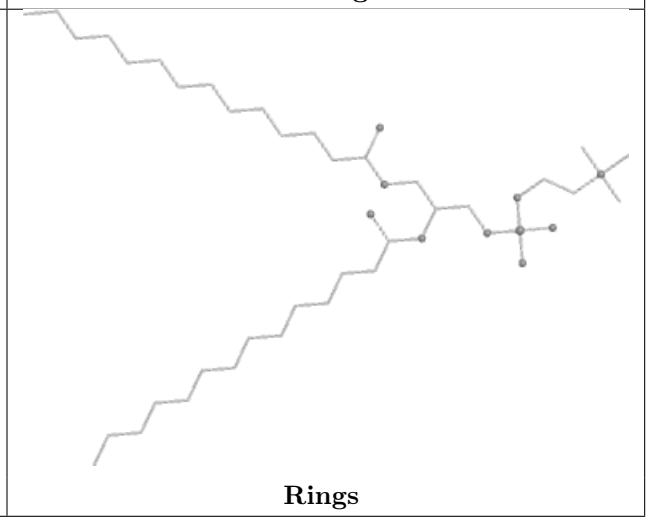
Bond lengths



Bond angles

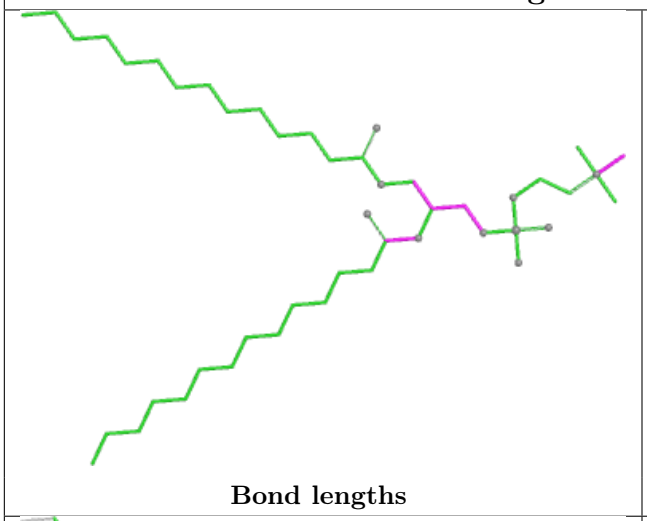


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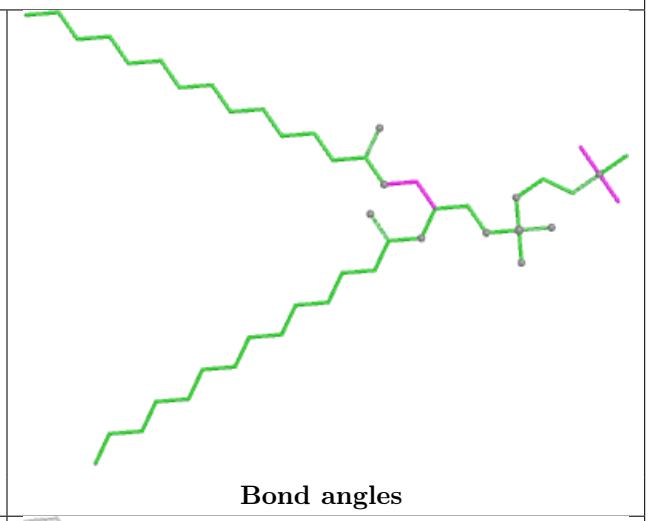


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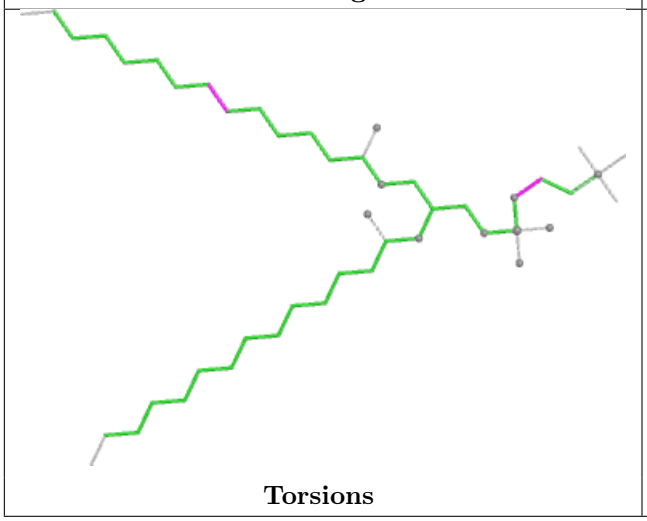
Ligand PX4 C 311



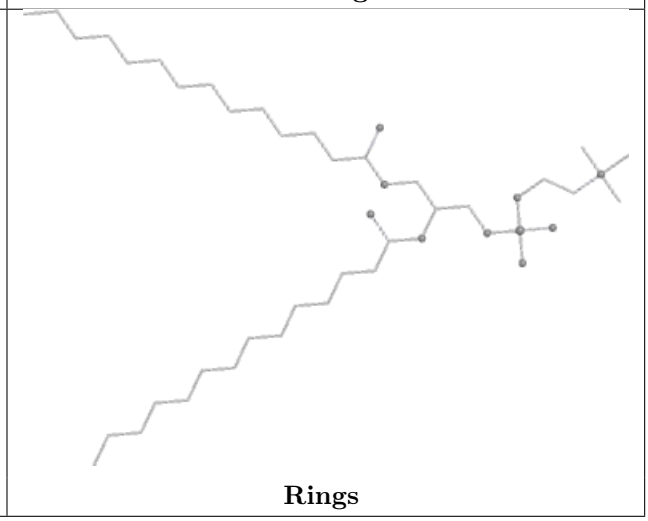
Bond lengths



Bond angles

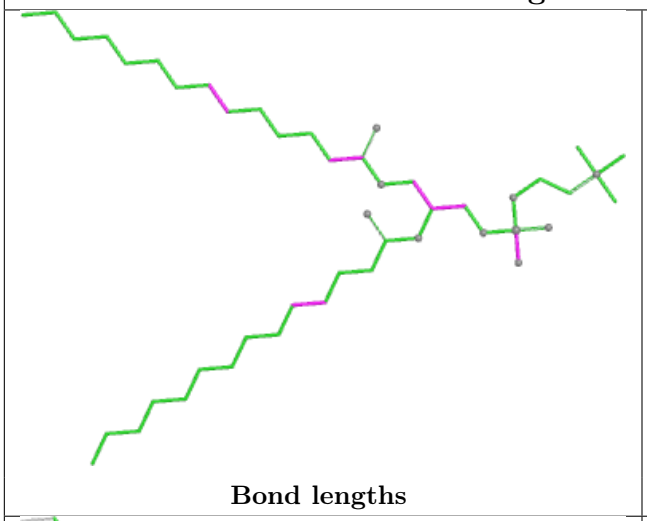


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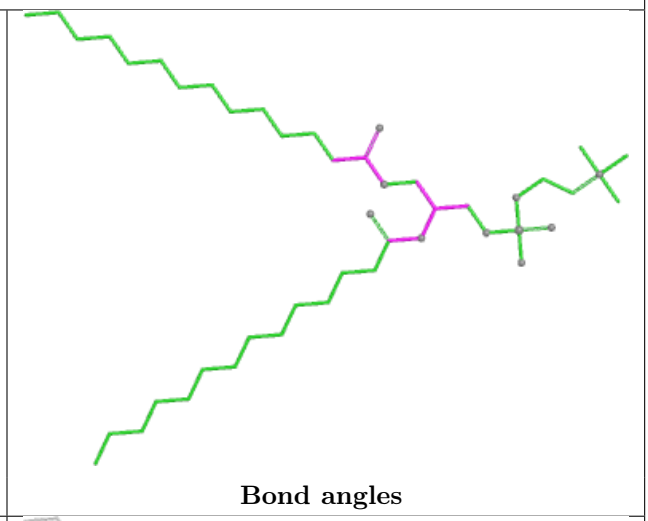


Rings

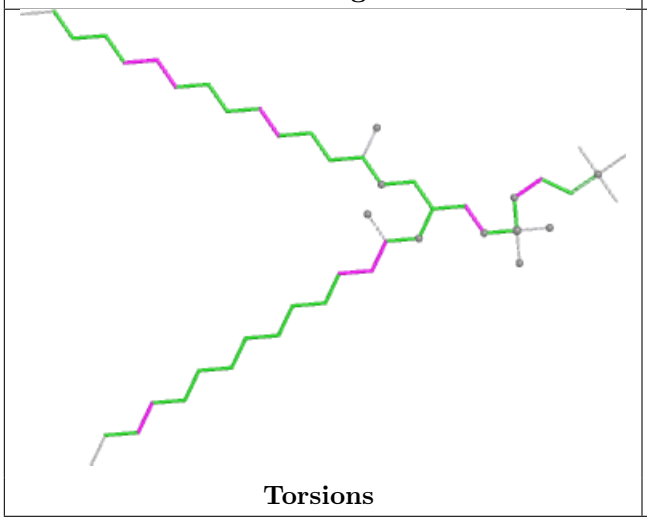
Ligand PX4 B 312



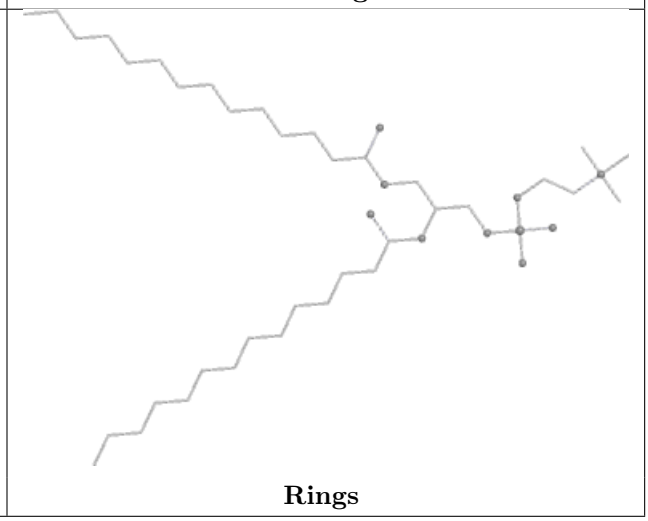
Bond lengths



Bond angles

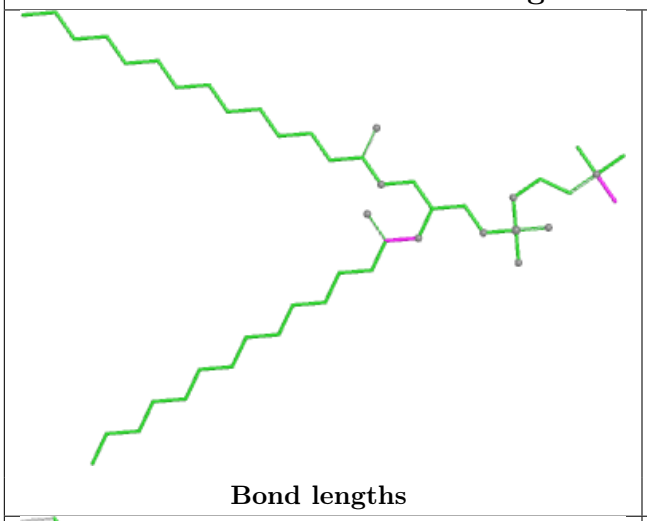


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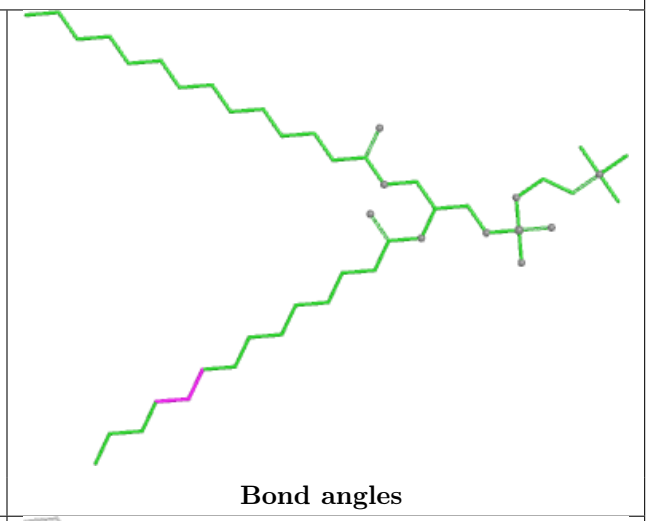


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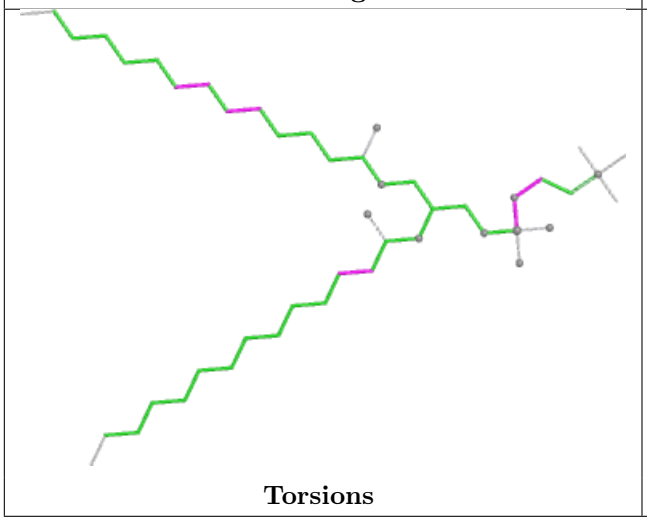
Ligand PX4 A 635



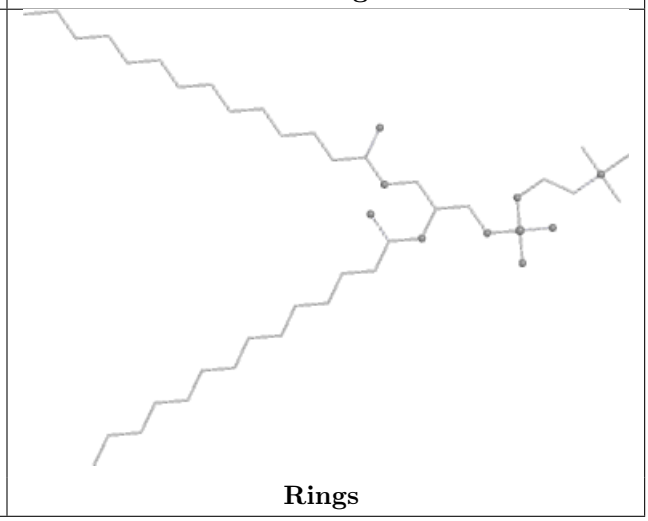
Bond lengths



Bond angles

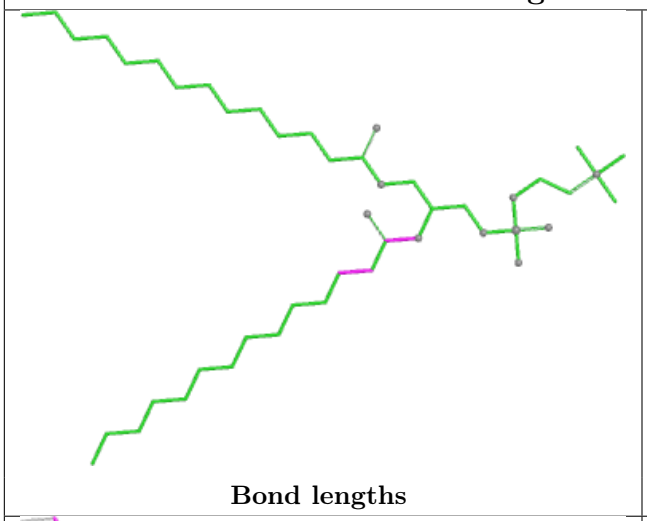


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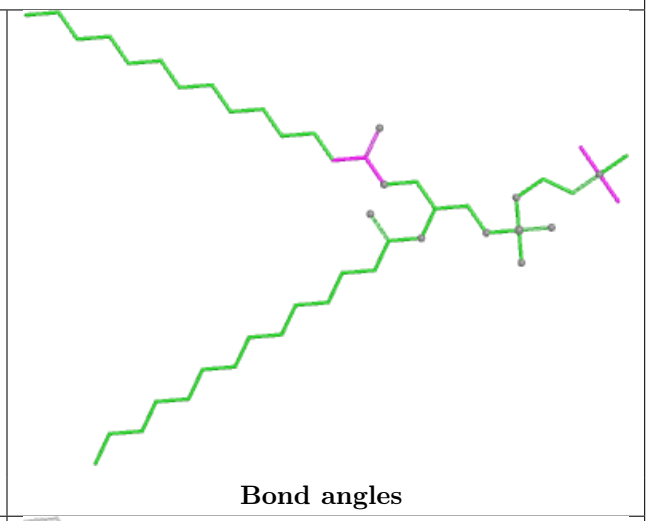


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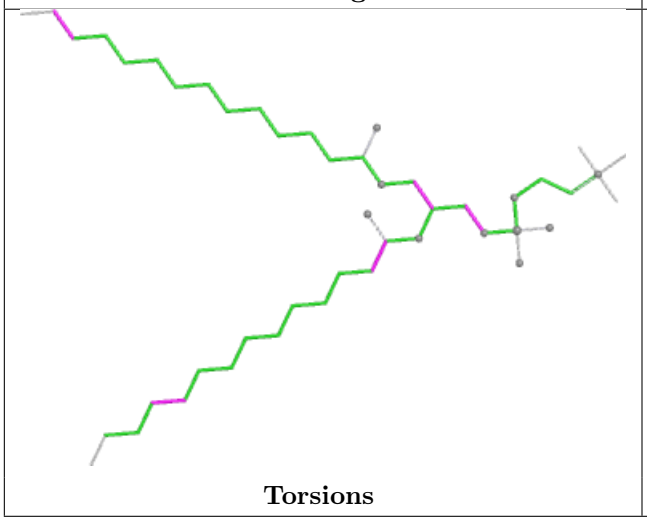
Ligand PX4 A 643



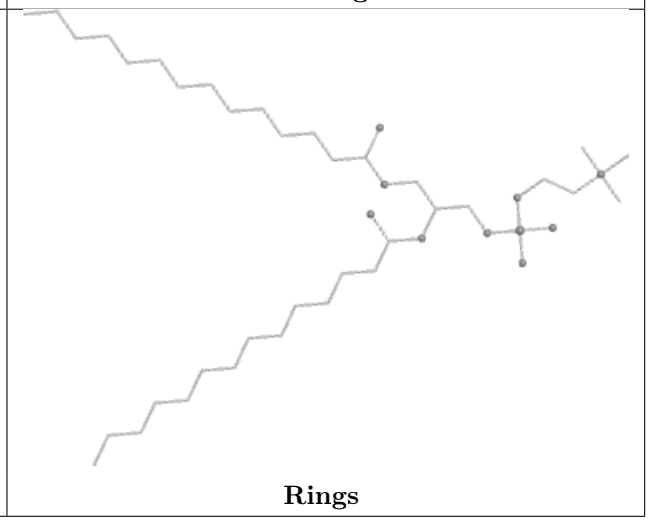
Bond lengths



Bond angles

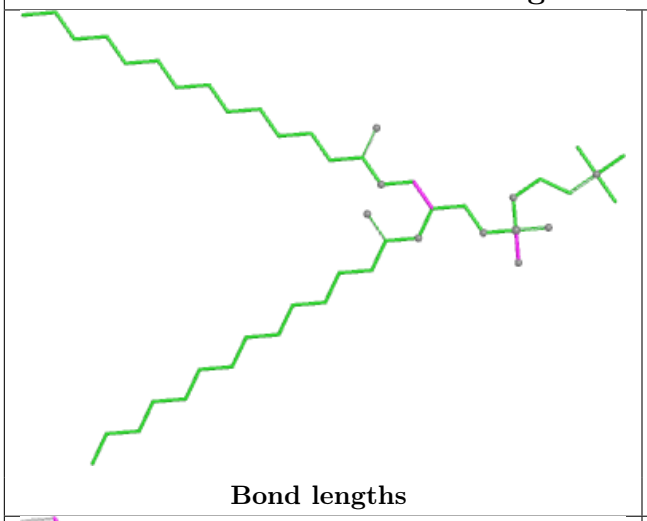


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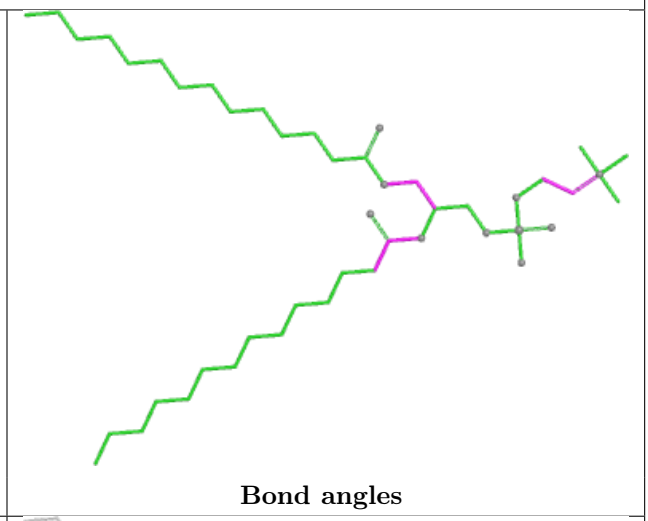


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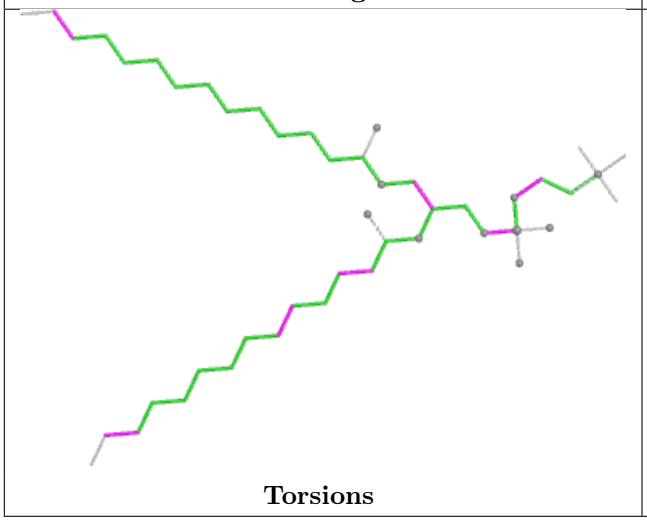
Ligand PX4 C 339



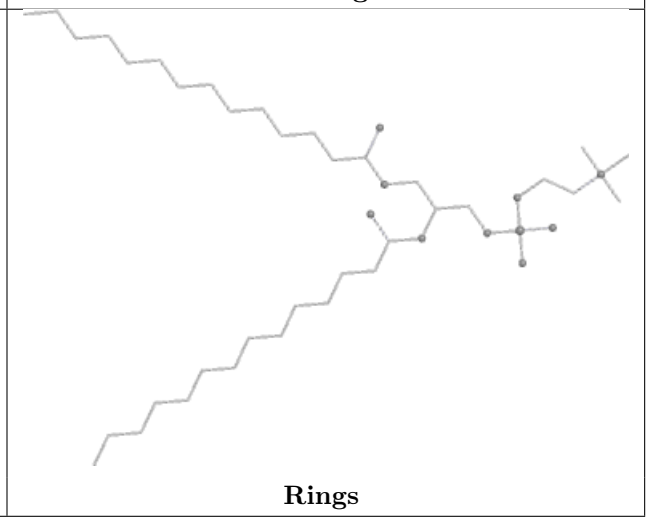
Bond lengths



Bond angles

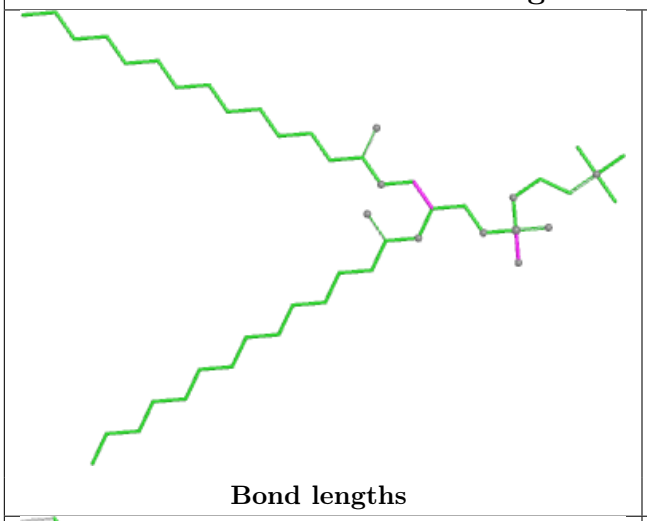


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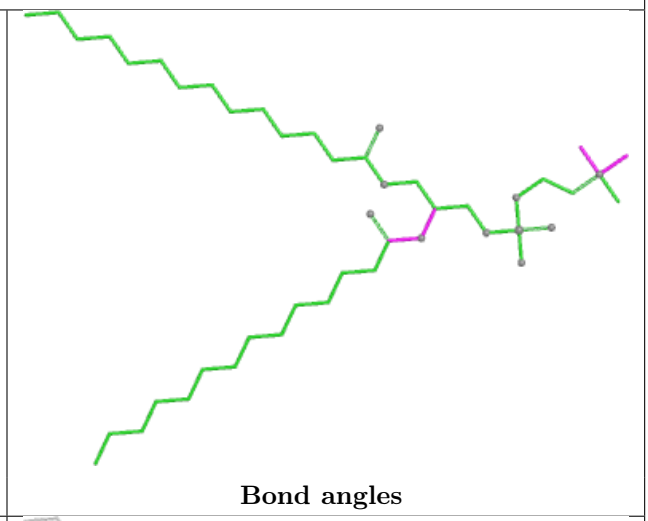


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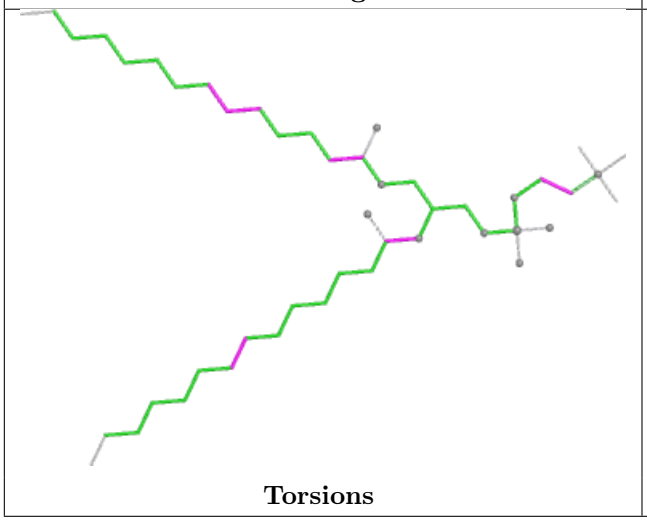
Ligand PX4 C 363



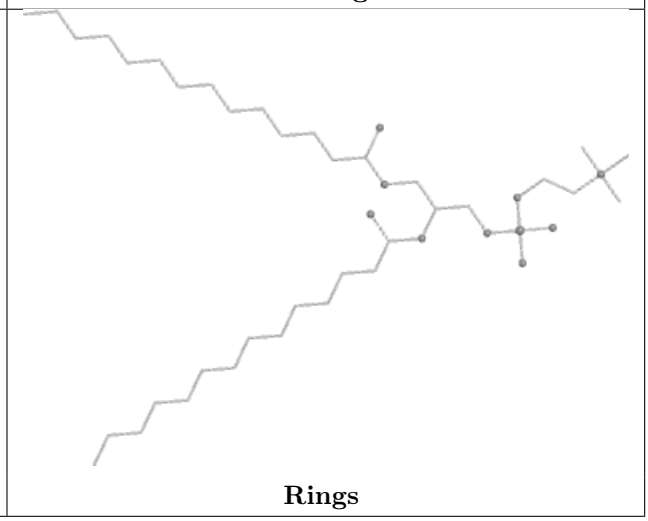
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Bond angles

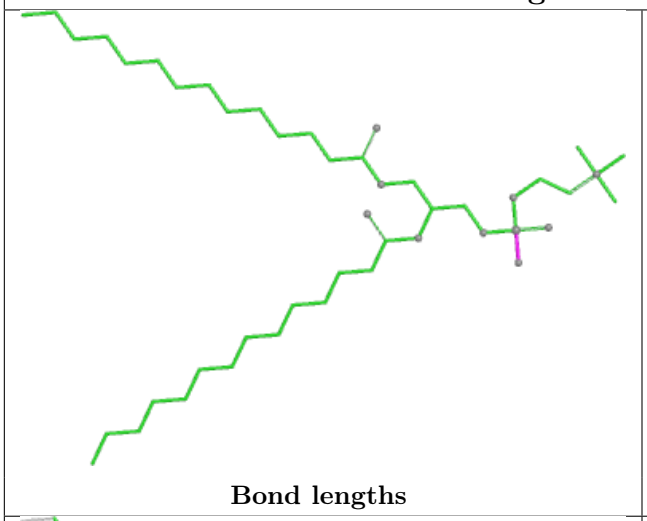


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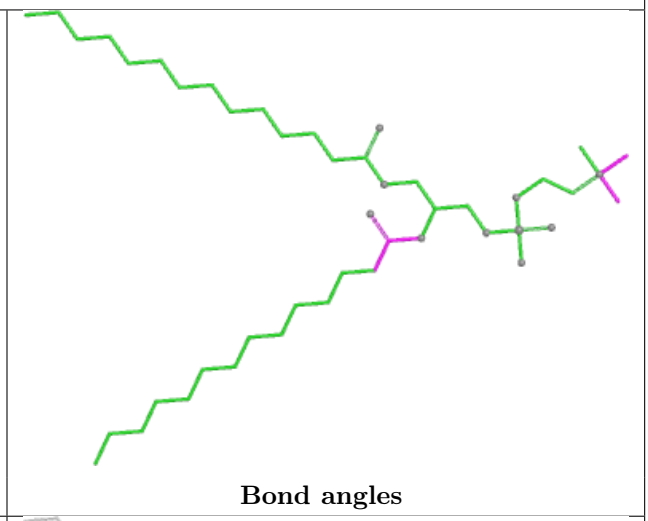


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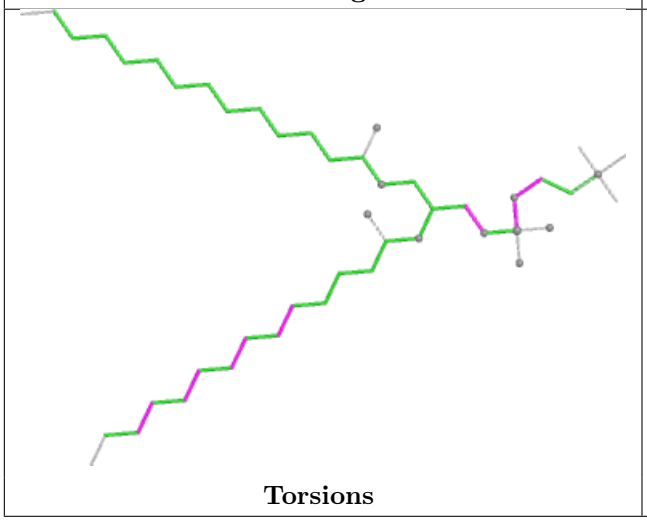
Ligand PX4 B 322



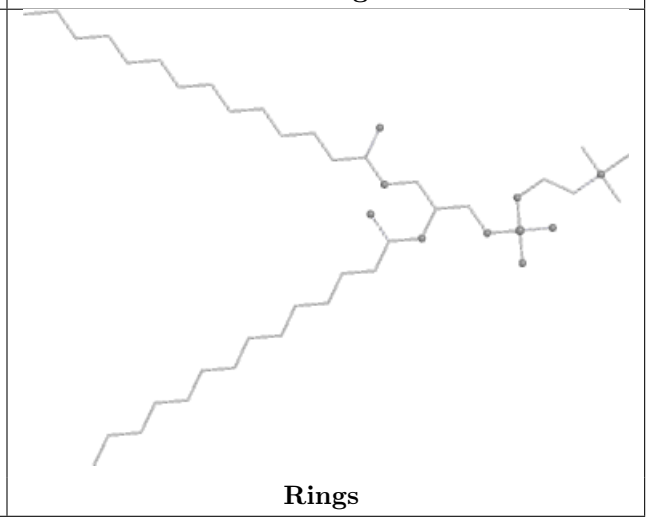
Bond lengths



Bond angles

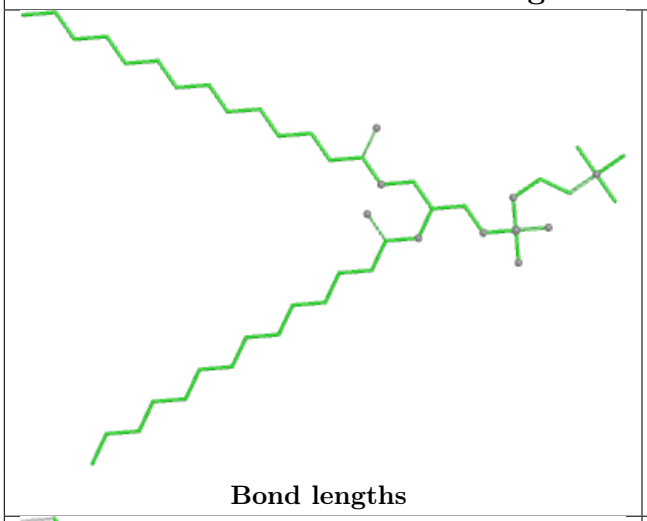


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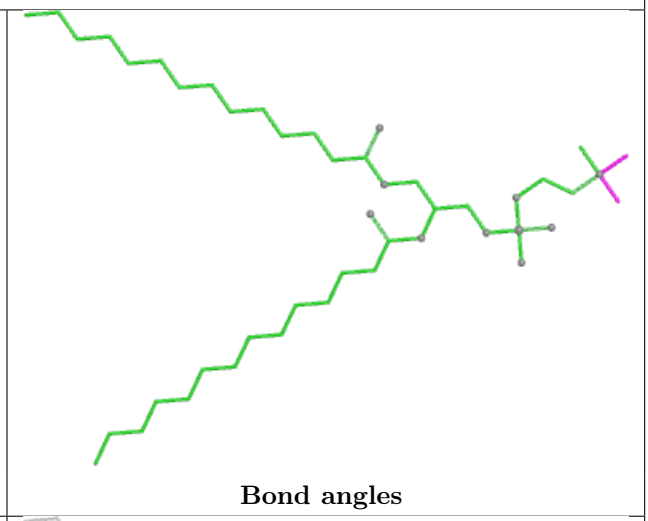


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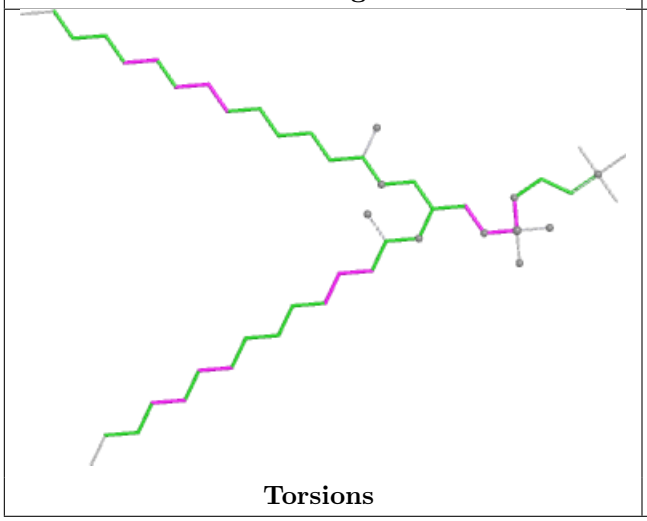
Ligand PX4 C 328



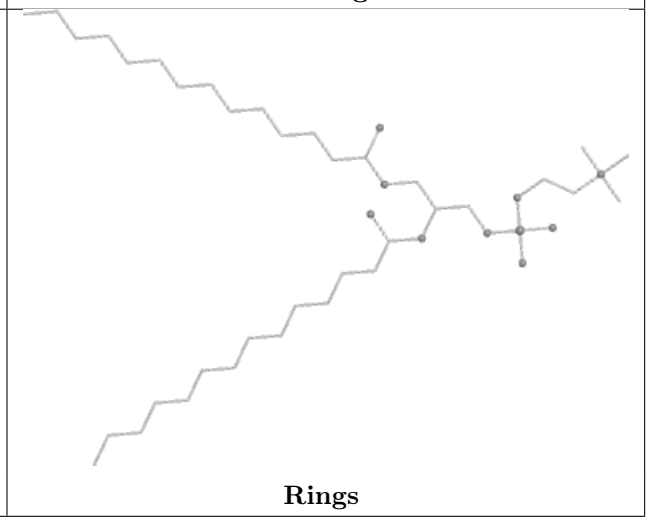
Bond lengths



Bond angles

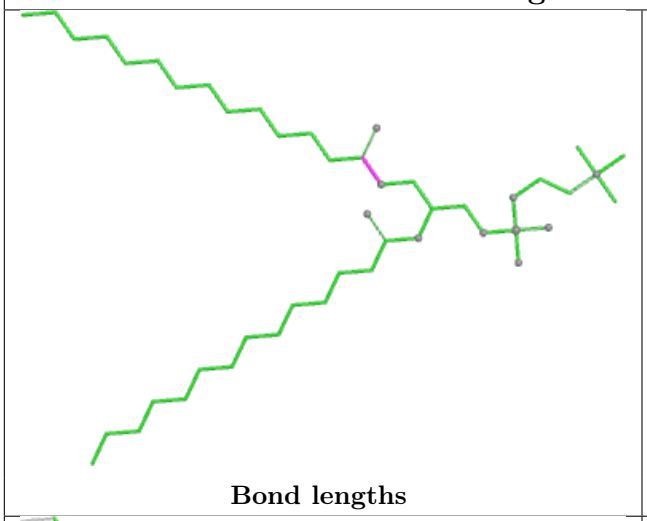


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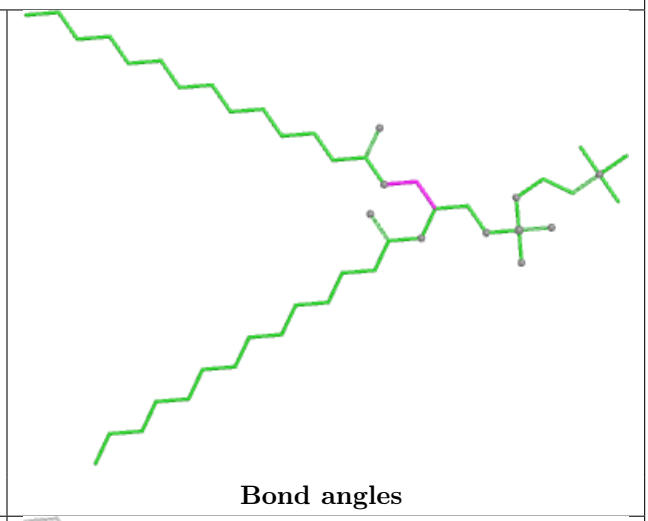


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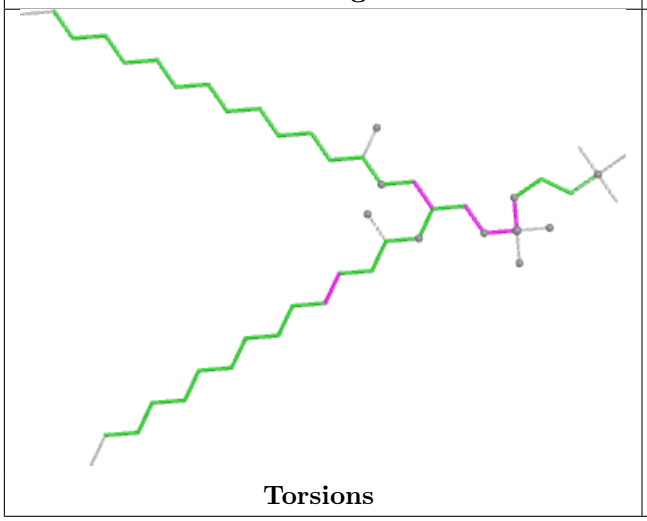
Ligand PX4 B 395



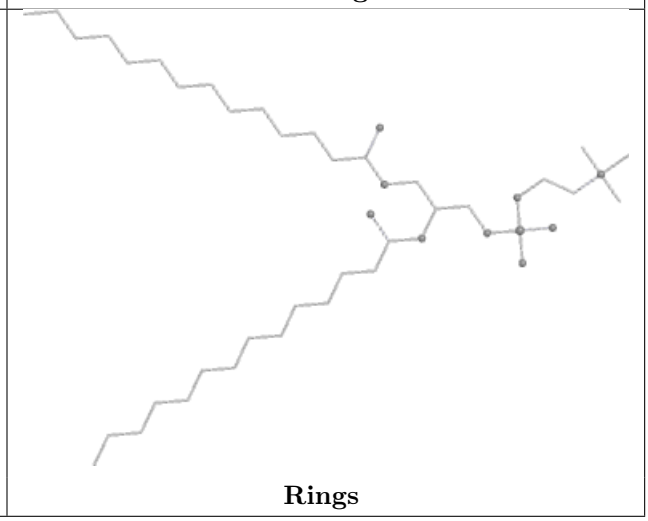
Bond lengths



Bond angles

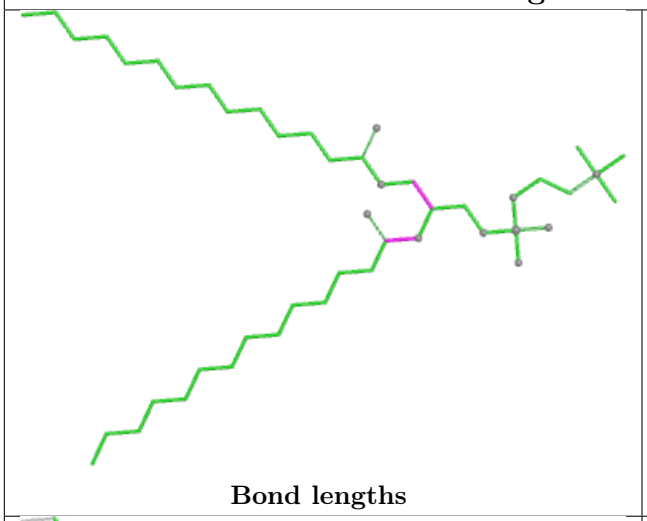


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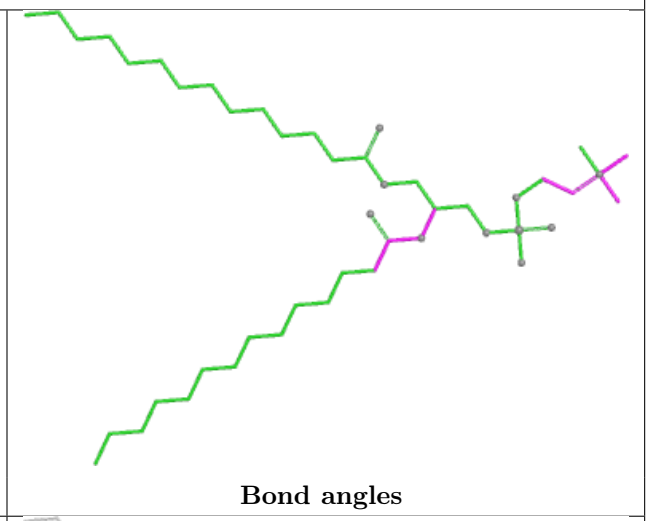


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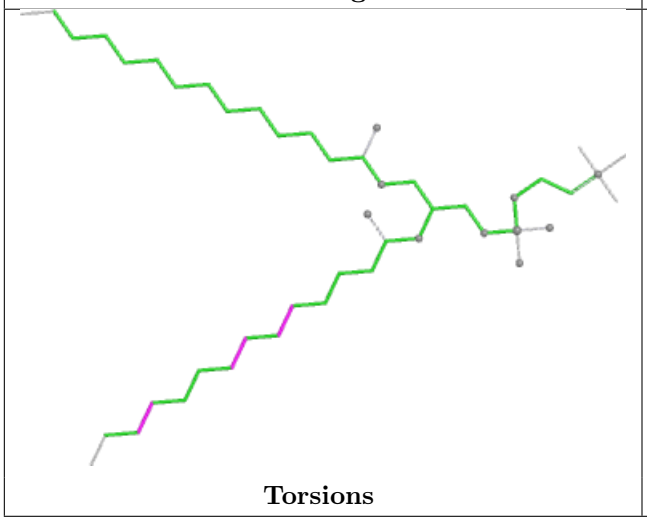
Ligand PX4 C 335



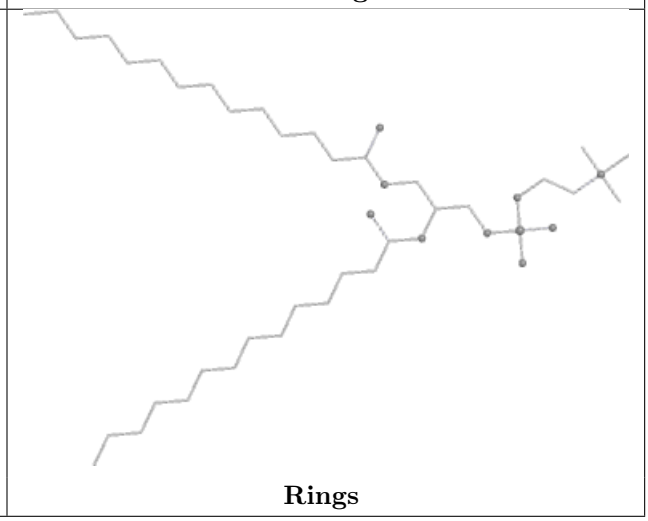
Bond lengths



Bond angles

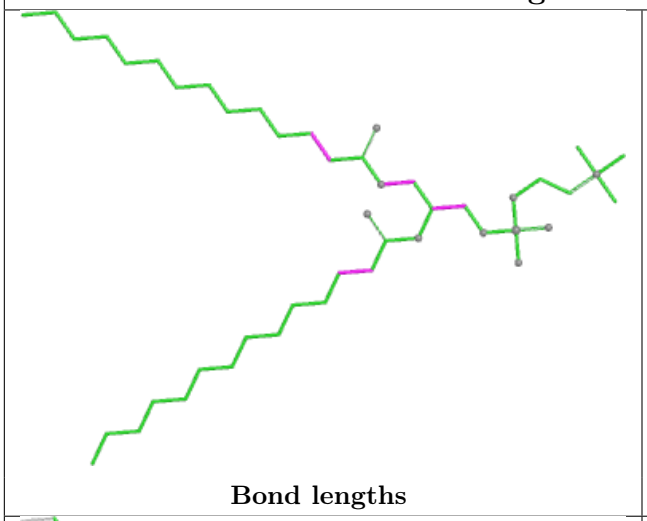


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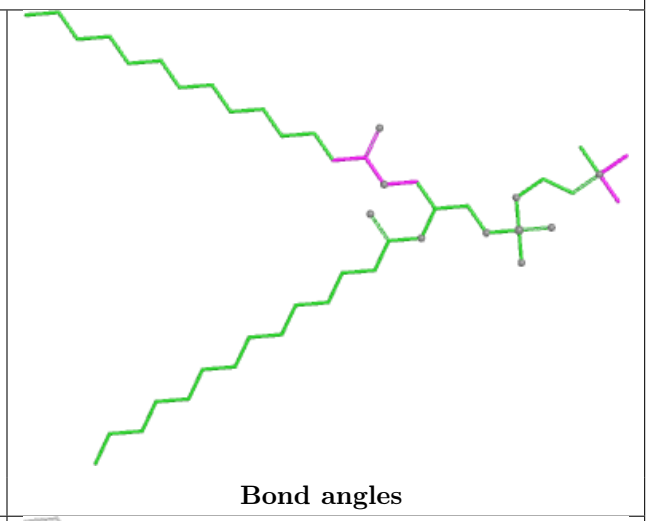


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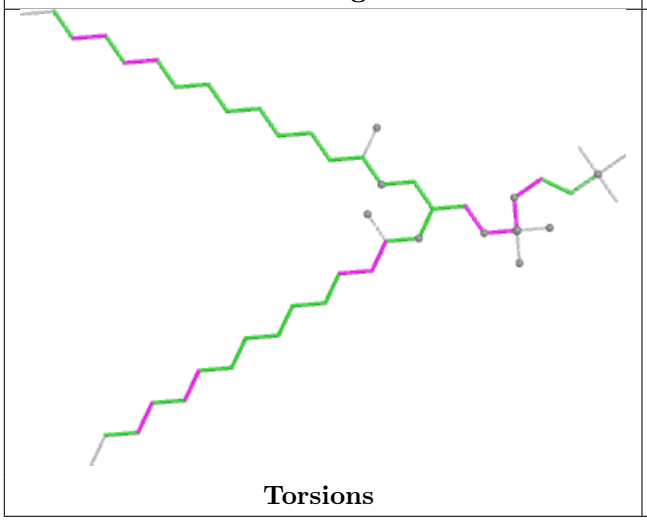
Ligand PX4 B 377



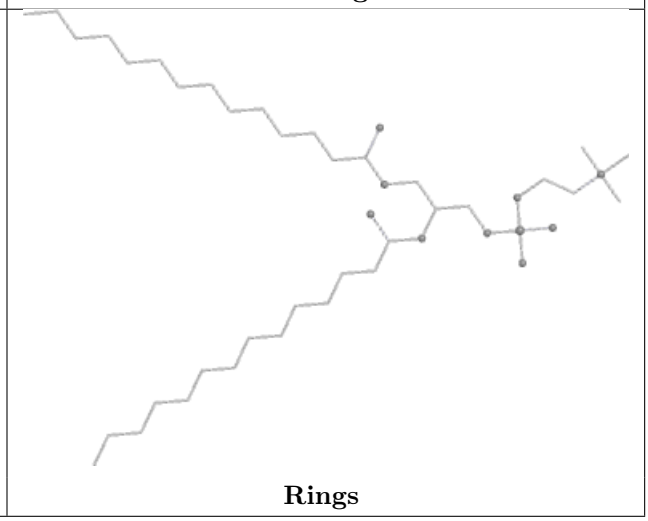
Bond lengths



Bond angles

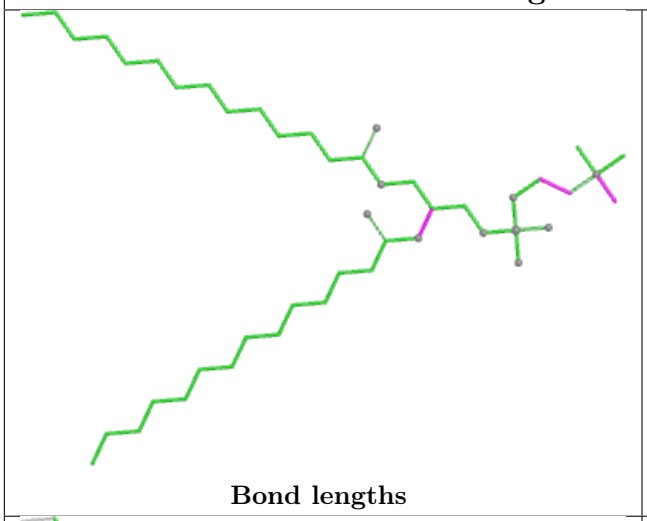


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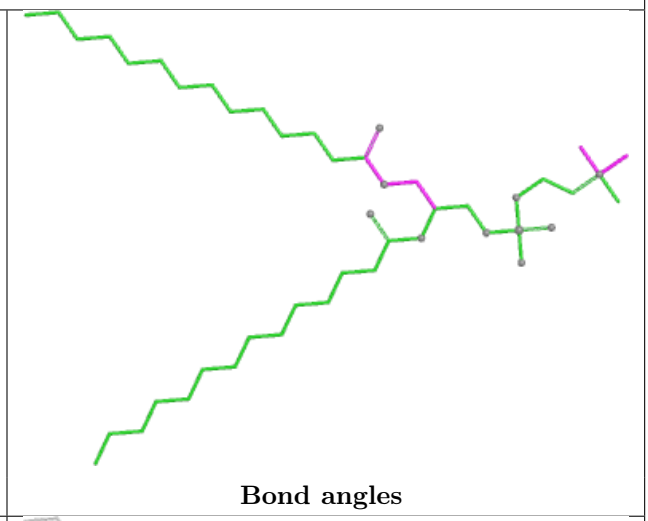


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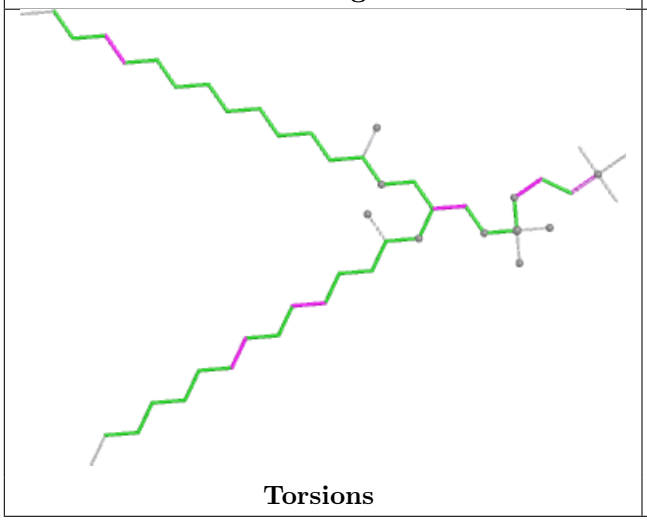
Ligand PX4 B 344



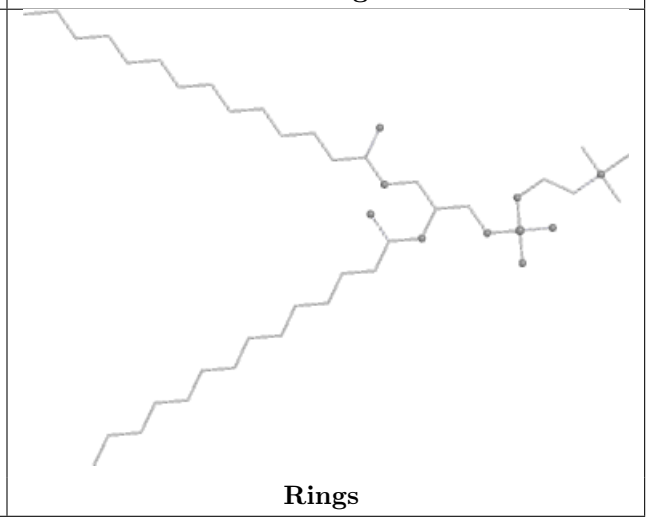
Bond lengths



Bond angles

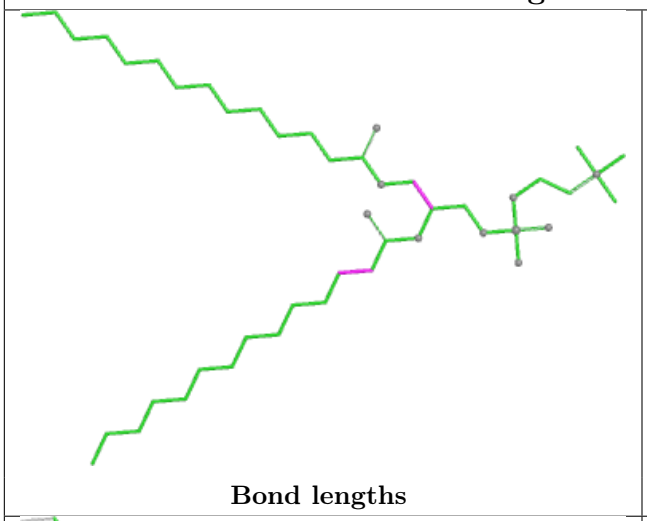


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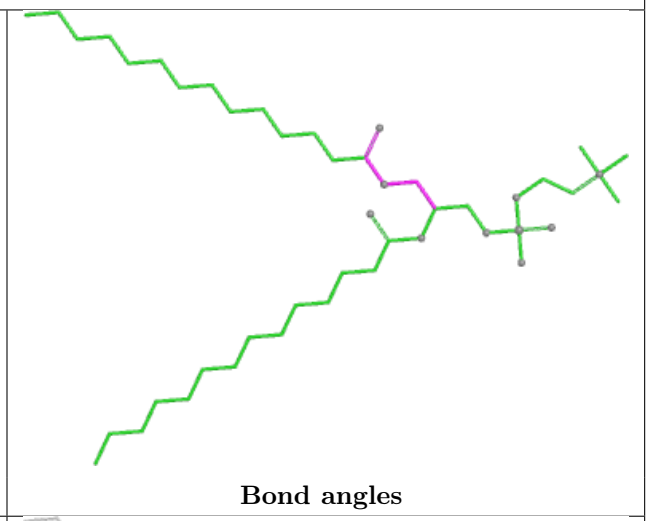


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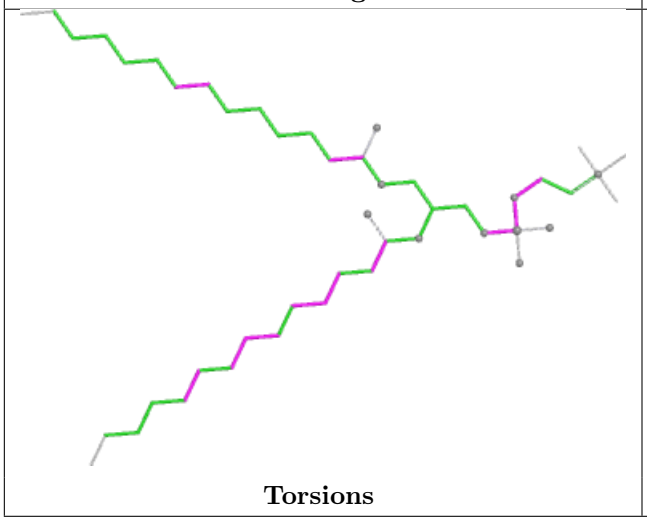
Ligand PX4 C 301



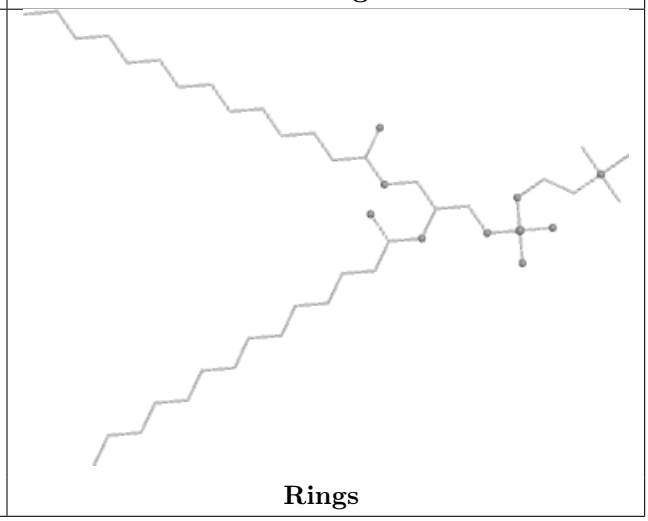
Bond lengths



Bond angles

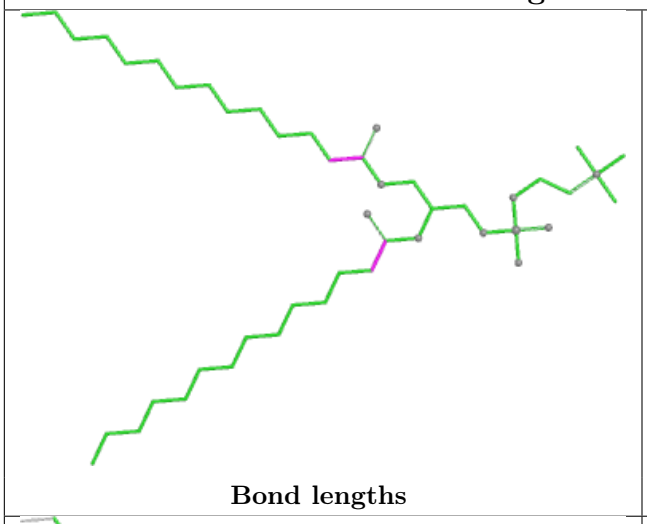


Torsions

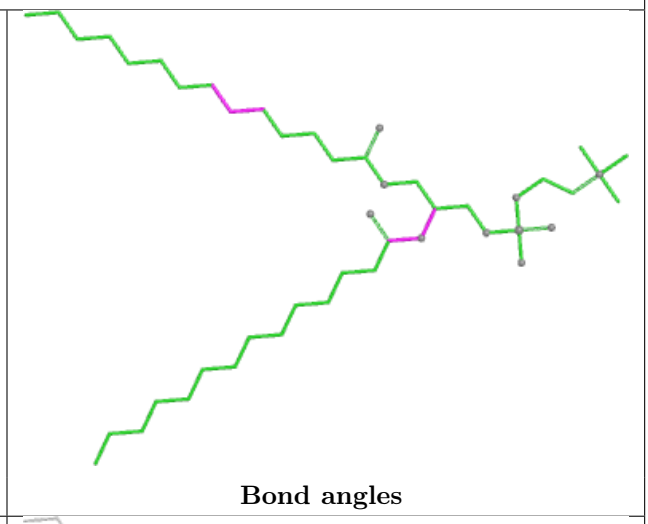


Rings

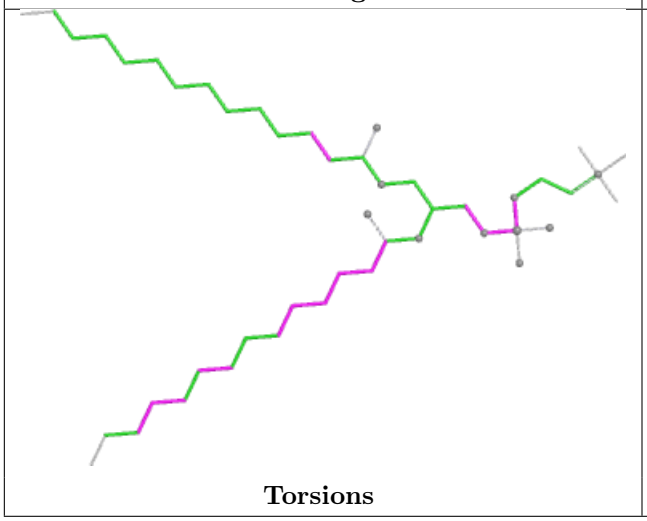
Ligand PX4 C 302



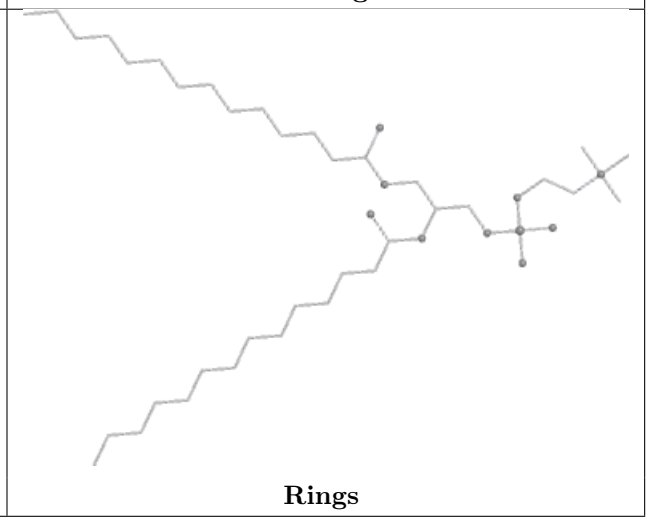
Bond lengths



Bond angles

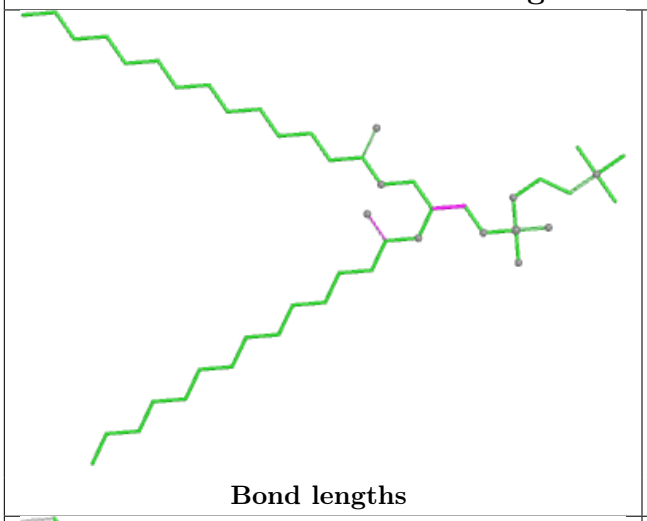


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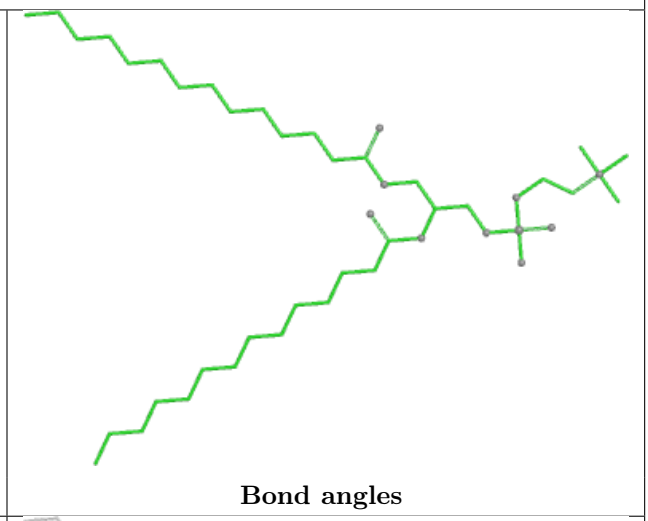


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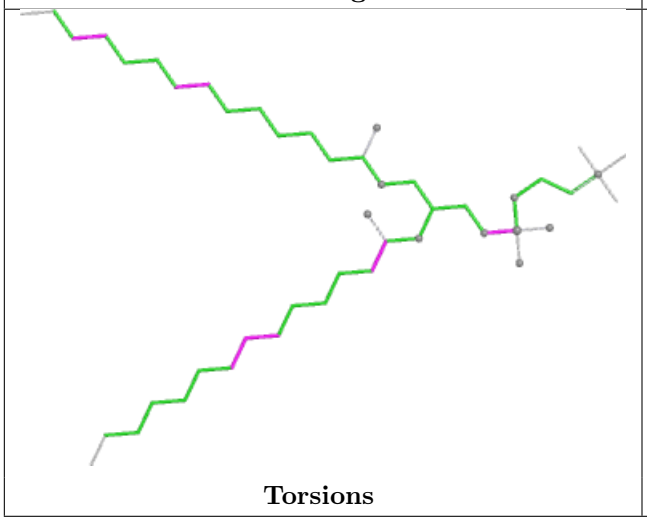
Ligand PX4 A 616



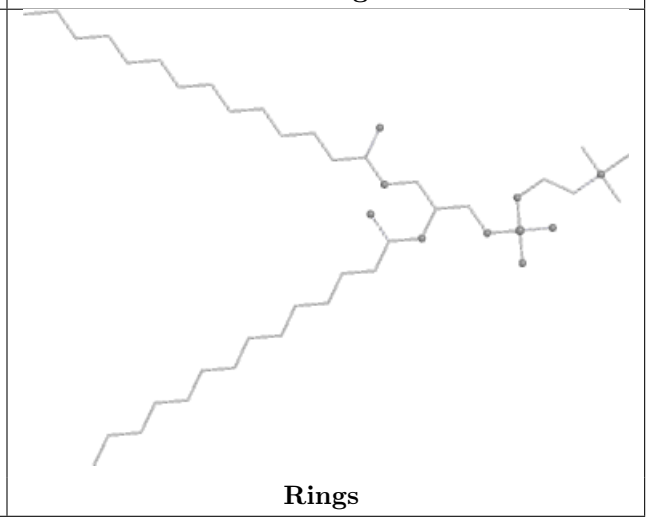
Bond lengths



Bond angles

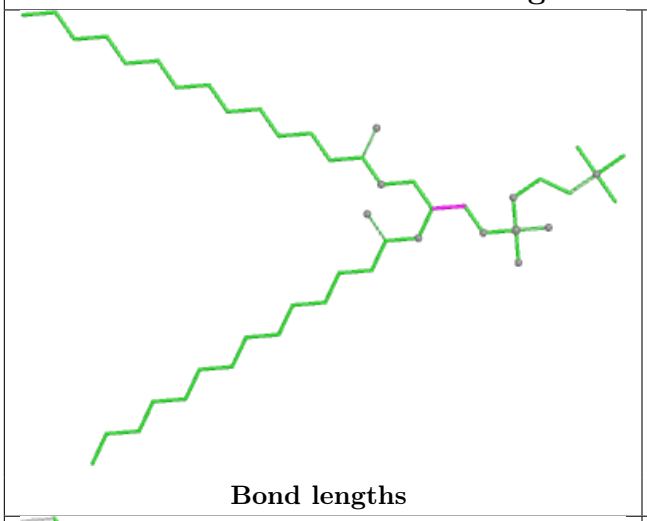


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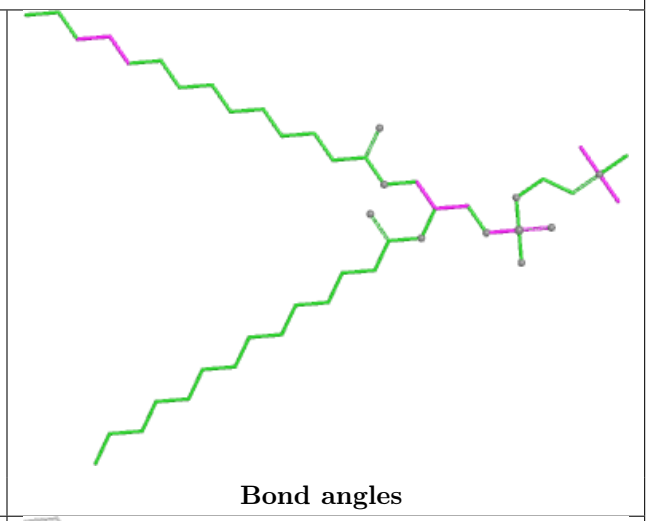


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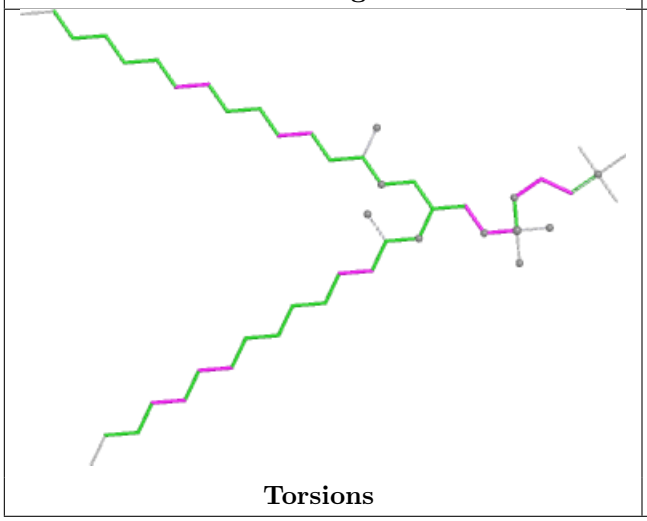
Ligand PX4 B 400



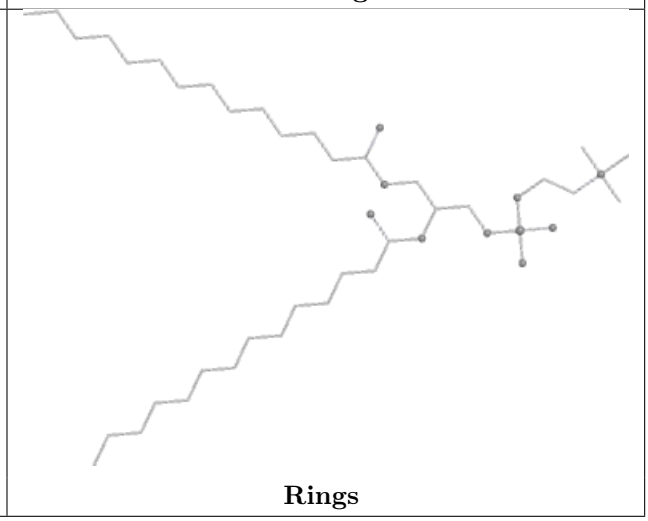
Bond lengths



Bond angles

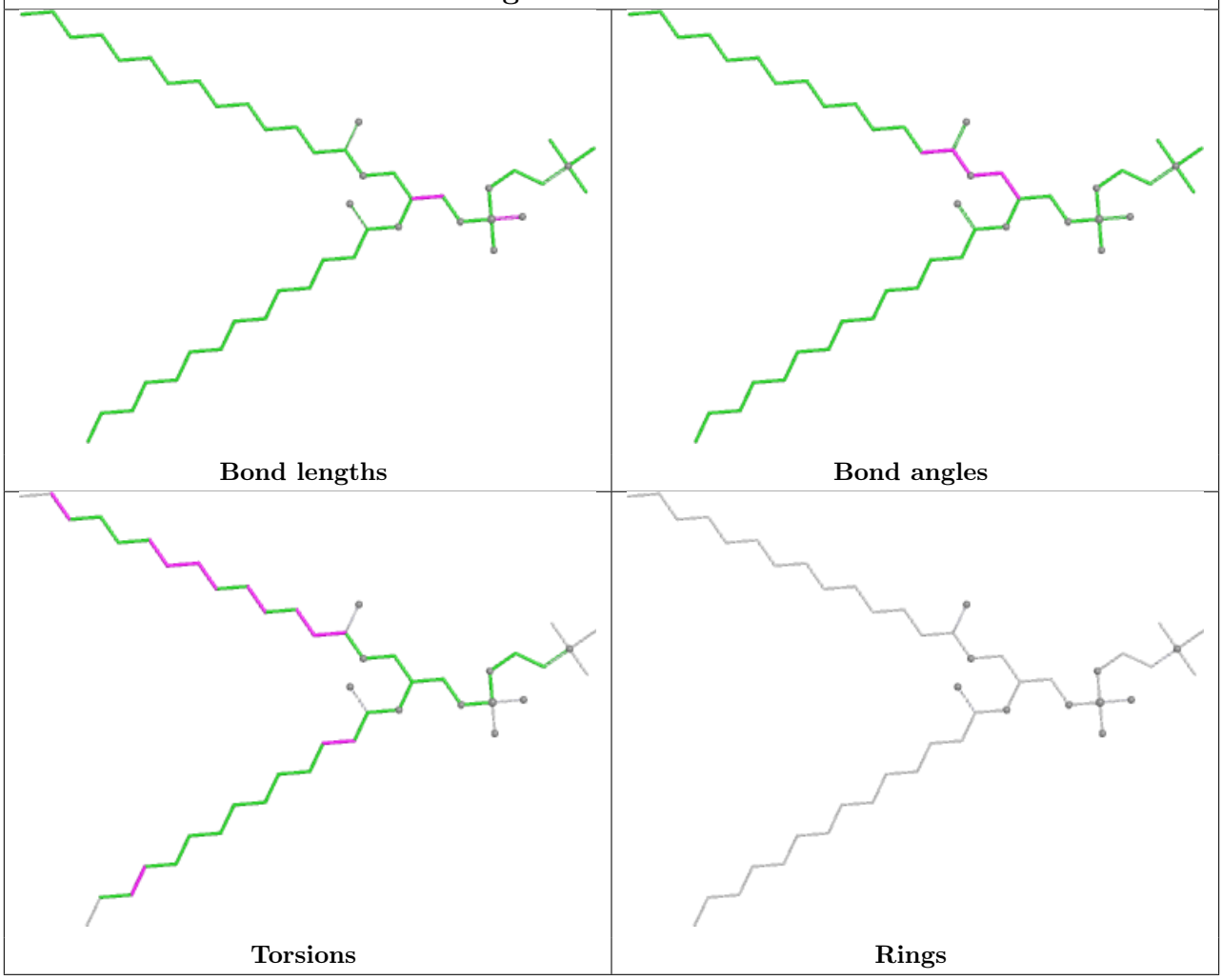


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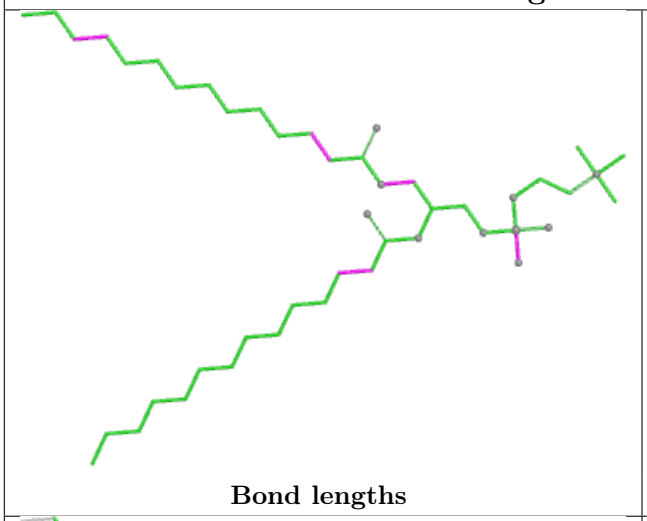


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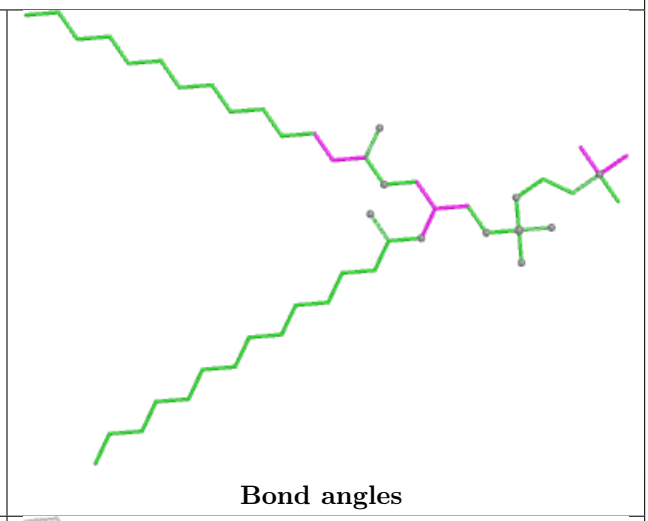
Ligand PX4 C 310



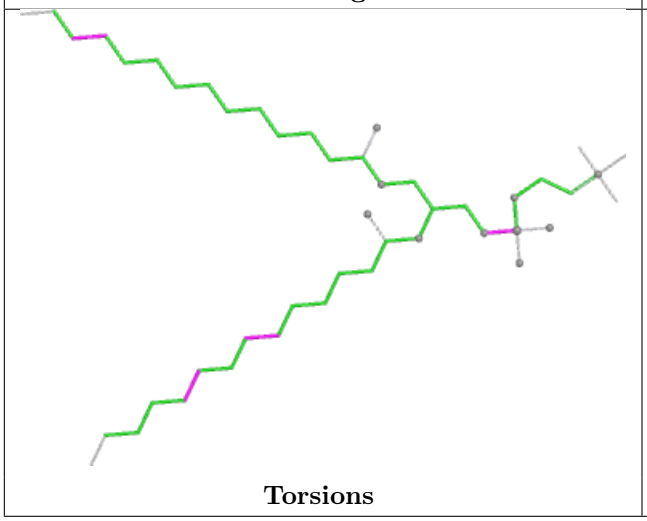
Ligand PX4 B 319



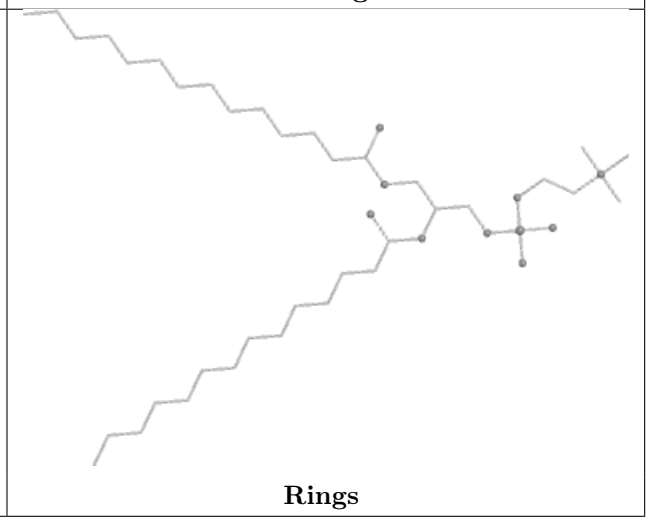
Bond lengths



Bond angles

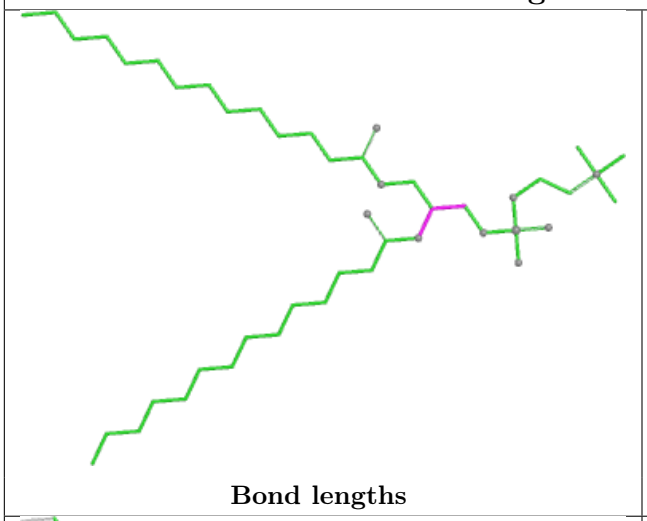


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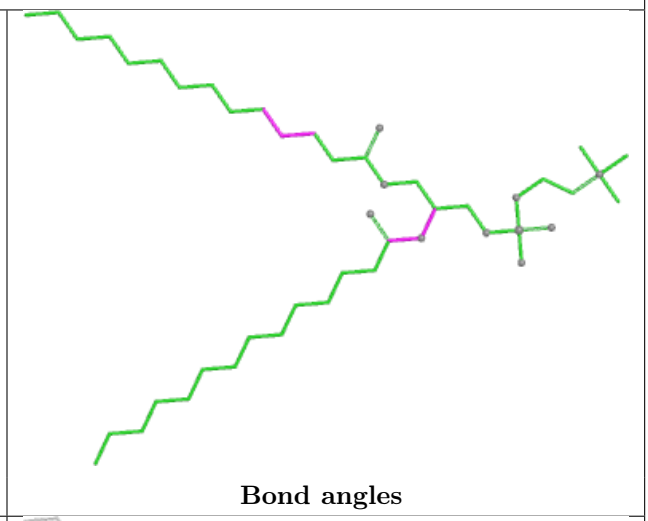


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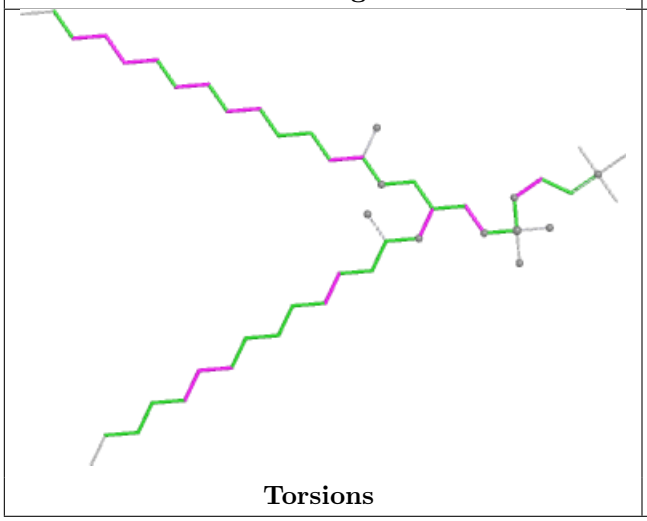
Ligand PX4 B 306



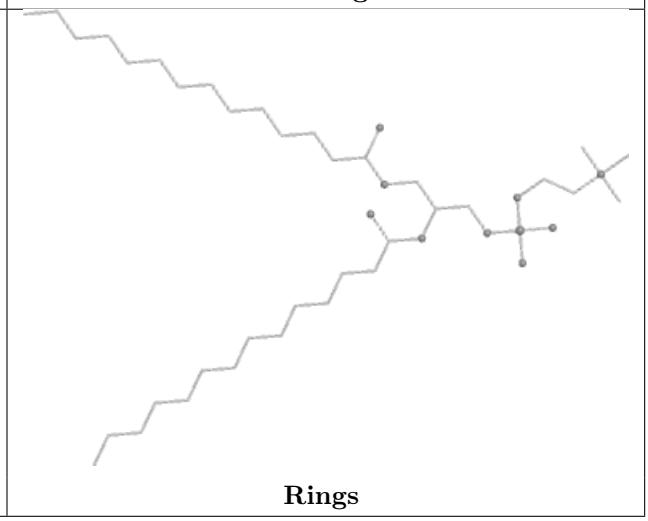
Bond lengths



Bond angles

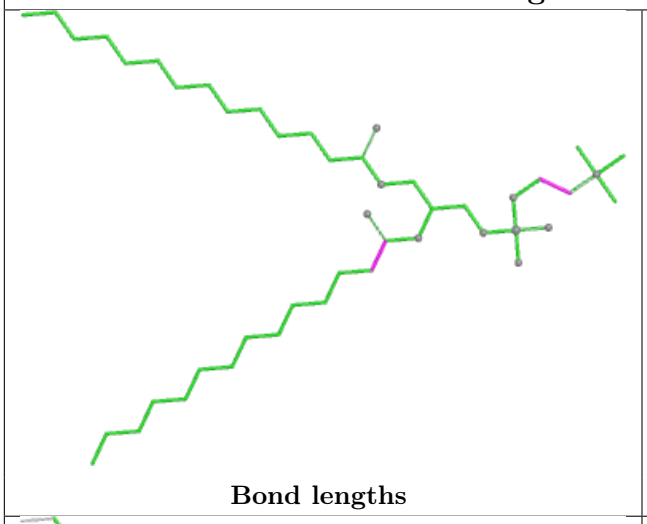


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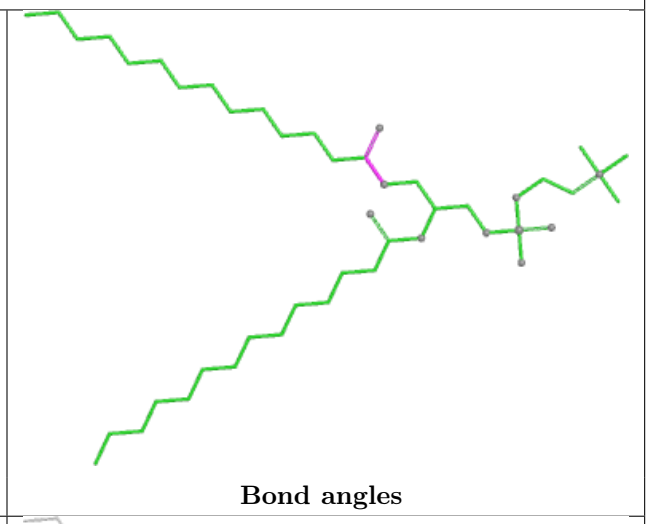


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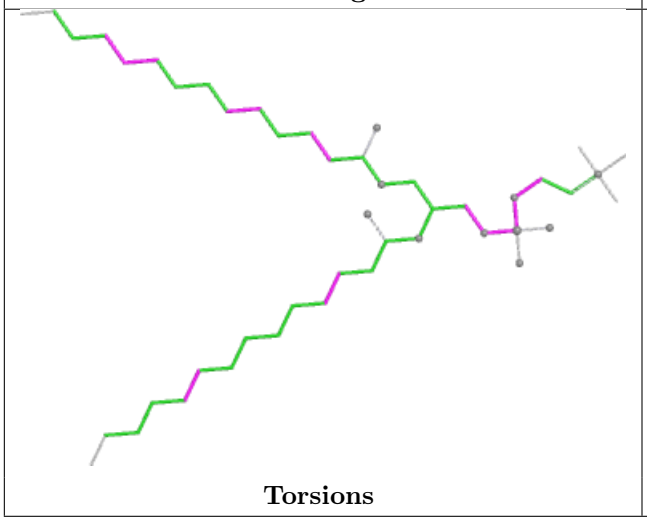
Ligand PX4 C 352



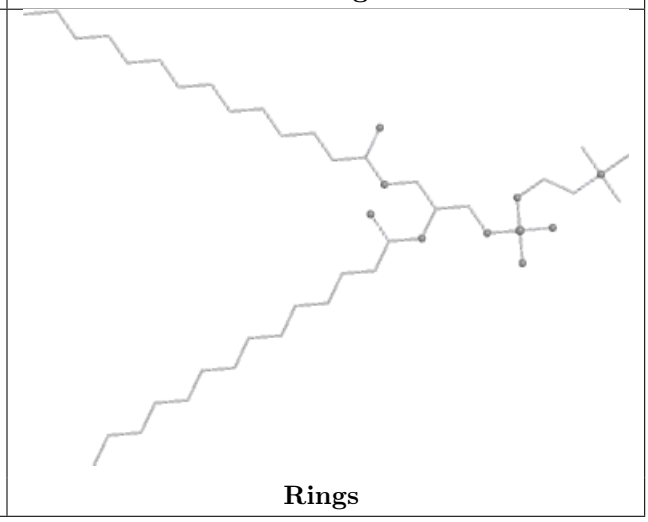
Bond lengths



Bond angles

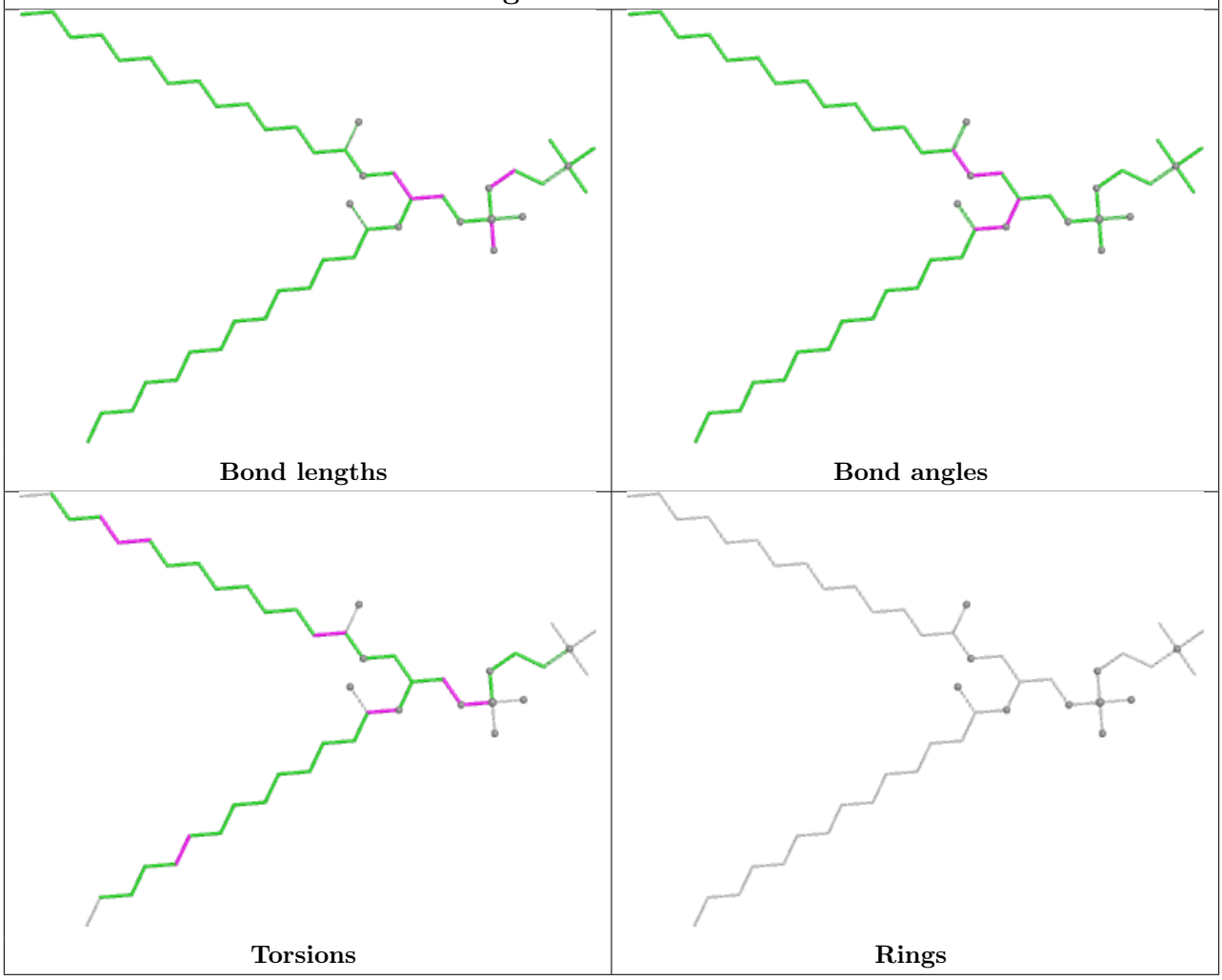


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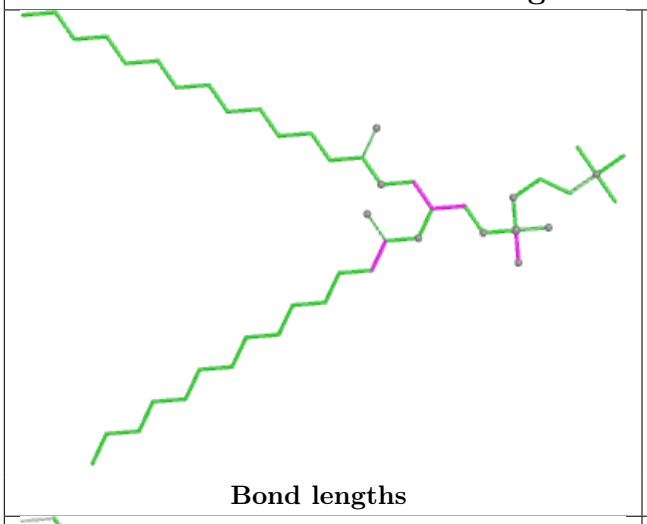


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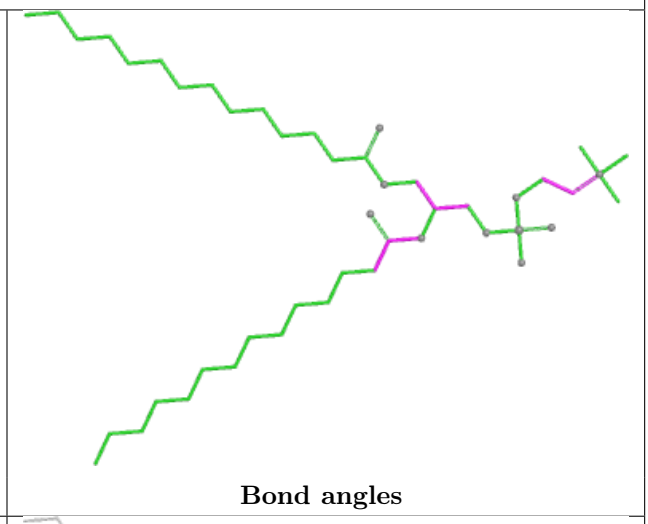
Ligand PX4 B 399



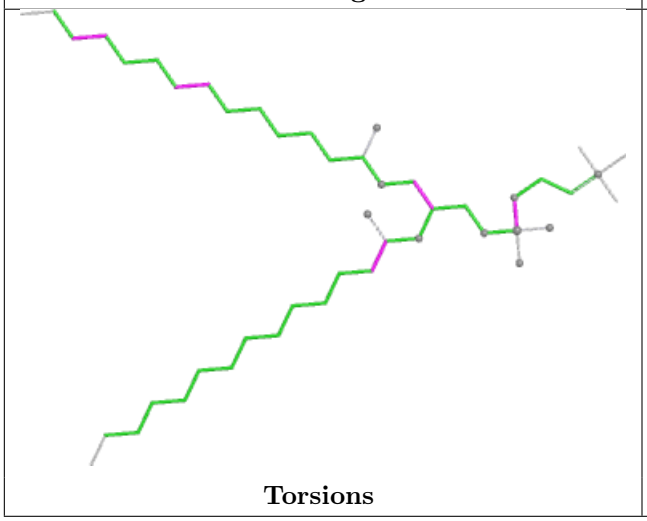
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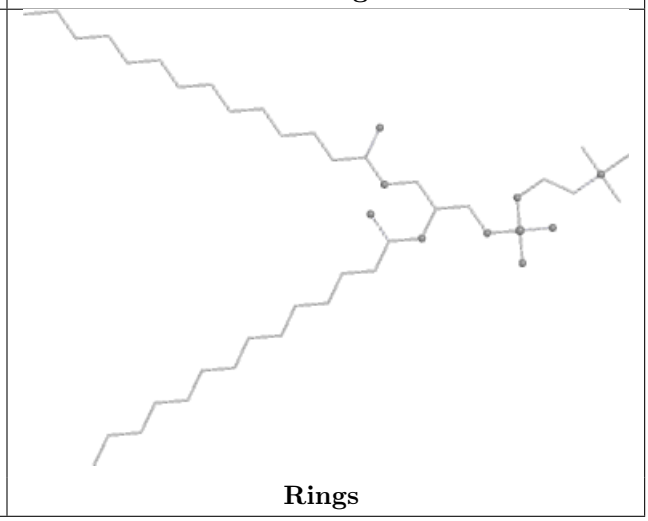
Bond lengths



Bond angles

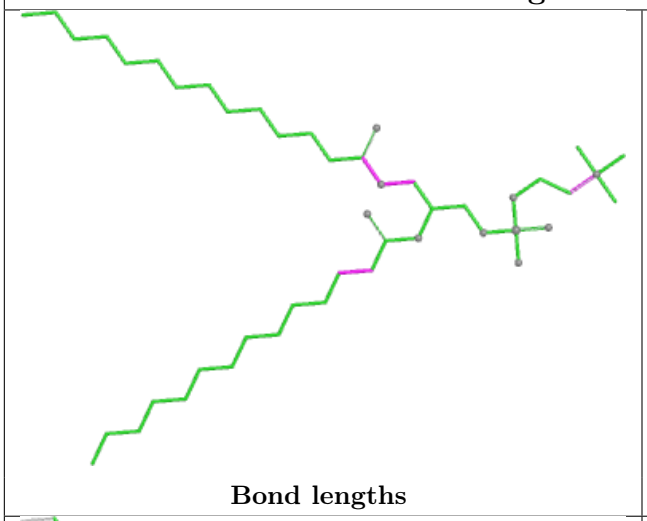


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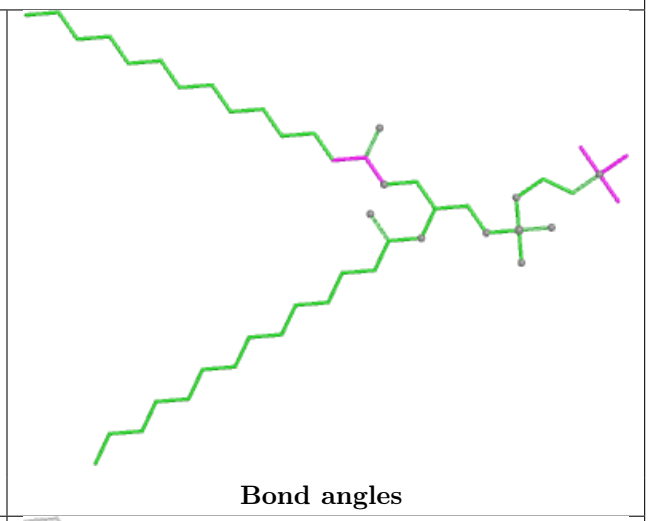


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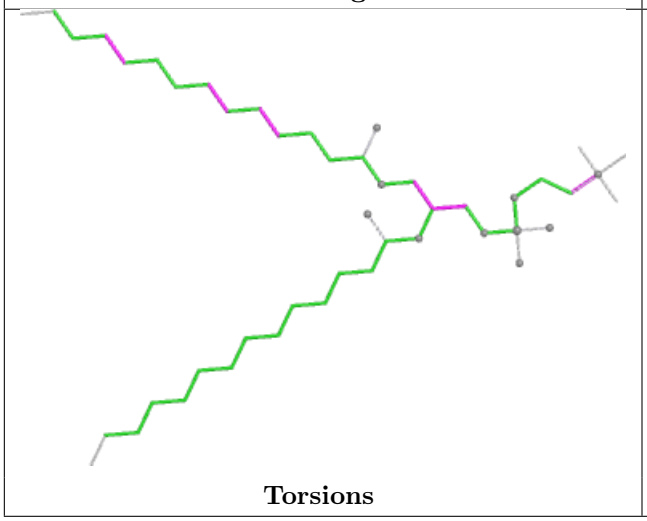
Ligand PX4 B 329



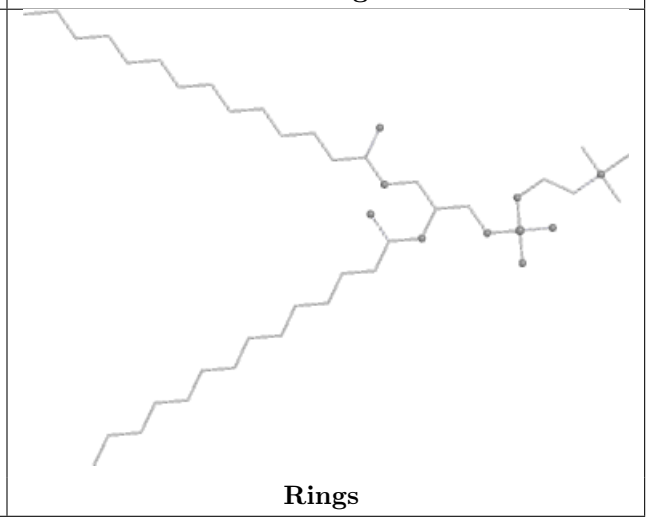
Bond lengths



Bond angles

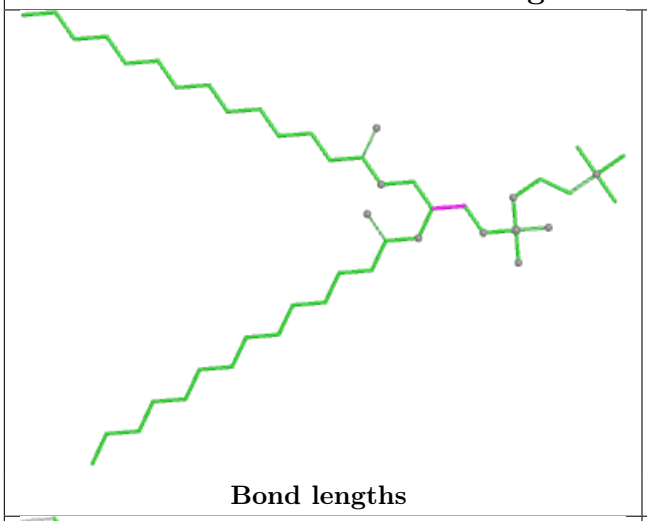


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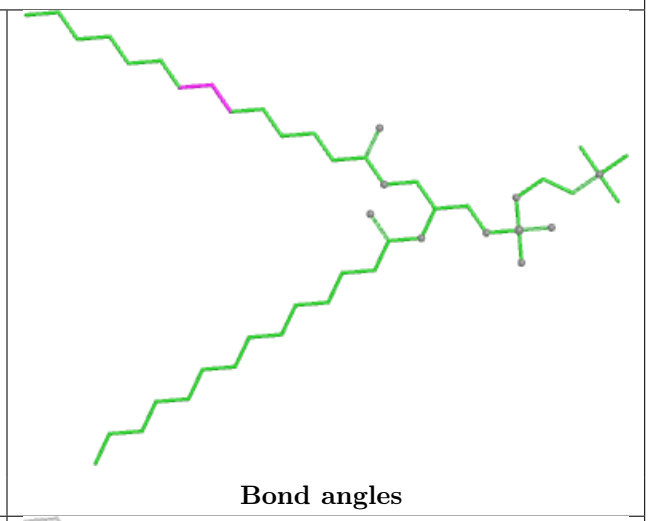


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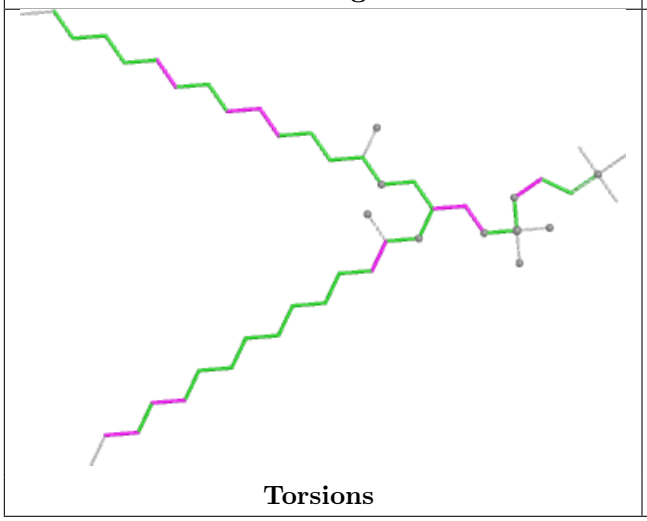
Ligand PX4 A 604



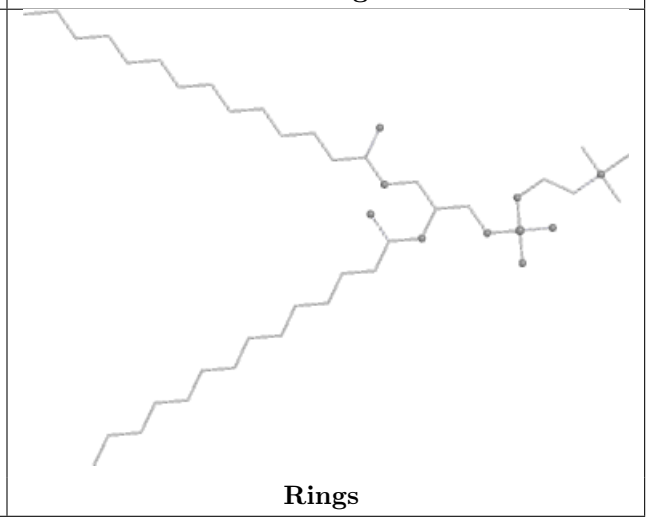
Bond lengths



Bond angles

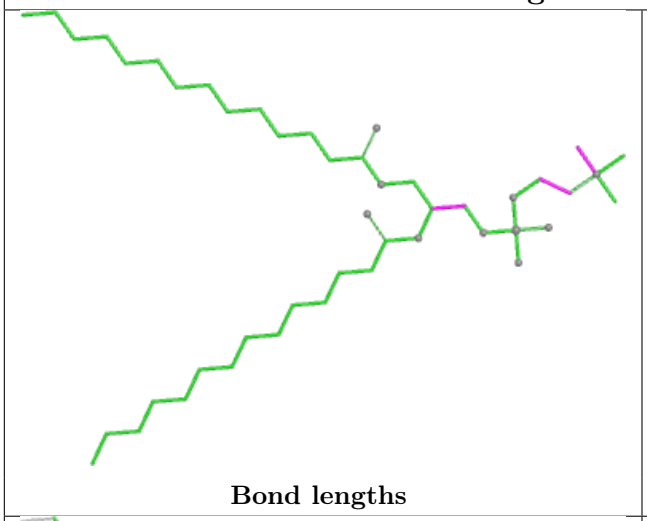


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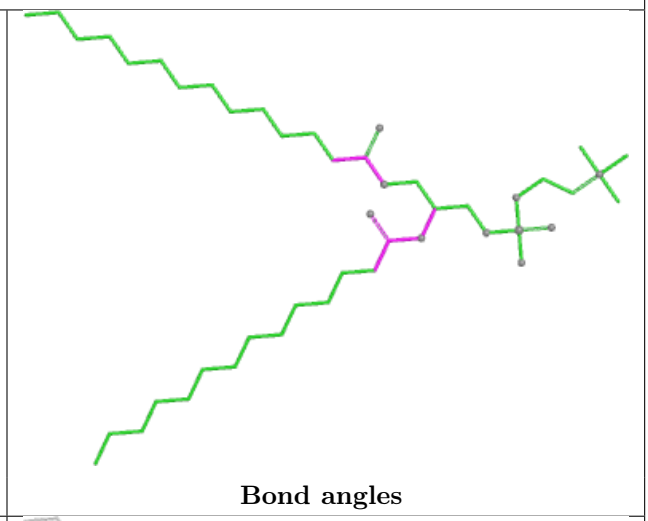


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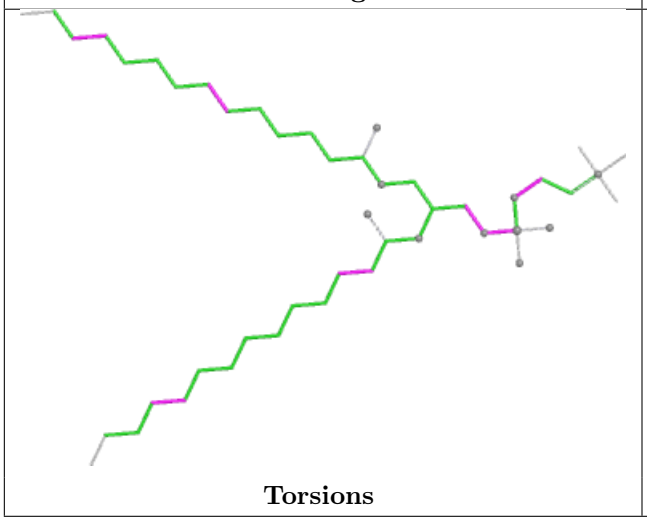
Ligand PX4 A 641



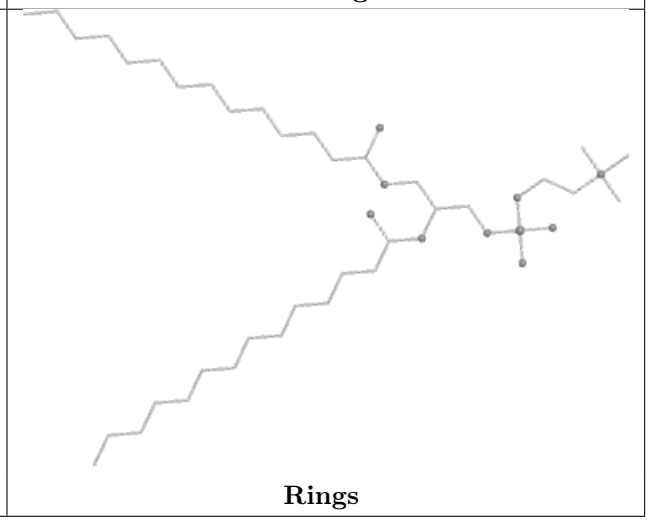
Bond lengths



Bond angles

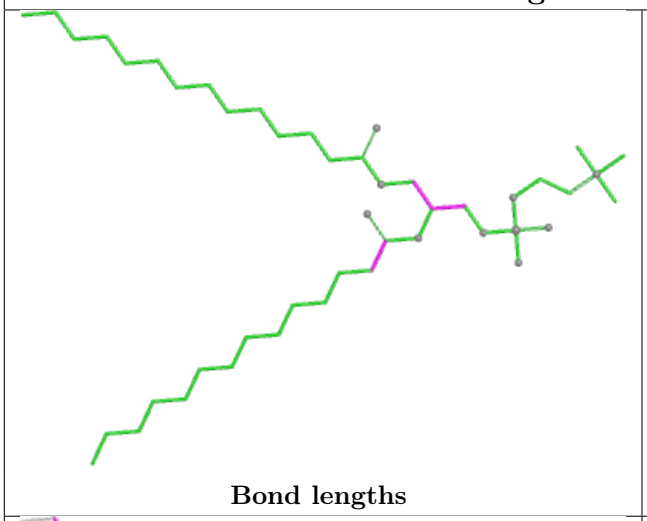


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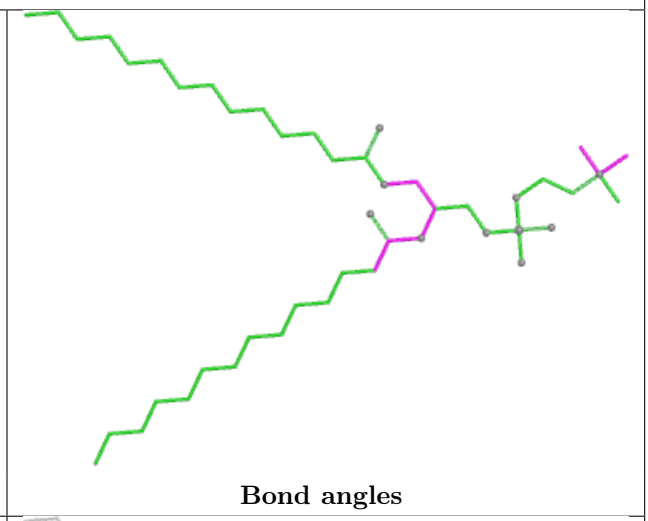


Rings

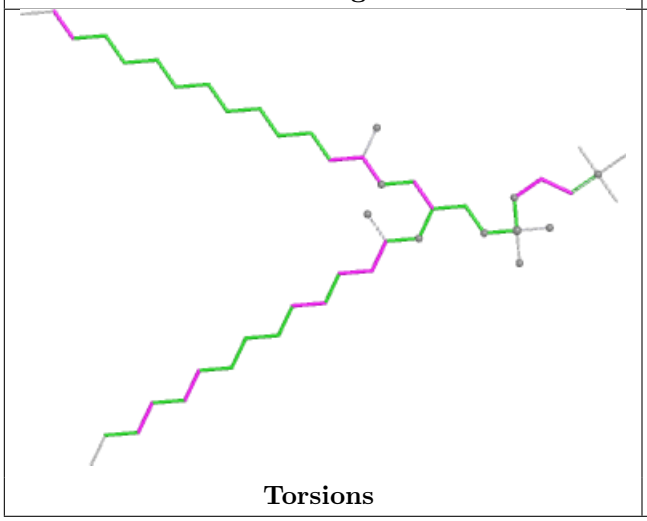
Ligand PX4 C 345



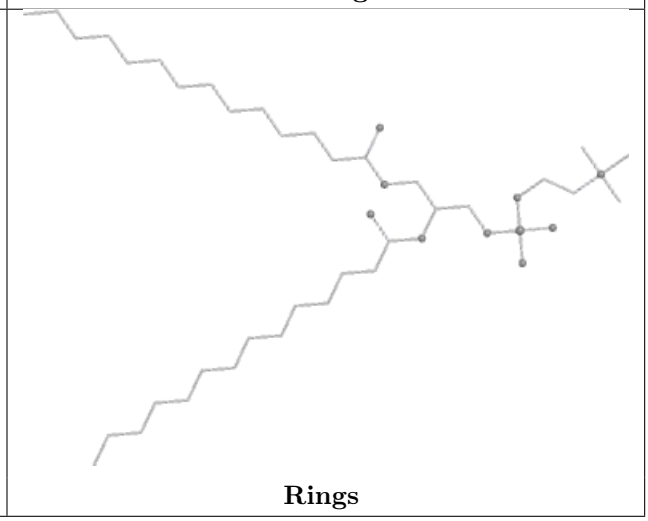
Bond lengths



Bond angles

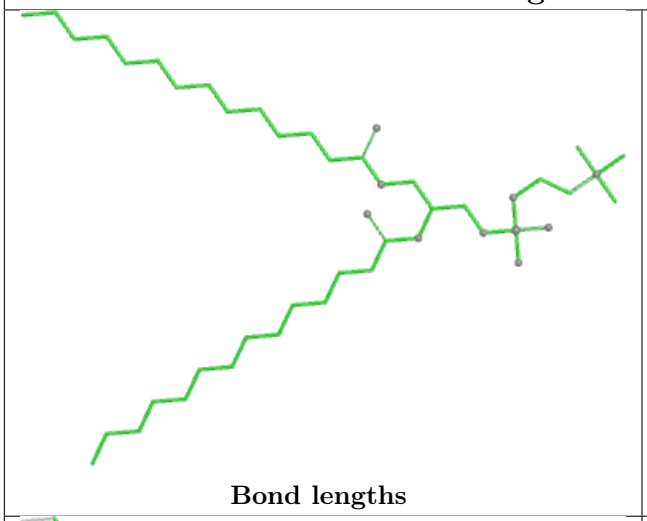


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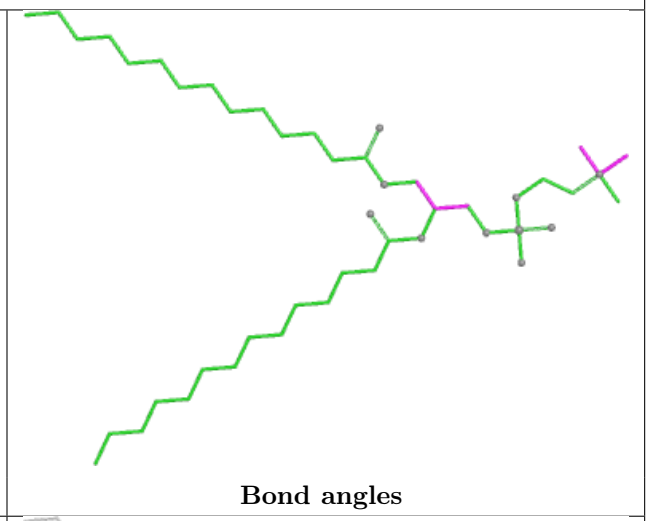


Rings

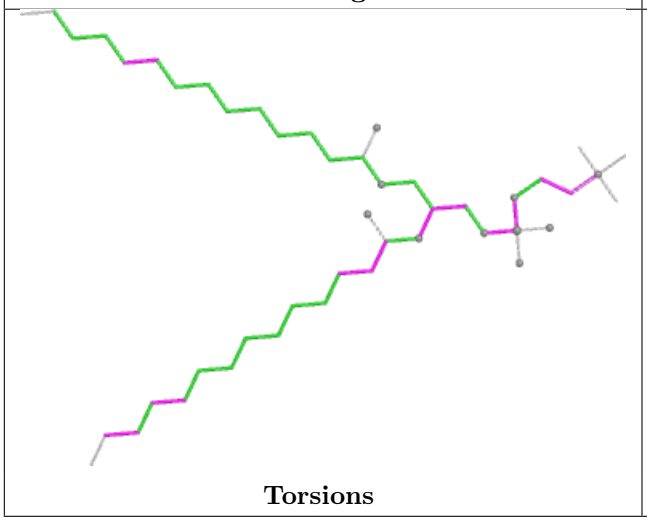
Ligand PX4 A 615



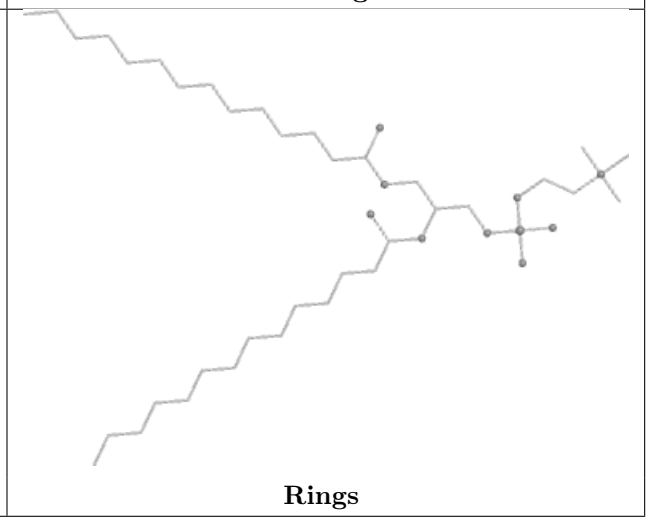
Bond lengths



Bond angles

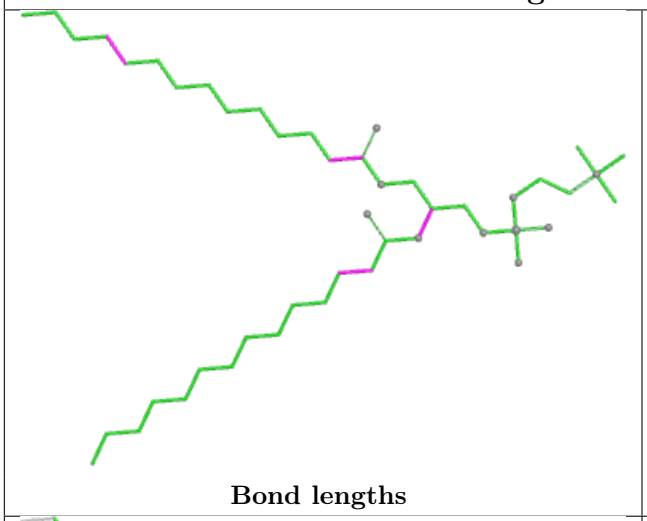


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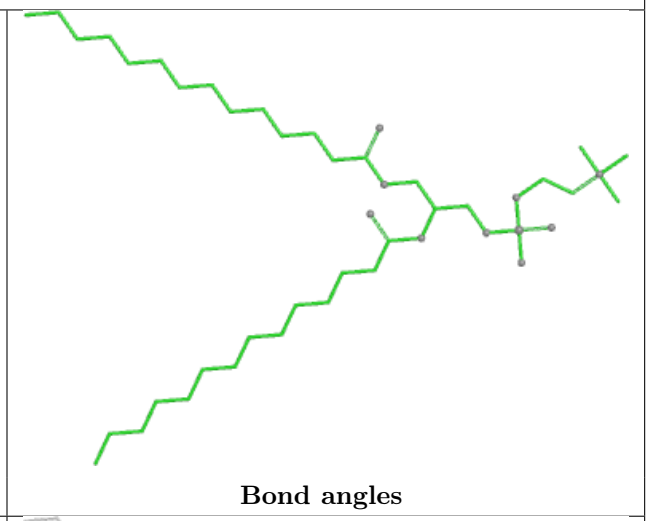


Rings

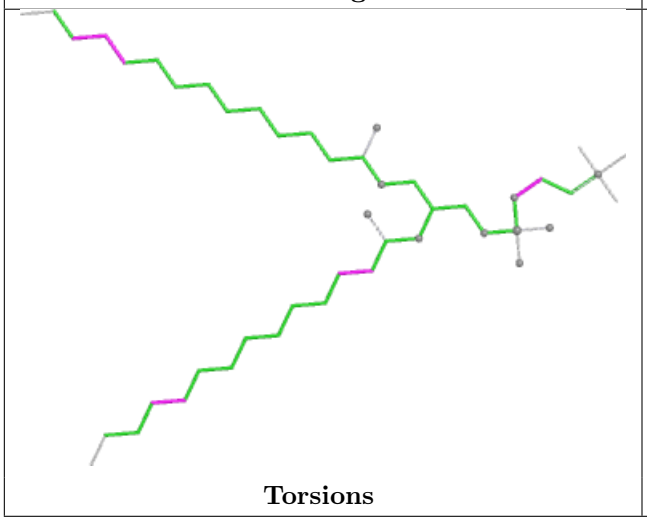
Ligand PX4 A 642



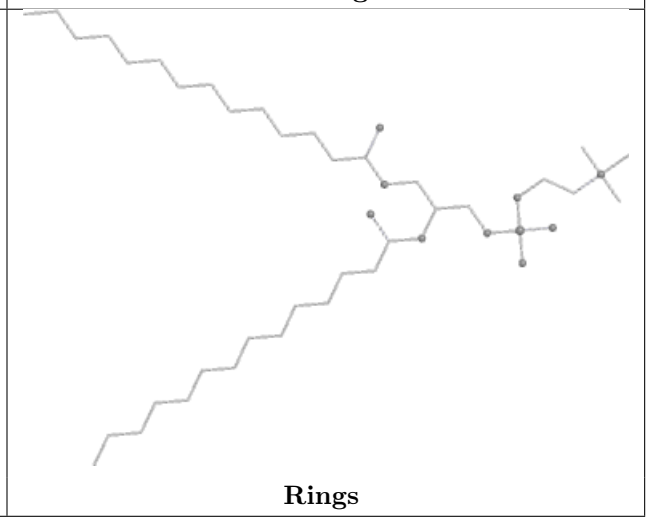
Bond lengths



Bond angles

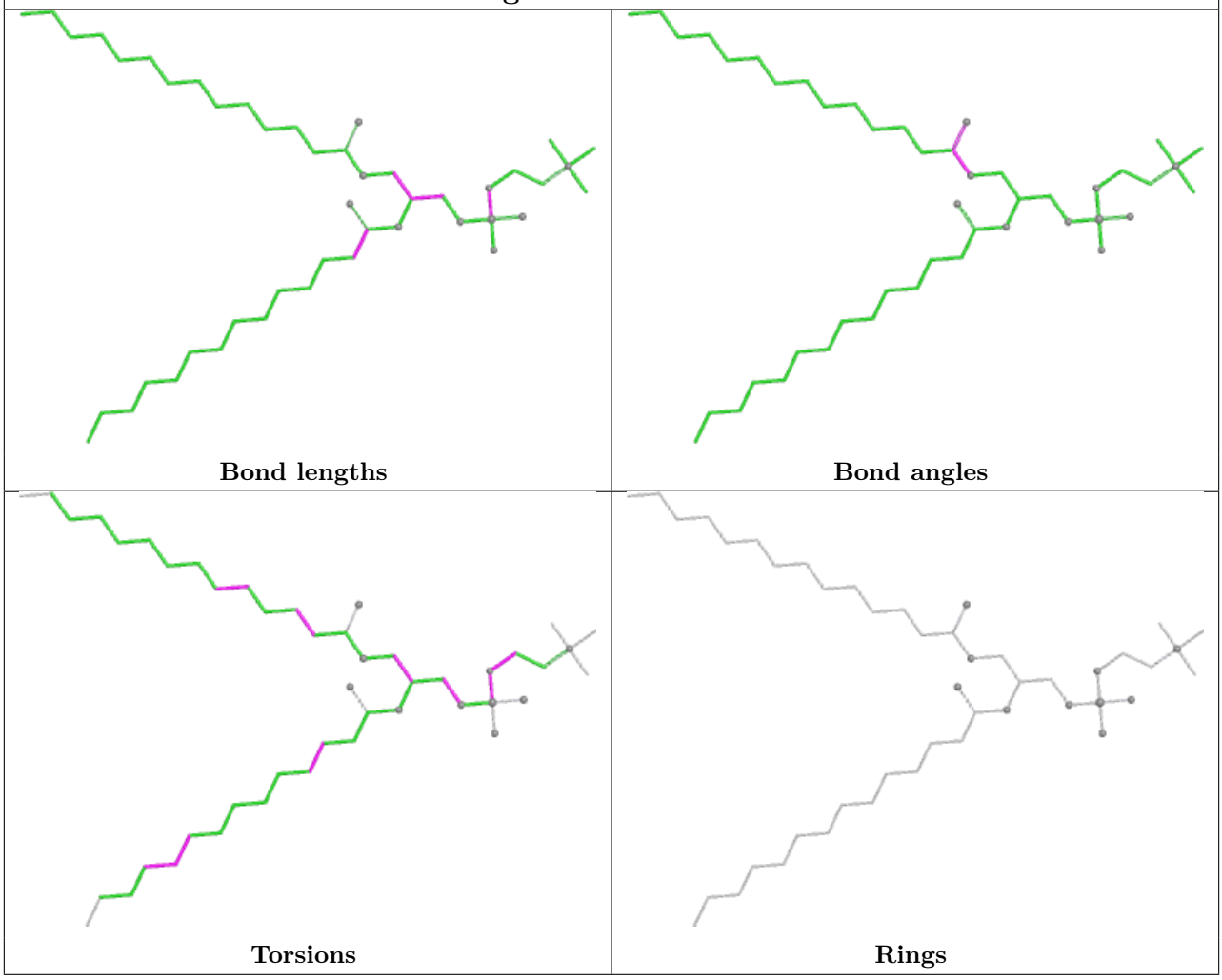


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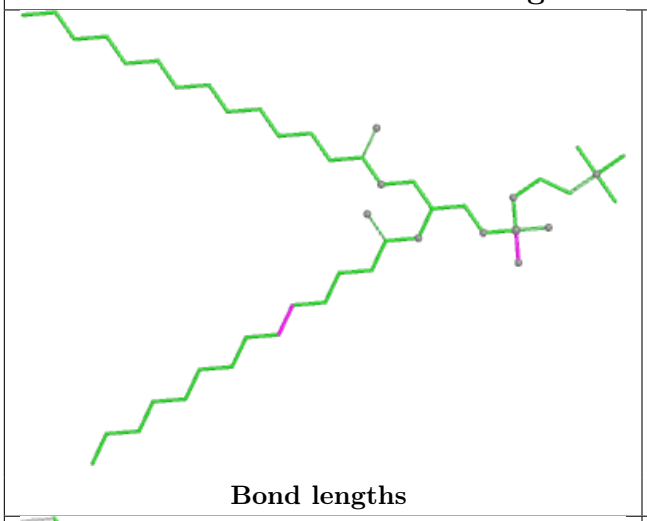


Rings

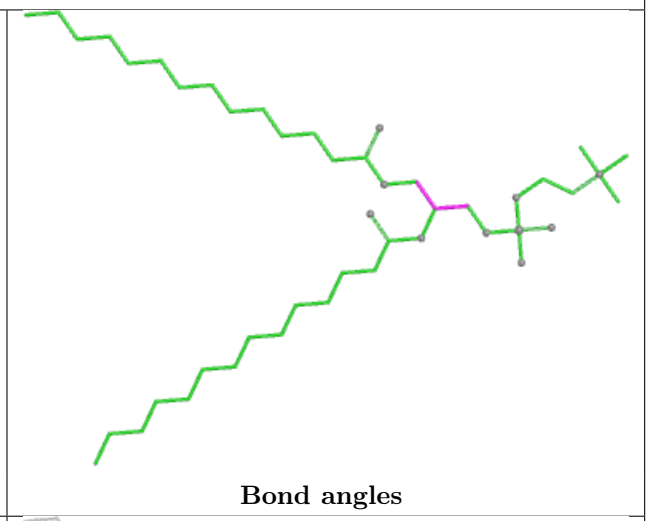
Ligand PX4 B 335



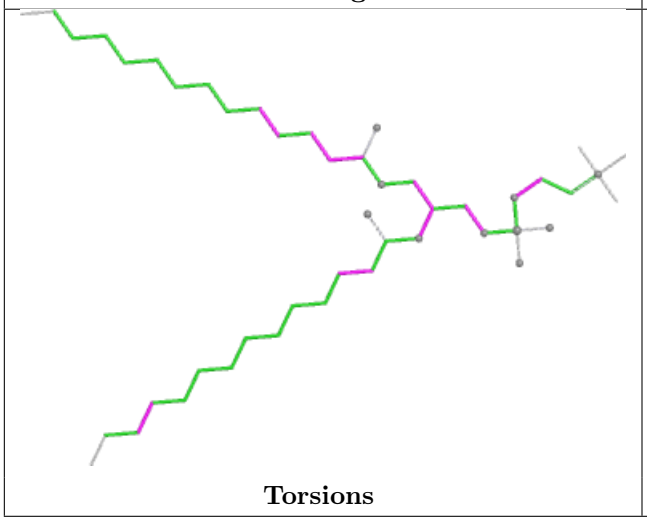
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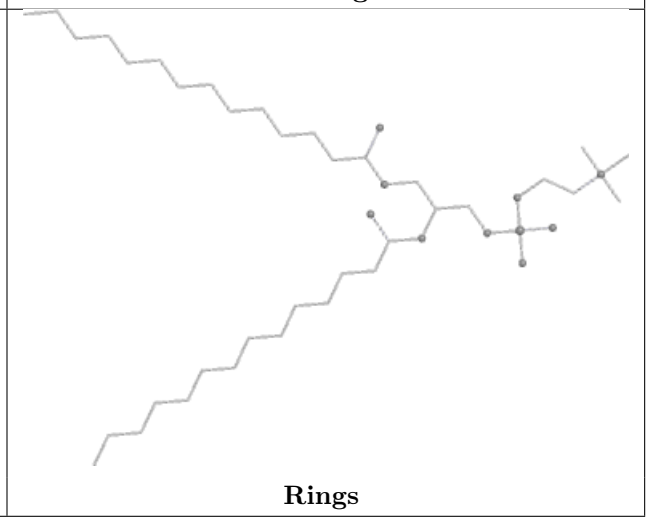
Bond lengths



Bond angles

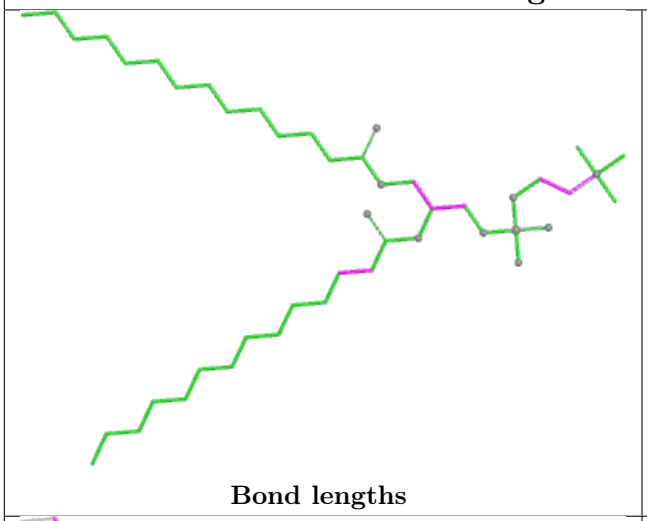


Torsions

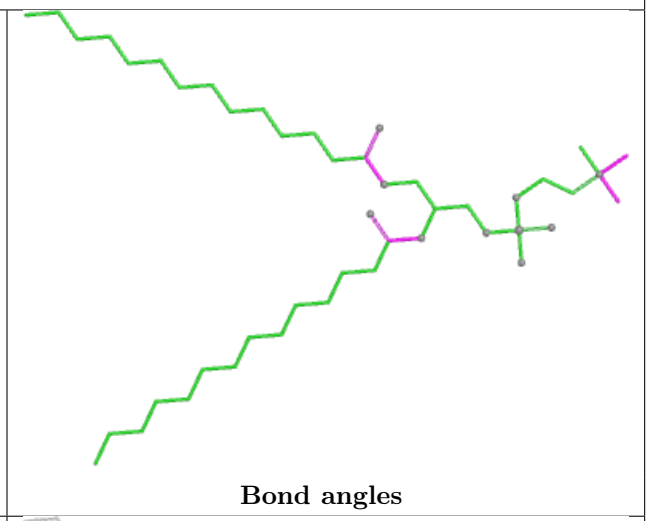


Rings

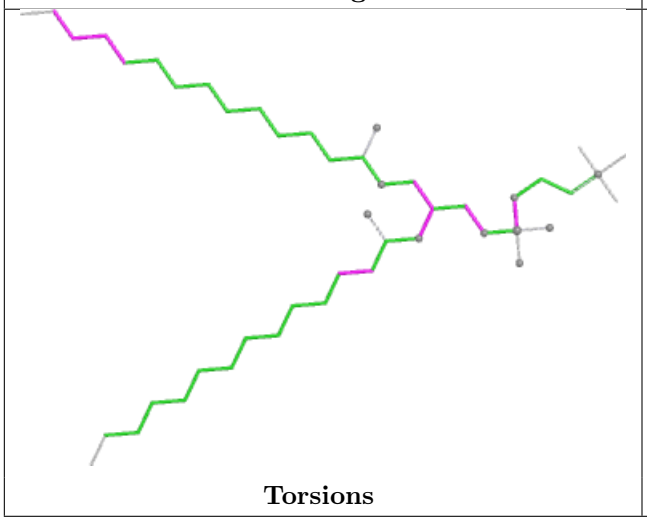
Ligand PX4 C 359



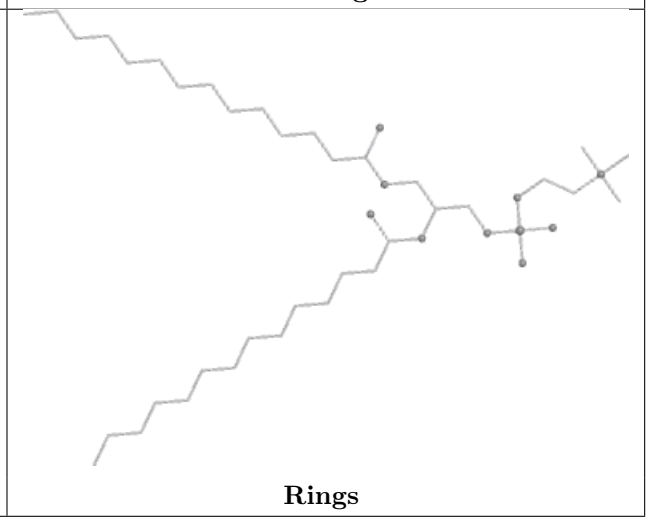
Bond lengths



Bond angles

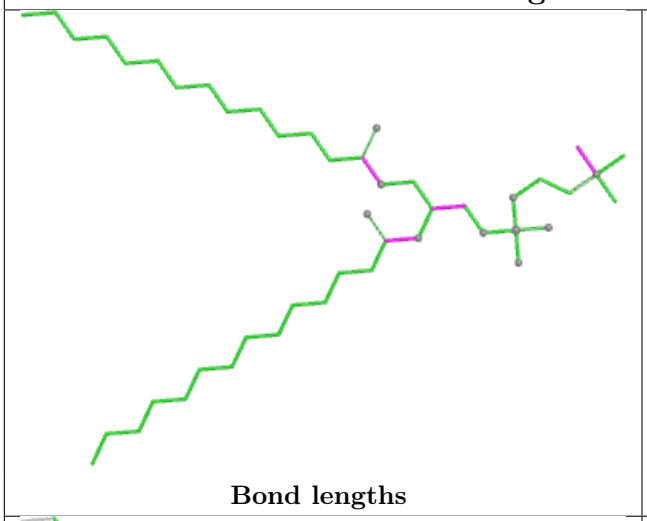


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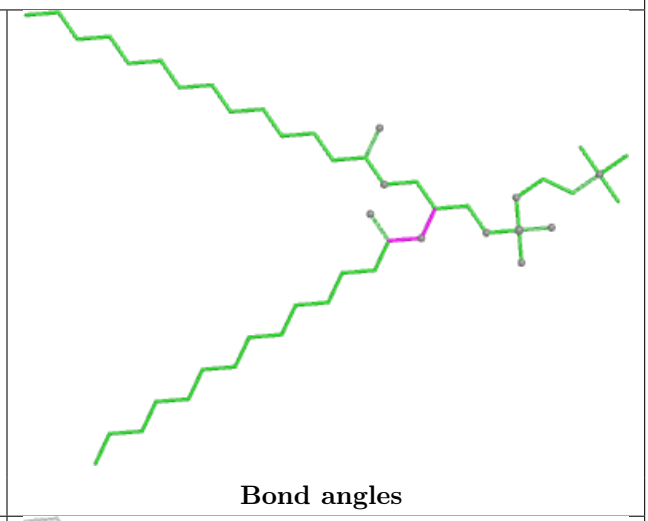


Rings

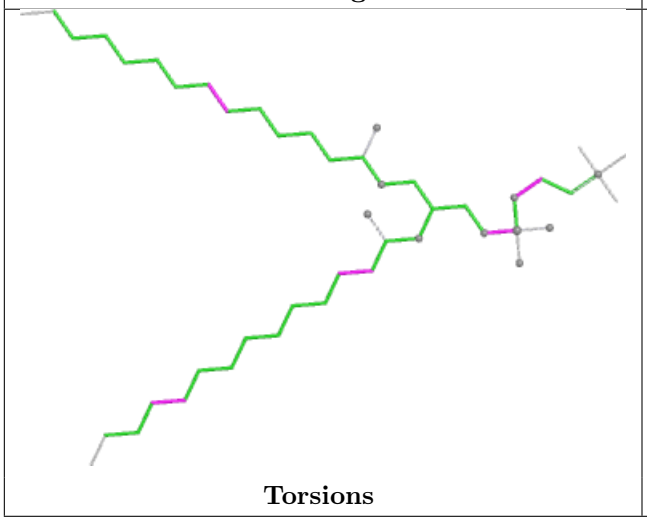
Ligand PX4 B 301



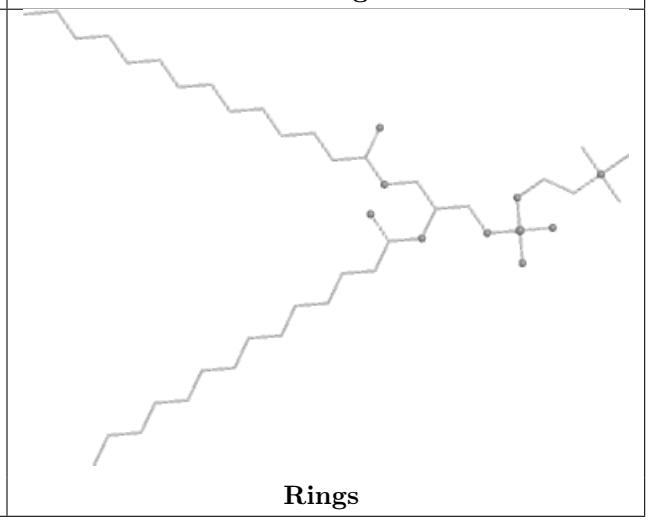
Bond lengths



Bond angles

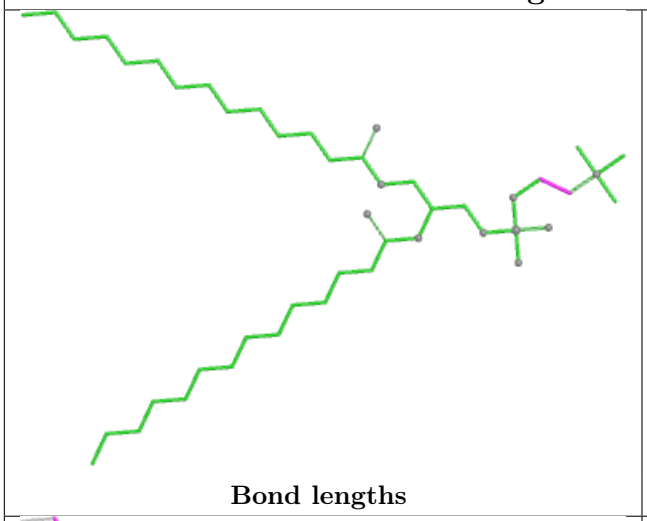


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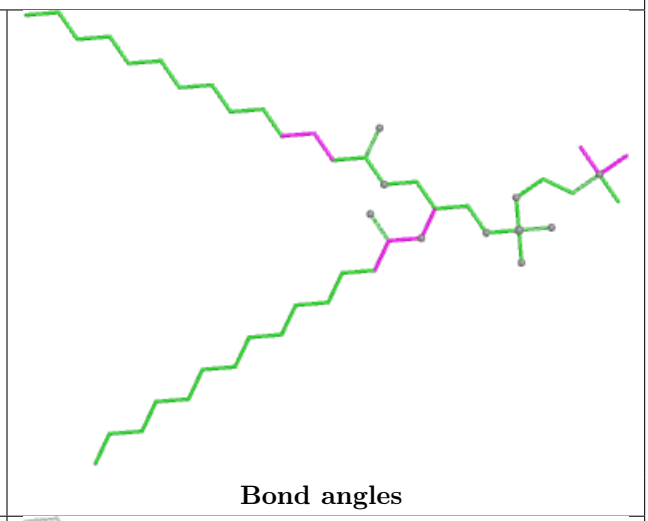


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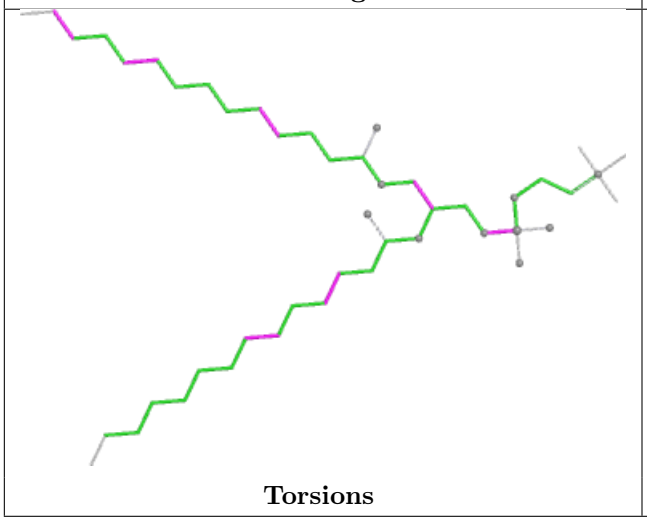
Ligand PX4 A 622



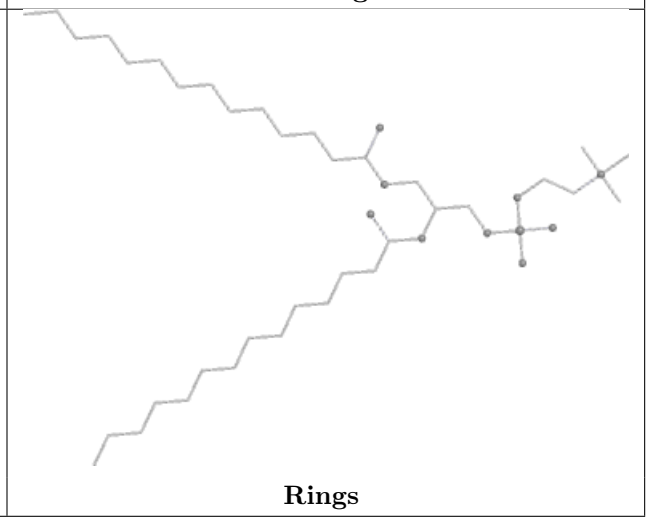
Bond lengths



Bond angles

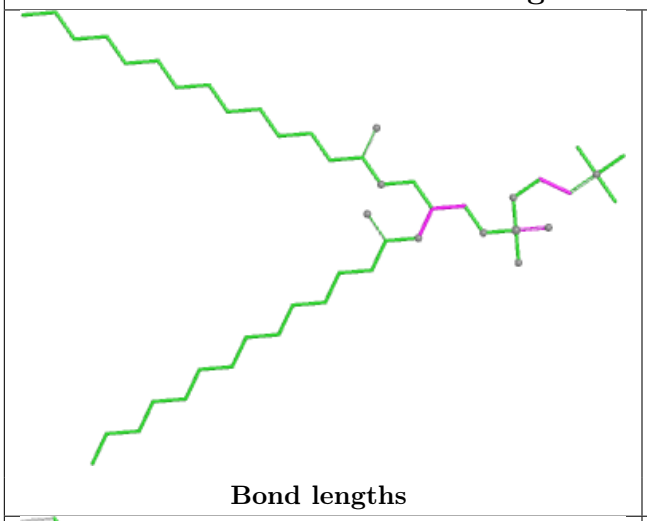


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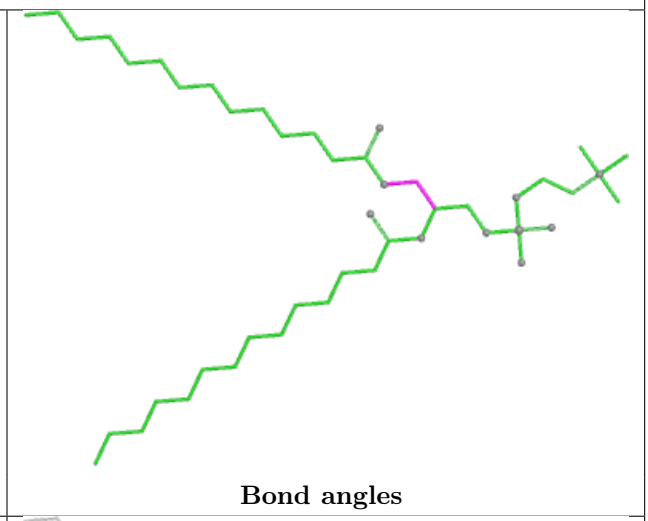


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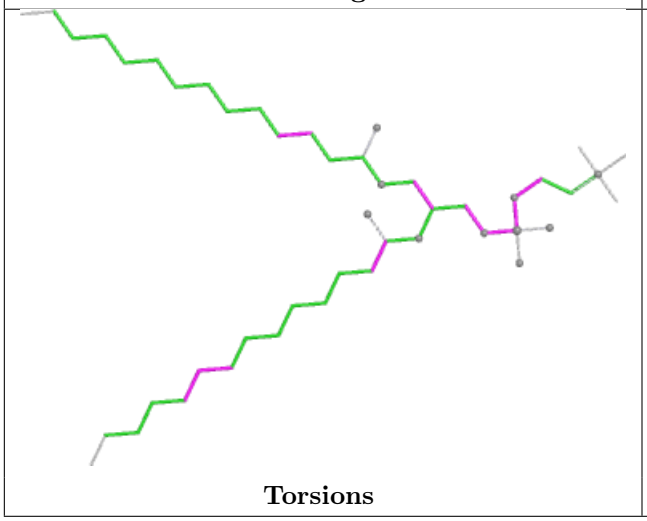
Ligand PX4 A 645



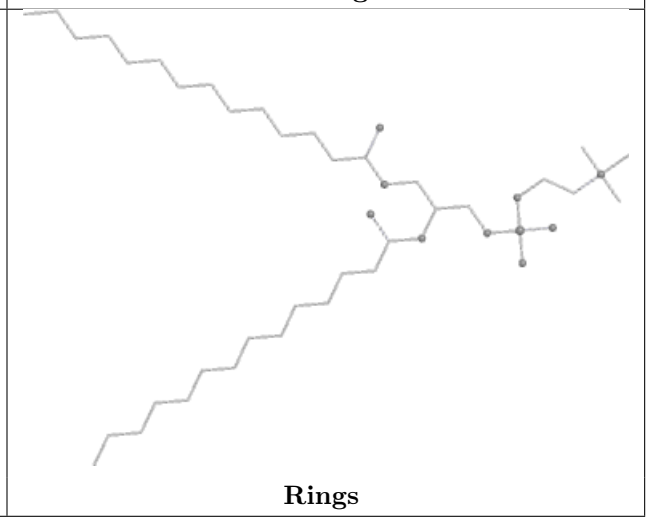
Bond lengths



Bond angles

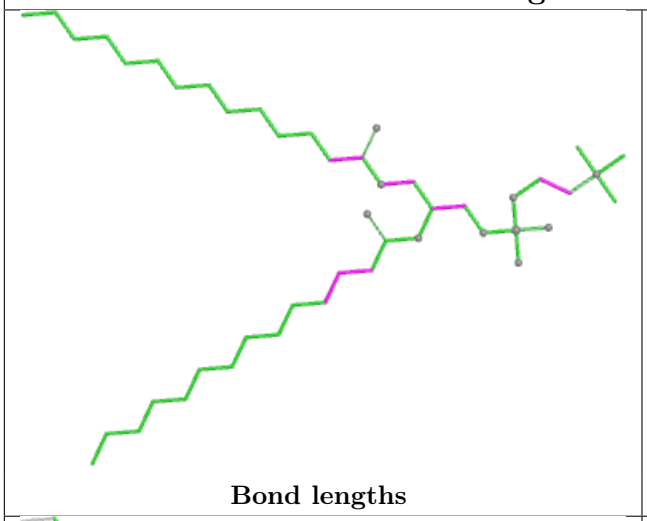


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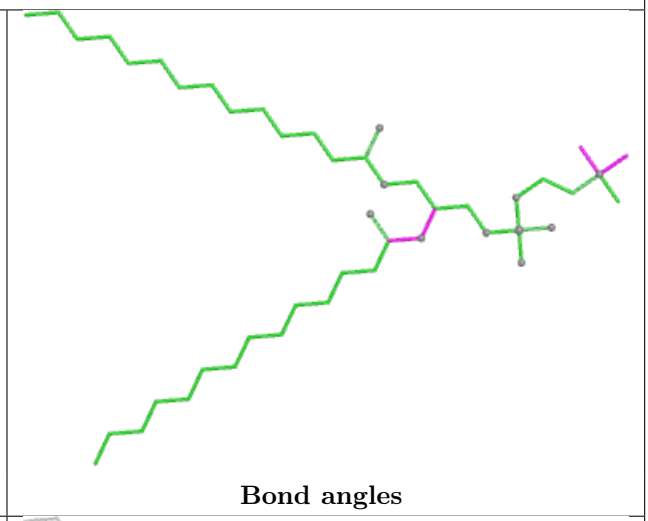


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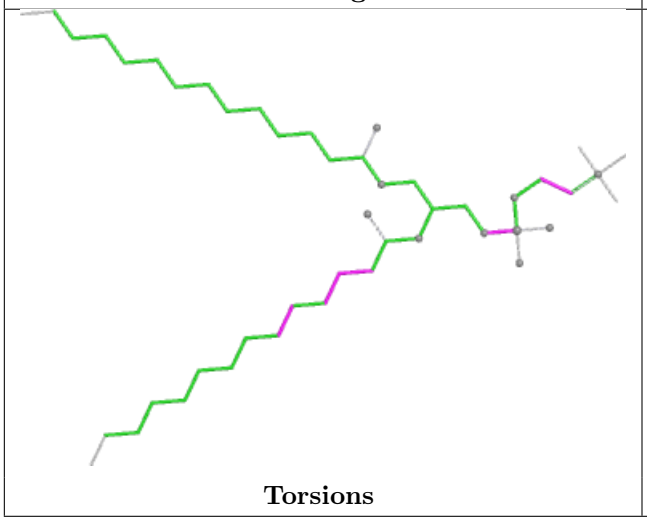
Ligand PX4 B 366



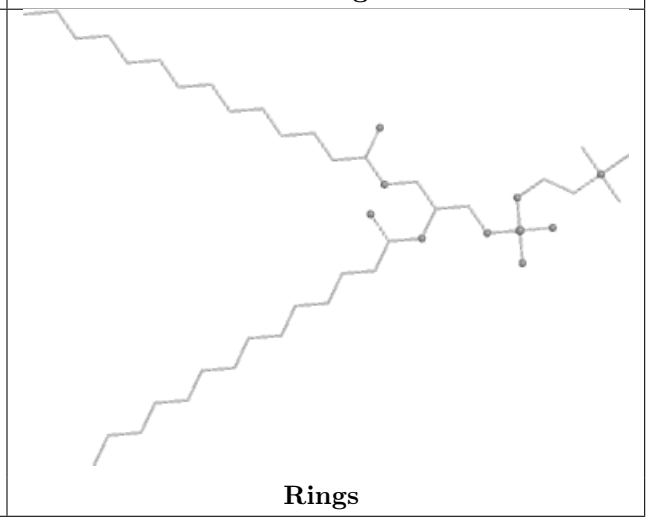
Bond lengths



Bond angles

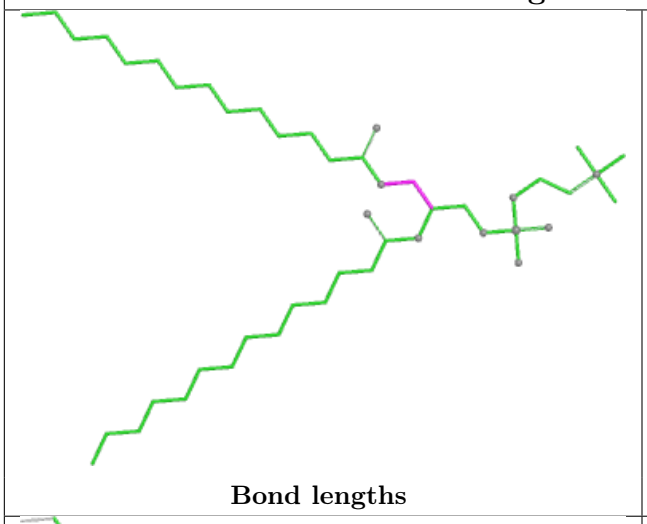


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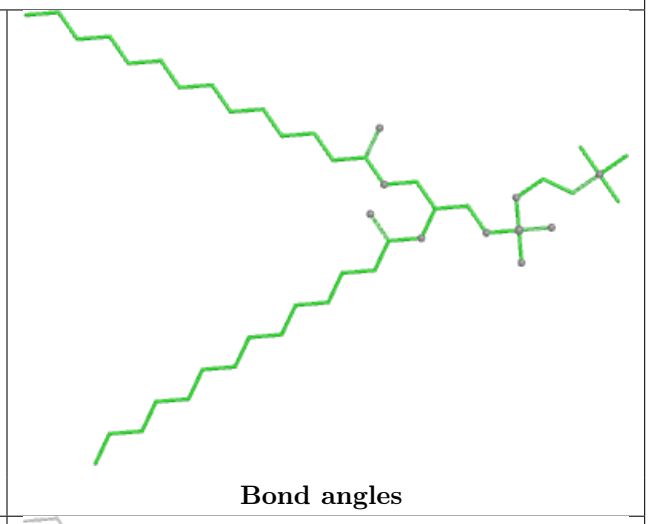


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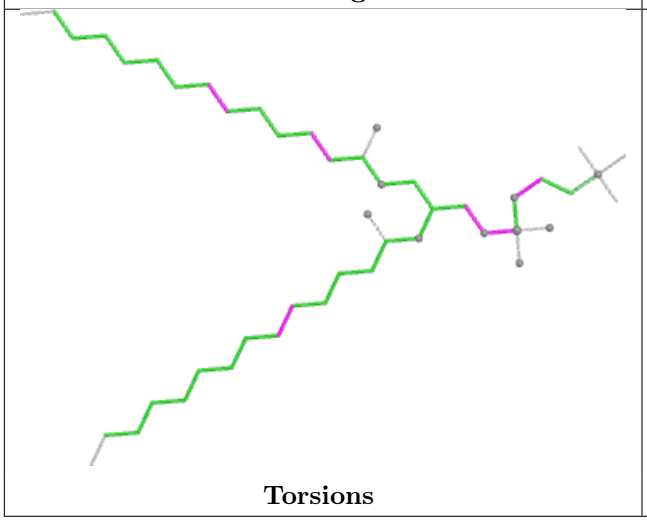
Ligand PX4 B 394



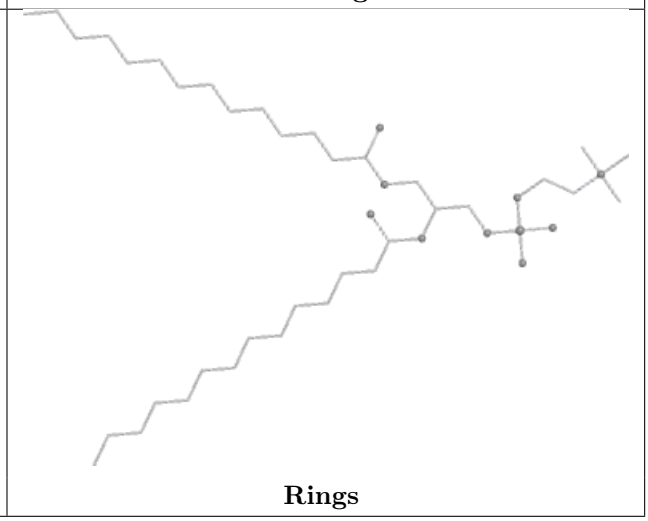
Bond lengths



Bond angles

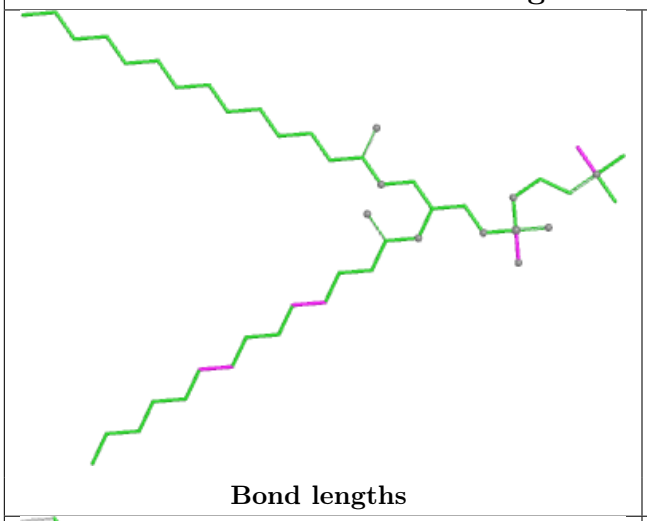


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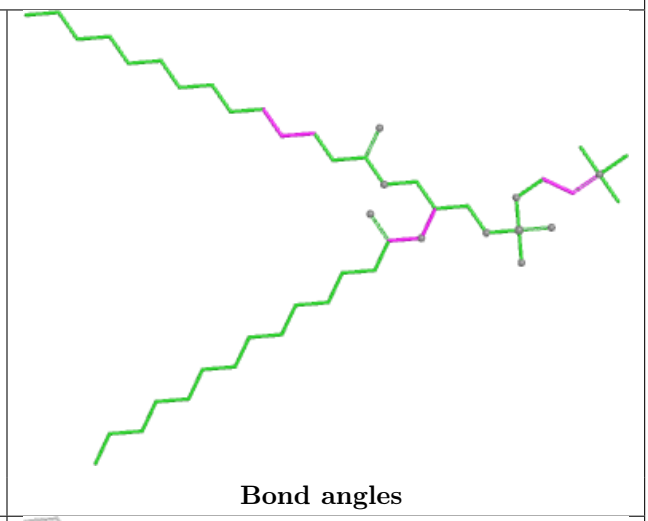


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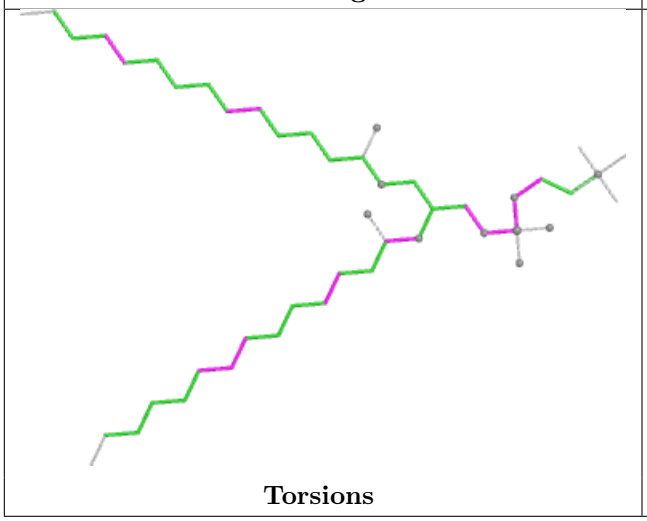
Ligand PX4 C 313



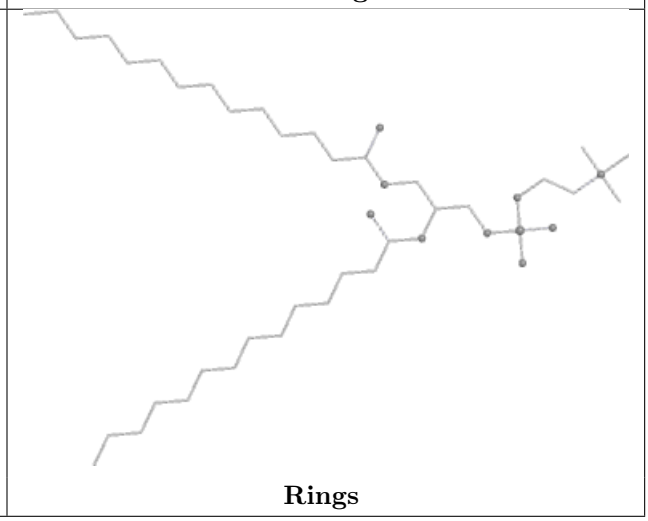
Bond lengths



Bond angles

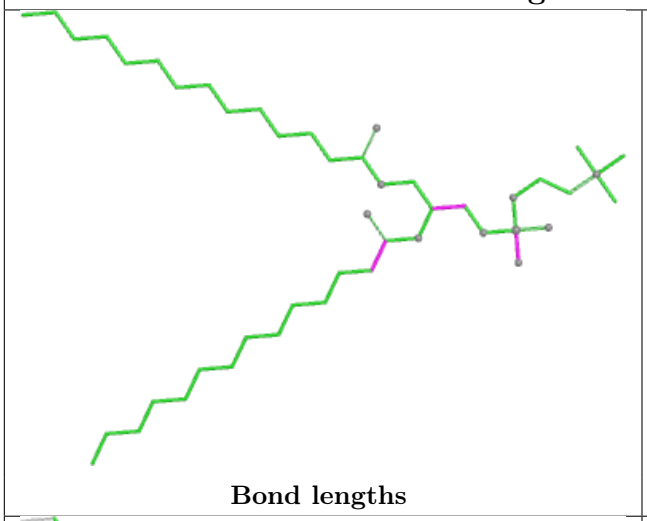


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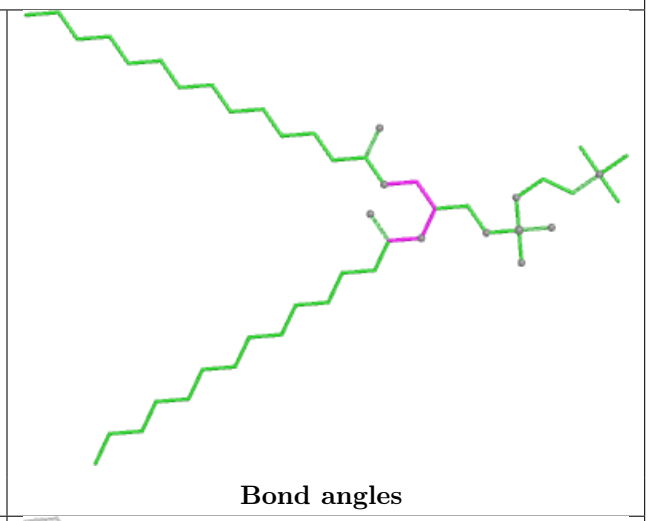


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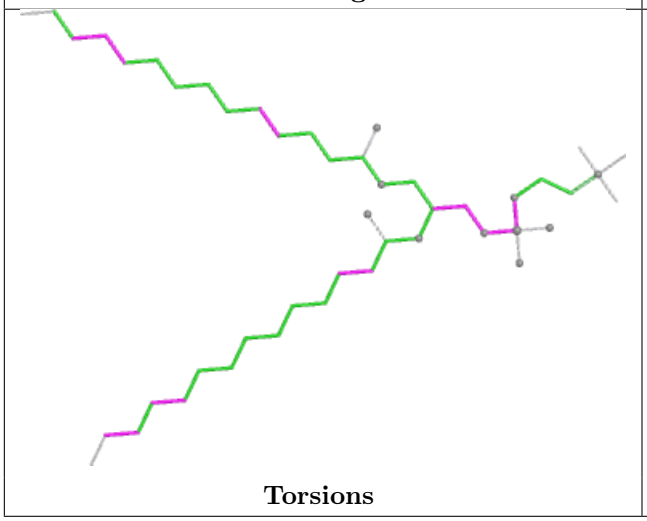
Ligand PX4 B 336



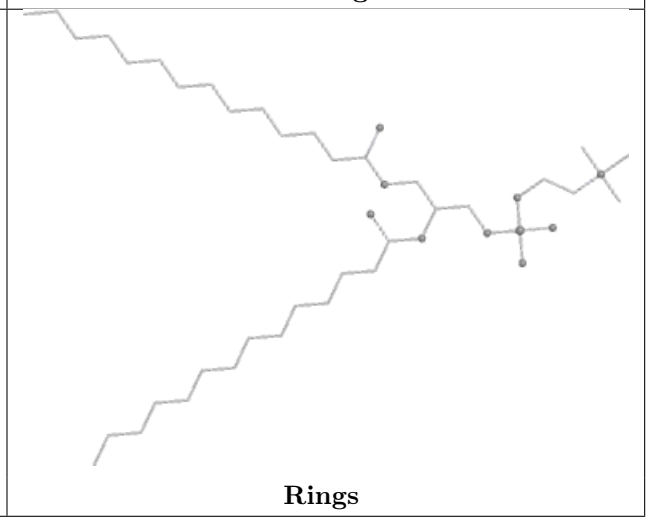
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Bond angles

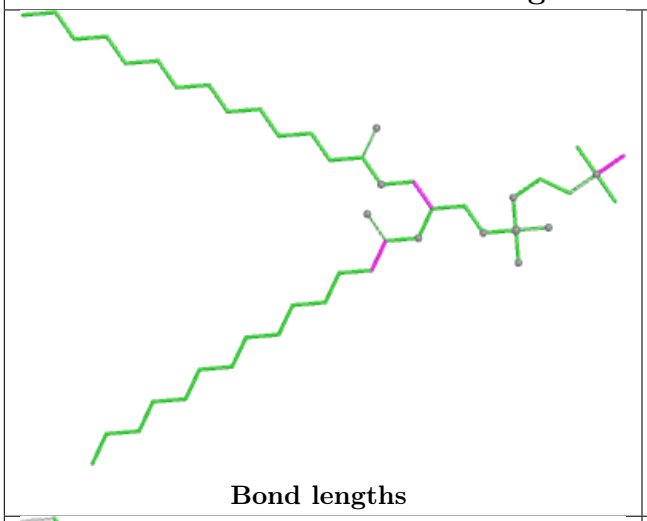


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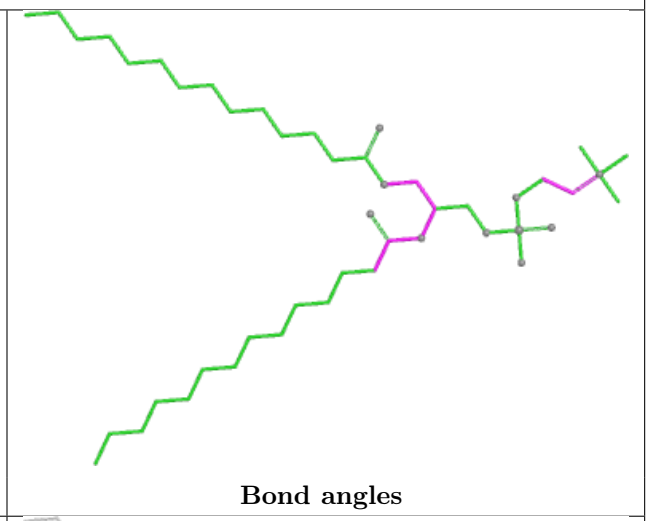


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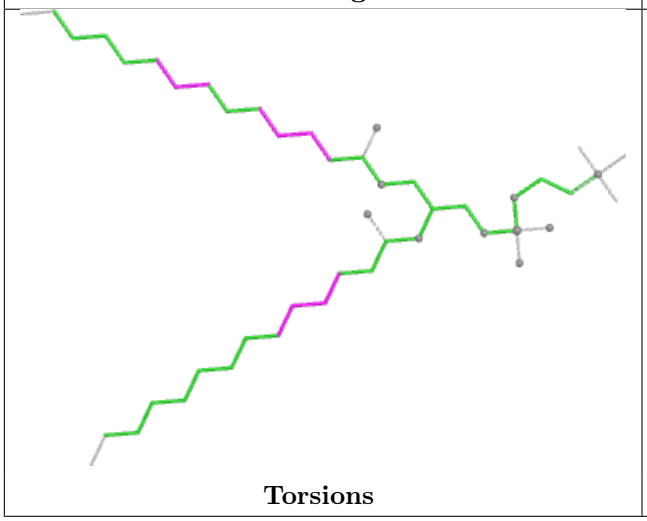
Ligand PX4 B 333



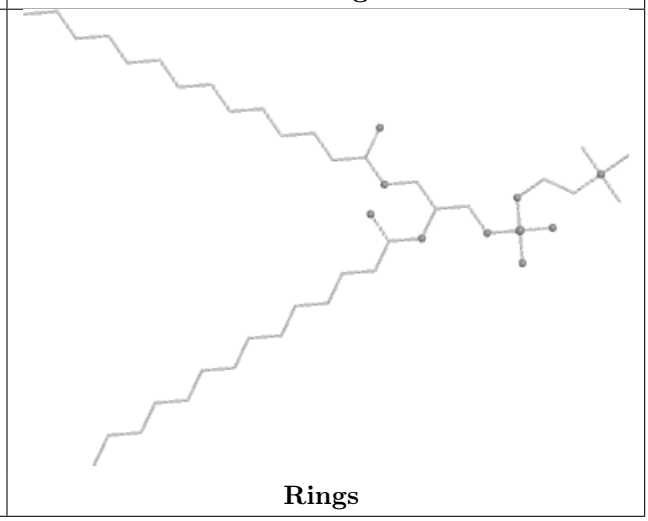
Bond lengths



Bond angles

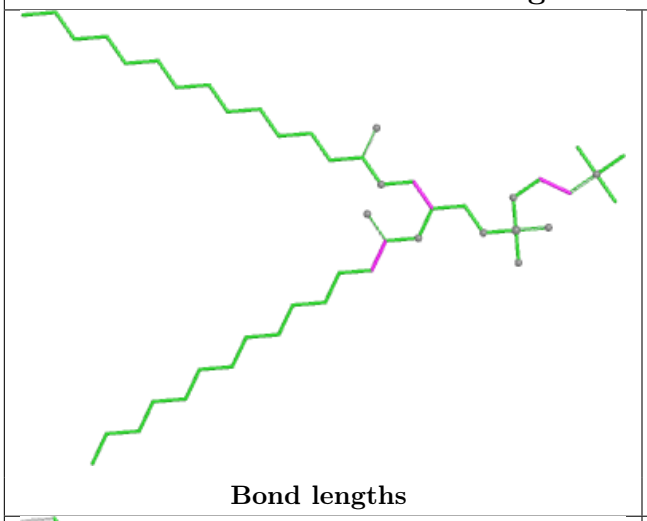


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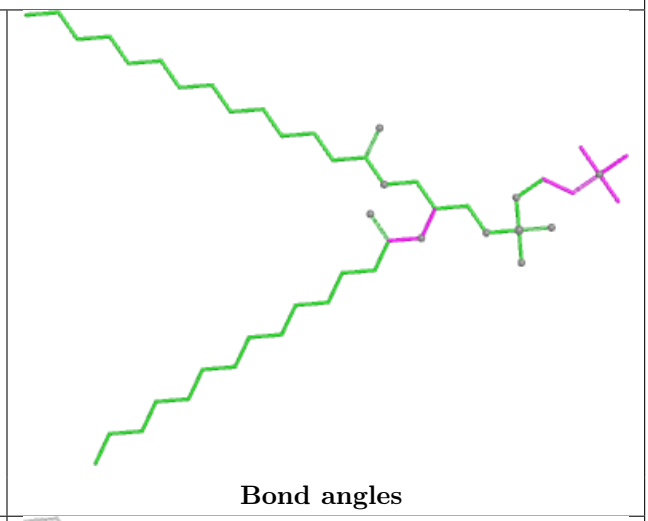


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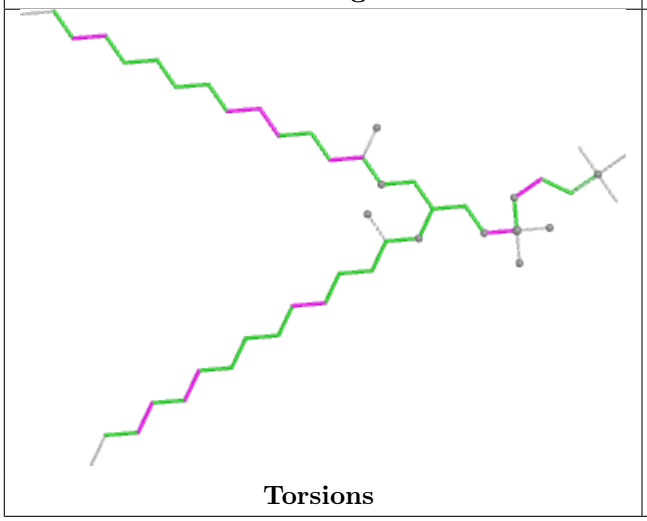
Ligand PX4 B 315



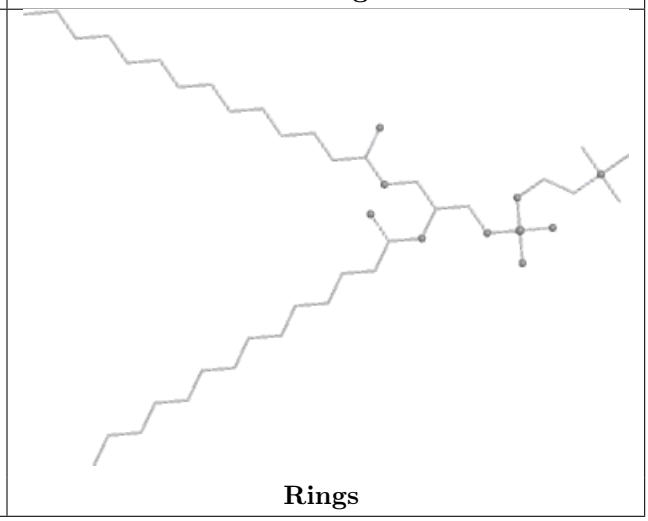
Bond lengths



Bond angles

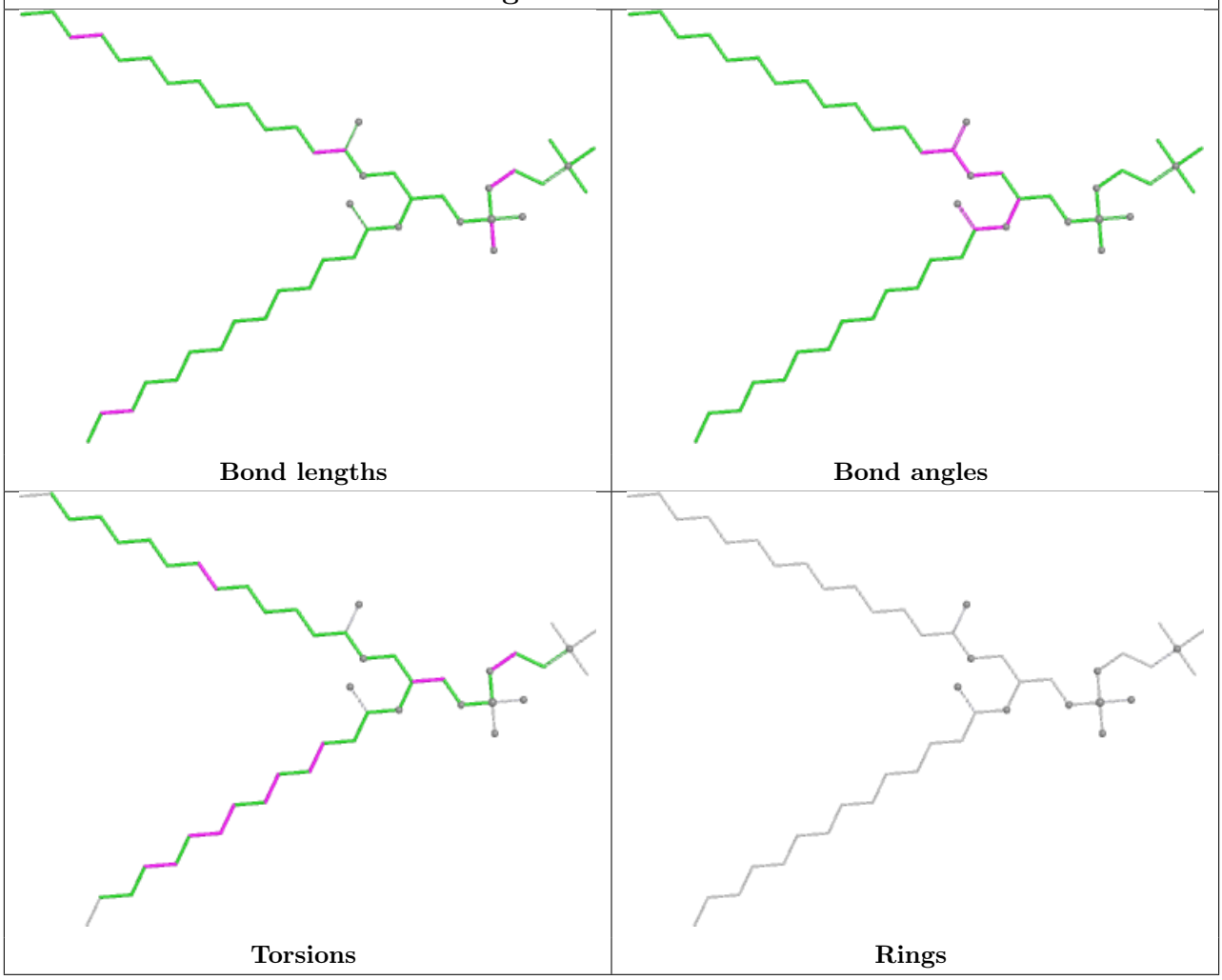


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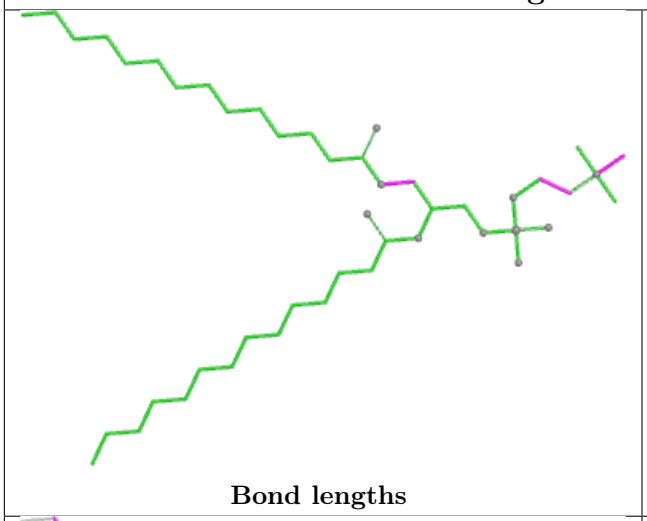


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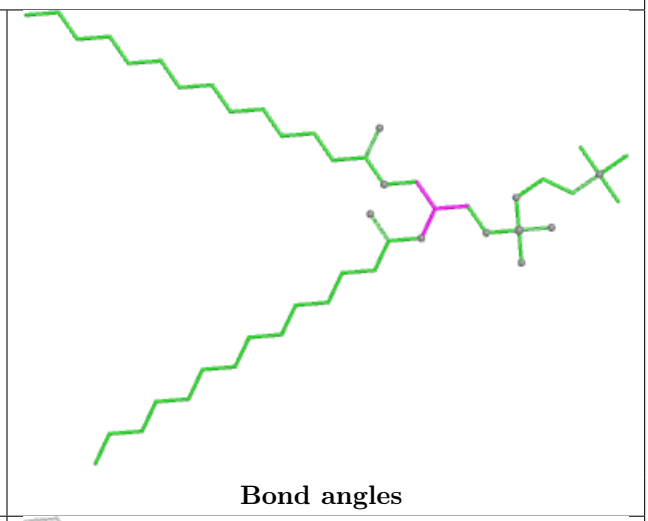
Ligand PX4 A 647



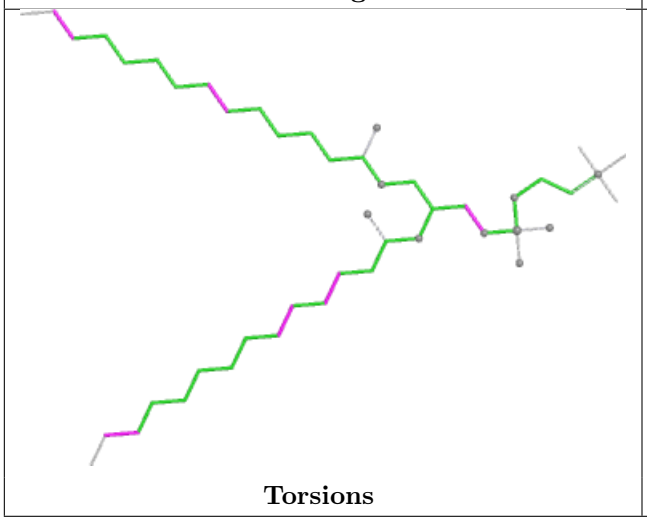
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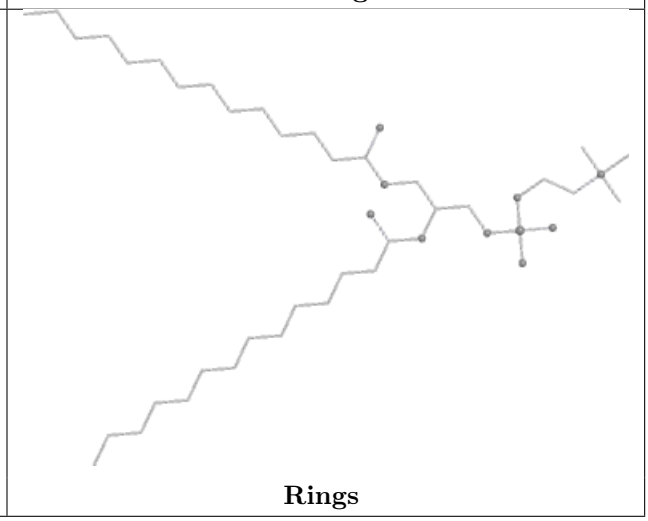
Bond lengths



Bond angles

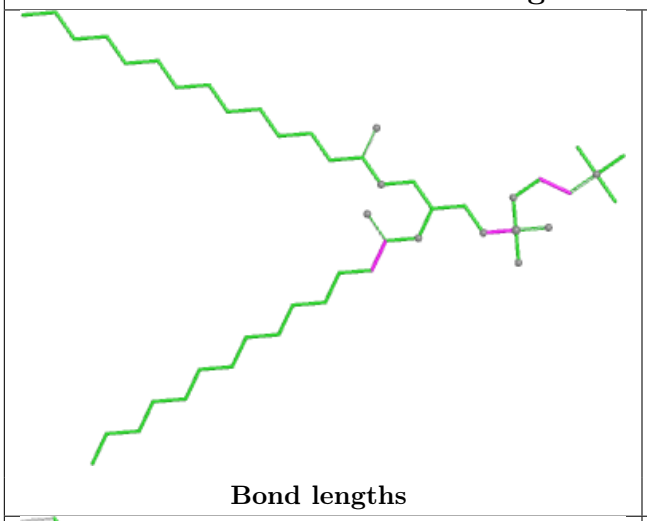


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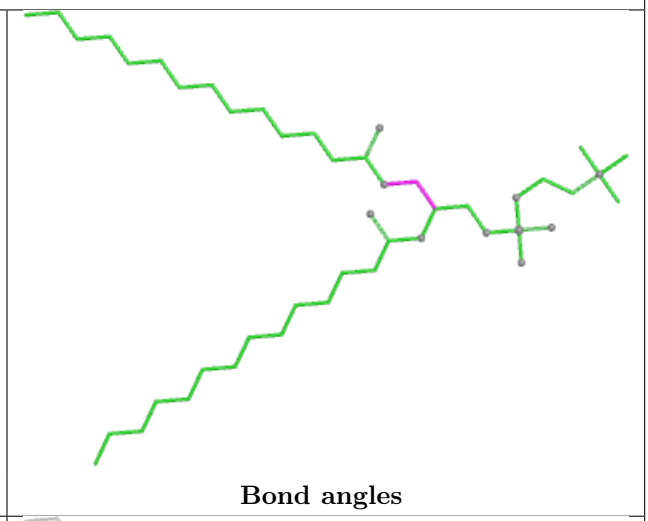


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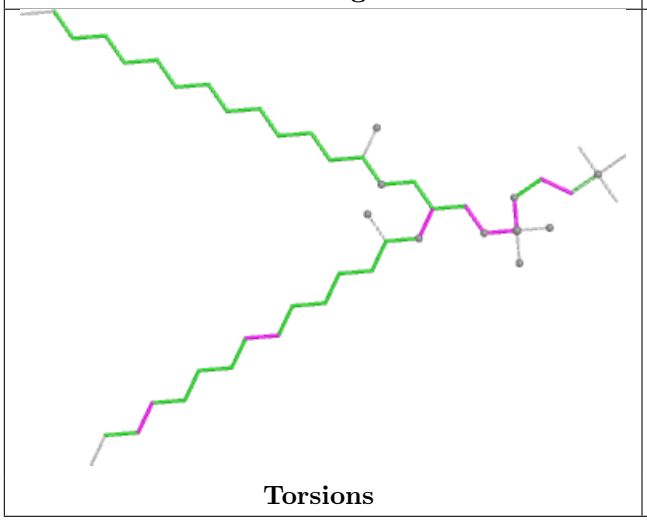
Ligand PX4 C 305



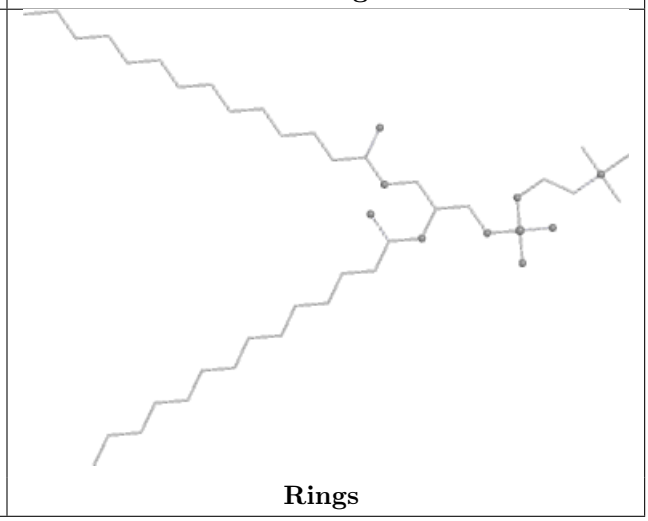
Bond lengths



Bond angles

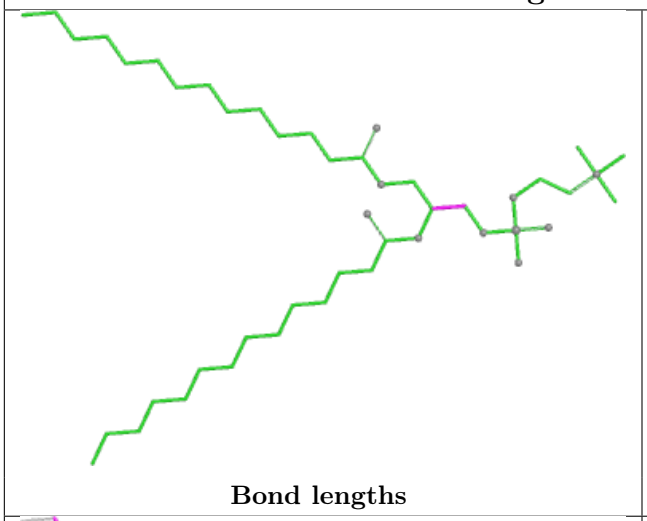


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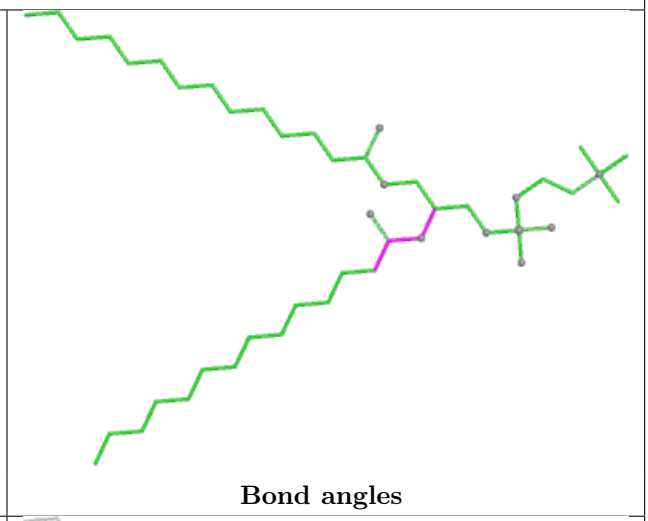


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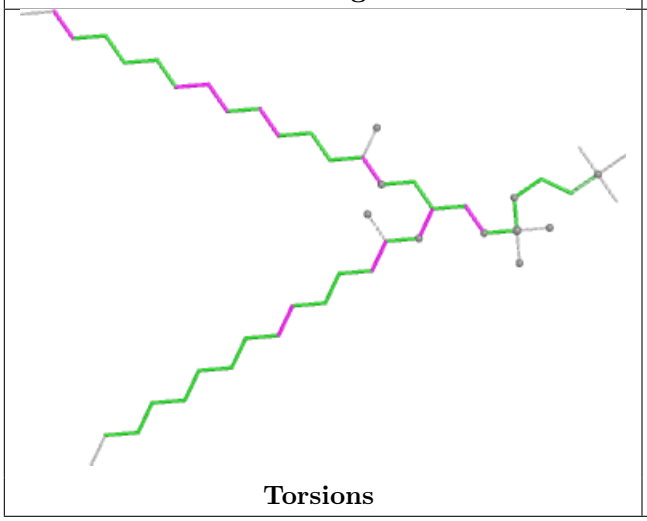
Ligand PX4 A 608



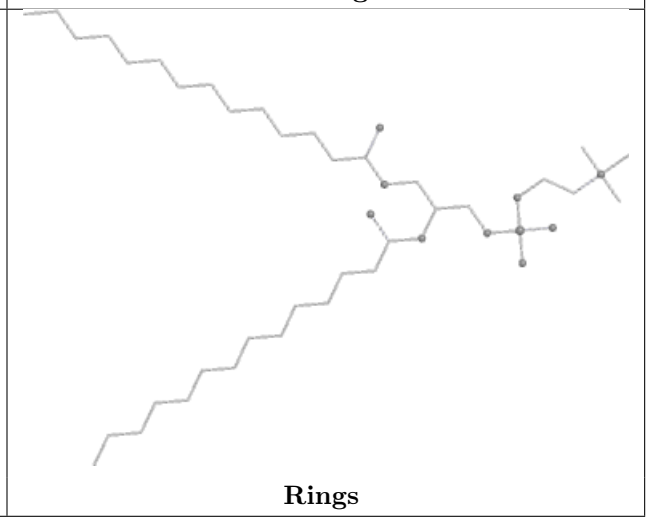
Bond lengths



Bond angles

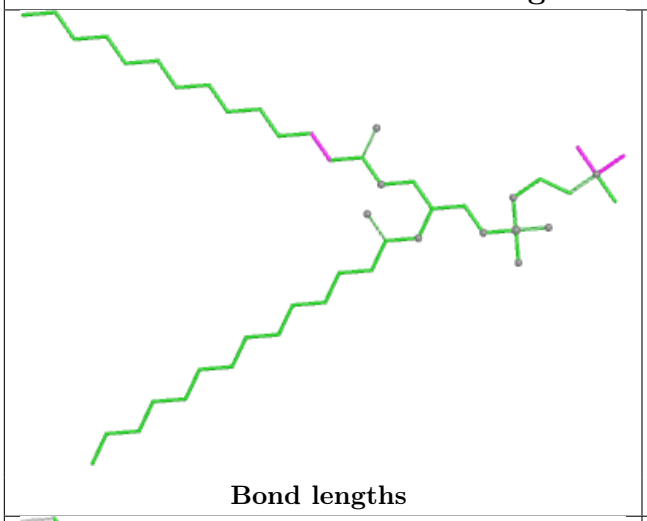


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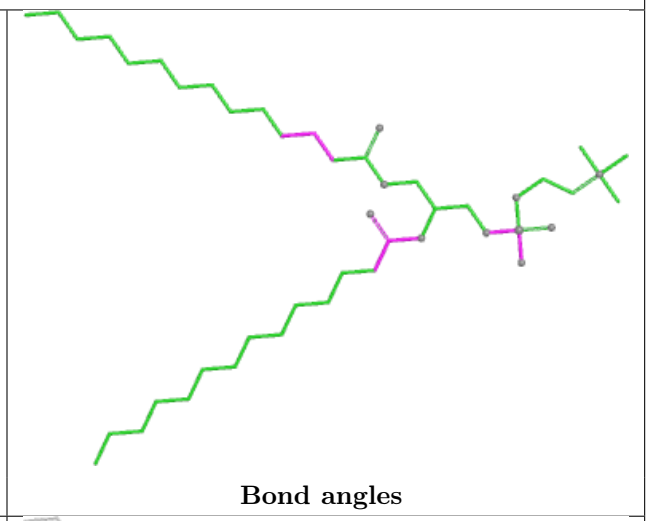


Rings

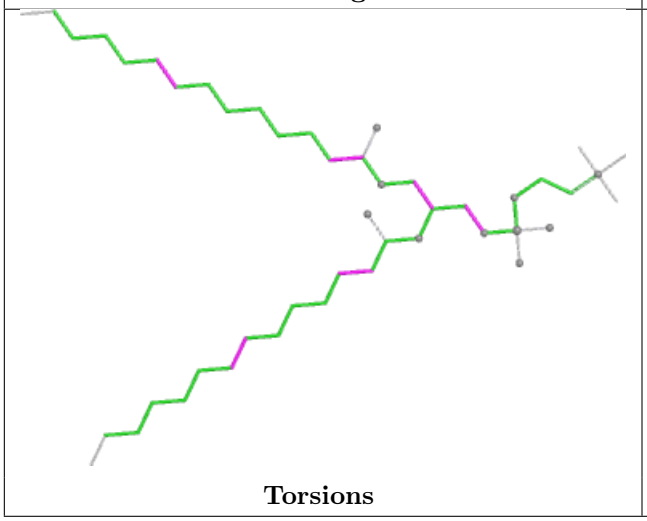
Ligand PX4 B 381



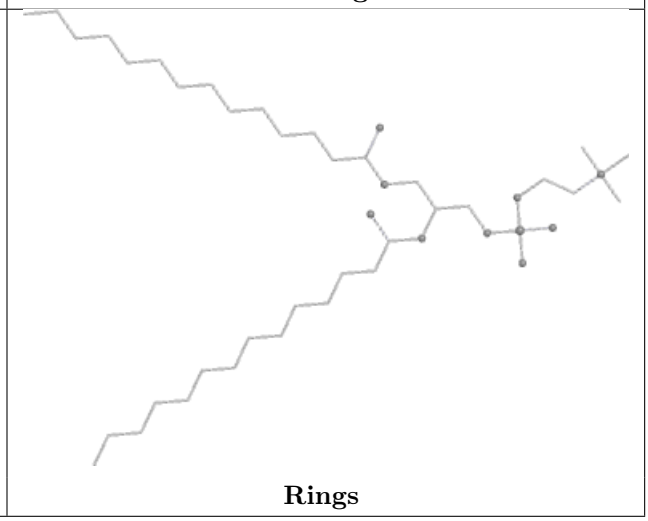
Bond lengths



Bond angles

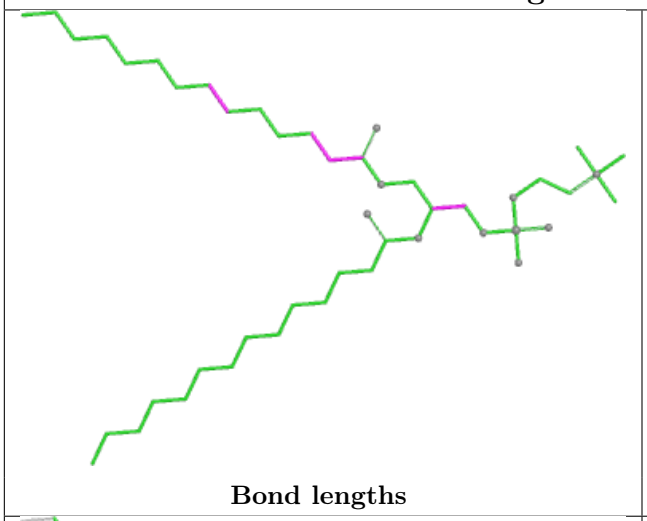


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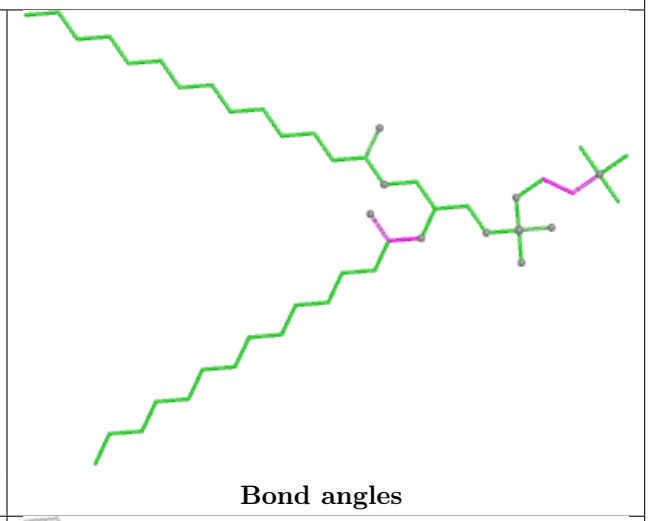


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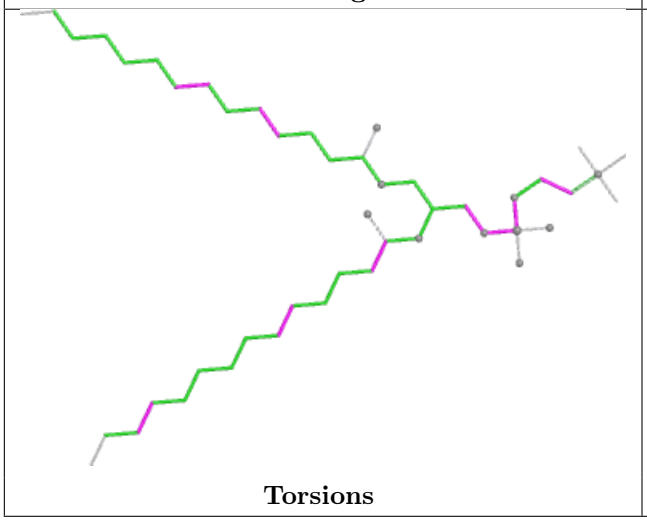
Ligand PX4 A 607



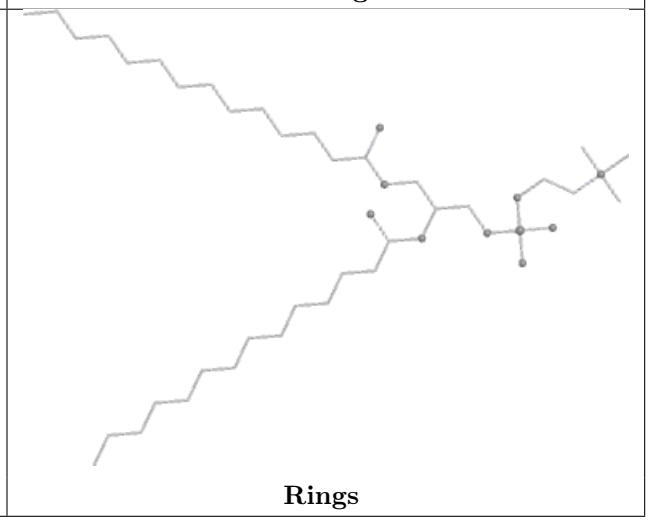
Bond lengths



Bond angles

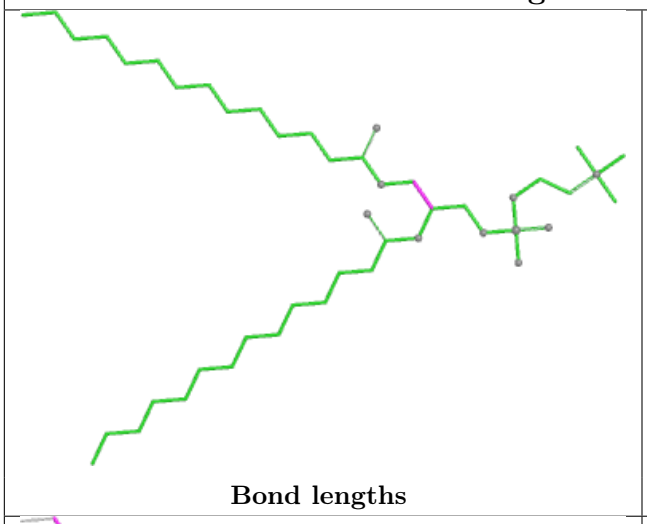


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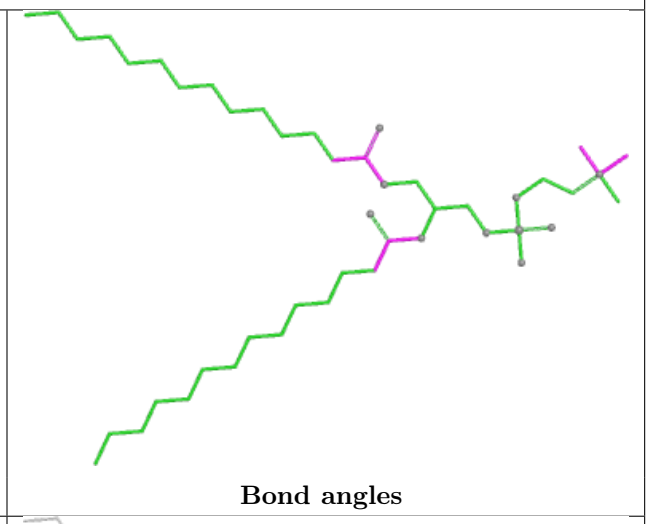


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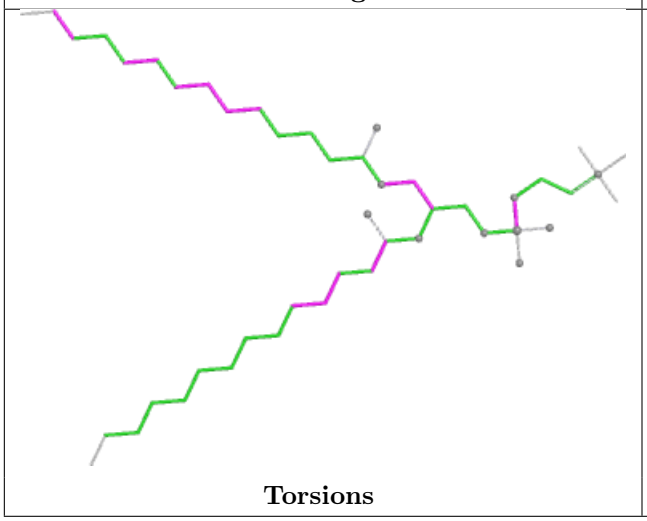
Ligand PX4 B 370



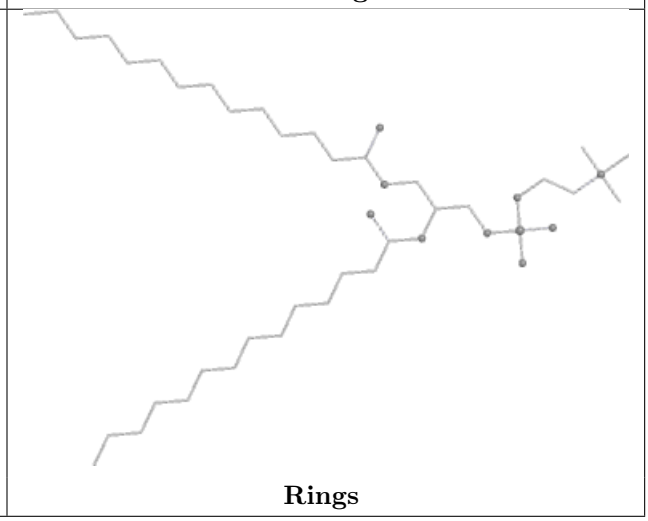
Bond lengths



Bond angles

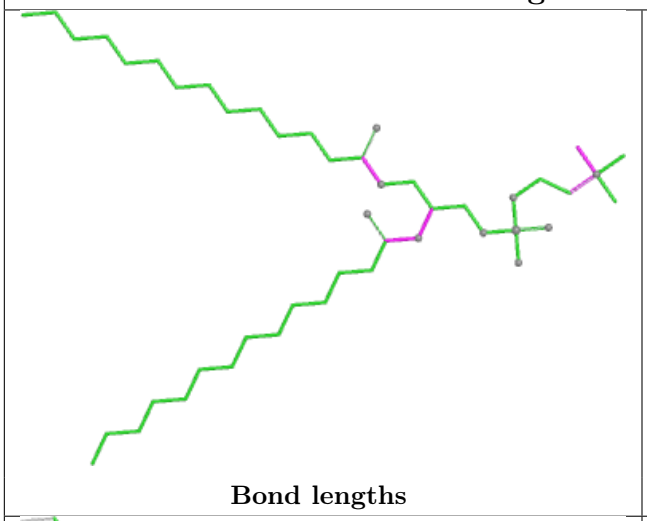


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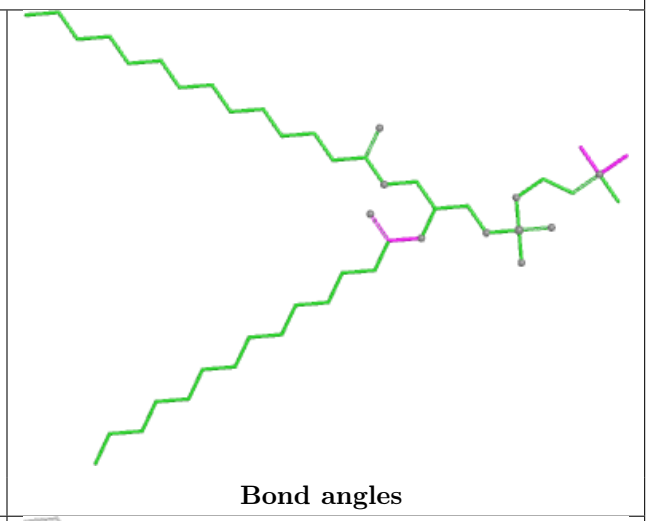


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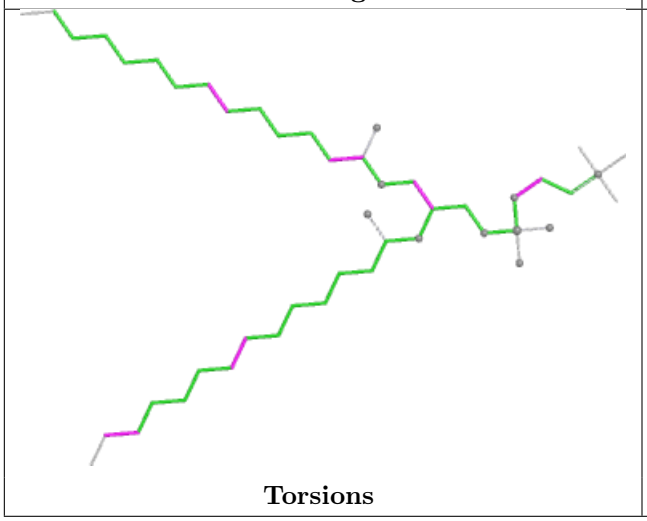
Ligand PX4 C 307



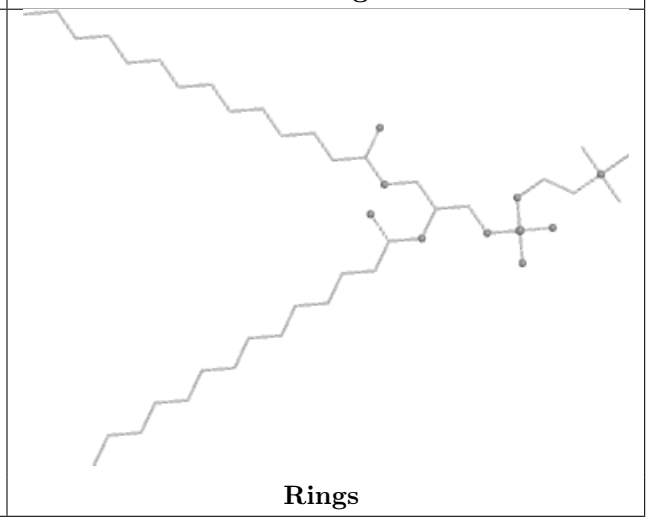
Bond lengths



Bond angles

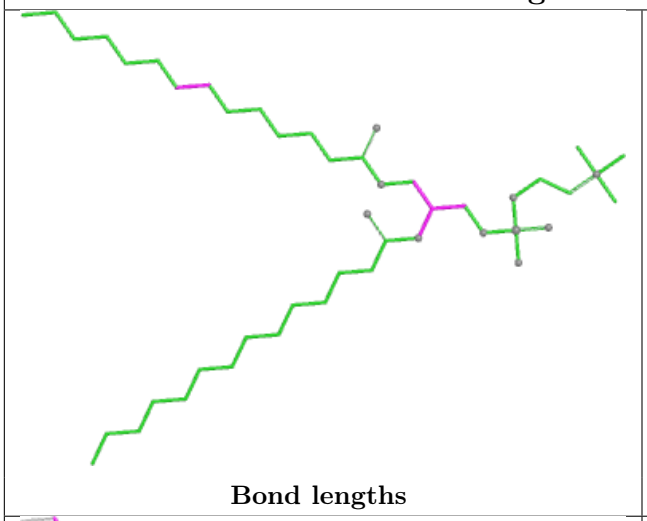


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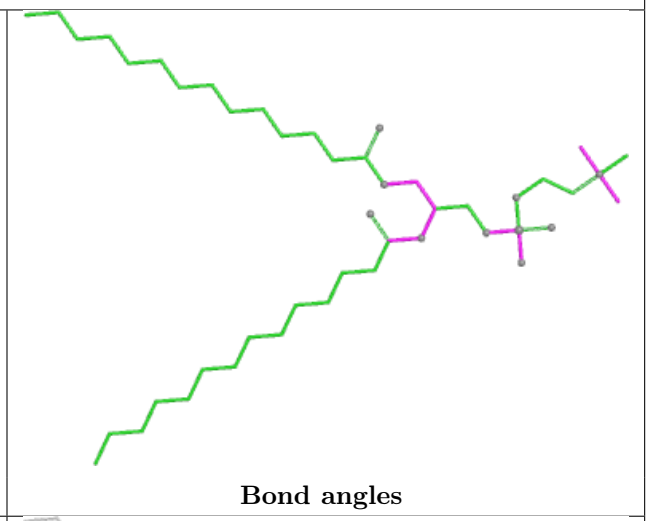


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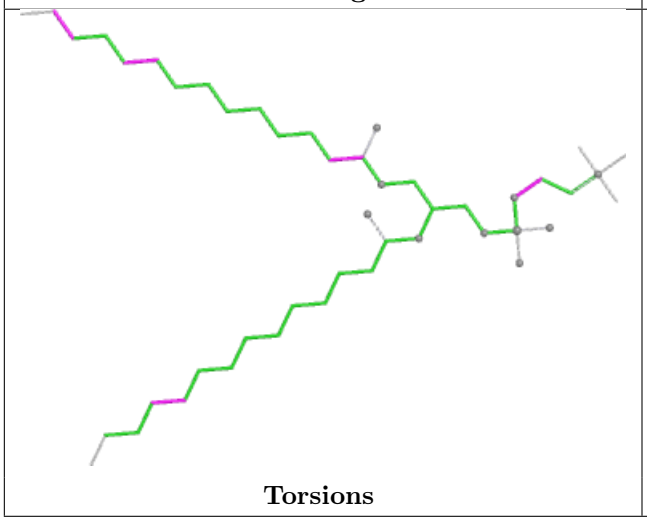
Ligand PX4 B 314



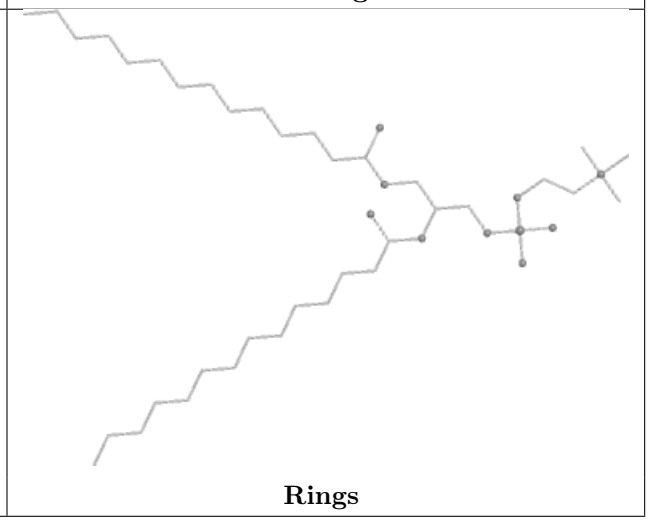
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Bond angles

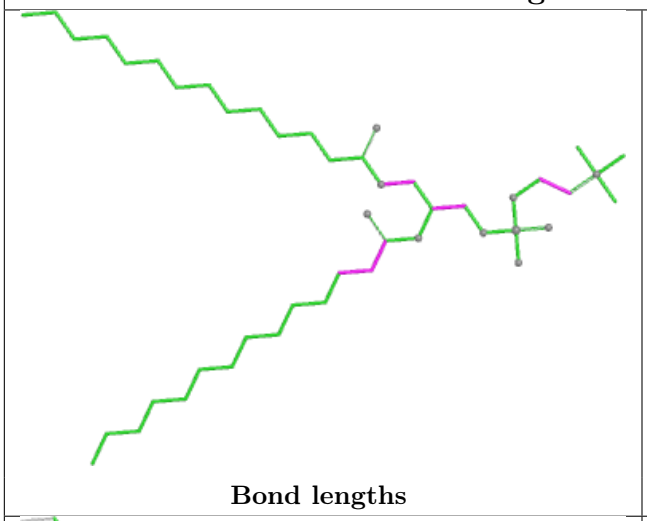


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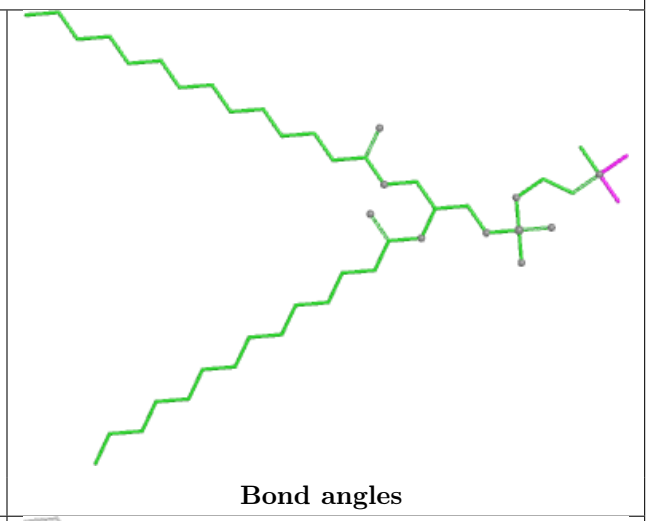


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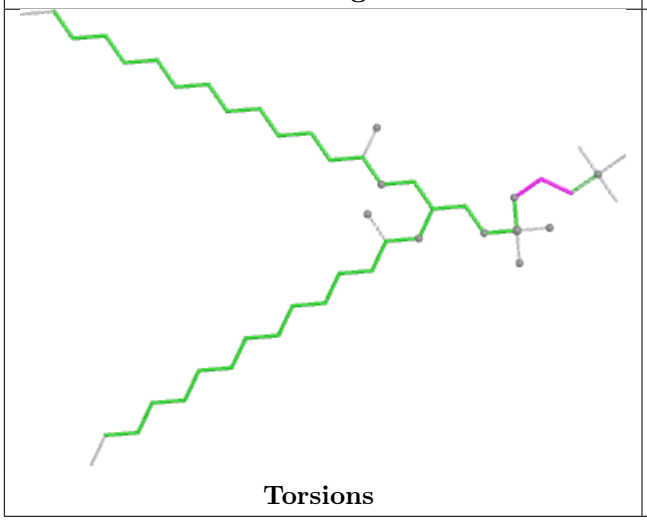
Ligand PX4 C 365



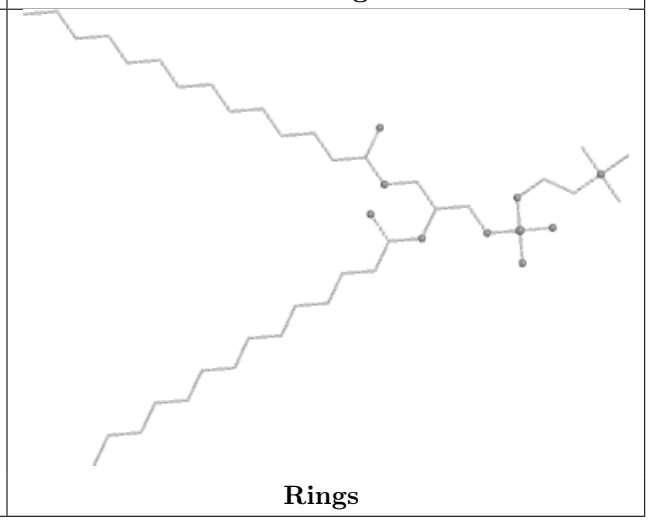
Bond lengths



Bond angles

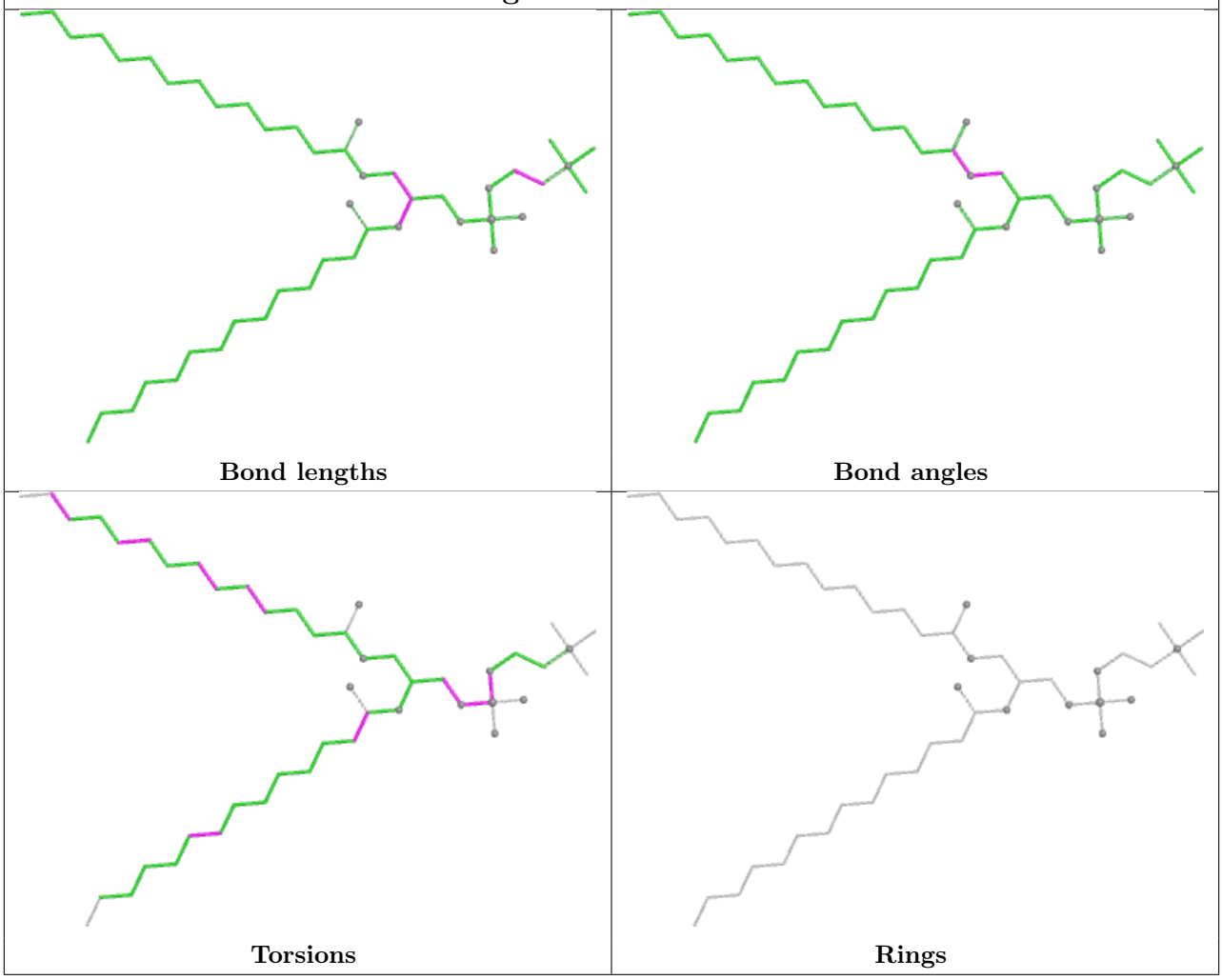


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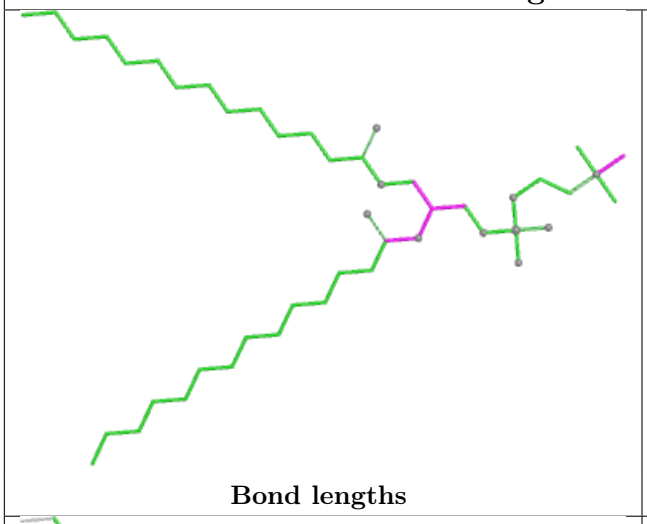


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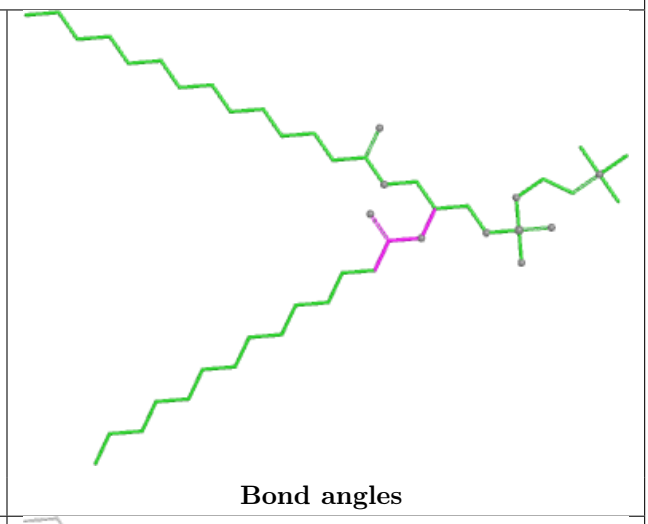
Ligand PX4 C 369



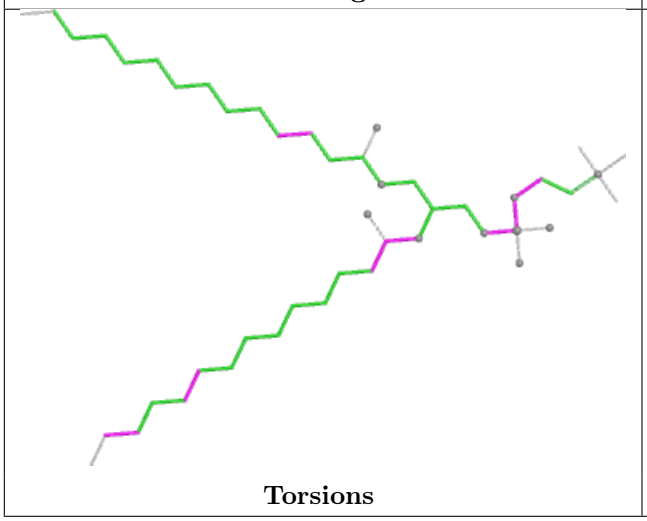
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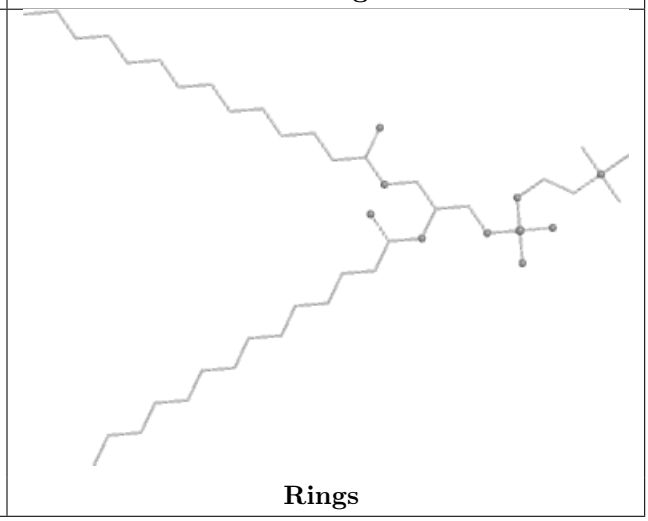
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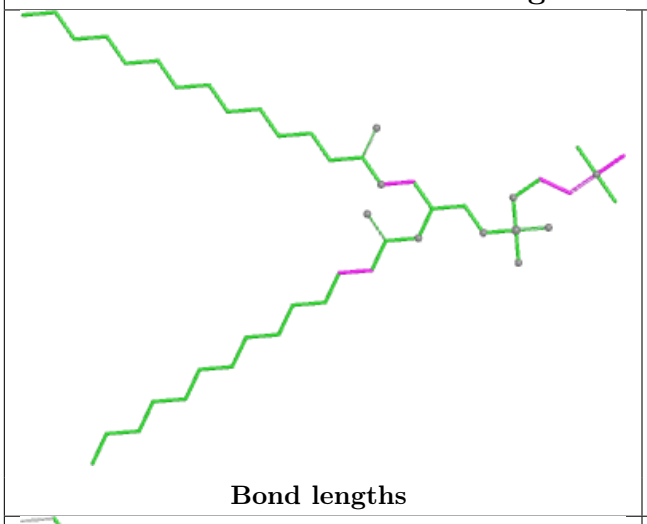


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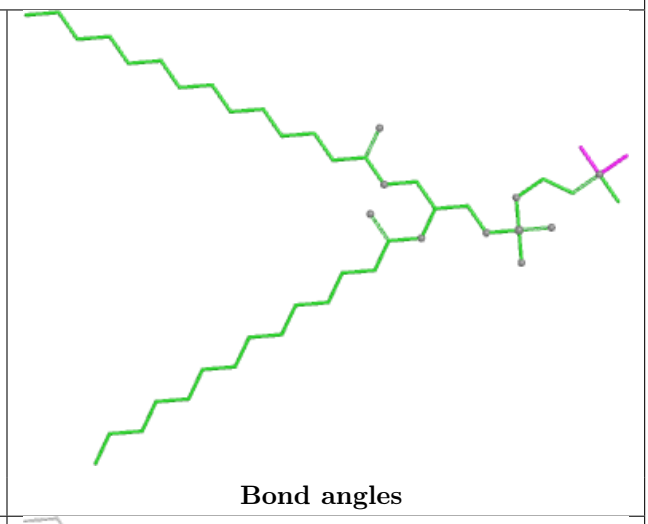


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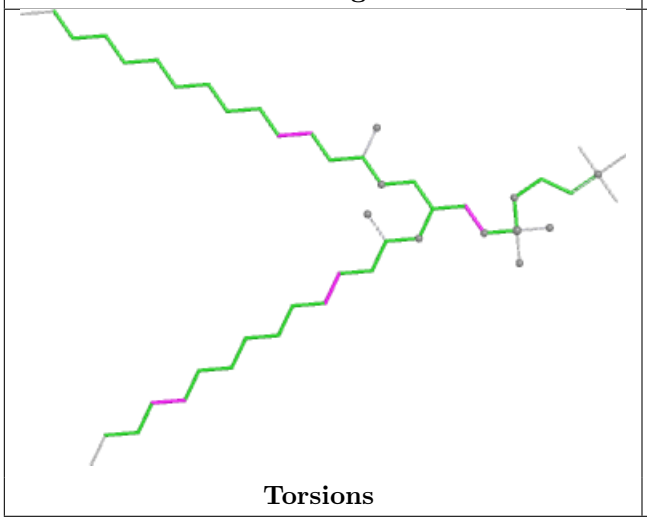
Ligand PX4 B 371



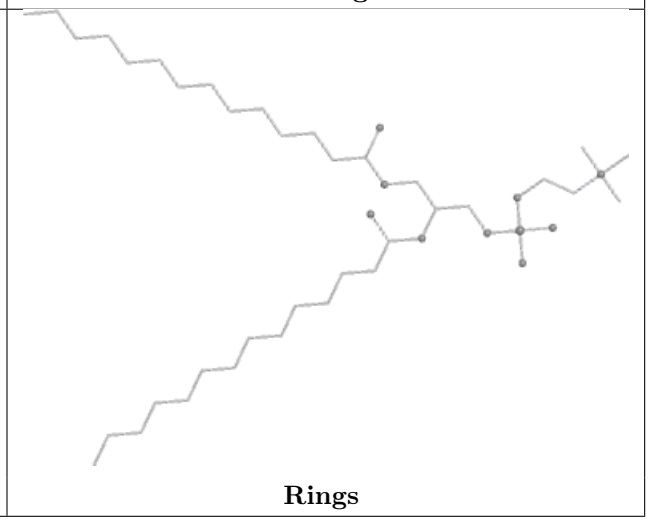
Bond lengths



Bond angles

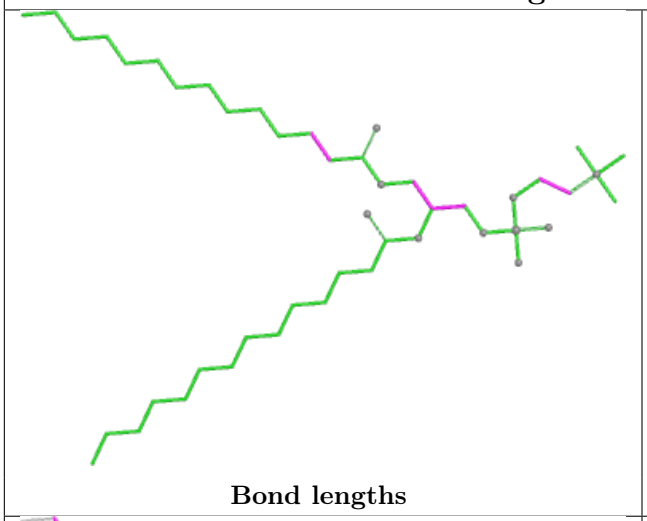


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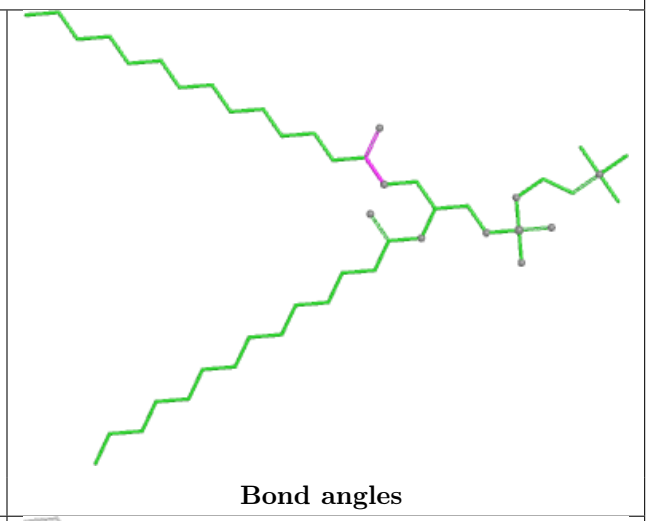


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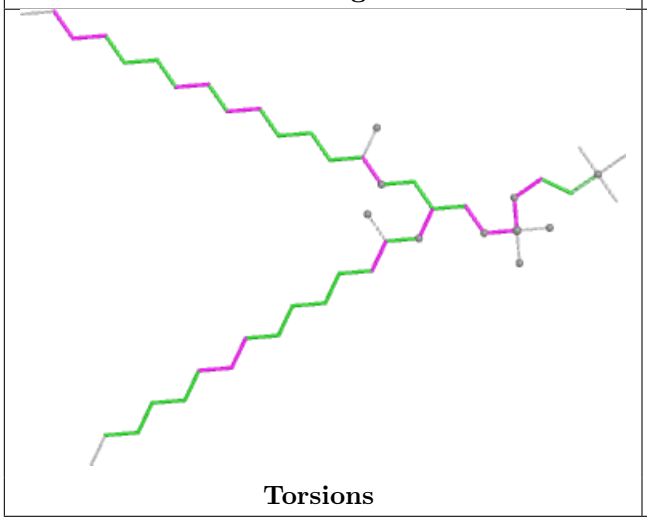
Ligand PX4 B 367



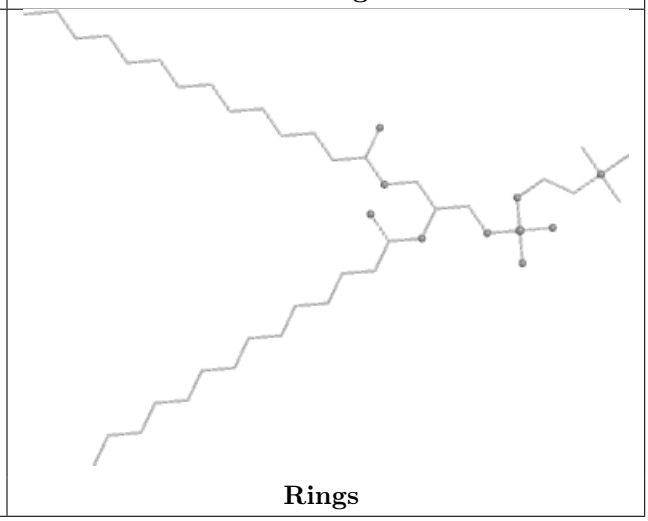
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Bond angles

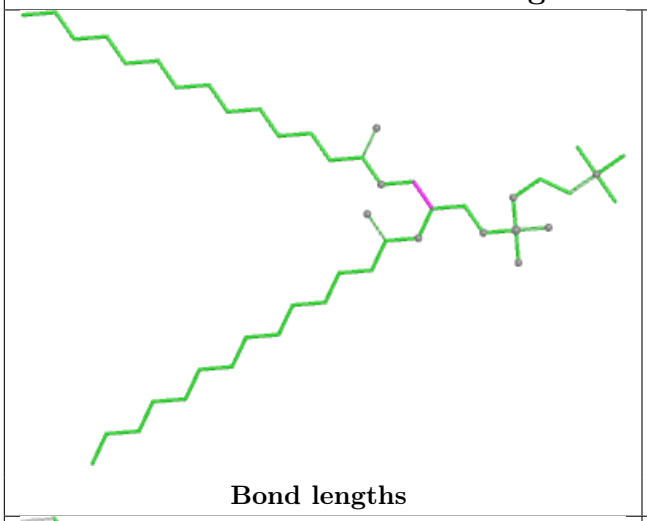


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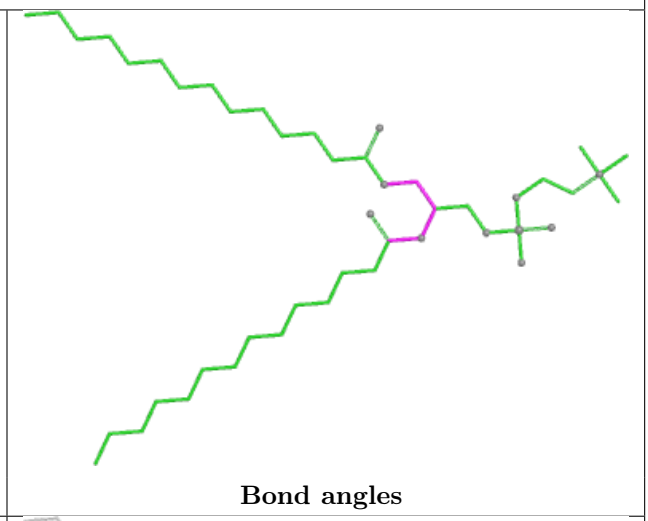


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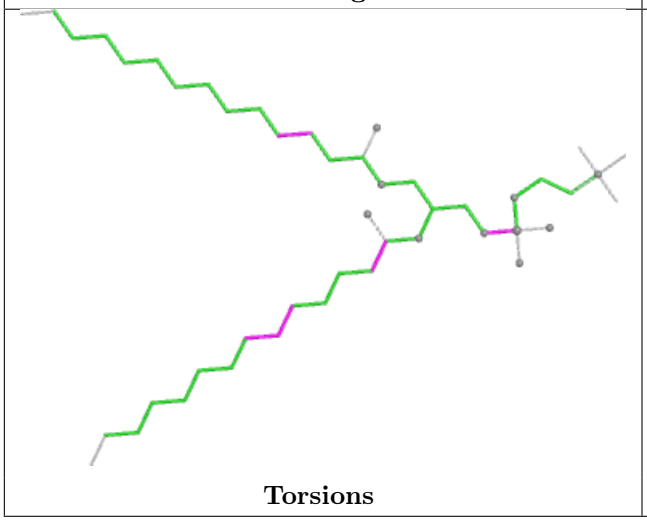
Ligand PX4 B 357



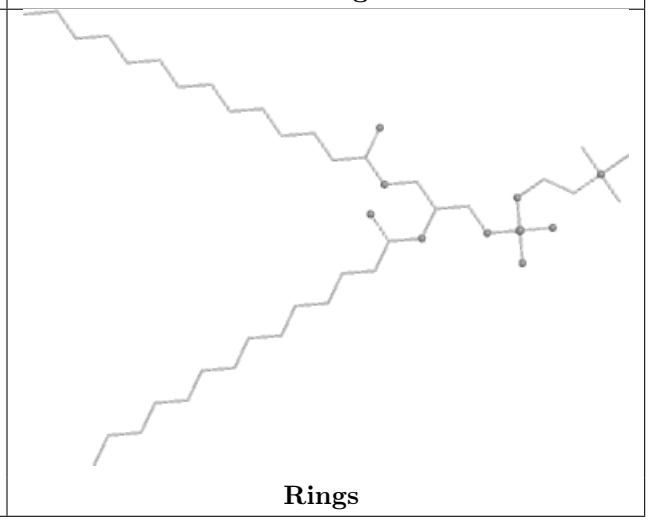
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Bond angles

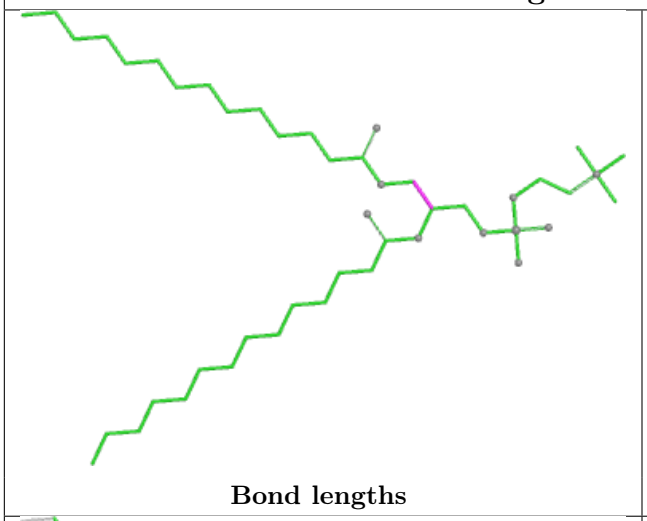


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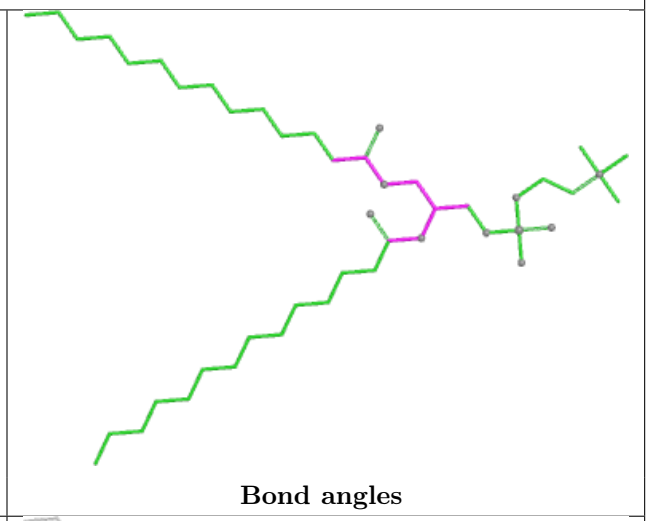


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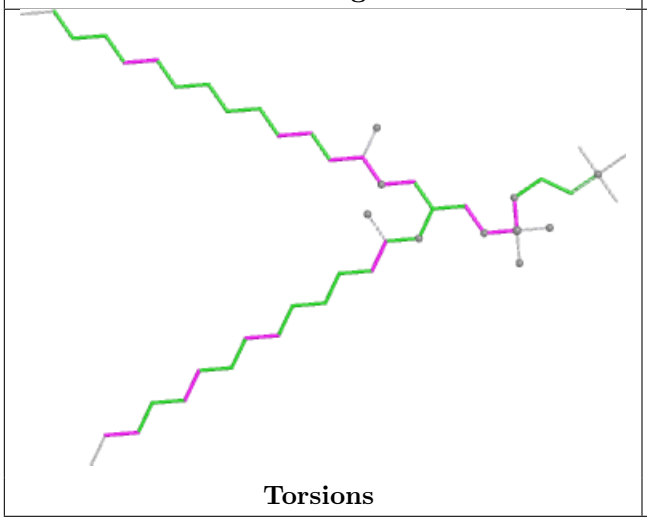
Ligand PX4 C 333



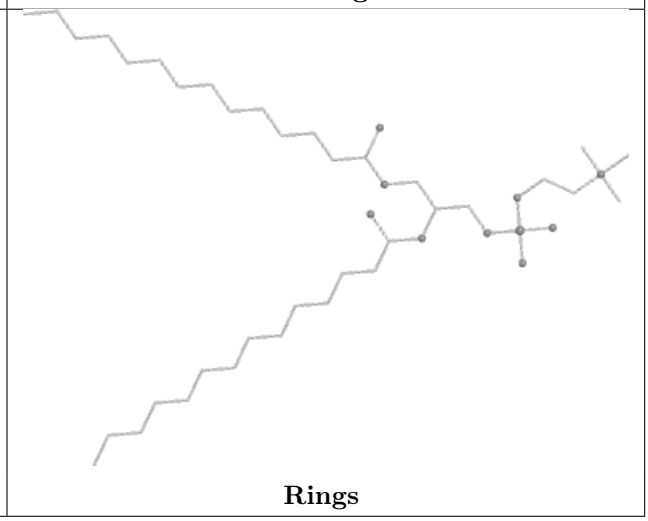
Bond lengths



Bond angles

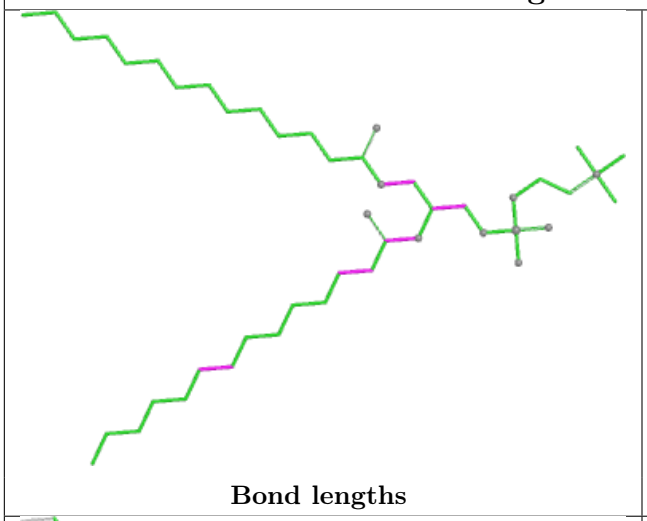


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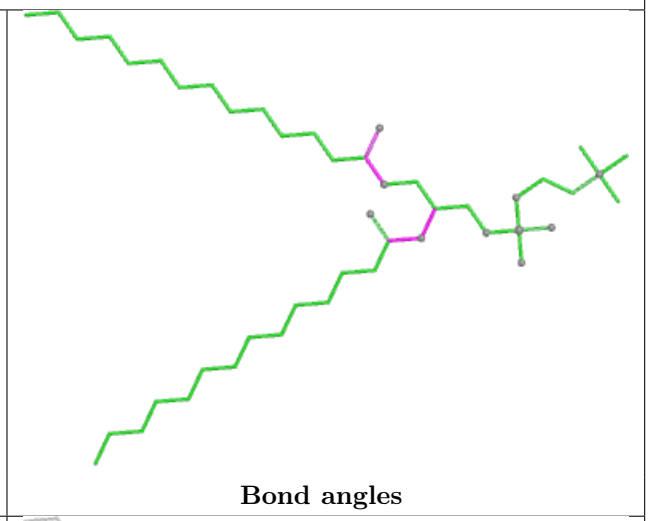


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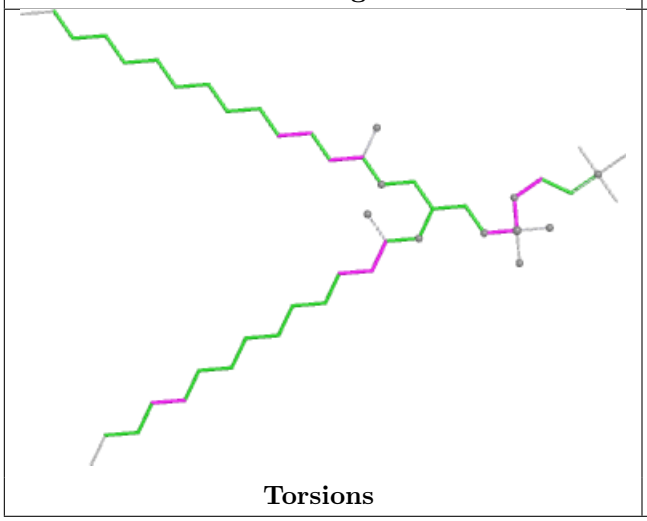
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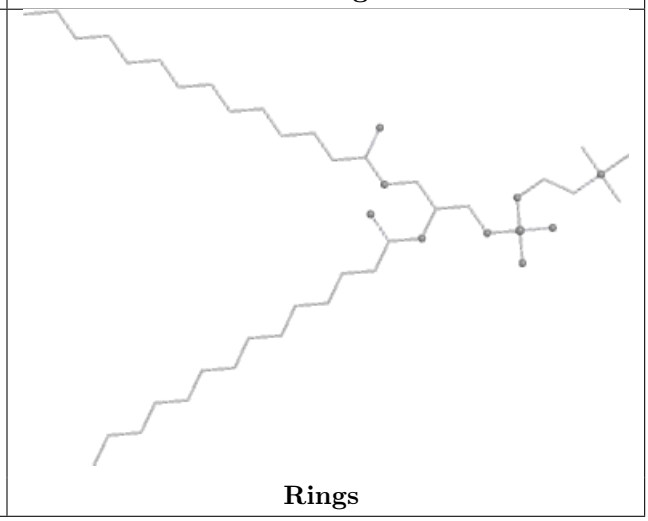
Bond lengths



Bond angles

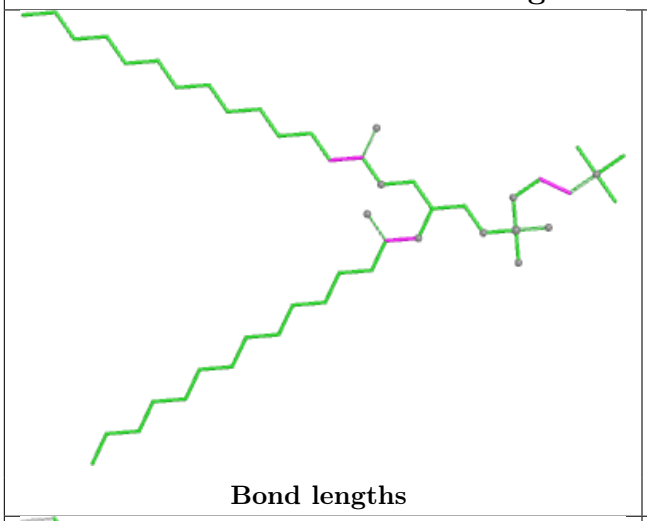


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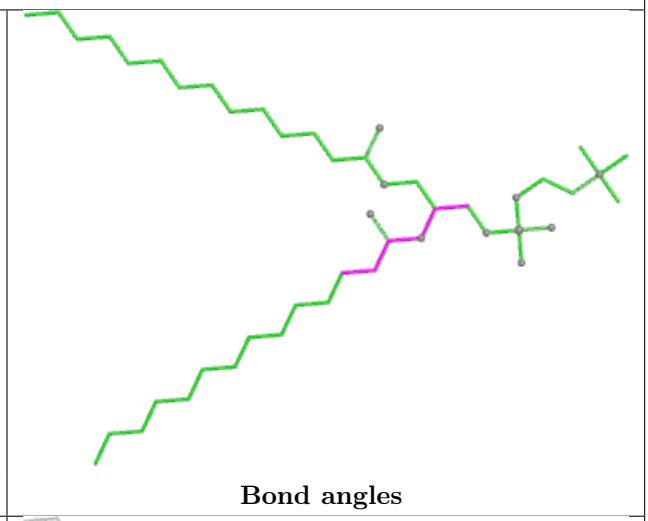


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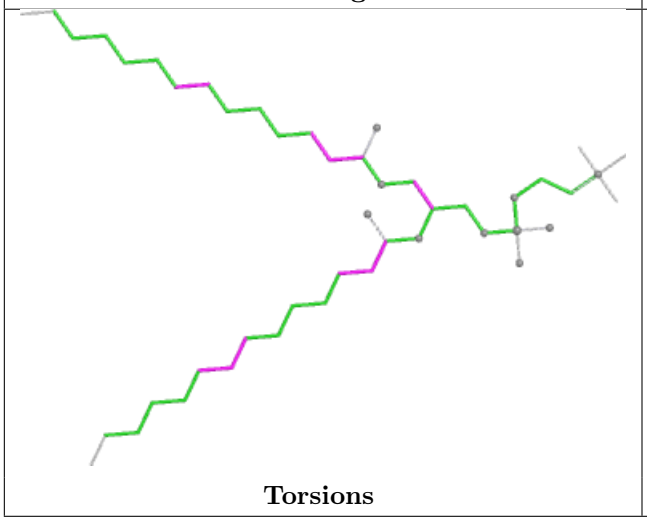
Ligand PX4 B 393



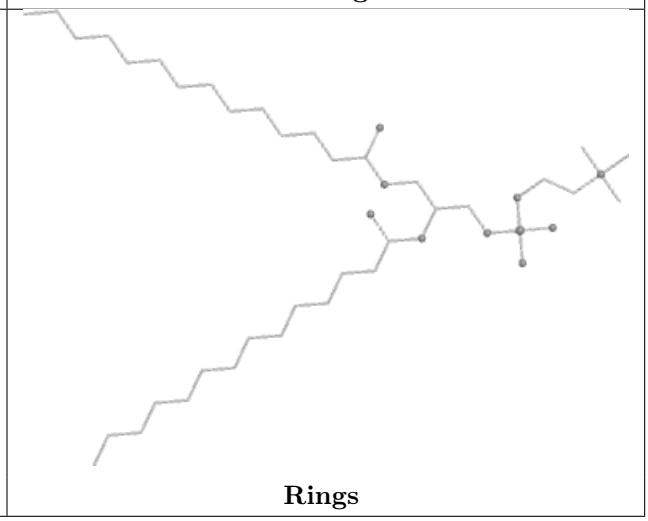
Bond lengths



Bond angles

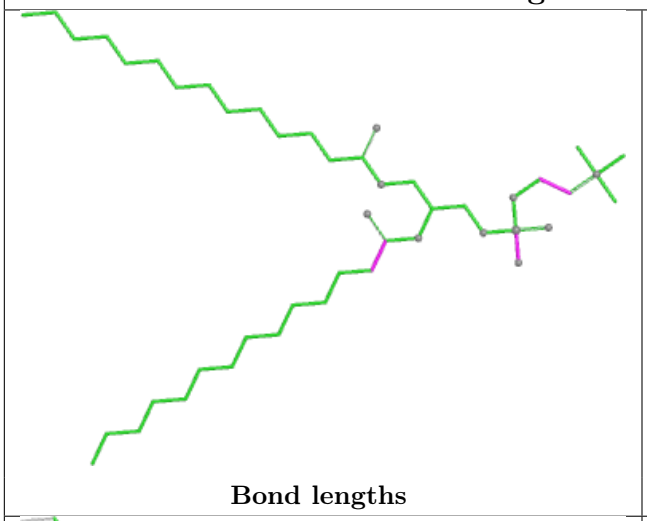


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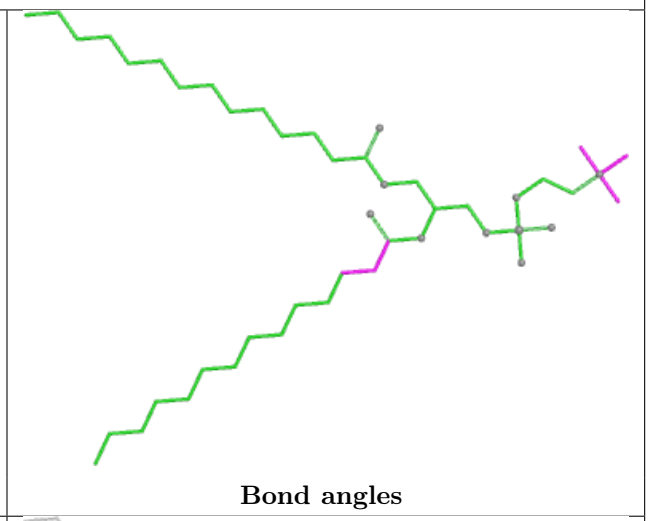


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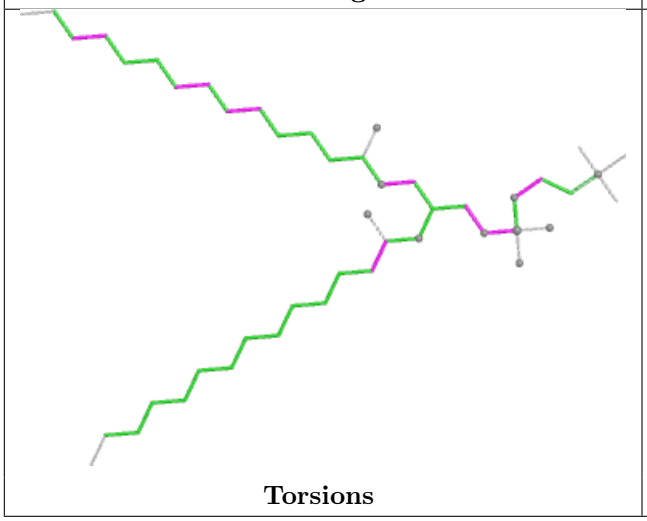
Ligand PX4 C 317



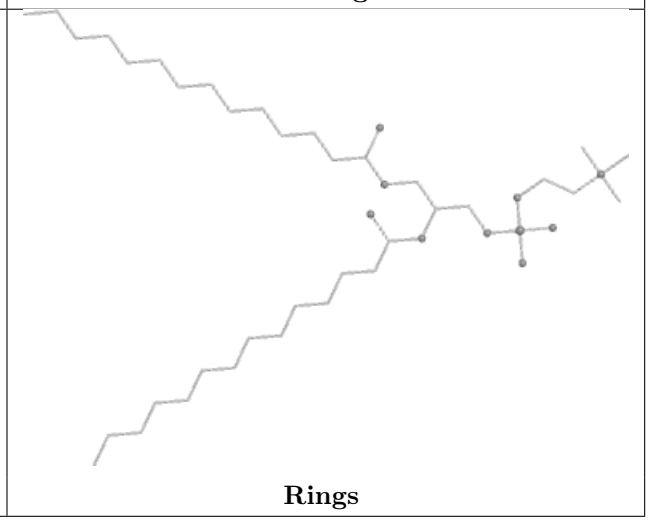
Bond lengths



Bond angles

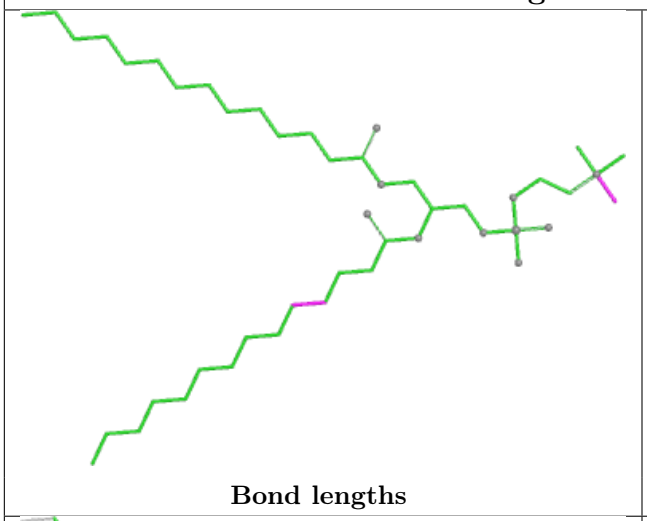


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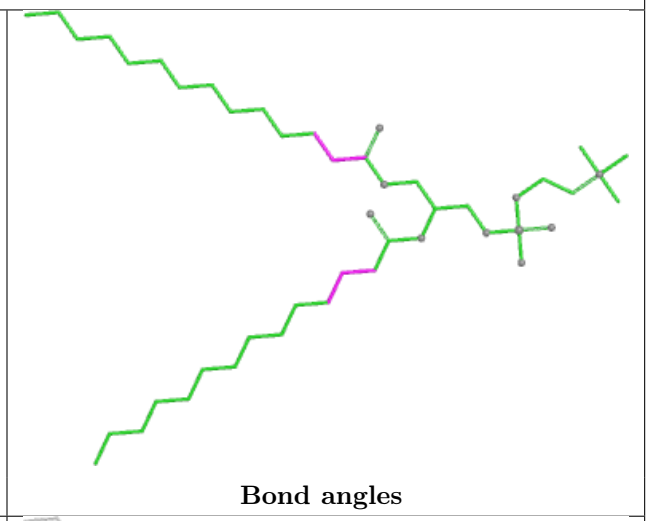


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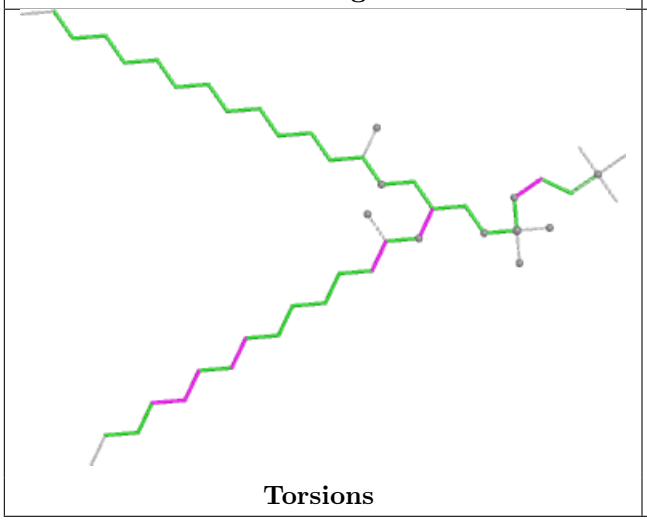
Ligand PX4 B 342



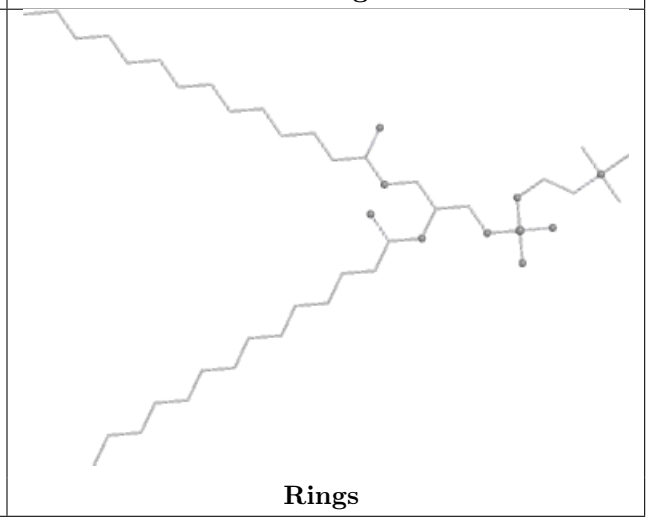
Bond lengths



Bond angles

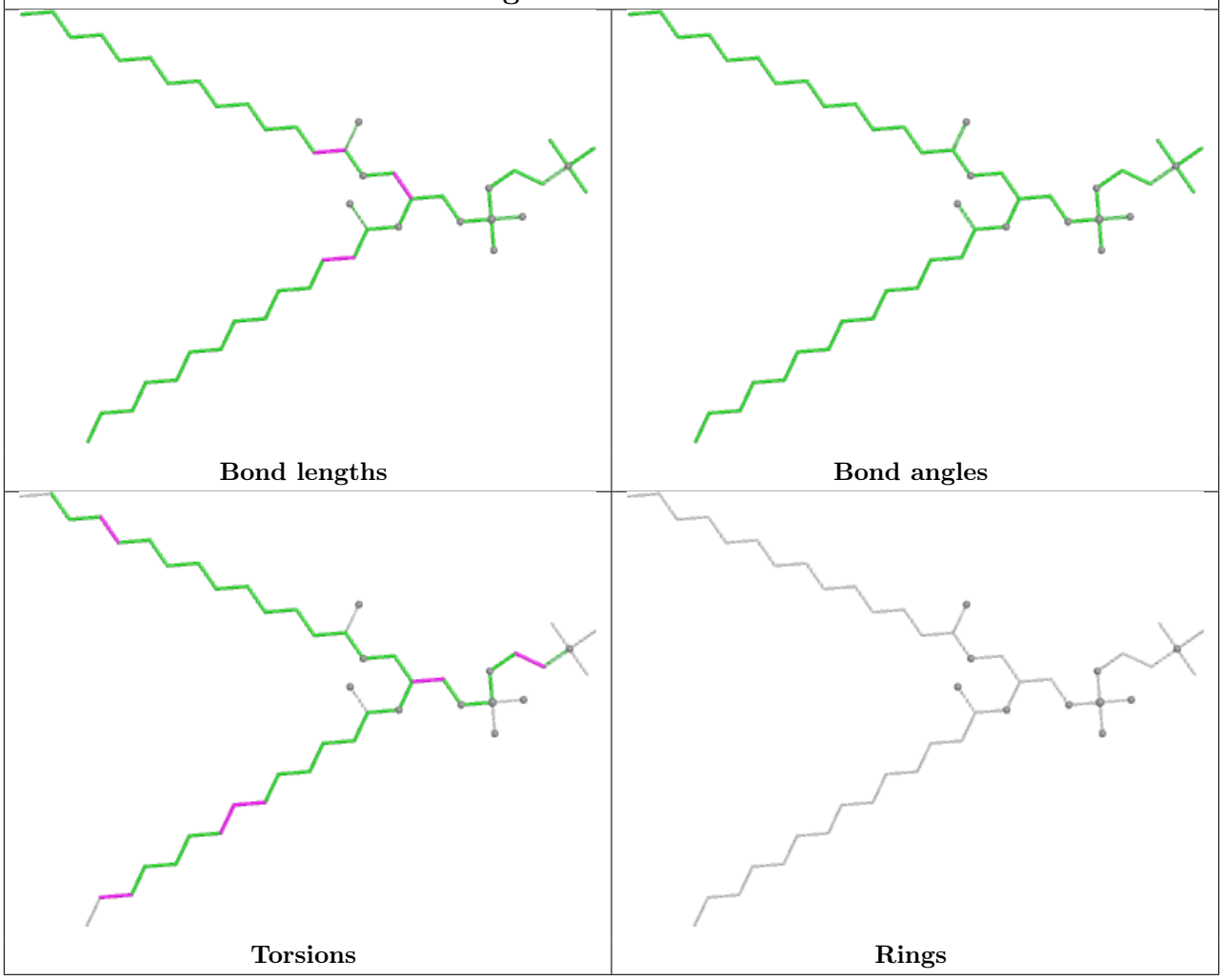


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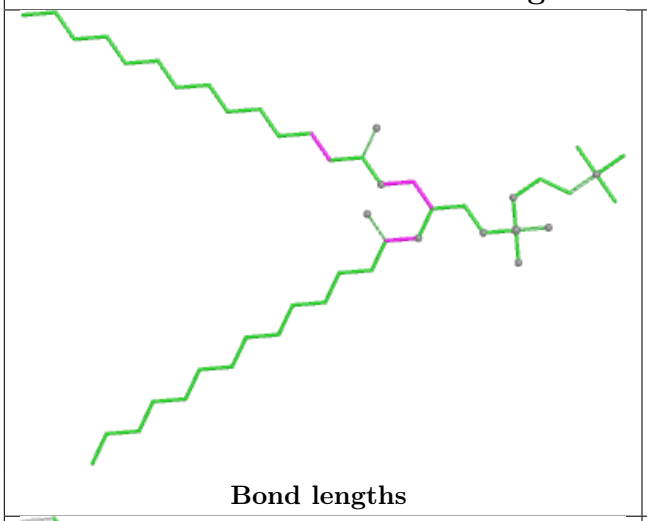


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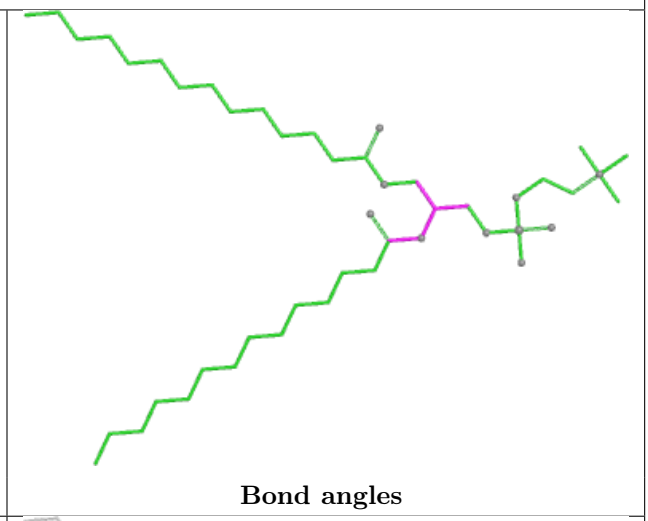
Ligand PX4 B 356



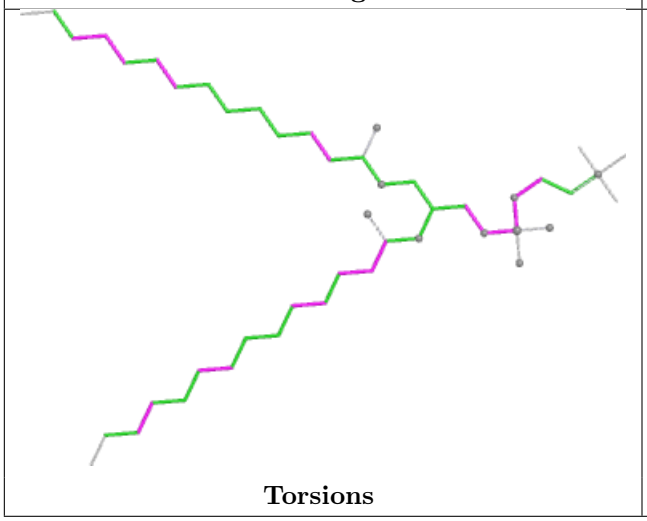
Ligand PX4 C 329



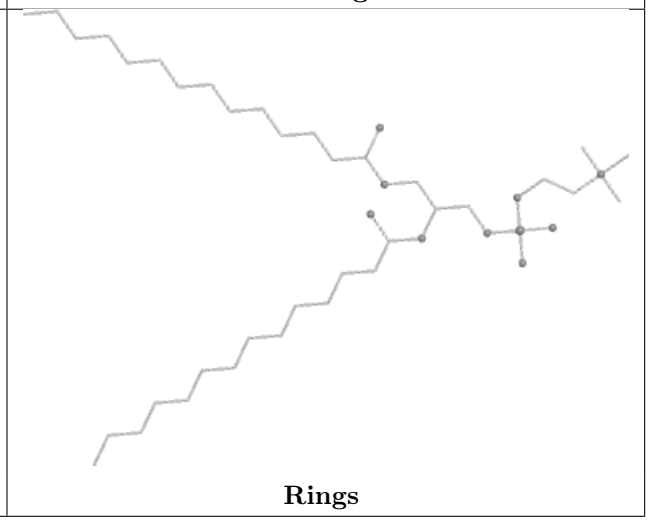
Bond lengths



Bond angles

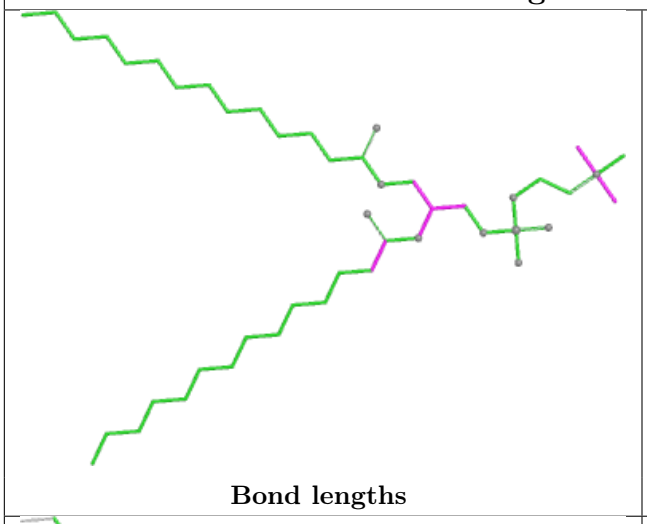


Torsions

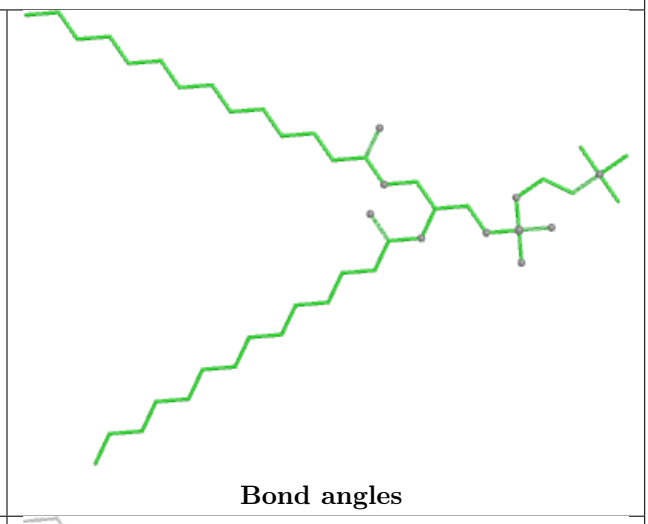


Rings

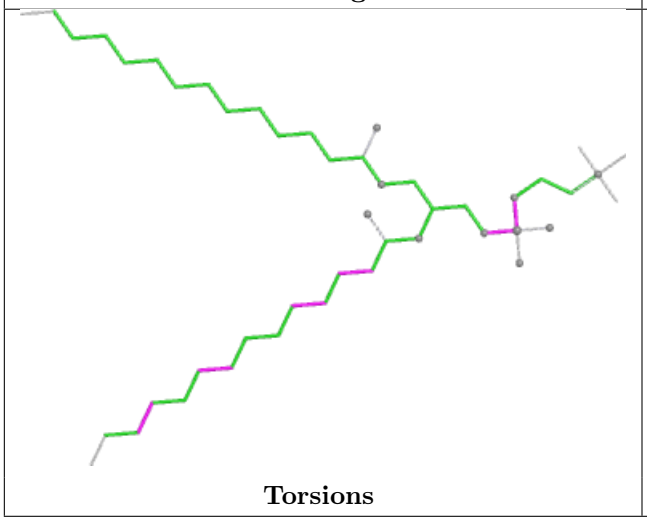
Ligand PX4 B 385



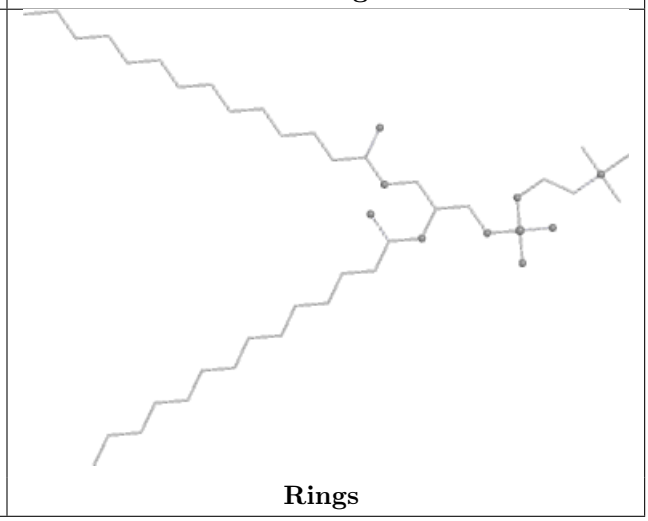
Bond lengths



Bond angles

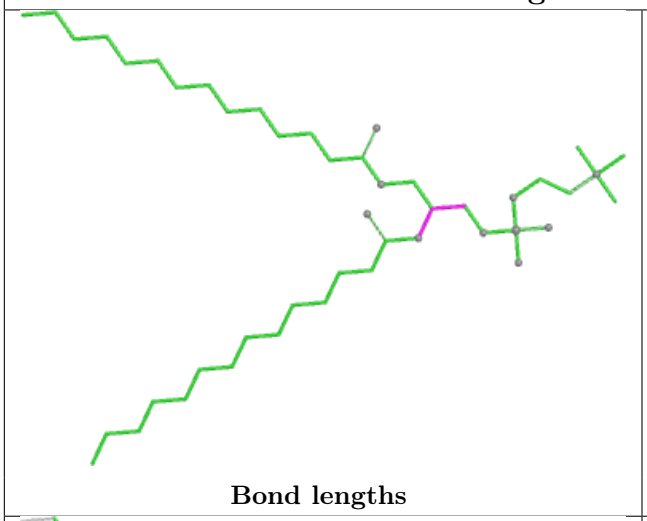


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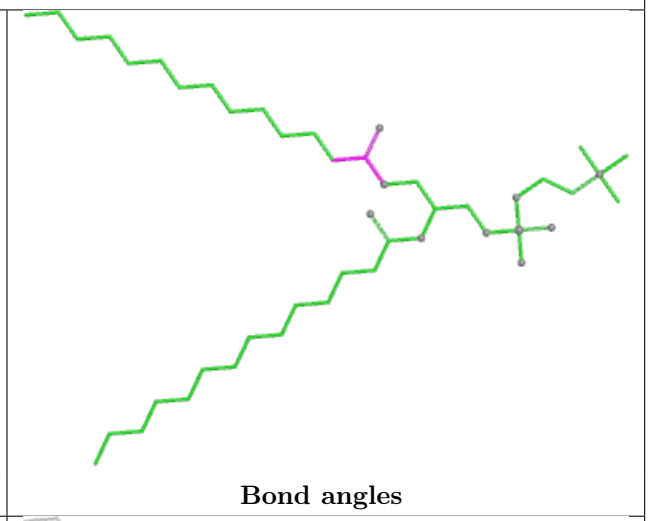


Rings

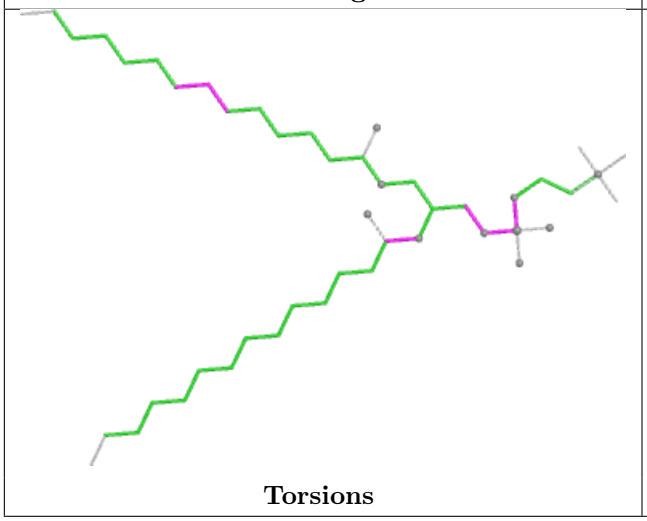
Ligand PX4 B 397



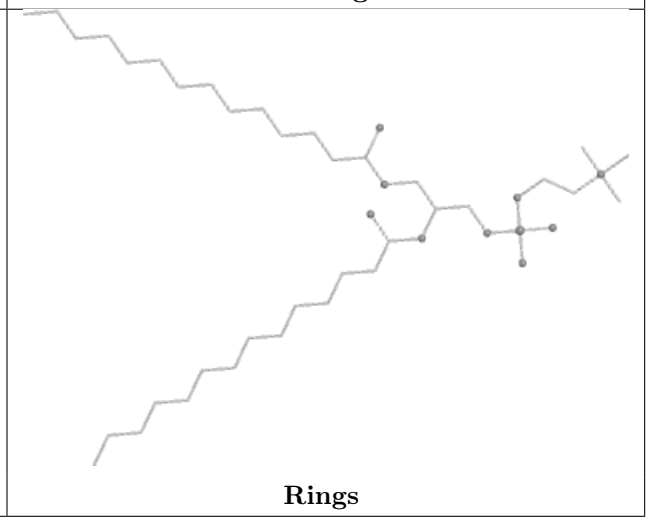
Bond lengths



Bond angles

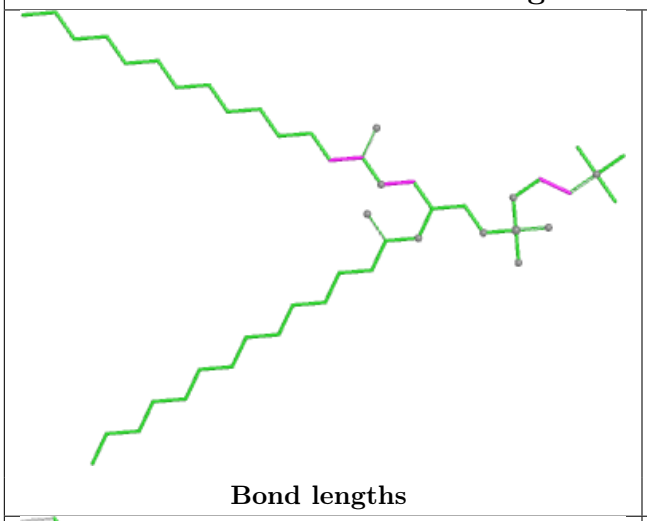


Torsions

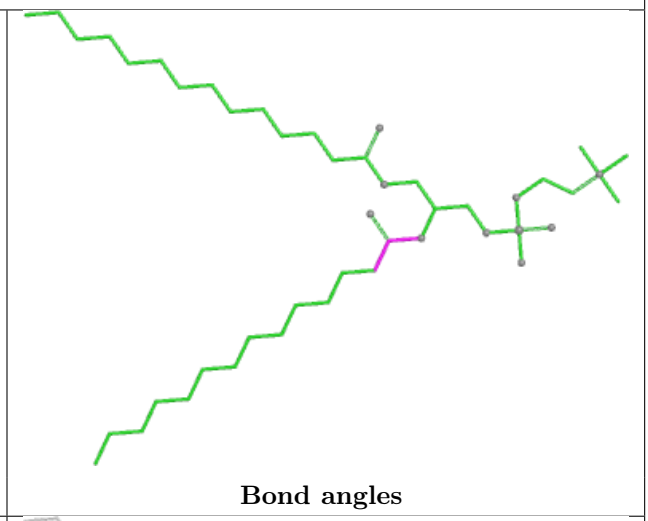


Rings

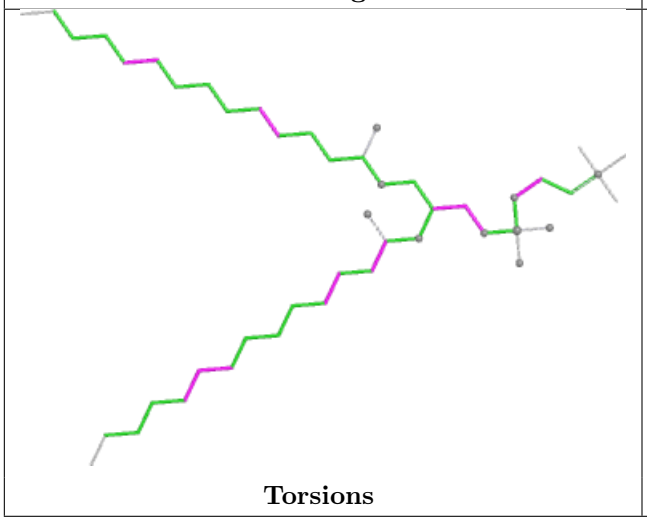
Ligand PX4 C 306



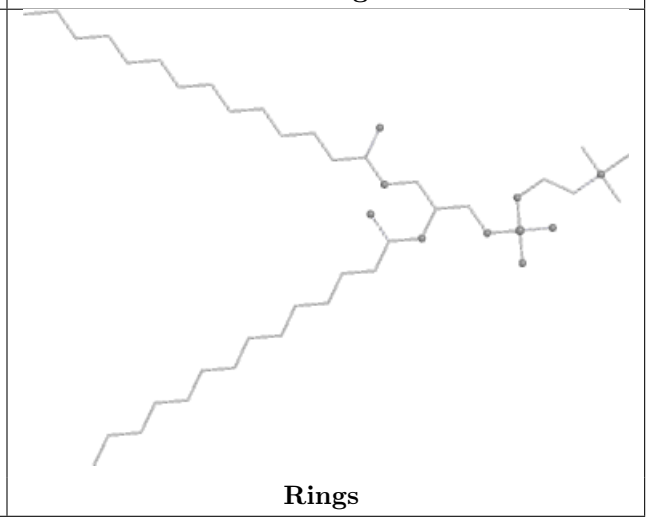
Bond lengths



Bond angles

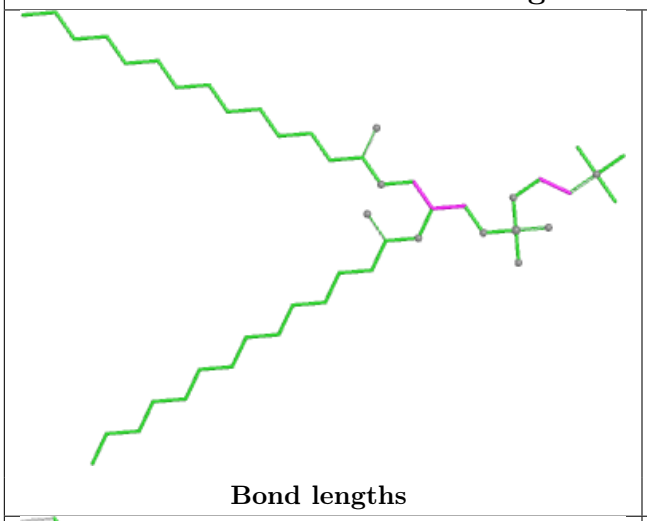


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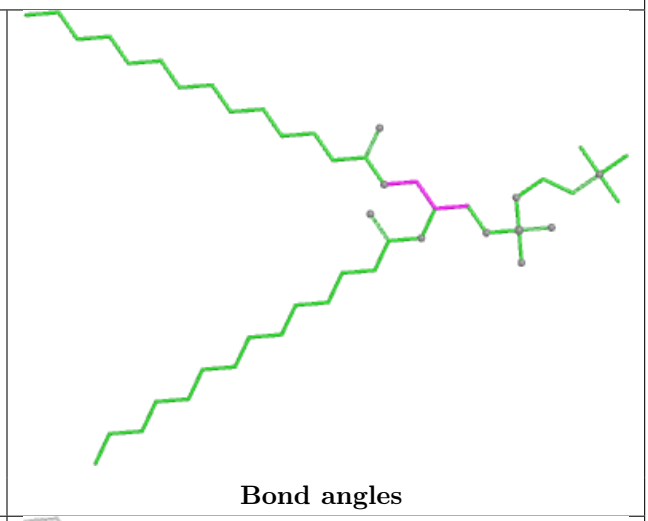


Rings

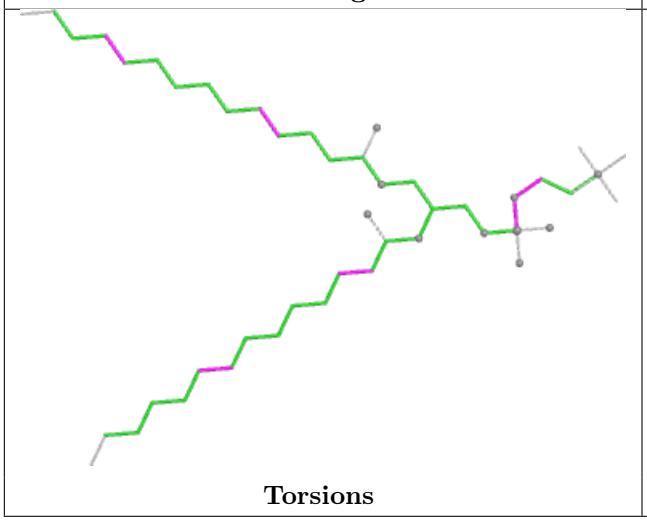
Ligand PX4 B 346



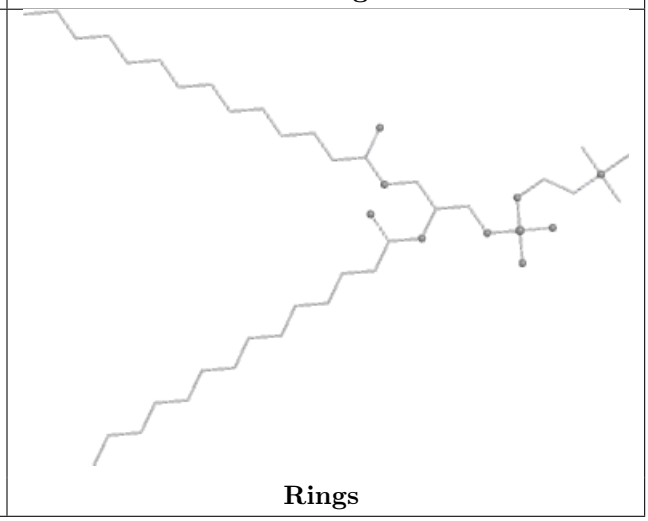
Bond lengths



Bond angles

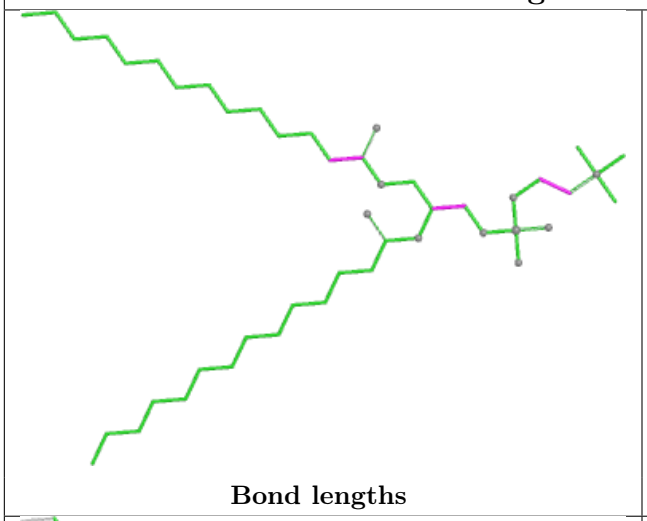


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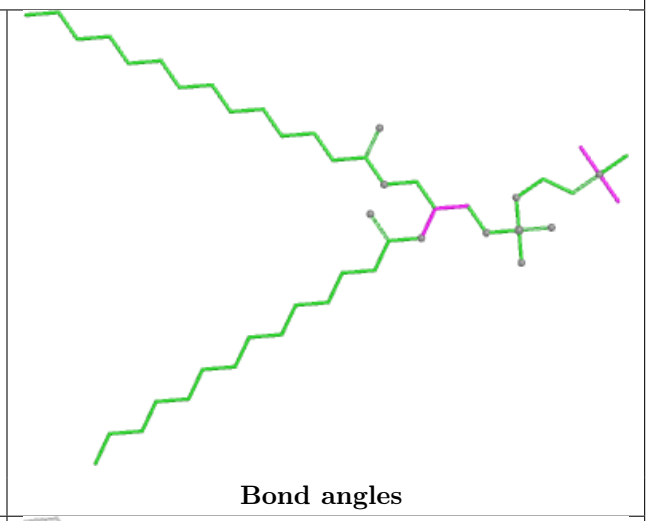


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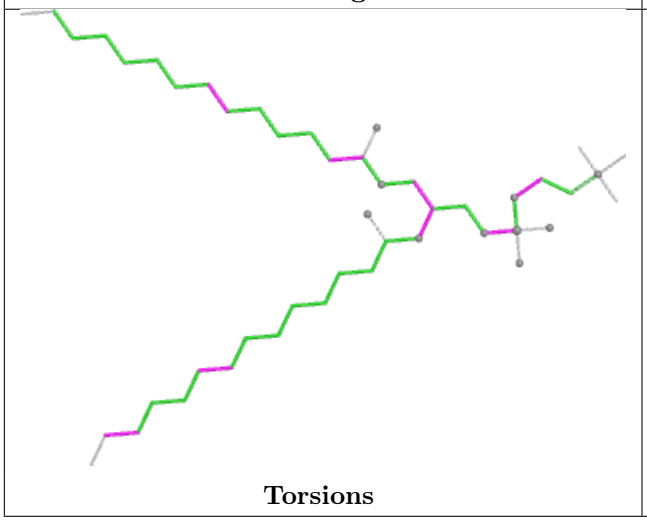
Ligand PX4 C 320



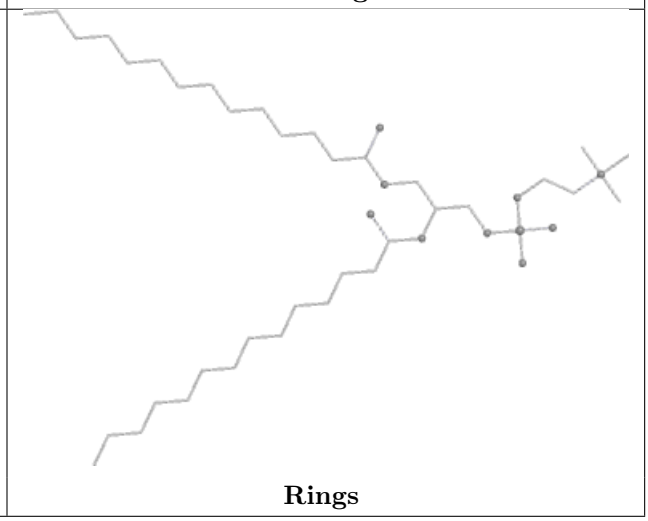
Bond lengths



Bond angles

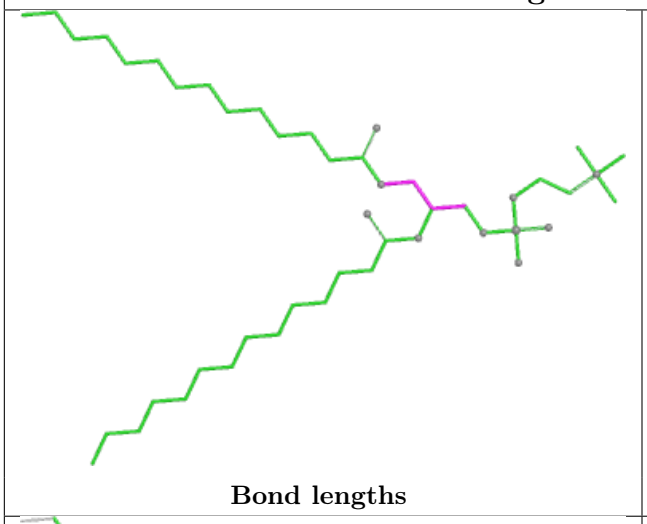


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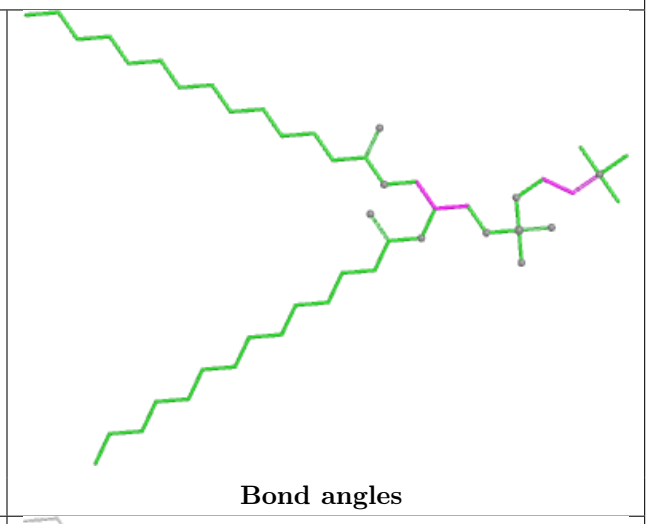


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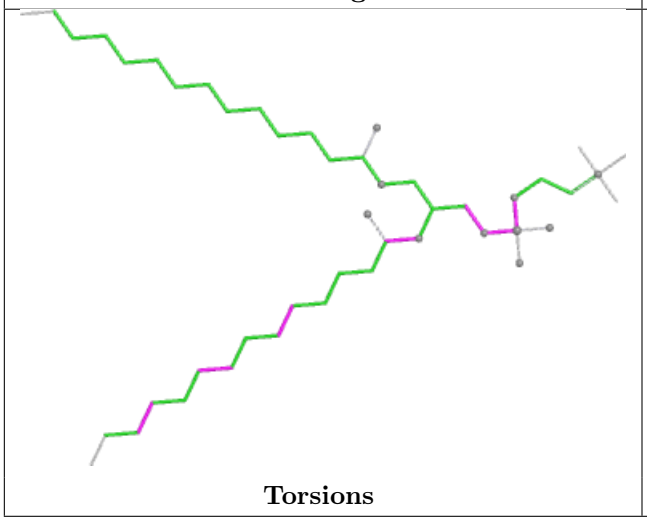
Ligand PX4 C 308



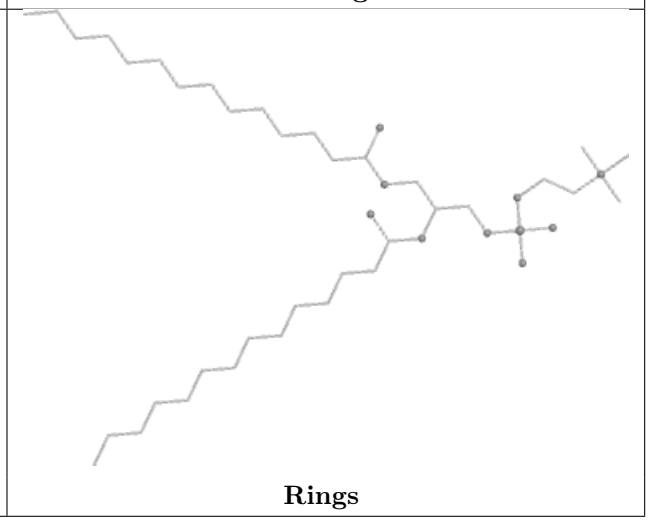
Bond lengths



Bond angles

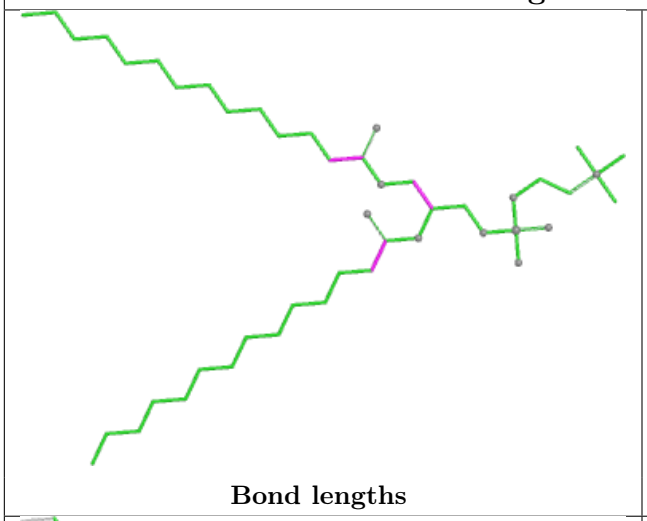


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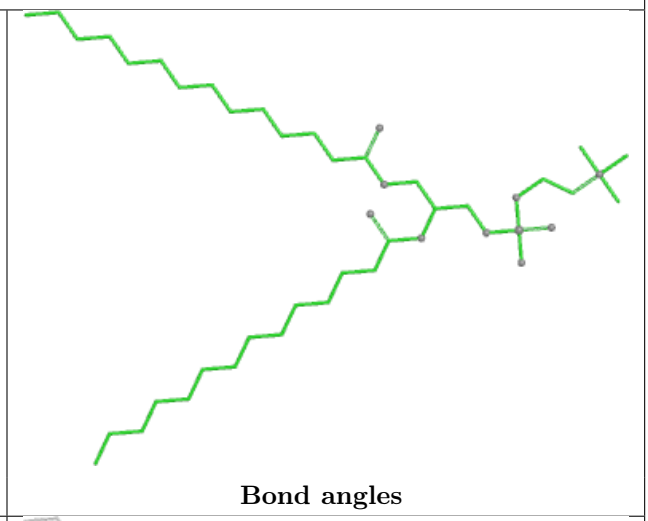


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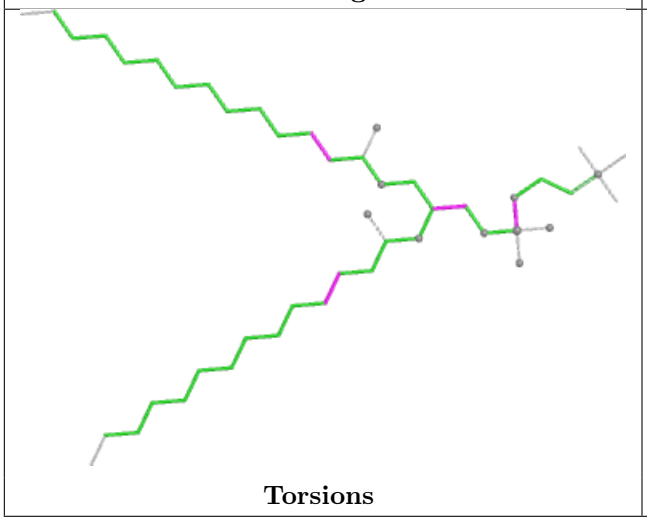
Ligand PX4 B 388



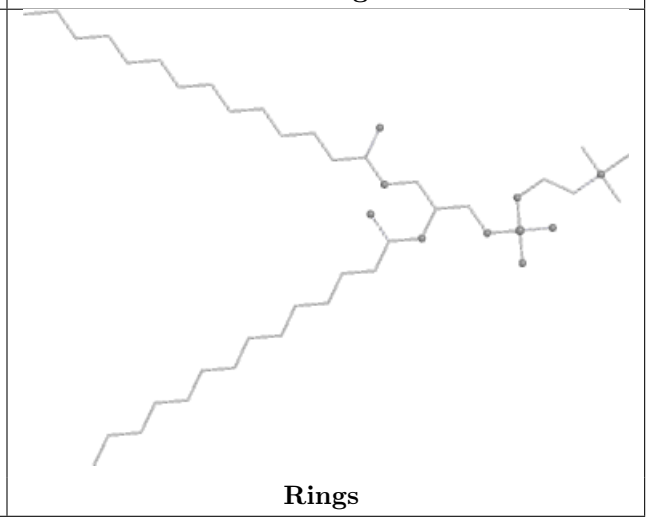
Bond lengths



Bond angles

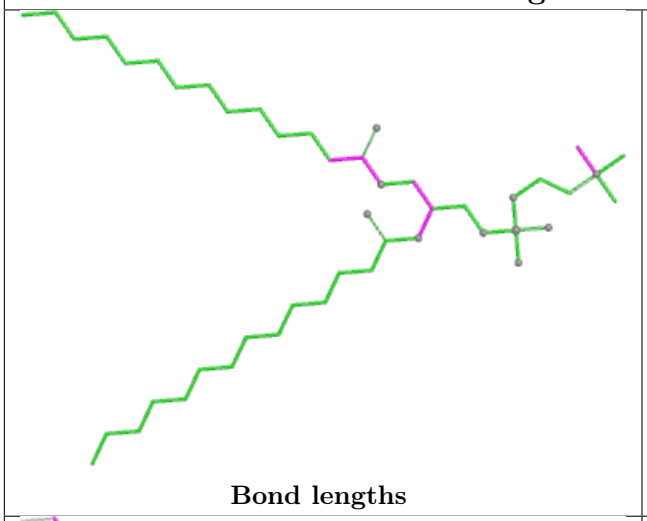


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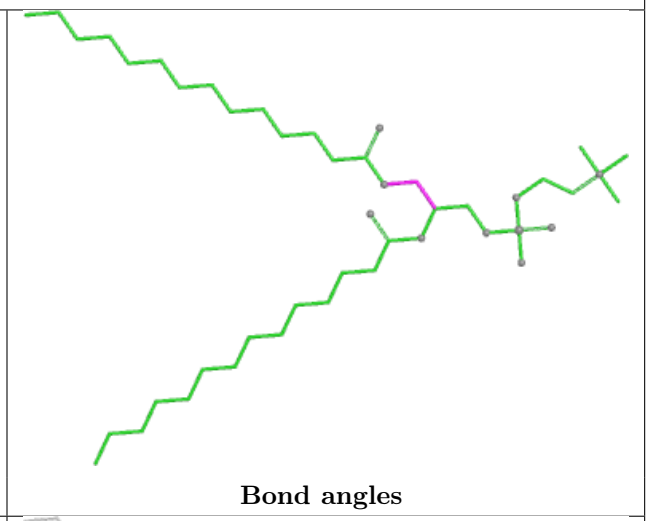


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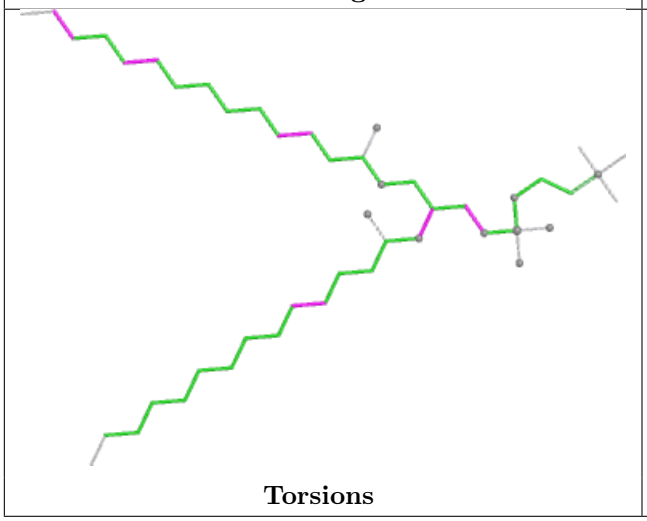
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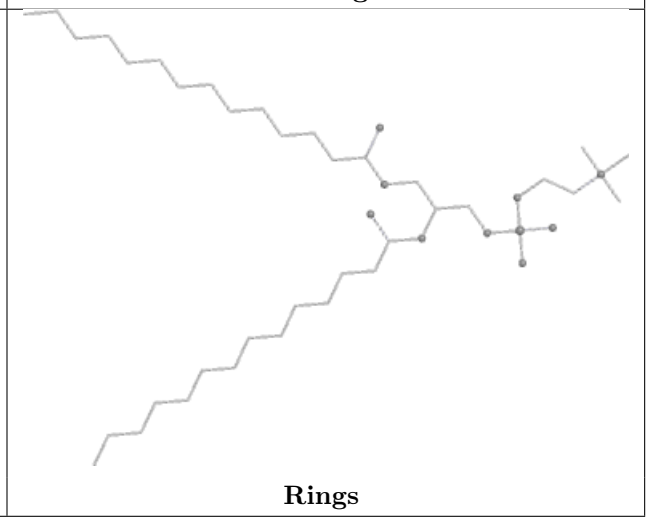
Bond lengths



Bond angles

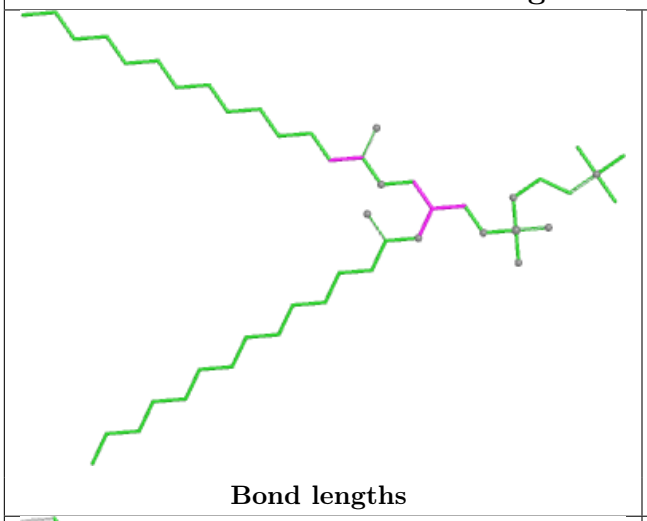


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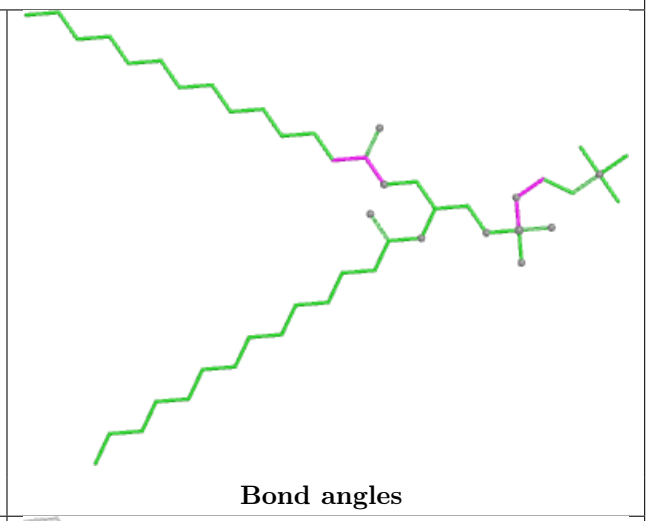


Rings

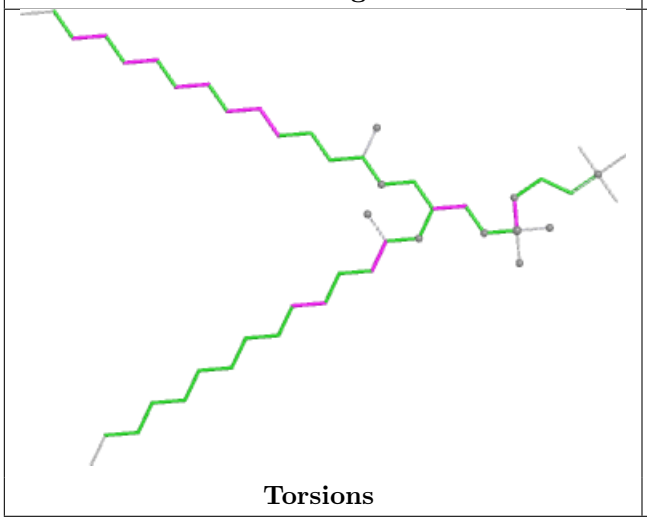
Ligand PX4 B 309



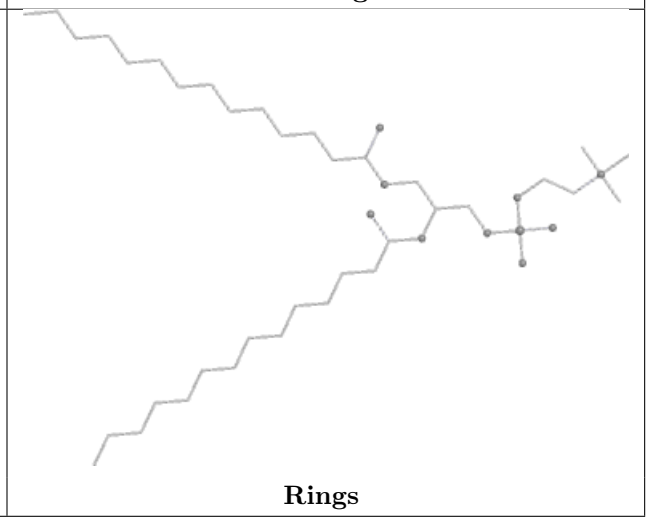
Bond lengths



Bond angles

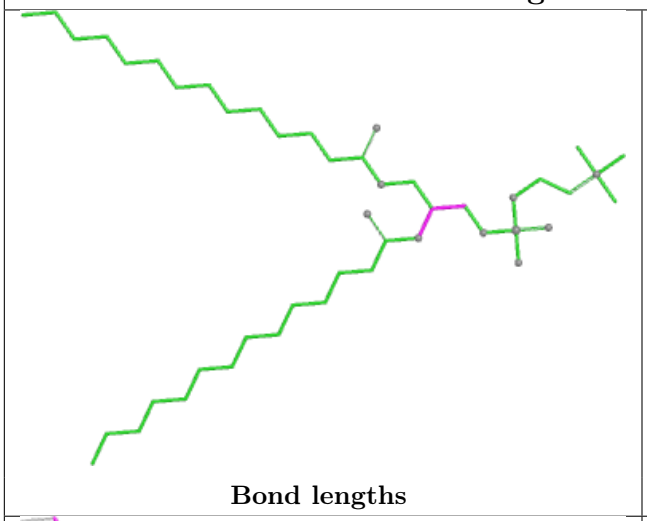


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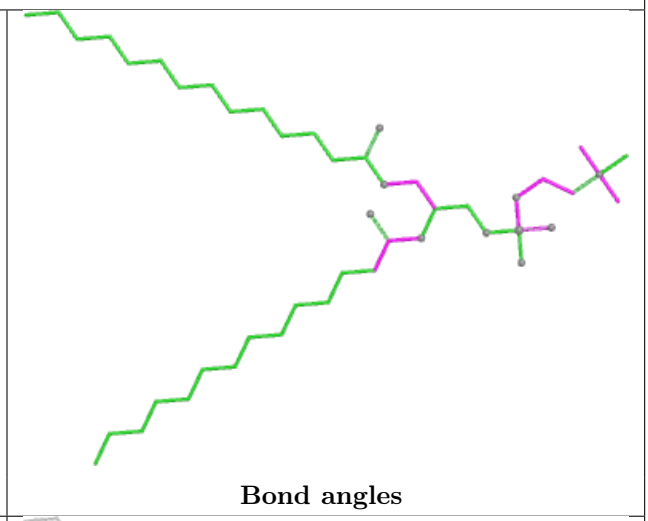


Rings

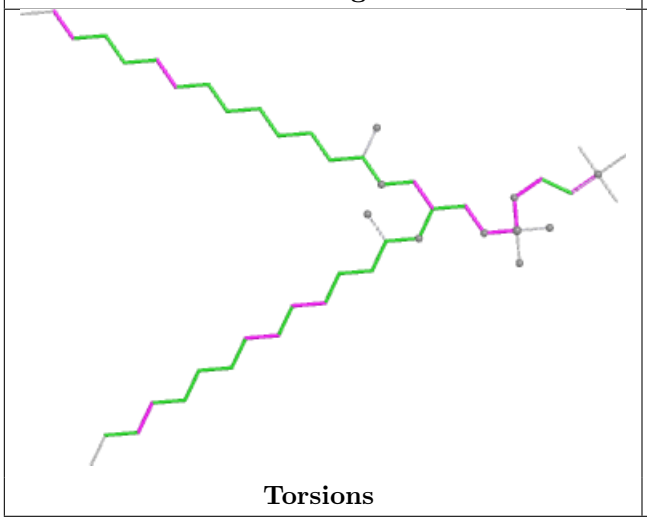
Ligand PX4 A 627



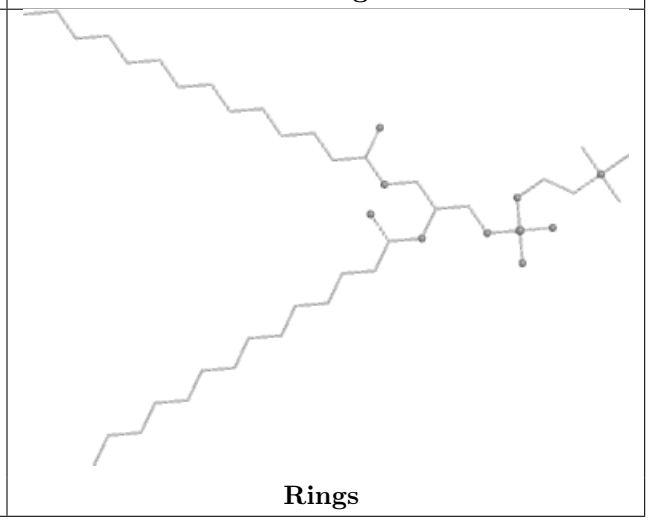
Bond lengths



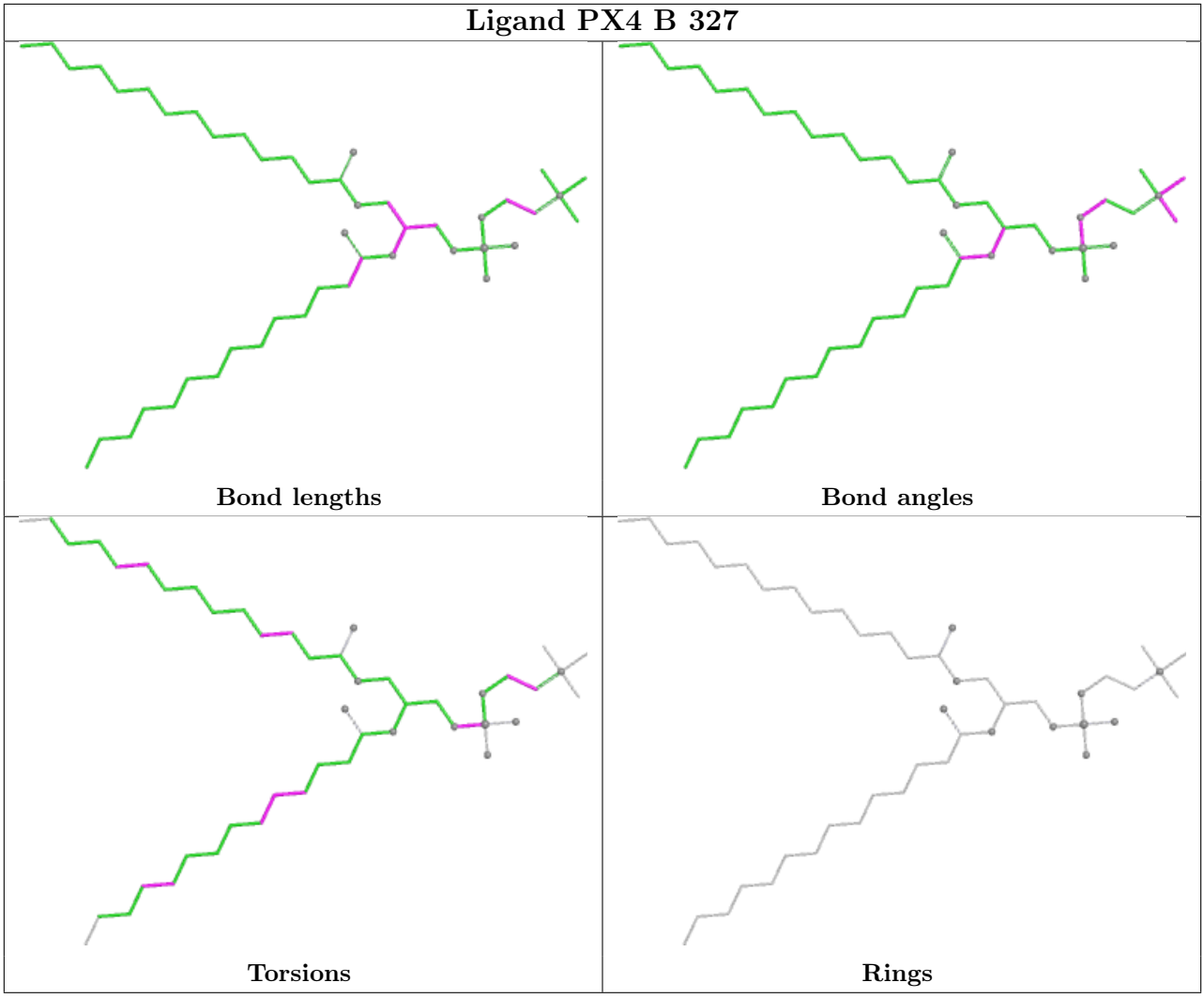
Bond angles



Torsions



Rings



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 4% for the well-defined parts and 4% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *showstar5.txt*

7.1.1 Bookkeeping

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

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

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	0	—	None (insufficient data)
$^{13}C_{\beta}$	0	—	None (insufficient data)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	92	1.11 ± 0.63	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 4%, i.e. 324 atoms were assigned a chemical shift out of a possible 8823. 0 out of 99 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	184/3063 (6%)	92/1239 (7%)	0/1236 (0%)	92/588 (16%)
Sidechain	140/4993 (3%)	105/3195 (3%)	35/1561 (2%)	0/237 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	0/767 (0%)	0/377 (0%)	0/364 (0%)	0/26 (0%)
Overall	324/8823 (4%)	197/4811 (4%)	35/3161 (1%)	92/851 (11%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 4%, i.e. 324 atoms were assigned a chemical shift out of a possible 8823. 0 out of 99 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	184/3063 (6%)	92/1239 (7%)	0/1236 (0%)	92/588 (16%)
Sidechain	140/4993 (3%)	105/3195 (3%)	35/1561 (2%)	0/237 (0%)
Aromatic	0/767 (0%)	0/377 (0%)	0/364 (0%)	0/26 (0%)
Overall	324/8823 (4%)	197/4811 (4%)	35/3161 (1%)	92/851 (11%)

7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.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:

